Lect 4: operator formalism, response function,

§1: perturbation theory

Consider a system with Hamiltonian H, and we add an external perturbation $f(t)\, O_1$, (H may contain interaction).

$$H + f(t)\, O_1 .$$

We assum that at $t=-\infty$, $f(t)\to 0$, and then the eigenstates $|\psi_n\rangle$ correspond to H. At time t, we have

$$|\psi_n(t)\rangle = T\left[e^{-i\int_{-\infty}^{t} dt' \left[H + f(t)\, O_1\right]} \right] |\psi_n\rangle ,$$

where T is the time-ordering operator.

Assuming $f(t)$ is small, we expand

$$T\left[e^{-i\int_{-\infty}^{t} dt' (H + f(t) O_1)}\right] = T\left[e^{-i\int_{-\infty}^{t} dt' H} \left(1 + (-i)\int_{-\infty}^{t} dt'' f(t'')\, O_1\right)\right]$$

$$= e^{-i(t-t_{-\infty})H} - i\int_{-\infty}^{t} dt'' \, e^{-i\int_{t''}^{t} dt' H} \left[f(t'')\, O_1\right] e^{-i\int_{-\infty}^{t''} dt' H}$$

$$= e^{-i(t-t_{-\infty})H} - i\int_{-\infty}^{t} dt' \, e^{-iH(t-t')} \left[f(t')\, O_1\right] e^{-iH(t'-t_{-\infty})}$$

$$\Rightarrow |\psi_n(t)\rangle = e^{-i\int_{t_{-\infty}}^{t} dt' H} |\psi_n(t)\rangle + \delta|\psi_n(t)\rangle$$

with $\delta|\psi_n(t)\rangle = -i\int_{t_{-\infty}}^{t} dt'\; e^{-iH(t-t')}\left[f(t')\, O_1\right] e^{-iH(t'-t_{-\infty})}\,|\psi_n\rangle$

$$\boxed{\begin{aligned}&\delta|\psi_n(t)\rangle = -i\int_{t_{-\infty}}^{t} dt'\; f(t')\; e^{-iH(t-t_{-\infty})}\; O_1(t')\;|\psi_n\rangle \\ &\text{where}\quad O_1(t) = e^{iH(t-t_{-\infty})}\, O_1\, e^{-iH(t-t_{-\infty})} \leftarrow \text{interaction picture.}\end{aligned}}$$

§. Calculation of Physical quantity O_2

$$\delta O_2(t) = \langle\psi_n(t)|\,O_2\,|\psi_n(t)\rangle - \langle\psi_n|\,e^{iH(t-t_{-\infty})}\,O_2\,e^{-iH(t-t_{-\infty})}\,|\psi_n\rangle$$

$$= -i\int_{t_{-\infty}}^{t} dt' \Big\{\langle\psi_n|\, e^{i(t-t_{-\infty})H}\, O_2\, e^{-iH(t-t_{-\infty})}\, f(t')\, O_1(t')\,|\psi_n\rangle - \langle\psi_n|\, O_1(t')f(t')\, e^{iH(t-t_{-\infty})}\, O_2\, e^{-i(t-t_{-\infty})H}\,|\psi_n\rangle$$

$$= -i\int_{t_{-\infty}}^{t} dt'\; \langle\psi_n|\,[\,O_2(t),\, O_1(t')\,]\,|\psi_n\rangle\; f(t')$$

we define retarded Green's function

$$\boxed{D(t-t') = -i\,\Theta(t-t')\,\langle\,|\,[\,O_2(t),\, O_1(t')\,]\,|\,\rangle},$$

where $\langle|\cdots|\rangle$ means $\langle\psi_0|\cdots|\psi_0\rangle$ at zero temperature, and thermal average at finite T. We have $\boxed{\delta O_2(t) = \int_{-\infty}^{+\infty} dt'\; D(t,t')\; f(t')}$

A simple example: Hamonic oscillater in an external E field

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 x^2, \quad \text{and} \quad H_1 = -exE$$

· Calculate polarizibility

① $|\psi_0\rangle = |0\rangle + \sum_n |n\rangle\langle n|H_1|0\rangle/(E_0 - E_n)$

$$d = \langle\psi_0|ex|\psi_0\rangle = -2E\sum_{n>0}\frac{\langle 0|ex|n\rangle\langle n|ex|0\rangle}{E_0 - E_n} = 2e^2E\frac{\langle 0|x^2|0\rangle}{\omega_0}$$

$$\Rightarrow \chi = 2e^2\frac{\langle 0|x^2|0\rangle}{\omega_0}.$$ — straight forward calculation.

② method of Green's function:

Set $H_1(t) = -exE\, e^{-\eta|t|}$, and $\eta \to 0^+$

$$d(t) = \int_{-\infty}^{+\infty} dt'\, e^2 D(t-t')\, e^{\eta t'} (-E)$$

$$D(t-t') = -i\Theta(t-t')\langle 0|[x(t), x(t')]|0\rangle$$

$$= -i\Theta(t-t')\left\{\langle 0|e^{iHt}x e^{-iH(t-t')}x e^{-iHt'}|0\rangle - \langle 0|e^{iHt'}x e^{-iH(t'-t)}x e^{-iHt}|0\rangle\right.$$

$$= -i\Theta(t-t')\left[\langle 0|x|1\rangle\langle 1|x|0\rangle\left(e^{-i(E_1-E_0)(t-t')} - e^{i(E_1-E_0)(t-t')}\right)\right.$$

$$= -2\Theta(t-t')\langle 0|x^2|0\rangle \sin\omega_0(t-t')$$

The d at zero frequency $\boxed{d(\omega=0) = -e^2 D(\omega=0)E}$, we need to calculate $D(\omega)$.

$$D(\omega) = \int_{-\infty}^{+\infty} d(t-t')\ e^{i(\omega+i\eta)(t-t')} (-i)\,\Theta(t-t')\langle 0|x^2|0\rangle\left(e^{-i\omega_0(t-t')} - e^{i\omega_0(t-t')}\right)$$

$\omega + i\eta \leftarrow$ control the convergence of the integral

$$\Rightarrow D(\omega) = -i\int_0^{+\infty} dt\ \langle 0|x^2|0\rangle\left[e^{i(\omega-\omega_0+i\eta)t} - e^{i(\omega+\omega_0+i\eta)t}\right]$$

$$= \langle 0|x^2|0\rangle\, i\left[\frac{1}{i(\omega-\omega_0+i\eta)} - \frac{1}{i(\omega+\omega_0+i\eta)}\right]$$

$$= \langle 0|x^2|0\rangle\left[\frac{1}{\omega-\omega_0+i\eta} - \frac{1}{\omega+\omega_0+i\eta}\right] = \langle 0|x^2|0\rangle\frac{2\omega_0}{\omega^2-\omega_0^2+i\,\mathrm{sgn}\,\omega\,\eta}$$

$$\Rightarrow D(\omega=0) = \frac{-2\langle 0|x^2|0\rangle}{\omega_0}, \quad \text{and } d(\omega=0) = \frac{2e^2\langle 0|x^2|0\rangle}{\omega_0}E.$$

§ Time-ordered correlation function and path integral harmonic oscillator

First assume $t>t'$, the first term of the retarded Green's function

$$\langle 0|O_2(t)O_1(t')|0\rangle = \langle 0|\mathcal{U}^\dagger(t,-\infty)\ O_2\ \mathcal{U}(t,t')\ O_1\ \mathcal{U}(t',-\infty)|0\rangle$$

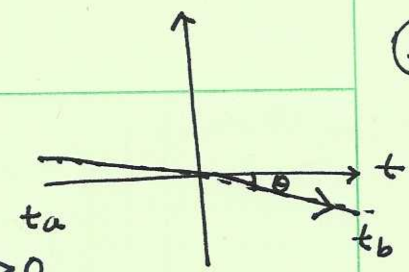
$$= \langle 0|\mathcal{U}^\dagger(+\infty,-\infty)\ \mathcal{U}(+\infty,t)\ O_2\ \mathcal{U}(t,t')\ O_1\ \mathcal{U}(t',-\infty)|0\rangle$$

- assume adibatic process, the system return to $|0\rangle$ at $t\to+\infty$,

$\langle 0|\mathcal{U}(+\infty,-\infty)|0\rangle$ is a phase.

$$\Rightarrow \boxed{\langle 0|O_2(t)O_1(t')|0\rangle = \frac{\langle 0|\mathcal{U}(+\infty,t)\,O_2\,\mathcal{U}(t,t')\,O_1\,\mathcal{U}(t',-\infty)|0\rangle}{\langle 0|\mathcal{U}(+\infty,-\infty)|0\rangle}}$$

we generalize the time-evolution to complex plane



$$\mathcal{U}^{\theta}(t_b, t_a) = e^{-i\{H(t_b-t_a)\, e^{-i\theta}\}}, \quad t_b > t_a \text{ and } \theta > 0.$$

we can choose arbitary state $|\psi\rangle$, after we apply $\mathcal{U}^{\theta}(t_b,t_a)|\psi\rangle$ as $t_b - t_a \to +\infty$, only the ground state is projected out. Then we have

$$\langle 0|\, O_2(t)\, O_1(t')|0\rangle = \frac{\langle\psi|\,\mathcal{U}^{\theta}(\infty,t)\, O_2\, \mathcal{U}^{\theta}(t,t')\, O_1\, \mathcal{U}^{\theta}(t',-\infty)|\psi\rangle}{\langle\psi|\,\mathcal{U}^{\theta}(\infty,-\infty)\,|\psi\rangle}$$

let's choose $|\psi\rangle = \delta(x-x_0) = |x_0\rangle$ as position eigenstate

$$\Rightarrow \langle x_0|\,\mathcal{U}^{\theta}(\infty,-\infty|x_0\rangle = \int \underset{\uparrow}{DX(t)}\; e^{i\int_{-\infty}^{+\infty} dt\, \mathcal{L}(x,\dot{x})}$$

path initial & final position at x_0

$$\langle x_0|\,\mathcal{U}^{\theta}(\infty t)\, \underbrace{O_2}_{(X(t))}\, \mathcal{U}^{\theta}(t\ t')\, O_1(X(t'))\, \mathcal{U}^{\theta}(t',-\infty)\,|x_0\rangle$$

$$= \int DX(t)\;\; e^{i\int_{t}^{+\infty} dt\, \mathcal{L}(x,\dot{x})}\; O_2(X(t))\; e^{i\int_{t'}^{t} dt\, \mathcal{L}(x x')}\; O_1(X(t'))\; e^{i\int_{-\infty}^{t'} dt\, \mathcal{L}(x x')}$$

$$= \int DX(t)\;\; O_2(X(t))\, O_1(X(t'))\;\; e^{i\int_{-\infty}^{+\infty} dt\; \mathcal{L}(x,x')}$$

where O_1, and O_2 are functions of coordinates. ~~the~~ The integral argument $t \to t\, e^{-i\theta}$

The key point of the expression of $\int Dx(t)\, O_2(x(t))\, O_1(x(t'))\, e^{i\int_{-\infty}^{+\infty} dt\, \mathcal{L}}$ is that: when we map it to operator formalism, the operator should be time-ordered! Thus if $t' > t$, we have

$$\int Dx(t)\, O_2(x(t)) O_1(x(t'))\, e^{i\int_{-\infty}^{+\infty} dt\, \mathcal{L}} = \int Dx(t)\, e^{i\int_{t'}^{+\infty} dt\, \mathcal{L}}\, O_1(x(t'))\, e^{i\int_{t}^{t'} dt\, \mathcal{L}}\, \overbrace{O_2(x(t))\, e^{i\int_{-\infty}^{t} dt\, \mathcal{L}}}$$

$$= \langle x_0 |\, U^\theta(\infty, t')\, O_1(x(t'))\, U^\theta(t', t)\, O_2(x(t))\, U^\theta(t, -\infty)\, | x_0 \rangle$$

$\Rightarrow$ Combine both cases of $t > t'$ and $t' > t$, we have

$$\boxed{\frac{\int Dx(t)\, O_2(x(t))\, O_1(x(t'))\, e^{i\int_{-\infty}^{+\infty} dt\, \mathcal{L}(x, x')}}{\int Dx(t)\, e^{i\int_{-\infty}^{+\infty} dt\, \mathcal{L}(x, x')}} = T\langle 0 |\, O_2(t)\, O_1(t')\, | 0 \rangle}$$

we define the time-ordered Green's function as

$$G(t_2, t_1) = -i \langle 0 |\, T(O_2(t_2)\, O_1(t_1))\, | 0 \rangle = \begin{cases} -i \langle 0 |\, O_2(t_2)\, O_1(t_1)\, | 0 \rangle & t_2 > t_1 \\ -i \langle 0 |\, O_1(t_1)\, O_2(t_2)\, | 0 \rangle & t_1 > t_2 \end{cases}$$

Example: For harmonic oscillator $H = \frac{p^2}{2m} + \frac{1}{2} m \omega_0^2 x^2$, we define

$$G(t_2 t_1) = -i \langle 0 | T\, x(t_2)\, x(t_1) | 0 \rangle, \text{ then}$$

$$iG(t_2 t_1) = \frac{\int Dx(t)\, x(t_2) x(t_1)\, e^{\, i \int_{-\infty}^{+\infty} dt\, -\frac{x}{2}\left(m \frac{d^2}{dt^2} x\right) - \frac{m}{2}\omega_0^2 x^2}}{\int Dx(t)\, e^{\, i \int_{-\infty}^{+\infty} dt\, -\frac{x}{2}\left(m \frac{d^2}{dt^2} x\right) - \frac{m}{2}\omega_0^2 x^2}}$$

"t" is understood as $t \to t e^{-i\theta}$ with $\theta = 0^+$,

and $\frac{d^2}{dt^2} \longrightarrow \frac{d^2}{dt^2} e^{2i\theta}$.

According to the formula of Gaussian integral

$$\int \prod_i dx_i \; x_{i_1} x_{i_2}\, e^{-\frac{1}{2} x_i A_{ij} x_j} \Big/ \int \prod_i dx_i\, e^{-\frac{1}{2} x_i A_{ij} x_j} = \left(A^{-1}\right)_{i_1 i_2}$$

the, A operator is just

$$\left\{ i \left[m \left(e^{i\theta} \frac{d}{dt}\right)^2 + \omega_0^2 e^{-i\theta} \right] \right\}^{-1}$$

$\Rightarrow$ $iG(t_2, t_1)$ satisfies the different equation

$$iG(t_2, t_1) = \left\{ i \left[m \left(e^{i\theta} \frac{d}{dt}\right)^2 + \omega_0^2 e^{-i\theta} \right] \right\}^{-1}_{t_2, t_1}$$

$$\Rightarrow \left[m e^{2i\theta} \frac{d^2}{dt_2^2} + \underbrace{m\omega_0^2}_{e^{-i\theta}} \right] G(t_2, t_1) = -\delta(t_2, t_1)$$

change to frequency space

$$G(\omega) = \int dt\, e^{i\omega t}\, G(t,0) \Rightarrow$$

$$\left(e^{i2\theta}\, m\, \omega^2 - m\omega_0^2\, e^{-i\theta}\right) G(\omega) = 1$$

only $\omega = \omega_0$, we need to worry, the imaginay part, and we only need to know the imaginary part $\rightarrow i0^+$, or $i0^-$.

Apparently, the above Eq. $\rightarrow$

$$\left\{ m(\omega^2 - \omega_0^2) + i0^+ \right\} G(\omega) = 1$$

or $$\boxed{G(\omega) = \frac{1/m}{\omega^2 - \omega_0^2 + i0^+}}$$

$G(\omega)$ is just the inverse of the operator $-m\frac{d^2}{dt^2} - m\omega_0^2$.

$G(\omega)$ canbe expressed as (time-ordered)

$$G(\omega) = \frac{1}{2\omega_0 m}\left[\frac{1}{\omega - \omega_0 + i\,\mathrm{sgn}\,\omega \cdot \eta} - \frac{1}{\omega + \omega_0 + i\,\mathrm{sgn}\,\omega \cdot \eta}\right]$$

Compare the retarded one, we derived before. Plug in $\langle 0 | x^2 | 0 \rangle = \frac{1}{2m\omega_0}$,

$$\Rightarrow D(\omega) = \frac{1}{2\omega_0 m}\left[\frac{1}{\omega - \omega_0 + i\eta} - \frac{1}{\omega + \omega_0 + i\eta}\right]$$

§ Relation between different Green functions

The response function (retaroted) is directly related to physical observables, but time-ordered one is easy to calculate through path integrals. Both of them can be connected by the imaginary Green's function, or, Matsubara Green's function, defined as

$$\boxed{\mathcal{G}(\tau) = -\langle T_\tau [O_2(\tau)\, O_1(0)] \rangle, \text{ where } O(\tau) = e^{H\tau} O\, e^{-H\tau} \quad (-\beta \le \tau \le \beta)}$$

if O_2, O_1 are bosonic operators, they satisfy

$$\mathcal{G}(\tau) = \mathcal{G}(\tau+\beta),$$

if O_2, O_1 are fermionic operators, they satisfy

$$\mathcal{G}(\tau) = -\mathcal{G}(\tau+\beta). \quad \leftarrow \text{ Please prove.}$$

$\Rightarrow$ For bosonic operators

$$\mathcal{G}(i\omega_n) = \frac{1}{2}\left[\int_{-\beta}^{0} d\tau\, \mathcal{G}(\tau)\, e^{i\tau\omega_n} + \int_0^\beta d\tau\, \mathcal{G}(\tau)\, e^{i\tau\omega_n}\right]$$

$$= \int_0^\beta d\tau\, \mathcal{G}(\tau)\, e^{i\tau\omega_n}\, \frac{1+e^{i\omega_n\beta}}{2}, \quad \text{only for } \omega_n = \frac{2n\pi}{\beta}$$

Fourier componets survies

$$\boxed{\mathcal{G}(i\omega_n) = \int_0^\beta d\tau\, \mathcal{G}(\tau)\, e^{i\tau\omega_n} \quad \text{for } \omega_n = \frac{2n\pi}{\beta}}$$

Similarly for fermionic operators

$$\boxed{\mathcal{G}(i\omega_n) = \int_0^\beta d\tau \; \mathcal{G}(\tau)\, e^{i\tau\omega_n} \quad \text{for } \omega_n = \frac{(2n+1)\pi}{\beta}}$$

At $\tau > 0$,

$$\mathcal{G}(\tau) = -\, e^{\beta\Omega} \sum_{nm} \langle n|\, e^{-\beta H} e^{H\tau}\, O_2\, e^{-H\tau} |m\rangle\langle m|\, O_1 \,|n\rangle$$

(where $Z = e^{\beta\Omega}$)

$$= -e^{\beta\Omega} \sum_{nm} e^{-\beta E_n}\, e^{(E_n - E_m)\tau} \langle n|\, O_2 \,|m\rangle\langle m|\, O_1 \,|n\rangle$$

$$\Rightarrow \mathcal{G}(i\omega_n) = -e^{\beta\Omega} \int_0^\beta d\tau\; e^{i\omega_n\tau}\, e^{(E_n - E_m)\tau} \langle n|\, O_2 \,|m\rangle\langle m|\, O_1 \,|n\rangle\, e^{-\beta E_n}$$

$$\boxed{\mathcal{G}(i\omega_n) = e^{\beta\Omega} \sum_{nm} \frac{\langle n|\, O_2 \,|m\rangle\langle m|\, O_1 \,|n\rangle}{i\omega_n + E_n - E_m} \left(e^{-\beta E_n} \mp e^{-\beta E_m}\right)}$$

$\mp$ for bosonic / fermionic operators, respectively.

This expression is often called Lehman - representation.

Now $D_{ret}(t-t') = -i\,\Theta(t-t') \left\langle \left| [\, O_2(t),\, O_1(t') \,]_{\mp} \right| \right\rangle$

$$= -i\,\Theta(t-t')\, e^{\beta\Omega} \sum_{nm} \langle n|\, O_2 \,|m\rangle\langle m|\, O_1 \,|n\rangle\, e^{i(E_n - E_m)(t-t')}$$

$$\times \left(e^{-\beta E_n} \mp e^{-\beta E_m} \right)$$

$$\boxed{\begin{aligned} D_{ret}(\omega) &= \int_{-\infty}^{+\infty} d(t-t')\; e^{i\omega(t-t')}\; D_{ret}(t-t') \\ &= \sum_{nm} e^{\beta\Omega}\, \frac{\langle n|O_2|m\rangle\langle m|O_1|n\rangle\,(e^{-\beta E_n} \mp e^{-\beta E_m})}{\omega + (E_n - E_m) + i\eta} \end{aligned}}$$

Next check the time-ordered Green's function

$$G(t-t') = -i\Theta(t-t')\langle\,|O_2(t)\,O_1(t')|0\rangle \mp (-i\Theta(t'-t)\langle|O_1(t')\,O_2(t)|\rangle$$

$$= -i\Theta(t-t')\,e^{\beta\Omega}\sum_{nm}\langle n|O_2|m\rangle\langle m|O_1|n\rangle\, e^{-\beta E_n}\, e^{i(E_n-E_m)(t-t')}$$

$$\pm(-i\Theta(t'-t)\,e^{\beta\Omega}\sum_{nm}\langle n|O_2|m\rangle\langle m|O_1|n\rangle\, e^{-\beta E_m}\; e^{i(E_n-E_m)(t-t')}$$

$$= e^{\beta\Omega}\sum_{nm}\langle n|O_2|m\rangle\langle m|O_1|n\rangle\, e^{i(E_n-E_m)(t-t')}\,\big(-i\Theta(t-t')\,e^{-\beta E_n} \pm (-i\Theta(t'-t)\,e^{-\beta E_m}\big)$$

$$\Rightarrow \boxed{G(\omega) = \sum_{nm} e^{\beta\Omega}\langle n|O_2|m\rangle\langle m|O_1|n\rangle \left\{ \frac{e^{-\beta E_n}}{\omega + E_n - E_m + i\eta} \mp \frac{e^{-\beta E_m}}{\omega + E_n - E_m - i\eta} \right\}.}$$

$$\cancel{G(\omega) = \sum_{nm} e^{\beta\Omega} \langle n|O_2|m\rangle\langle m|O_1|n\rangle \left\{ \frac{e^{-\beta E_n}}{\omega + E_n - E_m + i\eta} \mp \frac{e^{-\beta E_m}}{\omega + E_n - E_m - i\eta} \right\}}$$

thus:

$$\boxed{\begin{array}{l} D_{ret}(\omega) \text{ can be arrived by analytical continuition} \\ \qquad \mathcal{G}(i\omega_n)\big|_{i\omega_n \to \omega + i\eta}. \\ \text{at zero temperature: } \beta \to +\infty \\ G(\omega) = \sum \langle 0|O_2|m\rangle\langle m|O_1|0\rangle \dfrac{1}{\omega + (E_0 - E_m) + i\eta} \mp \langle n|O_2|0\rangle\langle 0|O_1|n\rangle \dfrac{1}{\omega + (E_n - E_0) - i\eta} \\ = \mathcal{G}(i\omega_n)\big|_{i\omega_n \to \omega + i\,\mathrm{sgn}(\omega)\eta}. \end{array}}$$

Define the spectral function as

$$A_+(\omega) = 2\pi \sum_{nm} e^{\beta\Omega} \langle n|O_2|m\rangle\langle m|O_1|n\rangle\, e^{-\beta E_n}\, \delta(\omega + E_n - E_m)$$

$$A_-(\omega) = 2\pi \sum_{nm} e^{\beta\Omega} \langle n|O_2|m\rangle\langle m|O_1|n\rangle\, e^{-\beta E_m}\, \delta(\omega + E_n - E_m)$$

$$= 2\pi \sum_{nm} e^{\beta\Omega} \langle m|O_2|n\rangle\langle n|O_1|m\rangle\, e^{-\beta E_n}\, \delta(\omega - (E_n - E_m))$$

$$A(\omega) = -2\,\mathrm{Im}\, D_{ret}(\omega) = A_+(\omega) \mp A_-(\omega)$$

$$A_+(\omega) = e^{\beta\omega} A_-(\omega)$$

we have $\quad i\,G(t)\big|_{t>0} = \displaystyle\int \frac{d\omega}{2\pi} A_+(\omega)\, e^{-i\omega t}$

$$i\,G(t)\big|_{t<0} = \pm \int \frac{d\omega}{2\pi} A_-(\omega)\, e^{-i\omega t}$$

if $O_1 = O_2^\dagger$, we have $A_+(\omega) = \frac{-1}{1 \pm e^{-\beta\omega}} \left(2\,\mathrm{Im}\, G(\omega) \right)$

$$= -[1 \pm n_{B/F}(\omega)] \left(2\,\mathrm{Im}\, D(\omega) \right)$$

Check: $-2\,\mathrm{Im}\, G(\omega) = A_+(\omega) \mp (-) A_-(\omega) = A_+(\omega) \left(1 \pm e^{-\beta\omega} \right)$

$$\Rightarrow A_+(\omega) = -2\,\mathrm{Im}\, G(\omega) \Big/ \left(1 \pm e^{-\beta\omega} \right)$$