Spectral representations / Lehmann representation

Relations between various GF's in Fourier or Matsubara domain can be made explicit using Lehmann-representations.

Thermal GF:

$$\mathcal{G}_{AB}(\tau>0) \overset{(23.2)}{=} -\frac{1}{\hbar Z}\sum_n \langle n| e^{-\hat{H}(\beta-\tau/\hbar)}\hat{A}\sum_m |m\rangle\langle m| e^{-\hat{H}\tau/\hbar}\hat{B}|n\rangle \quad (1)$$

$$= -\frac{1}{\hbar Z}\sum_{nm} \underbrace{\langle n|\hat{A}|m\rangle}_{\equiv A_{nm}}\underbrace{\langle m|\hat{B}|n\rangle}_{B_{mn}} e^{-E_n\beta}\, e^{\tau\left(-\frac{E_m}{\hbar}+\frac{E_n}{\hbar}\right)} \quad (2)$$

$$\bar{\mathcal{G}}_{AB}(i\omega_n) \overset{(23.3)}{=} \int_0^\beta d\tau\, e^{i\omega_n\tau}\,\mathcal{G}_{AB}(\tau) \quad (3)$$

$$= -\frac{1}{\hbar Z}\sum_{nm} A_{nm}B_{mn}\,e^{-E_n\beta}\times\frac{\overbrace{e^{i\beta\omega_\ell}}^{=\xi}e^{\beta(-E_m+E_n)}-1}{i\omega_\ell-(E_m-E_n)/\hbar} \quad (4)$$

$$\bar{\mathcal{G}}_{AB}(i\omega_\ell) = \frac{1}{Z}\sum_{nm} A_{nm}B_{mn}\frac{e^{-\beta E_n}-\xi e^{-\beta E_m}}{\hbar i\omega_\ell-(E_m-E_n)} \quad (1)$$

$$= \int d\bar{\omega}\,\frac{1}{i\omega_\ell-\bar{\omega}}\underbrace{\frac{1}{Z}\sum_{nm}A_{nm}B_{mn}\left(e^{-\beta E_n}-\xi e^{-\beta E_m}\right)\delta(\hbar\bar{\omega}-E_m+E_n)} \quad (2)$$

$$\equiv \mathcal{A}_{AB}(\bar{\omega}) = \text{“spectral function”} \quad (3)$$

$$\bar{\mathcal{G}}_{AB}(i\omega_\ell) = \int d\bar{\omega}\,\frac{\mathcal{A}_{AB}(\bar{\omega})}{i\omega_\ell-\bar{\omega}} \quad = \text{“spectral representation of } \bar{\mathcal{G}}_{AB}(i\omega_\ell)\text{”} \quad (4)$$

We will see that the spectral function $\mathcal{A}_{AB}(\bar{\omega})$ also governs the spectral representations of $\mathcal{G}^R$, $\mathcal{G}^A$ and $\mathcal{G}^C$!

Real-time GFs ($\mathcal{G}^R, \mathcal{G}^A, \mathcal{G}^C$) GF39

Fourier transformation convention:

$$\mathcal{G}_{AB}(t) \equiv \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \tilde{\mathcal{G}}_{AB}(\omega) \quad (1)$$

$$\tilde{\mathcal{G}}_{AB}(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} \mathcal{G}_{AB}(t) \quad (2)$$

FT of step function:

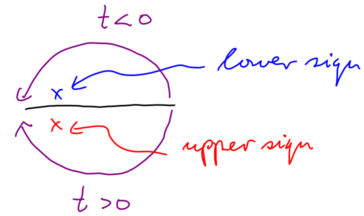
$$\tilde{\Theta}_{\pm}(\omega) = \int_{-\infty}^{\infty} dt\, e^{it(\omega \pm i\alpha)} \Theta(\pm t) = \begin{Bmatrix} \dfrac{0-1}{i(\omega+i\alpha)} \\ \dfrac{1-0}{i(\omega-i\alpha)} \end{Bmatrix} = \frac{\pm i}{\omega \pm i\alpha} \quad (3)$$

regularizer

Inverse:

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \underbrace{\frac{\pm i}{\omega \pm i\alpha}}_{\tilde{\Theta}_{\pm}(\omega)}$$

$$= \frac{\pm i}{2\pi} \begin{Bmatrix} -2\pi i\, \Theta(t) \\ +2\pi i\, \Theta(-t) \end{Bmatrix} = \Theta(\pm t) \quad (4)$$



GF40

$$\mathcal{G}^{>}_{AB}(t-t') \overset{(33.2)}{=} -i/\hbar\, \frac{1}{Z} \sum_n \langle n| e^{-\hat{H}(\beta - i(t-t')/\hbar)} \hat{A}\, e^{-i\hat{H}(t-t')/\hbar} \hat{B} |n\rangle \quad (1)$$

$\sum_m |m\rangle\langle m|$

$$= -(i/\hbar) \frac{1}{Z} \sum_{nm} e^{-\beta E_n} A_{nm} B_{mn} e^{-i(t-t')(E_m - E_n)/\hbar} \quad (2)$$

$\sum_n |n\rangle\langle n|$

$$\mathcal{G}^{<}_{AB}(t-t') \overset{(33.3)}{=} -i\zeta/\hbar\, \frac{1}{Z} \sum_m \langle m| e^{-\hat{H}(\beta + i(t-t')/\hbar)} \hat{B}\, e^{+i\hat{H}(t-t')/\hbar} \hat{A} |m\rangle \quad (3)$$

$$= -\zeta (i/\hbar) \frac{1}{Z} \sum_m e^{-\beta E_m} B_{mn} A_{nm} e^{-i(t-t')(E_m - E_n)/\hbar} \quad (4)$$

$$\text{FT:} \quad \tilde{\mathcal{G}}^{\gtrless}_{AB}(\omega) = -i \frac{1}{Z} \sum_{nm} A_{nm} B_{mn} \begin{Bmatrix} e^{-\beta E_n} \\ \zeta e^{-\beta E_m} \end{Bmatrix} \underbrace{\frac{1}{\hbar} \int dt\, e^{it\left(\omega - \frac{E_m}{\hbar} - \frac{E_n}{\hbar}\right)}}_{2\pi\, \delta(\hbar\omega - E_m + E_n)} \quad (5)$$

Now, let's consider FT of G^R, G^A, $G^<$, which all have similar structure : $\boxed{GF41}$

(30.4) G^R, (30.4) G^A, (32.2) $G^<$

$$\begin{Bmatrix} G^R(\omega) \\ G^A(\omega) \\ G^<(\omega)\end{Bmatrix}_{AB} = \int dt\, e^{i\omega t}\left[\begin{Bmatrix}\theta(t)\\ -\theta(-t)\\ \theta(t)\end{Bmatrix} G^>_{AB}(t) + \begin{Bmatrix}-\theta(t)\\ \theta(-t)\\ \theta(-t)\end{Bmatrix} G^<_{AB}(t)\right] \tag{5}$$

FT of product is convolution of FT's : $\left[\tilde\theta_\pm(\omega) \overset{(39.3)}{=} \frac{\pm i}{\omega \pm i\alpha} \right]$

$$= \int d\bar\omega \begin{Bmatrix}\tilde\theta_+(\omega-\bar\omega)\\ -\tilde\theta_-(\omega-\bar\omega)\\ \tilde\theta_+(\omega-\bar\omega)\end{Bmatrix} G^>_{AB}(\bar\omega) + \begin{Bmatrix}-\tilde\theta_+(\omega-\bar\omega)\\ \tilde\theta_-(\omega-\bar\omega)\\ \tilde\theta_-(\omega-\bar\omega)\end{Bmatrix} G^<_{AB}(\bar\omega) \tag{6}$$

$$= \frac{1}{Z}\sum_{nm} A_{nm} B_{mn} \int d\bar\omega\, \delta(\hbar\bar\omega - E_m + E_n)\left[\frac{e^{-\beta E_n}}{\omega - \bar\omega + \begin{Bmatrix}+\\-\\+\end{Bmatrix} i\alpha} - \frac{\zeta e^{-\beta E_m}}{\omega - \bar\omega + \begin{Bmatrix}+\\-\\-\end{Bmatrix} i\alpha}\right] \tag{7}$$

Thus, $G^R(\omega)$, $G^A(\omega)$, $G^<(\omega)$ differ only by pole structure in complex plane!

$\boxed{GF42}$

$$\begin{Bmatrix} G^R(\omega) \\ G^A(\omega)\end{Bmatrix} = \int d\bar\omega \frac{1}{\omega - \bar\omega \pm i\alpha} \underbrace{\frac{1}{Z}\sum_{nm} A_{nm} B_{mn}\left(e^{-\beta E_n} - \zeta e^{-\beta E_m}\right)\delta(\hbar\bar\omega - E_m + E_n)}_{= A_{AB}(\bar\omega) \,=\, (38.3)} \tag{1}$$

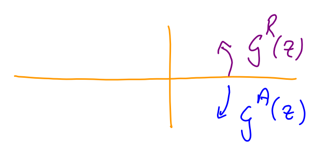
↑ same spectral function as for $\bar G_{AB}(i\omega_\ell)$!

$$= \int d\bar\omega \frac{A_{AB}(\bar\omega)}{\omega \pm i\alpha - \bar\omega} \quad = \text{"spectral representation of } G^{R/A}\text{"} \tag{2}$$

Remarks:

1. $G^{R/A}$ is analytic in upper/lower half plane, and thus can be continued into the complex plane using

$$G^{R/A}(z) \equiv \int d\bar\omega \frac{A_{AB}(\bar\omega)}{z \pm i\alpha - \bar\omega} \tag{3}$$



The poles of $G^{R/A}(z)$ all lie entirely in the lower/upper half-plane

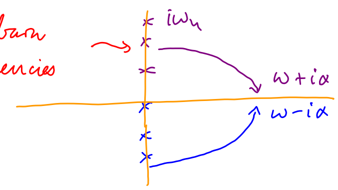
2. Reason: this ensures causality:

$$G^{R/A}(t) \overset{(42.2)}{=} \int d\bar{\omega}\, A_{AB}(\bar{\omega}) \underbrace{\int \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{\omega - \bar{\omega} \pm i\alpha}}_{\mp i e^{-i\bar{\omega} t}\, \theta(\pm t)} \qquad (1)$$

GF43

3. Comparing (2) with (38.4), we conclude

$$G^{R/A}_{AB}(\omega) = \bar{\mathcal{G}}_{AB}(i\omega_\ell \to \omega \pm i\alpha) \qquad (2)$$



$\Longrightarrow$ Retarded/advanced GF in frequency domain can be obtained from Matsubara GF by analytic continuation in complex frequency

4. Discontinuity of $\bar{\mathcal{G}}(i\omega_n)$ across real axis gives spectral function:

$$\frac{i}{2\pi}\left[G^R_{AB}(\omega) - G^A_{AB}(\omega)\right] = \frac{i}{2\pi}\left[\bar{\mathcal{G}}_{AB}(i\omega_\ell \to \omega + i\alpha) - \bar{\mathcal{G}}_{AB}(i\omega_\ell \to \omega - i\alpha)\right] \qquad (3)$$

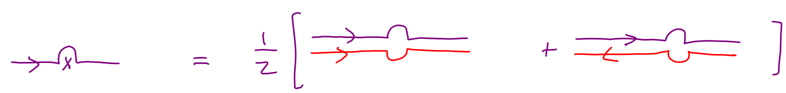
$$= \int d\bar{\omega}\, A_{AB}(\bar{\omega}) \frac{i}{2\pi}\Big[\underbrace{\frac{1}{\omega + i\alpha - \bar{\omega}} - \frac{1}{\omega - i\alpha - \bar{\omega}}}_{-2\pi i\, \delta(\omega - \bar{\omega})}\Big] = A_{AB}(\omega) \qquad (4)$$

Mnemonic for identity

GF48

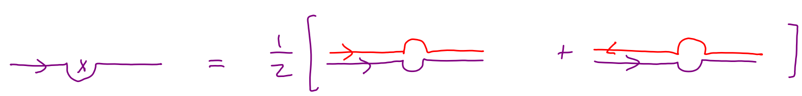
$$\frac{1}{\omega \pm i\alpha - \bar{\omega}} = \frac{P}{\omega - \bar{\omega}} \mp i\pi\, \delta(\omega - \bar{\omega}) \qquad (1)$$

upper sign:



(2)

$$= P + \tfrac{1}{2}(-i\,2\pi)\,\delta(\;) \qquad (3)$$



(4)

$$= P + \tfrac{1}{2}(i\,2\pi)\,\delta(\;) \qquad (5)$$

Interpretation of spectral function

GF49

$$A_{AB}(\omega) \overset{(38.3),(42.1)}{\equiv} \frac{1}{Z}\sum_{nm} A_{nm} B_{mn} \left(e^{-\beta E_n} - \xi e^{-\beta E_m}\right) \delta(\hbar\omega - E_m + E_n) \quad (1)$$

Consider $\hat A = \hat B^\dagger = c_k$, then $A_{nm} = \langle n | c_k | m\rangle$, $B_{mn} = \langle m | c_k^\dagger | n\rangle = A^*_{nm}$ (2)

and take limit $T \to 0$, such that $\frac{e^{-\beta E_n}}{Z} \to \delta_{ng}$ (3)

(only ground state contributes)

$$A_{c_k c_k^\dagger}(\omega > 0) = \sum_m |\langle m | \hat c_k^\dagger | g\rangle|^2 \, \delta(\hbar\omega - \underbrace{(E_m - E_g)}_{>0}) \quad (4)$$

$$A_{c_k c_k^\dagger}(\omega < 0) = -\xi \sum_n |\langle n | c_k | g\rangle|^2 \, \delta(\hbar\omega - \underbrace{(E_g - E_n)}_{<0}) \quad (5)$$

Golden-rule rate for perturbing ground state by creation/annihilation of a single particle with momentum $\bar k$, thereby exciting the system by $\pm\omega = |\omega|$ (6)

or: $A_{c_k c_k^\dagger}(\omega)$ counts the number of states with excitation energy $|\omega|$ that can be reached by adding/subtracting a single-particle excitation of momentum k $\Rightarrow$ "density of states" (7)

Spectral function for non-interacting free particles:

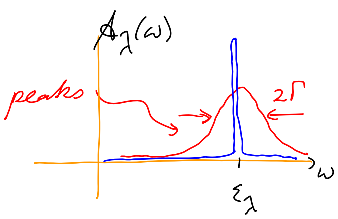
GF50

If $\hat H_0 = \sum_\lambda \varepsilon_\lambda c_\lambda^\dagger c_\lambda$, (1)

then $\bar{\mathcal{G}}_{\lambda\lambda'}(i\omega_\ell) = \bar{\mathcal{G}}_{c_\lambda c^\dagger_{\lambda'}}(i\omega_\ell) \overset{\text{(Problem Set 3.2)}}{=} \dfrac{\delta_{\lambda\lambda'}}{i\omega_\ell - \varepsilon_\lambda}$ (2)

spectral representation: $\overset{(38.4)}{=} \delta_{\lambda\lambda'} \int d\bar\omega \, \dfrac{A_\lambda(\bar\omega)}{i\omega_\ell - \bar\omega}$, with $A_\lambda(\omega) = \delta(\omega - \varepsilon_\lambda)$ (3)

Spectral function of free particles is a δ-function, peaked at single-particle excitation energy. Interactions will broaden these peaks.

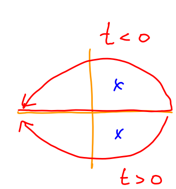


Broadening of spectral function gives finite life-time:

For example, if $A_\lambda(\omega) = \dfrac{\Gamma/\pi}{(\omega - \varepsilon_\lambda)^2 + \Gamma^2}$,

then $\mathcal{G}^{R/A}_\lambda(t) \overset{(43.1)}{=} \mp i\,\theta(\pm t) \int d\bar\omega \, A_\lambda(\bar\omega)\, e^{-i\bar\omega t}$ (6)

$= \theta(\pm t)\, e^{-i\varepsilon_\lambda t}\, e^{-\Gamma t}$ life-time $= 1/\Gamma$ (7)



Analogously to p. 49, the "local density of states" is defined by using $\boxed{GF51}$

$\hat{A} = \hat{\psi}(\vec{r}) = \hat{B}^{\dagger}$:

with $\hat{\psi}(\vec{r},\tau) = \sum_{\lambda} \varphi_{\lambda}(\vec{r}) \underbrace{c_{\lambda}(\tau)}_{= c_{\lambda} e^{-\varepsilon_{\lambda}\tau}}$, $\qquad \varphi_{\lambda}(\vec{r}) = \langle \vec{r} | c^{\dagger}_{\lambda} | \text{Vac} \rangle$ (1)

= single-particle wave function

$$\mathcal{N}(\vec{r},\omega) = \mathcal{A}_{\psi(\vec{r})\psi^{\dagger}(\vec{r})}(\omega) = -\frac{1}{\pi}\,\text{Im}\, \mathcal{G}^{R}(\vec{r},\vec{r};\omega) \qquad (2)$$

$$\left[\text{where } \mathcal{G}(\vec{r},\vec{r}';\tau) \equiv -\langle T_{\tau}\psi(\vec{r},\tau)\,\psi^{\dagger}(\vec{r}',0)\rangle\right] \qquad (3)$$

By analogy to (49.4), (49.5):

$$\mathcal{N}(\vec{r},\omega>0) \overset{T\to 0}{=} \sum_{m} |\langle m|\hat{\psi}^{\dagger}(r)|g\rangle|^2\, \delta(\hbar\omega - \underbrace{(E_m - E_g)}_{>0}) \qquad (4)$$

$$\mathcal{N}(\vec{r},\omega<0) \overset{T\to 0}{=} -\zeta \sum_{n} |\langle n|\hat{\psi}(r)|g\rangle|^2\, \delta(\hbar\omega - \underbrace{(E_g - E_n)}_{<0}) \qquad (5)$$

$\mathcal{N}(\vec{r},\omega \gtrless 0)$ counts the number of states with excitation energy $|\omega|$ that can be reached by adding/subtracting a particle at position $\vec{r}$: "local density of states".

"Total density of states": $\boxed{GF52}$

$$\mathcal{N}(\omega) \equiv \int d\vec{r}\ \mathcal{N}(\vec{r},\omega) \qquad (1)$$

$$\overset{(51.2)}{=} \int d\vec{r}\ \left(-\frac{1}{\pi}\right)\text{Im}\, \mathcal{G}^{R}(\vec{r},\vec{r};\omega) \qquad (2)$$

$$\overset{(51.1)}{=} \int d\vec{r}\ \sum_{\lambda\lambda'} \varphi_{\lambda}(\vec{r})\,\varphi^{*}_{\lambda'}(\vec{r})\ \underbrace{\left(-\frac{1}{\pi}\right)\text{Im}\, \mathcal{G}^{R}_{\lambda\lambda'}(\omega)}_{\overset{(50.3)}{=}\ \delta_{\lambda\lambda'}\underbrace{\mathcal{A}_{\lambda}(\omega)}_{\delta(\omega-\varepsilon_{\lambda})}} \qquad (3)$$

For non-interacting particles, we can use: (50.3) $\delta_{\lambda\lambda'}\, \mathcal{A}_{\lambda}(\omega)$, $\mathcal{A}_{\lambda}(\omega) = \delta(\omega-\varepsilon_{\lambda})$

$$= \sum_{\lambda} \underbrace{\int d\vec{r}\,|\varphi_{\lambda}(\vec{r})|^2}_{=1}\ \delta(\omega-\varepsilon_{\lambda}) \qquad (4)$$

$$= \sum_{\lambda} \delta(\omega-\varepsilon_{\lambda}) \qquad (5)$$

(counts the number of eigenstates with energy ω)

However, definition (2) can be used also for interacting systems.

Sum rules for spectral functions

GF53

$$A_{AB}(\omega) \equiv \frac{1}{Z}\sum_{nm} A_{nm} B_{mn} \left(e^{-\beta E_n} - \xi e^{-\beta E_m}\right) \delta(\hbar\omega - E_m + E_n) \tag{1}$$

$$\int d\omega\, A_{AB}(\omega) = \frac{1}{Z}\sum_{nm}\left(e^{-\beta E_n} A_{nm} B_{mn} - \xi \underset{n \leftrightarrow m}{e^{-\beta E_m} B_{mn} A_{nm}}\right) \tag{2}$$

$$= \langle \hat{A}\hat{B} - \xi \hat{B}\hat{A} \rangle = \langle [\hat{A}, \hat{B}]_\xi \rangle \quad \left[\begin{matrix}\text{exact} \\ \text{result}\end{matrix}\right] \tag{3}$$

Total weight of spectral function is fixed by a sum rule

For single-particle operators, e.g. $\hat{A} = \hat{c}_\lambda$, $\hat{B} = \hat{c}^\dagger_{\lambda'}$: (4)

$$\int d\omega\, A_{c_\lambda c^\dagger_{\lambda'}}(\omega) = \langle [\hat{c}_\lambda, \hat{c}^\dagger_{\lambda'}]_\xi \rangle = \delta_{\lambda\lambda'} \tag{5}$$

$\Rightarrow$ Single-particle spectral functions are usually normalized to unity.

Further useful relations :

GF54

$$A^*_{AB}(\omega) \overset{(38.3)}{=} \frac{1}{Z}\sum_{nm} A^*_{nm} B^*_{mn} \left(e^{-\beta E_n} - \xi e^{-\beta E_m}\right)\delta(\hbar\omega - E_m + E_n) = A_{B^\dagger A^\dagger}(\omega) \tag{1}$$

$$\langle n|A|m\rangle^* \langle m|B|n\rangle^* = \langle n|B^\dagger|m\rangle\langle m|A^\dagger|n\rangle \tag{2}$$

$$A^*_{AA^\dagger}(\omega) \overset{(1)}{=} A_{AA^\dagger}(\omega) = \text{real} \tag{3}$$

$$= \frac{1}{Z}\sum_{nm} |A_{nm}|^2 \left(e^{-\beta E_n} - \xi e^{-\beta E_m}\right)\delta(\hbar\omega - E_m + E_n) \tag{4}$$

$$= \begin{cases} \geq 0 & \text{for fermions } (\xi = -1) & (5) \\ \geq 0 & \text{for bosons if } \omega > 0 \; (\xi = +1) \text{ since then } E_m > E_n & (6) \end{cases}$$

$$G^{R*}_{AB}(\omega) = \int d\bar{\omega} \left(\frac{A_{AB}(\bar{\omega})}{\omega + i\alpha - \bar{\omega}}\right)^* = \int d\bar{\omega}\, \frac{A_{B^\dagger A^\dagger}(\bar{\omega})}{\omega - i\alpha - \bar{\omega}} = G^A_{B^\dagger A^\dagger}(\omega) \tag{7}$$

$$G^*_{AA^\dagger}(\omega) \overset{(8)}{=} G^R_{AA^\dagger}(\omega), \quad \Rightarrow \quad A_{AA^\dagger}(\omega) = \frac{i}{2\pi}\left[G^R - G^A\right]_{AA^\dagger}(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\, G^R_{AA^\dagger}(\omega) \tag{9}$$