

—Chapter 5—

Linear Response Theory

5-1 Linear Response Function

A. LINEAR RESPONSE

- (1) Time-dependent perturbation theory:

Consider the many-body Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}(t)$, where $\hat{H}_0$ is the unperturbed Hamiltonian and $\hat{V}(t) = \hat{O}(t)\eta(t)$ is the external perturbation driven by a small external field $\eta(t)$.

- (2) The expectation value of an observable $\hat{A}$ can be series expanded up to the first order as,

$$\langle \hat{A}(t) \rangle = \langle \hat{A} \rangle_0 + \int_0^t \frac{\delta \langle \hat{A}(t) \rangle}{\delta \eta(t')} \bigg|_{\eta=0} \eta(t') dt'$$

where $\langle \hat{A}(t) \rangle$ is the quantum and thermal average of $\hat{A}$ at time t , and $\langle \hat{A} \rangle_0$ is the equilibrium amount obtained when $\eta(t) = 0$.

A linear response is defined as

$$\delta \langle \hat{A}(t) \rangle = \langle \hat{A}(t) \rangle - \langle \hat{A} \rangle_0 = \int_0^\infty \chi(t, t') \eta(t') dt'$$

where

$$\chi(t, t') = \frac{\delta \langle \hat{A}(t) \rangle}{\delta \eta(t')} \bigg|_{\eta=0}$$

is called the response function.

NOTE:

In this definition, the upper boundary of the integral extends to $+\infty$, i.e., formally involves the generalized force in the future of the time t at which the effect $\langle \hat{A}(t) \rangle$ is considered, which violates causality. Causality requirement can be ensured by introducing a step function $\Theta(t - t')$.

EXAMPLES:

1. Time-independent perturbation theory:

Considering a harmonic oscillator in an applied electric field:

The Hamiltonian is

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2}_{\hat{H}_0} - \underbrace{ex\mathcal{E}}_{\hat{V}}$$

where $\hat{H}_0$ is the unperturbed Hamiltonian with

$$\hat{H}_0|\phi_n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|\phi_n\rangle$$

$\hat{V}$ is the polarization perturbation, and $\mathcal{E}$ is the electric field.

The induced dipole moment is given by

$$d = \langle\psi_n|ex|\psi_n\rangle,$$

where $|\psi_n\rangle$ is the eigenstate of $\hat{H}$.

The eigenstate up to the first order correction

$$|\psi_n\rangle = |\phi_n^{(0)}\rangle + \sum_{m \neq n} \frac{\langle\phi_m^{(0)}|\hat{V}|\phi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} |\phi_m^{(0)}\rangle$$

where $\langle\phi_m^{(0)}|\hat{V}|\phi_n^{(0)}\rangle \ll |E_n^{(0)} - E_m^{(0)}|$

The dipole moment up to the linear order is

$$\begin{aligned} d &= \langle\psi_n|ex|\psi_n\rangle \\ &= \left(\langle\phi_n^{(0)}| + \sum_{m \neq n} \frac{\langle\phi_n^{(0)}|\hat{V}|\phi_m^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} \langle\phi_m^{(0)}| \right) ex \\ &\quad \times \left(|\phi_n^{(0)}\rangle + \sum_{m \neq n} \frac{\langle\phi_m^{(0)}|\hat{V}|\phi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} |\phi_m^{(0)}\rangle \right) \\ &= \langle\phi_n^{(0)}|ex|\phi_n^{(0)}\rangle + \sum_{m \neq n} \frac{\langle\phi_m^{(0)}|-ex\mathcal{E}|\phi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} \langle\phi_n^{(0)}|ex|\phi_m^{(0)}\rangle \\ &\quad + \sum_{m \neq n} \frac{\langle\phi_n^{(0)}|-ex\mathcal{E}|\phi_m^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} \langle\phi_m^{(0)}|ex|\phi_n^{(0)}\rangle + \dots \\ &= \langle\phi_n^{(0)}|ex|\phi_n^{(0)}\rangle - 2\mathcal{E} \sum_{m \neq n} \frac{\langle\phi_n^{(0)}|ex|\phi_m^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} \langle\phi_m^{(0)}|ex|\phi_n^{(0)}\rangle \end{aligned}$$

Since $\langle\phi_n^{(0)}|\hat{x}|\phi_n^{(0)}\rangle = 0$

$$d = -2\mathcal{E} \sum_{m \neq n} \frac{\langle\phi_n^{(0)}|ex|\phi_m^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}} \langle\phi_m^{(0)}|ex|\phi_n^{(0)}\rangle$$

For the ground state ($n = 0$), $E_0^{(0)} - E_m^{(0)} \approx -\hbar\omega$

$$d = \frac{2e^2\mathcal{E}}{\hbar\omega} \sum_{m=0} \langle \phi_0^{(0)} | x | \phi_m^{(0)} \rangle \langle \phi_m^{(0)} | x | \phi_0^{(0)} \rangle = \frac{2e^2\mathcal{E} \langle \phi_0^{(0)} | x^2 | \phi_0^{(0)} \rangle}{\hbar\omega}$$

- (3) The calculation of the measurable response is set in the interaction picture with respect to the perturbation operator $\hat{V}_I(t)$, i.e.,

$$\begin{aligned} |\Phi(t)\rangle &= \hat{S}^\dagger(t, 0) |\Phi(0)\rangle \\ &= \hat{T} \left[\exp \left(\frac{i}{\hbar} \int_0^t \hat{V}_I(t') dt' \right) \right] |\Phi(0)\rangle \\ &= \left(\hat{1} - \frac{i}{\hbar} \int_0^t \hat{O}_I(t') \eta(t') dt' + \dots \right) |\Phi(0)\rangle \end{aligned}$$

We expand $|\Phi(t)\rangle$ to first order in $\hat{V}_I$ as

$$|\Phi(t)\rangle = |\Phi(0)\rangle - \frac{i}{\hbar} \int_0^t \hat{O}_I(t') \eta(t') dt' |\Phi(0)\rangle$$

The expectation value of $\hat{A}_I(t)$ in the interaction picture is

$$\begin{aligned} \langle \Phi(t) | \hat{A}_I(t) | \Phi(t) \rangle &= \langle \Phi(0) | \hat{A}_I(t) | \Phi(0) \rangle - \frac{i}{\hbar} \int_0^t \langle \Phi(0) | \hat{A}_I(t) \hat{O}_I(t') | \Phi(0) \rangle \eta(t') dt' \\ &\quad + \frac{i}{\hbar} \int_0^t \langle \Phi(0) | \hat{O}_I(t') \hat{A}_I(t) | \Phi(0) \rangle \eta(t') dt' \\ &= \langle \Phi(0) | \hat{A}_I(t) | \Phi(0) \rangle - \frac{i}{\hbar} \int_0^t \langle \Phi(0) | [\hat{A}_I(t), \hat{O}_I(t')] | \Phi(0) \rangle \eta(t') dt' \end{aligned}$$

The linear response function including the causality, the retarded response function, is

$$\chi(t, t') = -\frac{i}{\hbar} \Theta(t - t') \langle \Phi(0) | [\hat{A}_I(t), \hat{O}_I(t')] | \Phi(0) \rangle$$

which is also called Kubo formula.

EXAMPLES:

1. Time-dependent perturbation theory:

Considering a harmonic oscillator in an applied electric field:

The Hamiltonian is

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 x^2}_{\hat{H}_0} - \underbrace{ex\mathcal{E}}_{\hat{V}}$$

where $\hat{H}_0$ is the unperturbed Hamiltonian with

$$\hat{H}_0|\phi_n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|\phi_n\rangle$$

$\hat{V}$ is the polarization perturbation, and $\mathcal{E}$ is the electric field.

In the interaction picture, the response function of $\hat{A}_I(t)$ is

$$\begin{aligned}\chi(t, t') &= -\frac{i}{\hbar}\Theta(t - t')\langle\phi_0|[\hat{A}_I(t), \hat{O}_I(t')]| \phi_0\rangle \\ &= -\frac{i}{\hbar}\Theta(t - t')\left(\langle\phi_0|\hat{A}_I(t)\hat{O}_I(t')|\phi_0\rangle - \langle\phi_0|\hat{O}_I(t')\hat{A}_I(t)|\phi_0\rangle\right)\end{aligned}$$

Since

$$\begin{aligned}\hat{A}_I(t) &= e^{i\hat{H}_0 t/\hbar} x e^{-i\hat{H}_0 t/\hbar} \\ \hat{O}_I(t') &= e^{i\hat{H}_0 t'/\hbar} x \mathcal{E} e^{-i\hat{H}_0 t'/\hbar}\end{aligned}$$

we obtain

$$\begin{aligned}\langle\phi_0|\hat{A}_I(t)\hat{O}_I(t')|\phi_0\rangle &= e^2\mathcal{E}\left\langle\phi_0\left|e^{i\hat{H}_0 t/\hbar} x e^{-i\hat{H}_0 t/\hbar} e^{i\hat{H}_0 t'/\hbar} x e^{-i\hat{H}_0 t'/\hbar}\right|\phi_0\right\rangle \\ &= e^2\mathcal{E}\sum_n\langle\phi_0|e^{i\hat{H}_0 t/\hbar} x e^{-i\hat{H}_0 t/\hbar}|\phi_n\rangle\langle\phi_n|e^{i\hat{H}_0 t'/\hbar} x e^{-i\hat{H}_0 t'/\hbar}|\phi_0\rangle \\ &= e^2\mathcal{E}\sum_n e^{-i\omega_n(t-t')}\langle\phi_0|x|\phi_n\rangle\langle\phi_n|x|\phi_0\rangle\end{aligned}$$

Similarly,

$$\langle\phi_0|\hat{O}_I(t')\hat{A}_I(t)|\phi_0\rangle = e^2\mathcal{E}\sum_n e^{-i\omega_n(t'-t)}\langle\phi_0|x|\phi_n\rangle\langle\phi_n|x|\phi_0\rangle$$

Thus, we obtain

$$\begin{aligned}\chi(t - t') &= -\frac{i}{\hbar}\Theta(t - t')e^2\mathcal{E}\sum_n\left(e^{-i\omega_n(t-t')} - e^{-i\omega_n(t'-t)}\right) \\ &\quad \times \langle\phi_0|x|\phi_n\rangle\langle\phi_n|x|\phi_0\rangle \\ &= -\frac{2e^2\mathcal{E}}{\hbar}\Theta(t - t')\sum_n\sin\omega_n(t - t') \\ &\quad \times \langle\phi_0|x|\phi_n\rangle\langle\phi_n|x|\phi_0\rangle\end{aligned}$$

For the ground state, assume that $\omega_n \approx \omega$

$$\begin{aligned}\chi(t - t') &= -\frac{2e^2\mathcal{E}}{\hbar}\Theta(t - t')\sin\omega(t - t')\sum_n\langle\phi_0|x|\phi_n\rangle\langle\phi_n|x|\phi_0\rangle \\ &= -\frac{2e^2\mathcal{E}}{\hbar}\Theta(t - t')\sin\omega(t - t')\langle\phi_0|xx|\phi_0\rangle\end{aligned}$$

Assume that the electric field is turned on and off slowly, namely

$$\begin{aligned}
\eta(t) &= -e^{-0^+|t|} \\
d &= \int_{-\infty}^{\infty} \chi(t-t')\eta(t') dt' \\
&= \frac{2e^2 \mathcal{E} \langle \phi_0 | x^2 | \phi_0 \rangle}{\hbar} \int_{-\infty}^{\infty} \Theta(t-t') e^{-0^+|t'|} \sin \omega(t-t') dt' \\
&= \frac{2e^2 \mathcal{E} \langle \phi_0 | x^2 | \phi_0 \rangle}{\hbar \omega}
\end{aligned}$$

B. THE SUSCEPTIBILITY

- (1) The observed temporal behavior of the non-equilibrium system can be cast in the frequency domain as a susceptibility.

We can define a time-interval $\tau = t - t'$,

$$\delta \langle \hat{A}(t) \rangle = \int_0^{\infty} \chi(t-t')\eta(t') dt' = \int_0^{\infty} \chi(\tau)\eta(t-\tau) d\tau$$

The Fourier transform with respect to the frequency

$$\begin{aligned}
\delta \langle \hat{A}(\omega) \rangle &= \int_{-\infty}^{\infty} \delta \langle \hat{A}(t) \rangle e^{-i\omega t} dt \\
&= \int_{-\infty}^{\infty} \int_0^{\infty} \chi(\tau)\eta(t-\tau) e^{-i\omega t} d\tau dt \\
&= \int_{-\infty}^{\infty} \int_0^{\infty} \chi(\tau)\eta(t-\tau) e^{-i\omega(t-\tau)} e^{-i\omega\tau} d\tau dt \\
&= \int_0^{\infty} \chi(\tau) e^{-i\omega\tau} d\tau \int_{-\infty}^{\infty} \eta(t') e^{-i\omega t'} dt'
\end{aligned}$$

Let $\eta(\omega) = \int_{-\infty}^{\infty} \eta(t') e^{-i\omega t'} dt'$ and $\chi(\omega) = \int_0^{\infty} \chi(\tau) e^{-i\omega\tau} d\tau$

$$\delta \langle \hat{A}(\omega) \rangle = \chi(\omega) \eta(\omega)$$

where $\delta \langle \hat{A}(\omega) \rangle$ is the linear response, $\chi(\omega)$ is called the susceptibility, and $\eta(\omega)$ is the driving force.

Thus, we obtain

$$\chi = \frac{\text{response}}{\text{force}}$$

EXAMPLES:

1. For a polarized harmonic oscillator, $\mathcal{E}$ is the driving force, and d is the linear response. Thus, the susceptibility χ is given by

$$\chi = \frac{d}{\varepsilon} = \frac{\frac{2e^2 \mathcal{E} \langle \phi_0 | x^2 | \phi_0 \rangle}{\hbar \omega}}{\varepsilon} = \frac{2e^2 \langle \psi_0 | x^2 | \psi_0 \rangle}{\hbar \omega}$$

(2) Time-reversal symmetry:

The susceptibility $\chi(\omega)$ is a complex function of real frequency ω .

$$\chi(\omega) = \chi'(\omega) + i\chi''(\omega)$$

The real part:

$$\chi'(\omega) = \int_0^\infty \chi(\tau) \cos \omega \tau d\tau$$

$\Rightarrow \chi'(\omega)$ is an even function, i.e., $\chi'(-\omega) = \chi'(\omega)$

The imaginary part:

$$\chi''(\omega) = - \int_0^\infty \chi(\tau) \sin \omega \tau d\tau$$

$\Rightarrow \chi''(\omega)$ is an odd function, i.e., $\chi''(-\omega) = -\chi''(\omega)$

Thus, we get

$$\chi^*(\omega) = \chi'(\omega) - i\chi''(\omega) = \chi'(-\omega) + i\chi''(-\omega) = \chi(-\omega)$$

Since

$$\begin{aligned} \chi'(\omega) &= \frac{1}{2} [\chi(\omega) + \chi^*(\omega)] \\ &= \frac{1}{2} [\chi(\omega) + \chi(-\omega)] \\ &= \frac{1}{2} \int_{-\infty}^\infty [\chi(t) + \chi(-t)] e^{-i\omega t} dt \end{aligned}$$

Under the time reversal $t \rightarrow -t$, $\chi'(\omega)$ is invariant (symmetric). Here, $\chi'(\omega)$ is called the reactive part of the response function.

Since

$$\begin{aligned} \chi''(\omega) &= \frac{1}{2i} [\chi(\omega) - \chi^*(\omega)] \\ &= \frac{1}{2i} [\chi(\omega) - \chi(-\omega)] \\ &= \frac{1}{2i} \int_{-\infty}^\infty [\chi(t) - \chi(-t)] e^{-i\omega t} dt \end{aligned}$$

Under the time reversal $t \rightarrow -t$, $\chi''(\omega)$ is not invariant (antisymmetric). Since microscopic systems are invariant under time reversal, $\chi''(\omega)$ must be arising due to dissipative processes. $\chi''(\omega)$ is called the dissipative or absorptive part of the response function.

(3) Kramers-Krönig dispersion relations:

From the Cauchy integral

$$\begin{aligned}\chi(\omega) &= \lim_{\epsilon \rightarrow 0} \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\chi(\omega')}{\omega' - \omega - i\epsilon} d\omega' \\ &= \frac{1}{2\pi i} \text{P} \int_{-\infty}^{\infty} \frac{\chi(\omega')}{\omega' - \omega} d\omega' + \frac{1}{2} \int_{-\infty}^{\infty} \chi(\omega') \delta(\omega' - \omega) d\omega' \\ &= \frac{1}{2\pi i} \text{P} \int_{-\infty}^{\infty} \frac{\chi(\omega')}{\omega' - \omega} d\omega' + \frac{1}{2} \chi(\omega) \\ \Rightarrow \chi(\omega) - \frac{1}{2} \chi(\omega) &= \frac{1}{2\pi i} \text{P} \int_{-\infty}^{\infty} \frac{\chi(\omega')}{\omega' - \omega} d\omega' \\ \Rightarrow \chi(\omega) &= \frac{1}{\pi i} \text{P} \int_{-\infty}^{\infty} \frac{\chi(\omega')}{\omega' - \omega} d\omega'\end{aligned}$$

Since $\chi(\omega) = \chi'(\omega) + i\chi''(\omega)$

$$\begin{aligned}\chi(\omega) = \chi'(\omega) + i\chi''(\omega) &= \frac{1}{\pi i} \text{P} \int_{-\infty}^{\infty} \frac{\chi'(\omega) + i\chi''(\omega)}{\omega' - \omega} d\omega' \\ &= \frac{1}{\pi} \text{P} \int_{-\infty}^{\infty} \frac{\chi''(\omega)}{\omega' - \omega} d\omega' - i \frac{1}{\pi} \text{P} \int_{-\infty}^{\infty} \frac{\chi'(\omega)}{\omega' - \omega} d\omega'\end{aligned}$$

Consider real and imaginary parts of this relation separately:

$$\begin{aligned}\chi'(\omega) &= \frac{1}{\pi} \text{P} \int_{-\infty}^{\infty} \frac{\chi''(\omega')}{\omega' - \omega} d\omega' \\ \chi''(\omega) &= -\frac{1}{\pi} \text{P} \int_{-\infty}^{\infty} \frac{\chi'(\omega')}{\omega' - \omega} d\omega'\end{aligned}$$

The Kramers-Kronig relations are a consequence of the causality property of the response function.

5-2 Spectral Function

A. RETARDED GREEN'S FUNCTION

- (1) Define a retarded Green's function

$$G^R(r, t; r', t') = -\frac{i}{\hbar} \Theta(t - t') \langle \Psi(0) | [\hat{\Psi}(r, t), \hat{\Psi}^\dagger(r', t')] | \Psi(0) \rangle$$

where

$$\Theta(t - t') = \begin{cases} 1, & t \geq t' \\ 0, & t < t' \end{cases}$$

Let $x = r - r'$. The retarded Green's function in momentum space is

$$G^R(k, t, t') = -\frac{i}{\hbar} \Theta(t - t') \langle \Psi(0) | [\hat{\Psi}_k(t), \hat{\Psi}_k^\dagger(t')] | \Psi(0) \rangle$$

OS:

The problem is that calculation of the retarded function is usually rather cumbersome, whereas for time-ordered Green's functions one may obtain nice closed expressions (e.g., the very intuitive ones represented by the Feynmann diagrams). One therefore usually calculates the time-ordered Green's function and then passes to the retarded Green's function using Lehmann representation.

- (2) Considering a set of eigenstates $\{|\Psi_n^N\rangle\}$ of the full Hamiltonian $\hat{H}$ for N -particles, as basis set, i.e., $\hat{H}|\Psi_n^N\rangle = \varepsilon_n|\Psi_n^N\rangle$.

Let $|\Psi(0)\rangle \equiv |\Psi_0^N\rangle$

$$\begin{aligned} G^R(k, t, t') &= -\frac{i}{\hbar} \Theta(t - t') \langle \Psi_0^N | [\hat{\Psi}_k(t), \hat{\Psi}_k^\dagger(t')] | \Psi_0^N \rangle \\ &= -\frac{i}{\hbar} \Theta(t - t') \langle \Psi_0^N | \hat{\Psi}_k(t) \hat{\Psi}_k^\dagger(t') | \Psi_0^N \rangle \\ &\quad + \frac{i}{\hbar} \Theta(t - t') \langle \Psi_0^N | \hat{\Psi}_k^\dagger(t') \hat{\Psi}_k(t) | \Psi_0^N \rangle \end{aligned}$$

Insert a complete set of Heisenberg states $\sum_n |\Psi_n^N\rangle \langle \Psi_n^N| = \hat{1}$ between the field operators,

$$\begin{aligned} G^R(k, t, t') &= -\frac{i}{\hbar} \Theta(t - t') \sum_n \langle \Psi_0^N | \hat{\Psi}_k(t) \underbrace{|\Psi_{n+1}^N\rangle \langle \Psi_{n+1}^N|}_{\hat{1}} \hat{\Psi}_k^\dagger(t') | \Psi_0^N \rangle \\ &\quad + \frac{i}{\hbar} \Theta(t - t') \sum_n \langle \Psi_0^N | \hat{\Psi}_k^\dagger(t') \underbrace{|\Psi_{n-1}^N\rangle \langle \Psi_{n-1}^N|}_{\hat{1}} \hat{\Psi}_k(t) | \Psi_0^N \rangle \end{aligned}$$

- (3) The Heisenberg operators with time-independent $\hat{H}$ can be rewritten in the form

$$\begin{aligned}\hat{\Phi}_k(t) &= \hat{U}^\dagger(t) \hat{\psi}_k \hat{U}(t) = e^{i\hat{H}t/\hbar} \hat{\psi}_k e^{-i\hat{H}t/\hbar} \\ \hat{\Phi}_k^\dagger(t) &= \hat{U}^\dagger(t) \hat{\psi}_k^\dagger \hat{U}(t) = e^{i\hat{H}t/\hbar} \hat{\psi}_k^\dagger e^{-i\hat{H}t/\hbar}\end{aligned}$$

Thus, we obtain

$$\begin{aligned}G^R(k, t, t') &= -\frac{i}{\hbar} \Theta(t - t') \sum_n \left\langle \Psi_0^N \left| e^{i\hat{H}t/\hbar} \hat{\psi}_k e^{-i\hat{H}t/\hbar} \right| \Psi_n^{N+1} \right\rangle \\ &\quad \times \left\langle \Psi_n^{N+1} \left| e^{i\hat{H}t'/\hbar} \hat{\psi}_k^\dagger e^{-i\hat{H}t'/\hbar} \right| \Psi_0^N \right\rangle \\ &\quad + \frac{i}{\hbar} \Theta(t - t') \sum_n \left\langle \Psi_0^N \left| e^{i\hat{H}t'/\hbar} \hat{\psi}_k^\dagger e^{-i\hat{H}t'/\hbar} \right| \Psi_n^{N-1} \right\rangle \\ &\quad \times \left\langle \Psi_n^{N-1} \left| e^{i\hat{H}t/\hbar} \hat{\psi}_k e^{-i\hat{H}t/\hbar} \right| \Psi_0^N \right\rangle\end{aligned}$$

Since

$$\begin{aligned}\left\langle \Psi_0^N \left| e^{i\hat{H}t/\hbar} \hat{\psi}_k e^{-i\hat{H}t/\hbar} \right| \Psi_n^{N+1} \right\rangle &= \left\langle \Psi_0^N \left| \hat{\psi}_k \right| \Psi_n^{N+1} \right\rangle e^{-i(\varepsilon_n^{N+1} - \varepsilon_0^N)t/\hbar} \\ \left\langle \Psi_n^{N+1} \left| e^{i\hat{H}t/\hbar} \hat{\psi}_k^\dagger e^{-i\hat{H}t/\hbar} \right| \Psi_0^N \right\rangle &= \left\langle \Psi_0^N \left| \hat{\psi}_k^\dagger \right| \Psi_n^{N+1} \right\rangle e^{i(\varepsilon_n^{N+1} - \varepsilon_0^N)t/\hbar}\end{aligned}$$

we obtain

$$\begin{aligned}G^R(k, t, t') &= -\frac{i}{\hbar} \Theta(t - t') \sum_n \left\langle \Psi_0^N \left| \hat{\psi}_k \right| \Psi_n^{N+1} \right\rangle e^{-i(\varepsilon_n^{N+1} - \varepsilon_0^N)t/\hbar} \\ &\quad \times \left\langle \Psi_n^{N+1} \left| \hat{\psi}_k^\dagger \right| \Psi_0^N \right\rangle e^{i(\varepsilon_n^{N+1} - \varepsilon_0^N)t'/\hbar} \\ &\quad + \frac{i}{\hbar} \Theta(t - t') \sum_n \left\langle \Psi_0^N \left| \hat{\psi}_k^\dagger \right| \Psi_n^{N-1} \right\rangle e^{-i(\varepsilon_n^{N-1} - \varepsilon_0^N)t'/\hbar} \\ &\quad \times \left\langle \Psi_n^{N-1} \left| \hat{\psi}_k \right| \Psi_0^N \right\rangle e^{i(\varepsilon_n^{N-1} - \varepsilon_0^N)t/\hbar} \\ &= -\frac{i}{\hbar} \Theta(t - t') \sum_n \left| \left\langle \Psi_n^{N+1} \left| \hat{\psi}_k^\dagger \right| \Psi_0^N \right\rangle \right|^2 e^{-i(\varepsilon_n^{N+1} - \varepsilon_0^N)(t-t')/\hbar} \\ &\quad + \frac{i}{\hbar} \Theta(t - t') \sum_n \left| \left\langle \Psi_n^{N-1} \left| \hat{\psi}_k \right| \Psi_0^N \right\rangle \right|^2 e^{i(\varepsilon_n^{N-1} - \varepsilon_0^N)(t-t')/\hbar}\end{aligned}$$

Fourier transform with respect to $\tau = t - t'$

$$G^R(k, \omega) = \int_{-\infty}^{\infty} G^R(k, \tau) e^{i\omega\tau} d\tau$$

Since

$$G^R(k, \tau) = -\frac{i}{\hbar} \Theta(\tau) \sum_n \left| \langle \Psi_n^{N+1} | \hat{\psi}_k^\dagger | \Psi_0^N \rangle \right|^2 e^{-i(\varepsilon_n^{N+1} - \varepsilon_0^N)\tau/\hbar} \\ + \frac{i}{\hbar} \Theta(-\tau) \sum_n \left| \langle \Psi_n^{N-1} | \hat{\psi}_k | \Psi_0^N \rangle \right|^2 e^{i(\varepsilon_n^{N-1} - \varepsilon_0^N)\tau/\hbar}$$

we obtain

$$G^R(k, \omega) = -\frac{i}{\hbar} \int_0^\infty \sum_n \left| \langle \Psi_n^{N+1} | \hat{\psi}_k^\dagger | \Psi_0^N \rangle \right|^2 e^{-i(\varepsilon_n^{N+1} - \varepsilon_0^N)\tau/\hbar} e^{i\omega\tau} e^{-\eta\tau} d\tau \\ + \frac{i}{\hbar} \int_{-\infty}^0 \sum_n \left| \langle \Psi_n^{N-1} | \hat{\psi}_k | \Psi_0^N \rangle \right|^2 e^{i(\varepsilon_n^{N-1} - \varepsilon_0^N)\tau/\hbar} e^{i\omega\tau} e^{\eta\tau} d\tau \\ = -\frac{i}{\hbar} \sum_n \left| \langle \Psi_n^{N+1} | \hat{\psi}_k^\dagger | \Psi_0^N \rangle \right|^2 \frac{-1}{i\omega - i(\varepsilon_n^{N+1} - \varepsilon_0^N)/\hbar - \eta} \\ + \frac{i}{\hbar} \sum_n \left| \langle \Psi_n^{N-1} | \hat{\psi}_k | \Psi_0^N \rangle \right|^2 \frac{1}{i\omega + i(\varepsilon_n^{N-1} - \varepsilon_0^N)/\hbar + \eta} \\ = \frac{1}{\hbar} \sum_n \left| \langle \Psi_n^{N+1} | \hat{\psi}_k^\dagger | \Psi_0^N \rangle \right|^2 \frac{1}{\omega - (\varepsilon_n^{N+1} - \varepsilon_0^N)/\hbar + i\eta} \\ + \frac{1}{\hbar} \sum_n \left| \langle \Psi_n^{N-1} | \hat{\psi}_k | \Psi_0^N \rangle \right|^2 \frac{1}{\omega + (\varepsilon_n^{N-1} - \varepsilon_0^N)/\hbar - i\eta} \\ = \sum_n \frac{1}{\hbar} \left[\frac{\left| \langle \Psi_n^{N+1} | \hat{\psi}_k^\dagger | \Psi_0^N \rangle \right|^2}{\omega - (\varepsilon_n^{N+1} - \varepsilon_0^N)/\hbar + i\eta} + \frac{\left| \langle \Psi_n^{N-1} | \hat{\psi}_k | \Psi_0^N \rangle \right|^2}{\omega + (\varepsilon_n^{N-1} - \varepsilon_0^N)/\hbar - i\eta} \right]$$

This is the Lehmann representation of the retarded Green's function.

OS:

Alternative method:

$$\Theta(\tau) = \lim_{\eta \rightarrow 0^+} -\frac{1}{i} \int_{-\infty}^\infty \frac{e^{-i\omega\tau}}{\omega + i\eta} \frac{d\omega}{2\pi} \\ \Theta(-\tau) = \lim_{\eta \rightarrow 0^+} \frac{1}{i} \int_{-\infty}^\infty \frac{e^{-i\omega\tau}}{\omega - i\eta} \frac{d\omega}{2\pi}$$

$$\begin{aligned}
& \frac{1}{\hbar} \int_{-\infty}^{\infty} \frac{e^{-i\omega'\tau}}{\omega' + i\eta} \frac{d\omega'}{2\pi} \sum_n \left| \left\langle \Psi_n^{N+1} \left| \hat{\psi}_k^\dagger \right| \Psi_0^N \right\rangle \right|^2 e^{-i(\varepsilon_n^{N+1} - \varepsilon_0^N)\tau/\hbar} e^{i\omega\tau} d\tau \\
&= \frac{1}{\hbar} \int_{-\infty}^{\infty} \sum_n \frac{\left| \left\langle \Psi_n^{N+1} \left| \hat{\psi}_k^\dagger \right| \Psi_0^N \right\rangle \right|^2}{\omega' + i\eta} \delta(\omega' + (\varepsilon_n^{N+1} - \varepsilon_0^N)\tau/\hbar - \omega) d\omega' \\
&= \frac{1}{\hbar} \sum_n \frac{\left| \left\langle \Psi_n^{N+1} \left| \hat{\psi}_k^\dagger \right| \Psi_0^N \right\rangle \right|^2}{\omega - (\varepsilon_n^{N+1} - \varepsilon_0^N)\tau/\hbar + i\eta}
\end{aligned}$$

B. FINITE TEMPERATURE GREEN'S FUNCTION

- (1) The Lehmann representation of the retarded Green's function at finite temperature still with real time

$$G^R(k, t, t') = -\frac{i}{\hbar} \Theta(t - t') \left\langle \hat{\Psi}_k(t) \hat{\Psi}_k^\dagger(t') \right\rangle - \frac{i}{\hbar} \Theta(t - t') \left\langle \hat{\Psi}_k^\dagger(t') \hat{\Psi}_k(t) \right\rangle$$

Since

$$\begin{aligned}
\left\langle \hat{\Psi}_k(t) \hat{\Psi}_k^\dagger(t') \right\rangle &= \frac{1}{Z} \text{Tr} \left[e^{-\beta(\hat{H} - \mu\hat{N})} \hat{\Psi}_k(t) \hat{\Psi}_k^\dagger(t') \right] \\
&= \frac{1}{Z} \text{Tr} \left[\hat{\Psi}_k(t) \hat{\Psi}_k^\dagger(t') e^{-\beta(\hat{H} - \mu\hat{N})} \right] \\
&= \frac{1}{Z} \sum_n \left\langle \Psi_n \left| \hat{\Psi}_k(t) \hat{\Psi}_k^\dagger(t') e^{-\beta(\hat{H} - \mu\hat{N})} \right| \Psi_n \right\rangle \\
&= \frac{1}{Z} \sum_n \left\langle \Psi_n \left| \hat{\Psi}_k(t) \hat{\Psi}_k^\dagger(t') \right| \Psi_n \right\rangle e^{-\beta\xi_n} \\
&= \frac{1}{Z} \sum_{nm} \langle \Psi_n | \hat{\Psi}_k(t) | \Psi_m \rangle \langle \Psi_m | \hat{\Psi}_k^\dagger(t') | \Psi_n \rangle e^{-\beta\xi_n}
\end{aligned}$$

where $\xi_n = \varepsilon_n - \mu$, and

$$\hat{\Psi}_k(t) = \hat{U}^\dagger(t) \hat{\psi}_k \hat{U}(t) = e^{i(\hat{H} - \mu\hat{N})t/\hbar} \hat{\psi}_k e^{-i(\hat{H} - \mu\hat{N})t/\hbar}$$

$$\hat{\Psi}_k^\dagger(t) = \hat{U}^\dagger(t) \hat{\psi}_k^\dagger \hat{U}(t) = e^{i(\hat{H} - \mu\hat{N})t/\hbar} \hat{\psi}_k^\dagger e^{-i(\hat{H} - \mu\hat{N})t/\hbar}$$

we obtain

$$\begin{aligned}
G^R(k, t, t') &= -\frac{i}{\hbar} \Theta(t - t') \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} \langle \Psi_n | \hat{\psi}_k | \Psi_m \rangle \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \\
&\quad \times e^{-i(\xi_m - \xi_n)(t - t')/\hbar} \\
&\quad - \frac{i}{\hbar} \Theta(t - t') \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} \langle \Psi_n | \hat{\psi}_k^\dagger | \Psi_m \rangle \langle \Psi_m | \hat{\psi}_k | \Psi_n \rangle \\
&\quad \times e^{i(\xi_m - \xi_n)(t - t')/\hbar}
\end{aligned}$$

Let $\tau = t - t'$

$$\begin{aligned}
G^R(k, \tau) &= -\frac{i}{\hbar} \Theta(\tau) \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} \left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2 e^{-i(\xi_m - \xi_n)\tau/\hbar} \\
&\quad - \frac{i}{\hbar} \Theta(\tau) \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} |\langle \Psi_m | \hat{\psi}_k | \Psi_n \rangle|^2 e^{i(\xi_m - \xi_n)\tau/\hbar}
\end{aligned}$$

Fourier transform with respect to τ

$$\begin{aligned}
G^R(k, \omega) &= -\frac{i}{\hbar} \int_0^\infty \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} \left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2 e^{-i(\xi_m - \xi_n)\tau/\hbar} e^{i\omega\tau} e^{-\eta\tau} d\tau \\
&\quad - \frac{i}{\hbar} \int_0^\infty \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} |\langle \Psi_m | \hat{\psi}_k | \Psi_n \rangle|^2 e^{i(\xi_m - \xi_n)\tau/\hbar} e^{i\omega\tau} e^{-\eta\tau} d\tau \\
&= -\frac{i}{\hbar} \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} \left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2 \frac{-1}{i\omega - i(\xi_m - \xi_n)/\hbar - \eta} \\
&\quad - \frac{i}{\hbar} \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} |\langle \Psi_m | \hat{\psi}_k | \Psi_n \rangle|^2 \frac{-1}{i\omega + i(\xi_m - \xi_n)/\hbar - \eta} \\
&= \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} \frac{1}{\hbar} \frac{\left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2}{\omega - (\xi_m - \xi_n)/\hbar + i\eta} \\
&\quad + \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} \frac{1}{\hbar} \frac{|\langle \Psi_m | \hat{\psi}_k | \Psi_n \rangle|^2}{\omega + (\xi_m - \xi_n)/\hbar + i\eta}
\end{aligned}$$

Since

$$|\langle \Psi_m | \hat{\psi}_k | \Psi_n \rangle|^2 = \langle \Psi_n | \hat{\psi}_k^\dagger | \Psi_m \rangle \langle \Psi_m | \hat{\psi}_k | \Psi_n \rangle = \left| \langle \Psi_n | \hat{\psi}_k^\dagger | \Psi_m \rangle \right|^2$$

we obtain

$$\begin{aligned}
G^R(k, \omega) &= \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} \frac{1}{\hbar \omega - (\xi_m - \xi_n)/\hbar + i\eta} \frac{\left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2}{\hbar \omega - (\xi_m - \xi_n)/\hbar + i\eta} \\
&\quad + \frac{1}{Z} \sum_{nm} e^{-\beta \xi_m} \frac{1}{\hbar \omega - (\xi_n - \xi_m)/\hbar + i\eta} \frac{\left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2}{\hbar \omega - (\xi_n - \xi_m)/\hbar + i\eta} \\
&= \frac{1}{Z} \sum_{nm} \frac{1}{\hbar \omega - (\xi_m - \xi_n)/\hbar + i\eta} \frac{\left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2}{\hbar \omega - (\xi_m - \xi_n)/\hbar + i\eta} (e^{-\beta \xi_n} + e^{-\beta \xi_m})
\end{aligned}$$

(2) The Lehmann representation of the Matsubara Green's function.

$$\begin{aligned}
G(k, \tau) &= -\Theta(\tau) \left\langle \hat{\Psi}_k(\tau) \hat{\Psi}_k^\dagger(0) \right\rangle + \Theta(-\tau) \left\langle \hat{\Psi}_k^\dagger(0) \hat{\Psi}_k(\tau) \right\rangle \\
&= -\Theta(\tau) \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} \langle \Psi_n | \hat{\Psi}_k(\tau) | \Psi_m \rangle \left\langle \Psi_m | \hat{\Psi}_k^\dagger(0) | \Psi_n \right\rangle \\
&\quad + \Theta(-\tau) \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} \left\langle \Psi_n | \hat{\Psi}_k^\dagger(0) | \Psi_m \right\rangle \langle \Psi_m | \hat{\Psi}_k(\tau) | \Psi_n \rangle
\end{aligned}$$

Since

$$\hat{\Psi}_k(\tau) = e^{(\hat{H} - \mu \hat{N})\tau/\hbar} \hat{\psi}_k e^{-(\hat{H} - \mu \hat{N})\tau/\hbar}$$

we obtain

$$\begin{aligned}
G(k, \tau) &= -\Theta(\tau) \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} \left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2 e^{-(\xi_m - \xi_n)\tau/\hbar} \\
&\quad + \Theta(-\tau) \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} \left| \langle \Psi_m | \hat{\psi}_k | \Psi_n \rangle \right|^2 e^{(\xi_m - \xi_n)\tau/\hbar}
\end{aligned}$$

Fourier transform with respect to τ

$$\begin{aligned}
G(k, i\omega_n) &= -\frac{1}{2} \frac{1}{Z} \int_0^{\beta \hbar} \sum_{nm} e^{-\beta \xi_n} \left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2 e^{-(\xi_m - \xi_n)\tau/\hbar} e^{i\omega_n \tau} d\tau \\
&\quad + \frac{1}{2} \frac{1}{Z} \int_{-\beta \hbar}^0 \sum_{nm} e^{-\beta \xi_n} \left| \langle \Psi_m | \hat{\psi}_k | \Psi_n \rangle \right|^2 e^{(\xi_m - \xi_n)\tau/\hbar} e^{i\omega_n \tau} d\tau \\
&= -\frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} \frac{1}{\hbar} \left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2 \frac{e^{\beta \hbar (i\omega_n - (\xi_m - \xi_n)/\hbar)} - 1}{i\omega_n - (\xi_m - \xi_n)/\hbar} \\
&\quad + \frac{1}{Z} \sum_{nm} e^{-\beta \xi_n} \frac{1}{\hbar} \left| \langle \Psi_m | \hat{\psi}_k | \Psi_n \rangle \right|^2 \frac{1 - e^{-\beta \hbar (i\omega_n + (\xi_m - \xi_n)/\hbar)}}{i\omega_n + (\xi_m - \xi_n)/\hbar}
\end{aligned}$$

Since

$$e^{\pm i\beta\hbar\omega_n} = -1$$

we obtain

$$\begin{aligned} G(k, i\omega_n) &= -\frac{1}{2Z} \sum_{nm} e^{-\beta\xi_n} \frac{1}{\hbar} \left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2 \frac{-e^{-\beta(\xi_m - \xi_n)} - 1}{i\omega_n - (\xi_m - \xi_n)/\hbar} \\ &\quad + \frac{1}{2Z} \sum_{nm} e^{-\beta\xi_n} \frac{1}{\hbar} \left| \langle \Psi_m | \hat{\psi}_k | \Psi_n \rangle \right|^2 \frac{1 + e^{-\beta(\xi_m - \xi_n)}}{i\omega_n + (\xi_m - \xi_n)/\hbar} \\ G(k, i\omega_n) &= \frac{1}{2Z} \sum_{nm} \frac{1}{\hbar} \left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2 \frac{e^{-\beta\xi_m} + e^{-\beta\xi_n}}{i\omega_n - (\xi_m - \xi_n)/\hbar} \\ &\quad + \frac{1}{2Z} \sum_{nm} \frac{1}{\hbar} \left| \langle \Psi_m | \hat{\psi}_k | \Psi_n \rangle \right|^2 \frac{e^{-\beta\xi_n} + e^{-\beta\xi_m}}{i\omega_n + (\xi_m - \xi_n)/\hbar} \\ &= \frac{1}{Z} \sum_{nm} \frac{1}{\hbar} \frac{\left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2}{i\omega_n - (\xi_m - \xi_n)/\hbar} (e^{-\beta\xi_n} + e^{-\beta\xi_m}) \end{aligned}$$

- (3) The analytic continuation in the upper-half plane, i.e., $i\omega_n \rightarrow \omega + i\eta$
 $G^R(k, \omega) = G(k, i\omega_n \rightarrow \omega + i\eta)$

C. SPECTRAL FUNCTION

- (1) The retarded Green's function can be written as

$$G^R(k, \omega) = \int \frac{A(k, \omega')}{\omega - \omega' + i\eta} d\omega'$$

where

$$\begin{aligned} A(k, \omega) &= \sum_n \left[\left| \langle \Psi_n^{N+1} | \hat{\psi}_k^\dagger | \Psi_0^N \rangle \right|^2 \delta \left(\omega - \frac{\varepsilon_n^{N+1} - \varepsilon_0^N}{\hbar} \right) \right. \\ &\quad \left. + \left| \langle \Psi_n^{N-1} | \hat{\psi}_k | \Psi_0^N \rangle \right|^2 \delta \left(\omega + \frac{\varepsilon_n^{N-1} - \varepsilon_0^N}{\hbar} \right) \right] \end{aligned}$$

From Cauchy's principal value

$$\frac{1}{x \pm i\epsilon} = \mathcal{P} \frac{1}{x} \mp i\pi\delta(x)$$

The spectral function of the retarded Green's function is

$$A(k, \omega) = -\frac{1}{\pi} \text{Im } G^R(k, \omega)$$

- (2) The finite temperature spectral function of the retarded Green's function

$$\begin{aligned}
 A(k, \omega) &= -\frac{1}{\pi} \text{Im } G^R(k, \omega) \\
 &= -\frac{1}{\pi} \text{Im } G(k, \omega + i\delta) \\
 &= \frac{1}{Z} \sum_n \left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2 (e^{-\beta \varepsilon_n} + e^{-\beta \varepsilon_m}) \delta \left(\omega - \frac{\xi_m - \xi_n}{\hbar} \right)
 \end{aligned}$$

- (3) Density of states

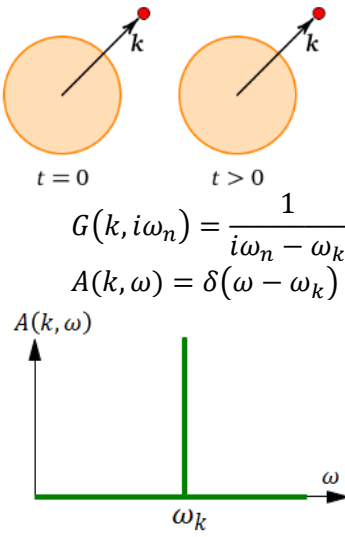
$$\begin{aligned}
 N(\omega) &= \frac{1}{V} \sum_k A(k, \omega) \\
 &= -\frac{1}{\pi V} \sum_k \text{Im } G^R(k, \omega) \\
 &= -\frac{1}{\pi V} \sum_k \text{Im } G(k, i\omega_m \rightarrow \omega + i\delta)
 \end{aligned}$$

- (4) Probabilistic interpretation

$$\begin{aligned}
 &\int_{-\infty}^{\infty} A(k, \omega) d\omega \\
 &= \frac{1}{Z} \sum_{nm} \left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2 (e^{-\beta \xi_n} + e^{-\beta \xi_m}) \underbrace{\int_{-\infty}^{\infty} \delta \left(\omega - \frac{\xi_m - \xi_n}{\hbar} \right) d\omega}_{=1} \\
 &= \frac{1}{Z} \sum_{nm} \left[e^{-\beta \xi_n} \left| \langle \Psi_m | \hat{\psi}_k^\dagger | \Psi_n \rangle \right|^2 + e^{-\beta \xi_n} \left| \langle \Psi_n | \hat{\psi}_k | \Psi_m \rangle \right|^2 \right] \\
 &= \frac{1}{Z} \sum_n \left[e^{-\beta \xi_n} \langle \Psi_n | \hat{\psi}_k \hat{\psi}_k^\dagger | \Psi_n \rangle + e^{-\beta \xi_n} \langle \Psi_n | \hat{\psi}_k^\dagger \hat{\psi}_k | \Psi_n \rangle \right] \\
 &= \frac{1}{Z} \sum_n e^{-\beta \xi_n} \langle \Psi_n | \hat{\psi}_k \hat{\psi}_k^\dagger + \hat{\psi}_k^\dagger \hat{\psi}_k | \Psi_n \rangle \\
 &= \frac{1}{Z} \sum_n e^{-\beta \xi_n} \\
 &= 1
 \end{aligned}$$

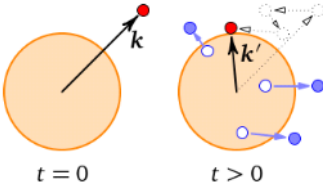
- (5) Bare particles

If a particle injected at time $t = 0$ keeps its identity at time $t > 0$,



(6) Quasiparticles

If the injected electron loses momentum and energy by exciting electron-hole pairs across the Fermi surface,



The retarded Green's function

$$G^R(k, \omega) = \frac{1}{\omega - \omega_k - \Sigma^R(k, \omega) + i\delta}$$

Here $\Sigma^R(k, \omega) = \Sigma'(k, \omega) + i\Sigma''(k, \omega)$

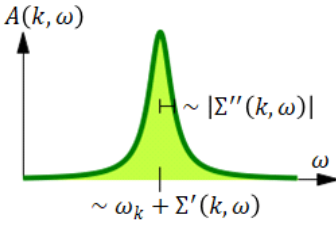
The spectral function

$$A(k, \omega) = -\frac{1}{\pi} \text{Im } G^R(k, \omega)$$

$$= \frac{-\Sigma''(k, \omega)}{(\omega - \omega_k - \Sigma'(k, \omega))^2 + (\Sigma''(k, \omega))^2}$$

If the imaginary part of the self-energy is not too large and varies smoothly with frequency, the $A(k, \omega)$ will have a maximum

The maximum is given by the equation, $\omega - \omega_k - \Sigma'(k, \omega) = 0$



Define the Fermi “surface”: the locus of zero-energy excitations in momentum space, i.e., the maximum of $A(k, 0)$ and $\omega_{k_F} + \Sigma'(k_F, 0) = 0$. For studying the low-energy one-particle excitations in weakly-interacting systems, expanding the Green's function around $k = k_F$ and $\omega = 0$

$$\begin{aligned}
 \frac{1}{G^R(k, \omega)} &= \omega - \omega_k - \Sigma'(k, \omega) - i\Sigma''(k, \omega) \\
 &= \omega - \left[\omega_{k_F} + (k - k_F) \cdot \nabla \omega_k \Big|_{k_F} \right] \\
 &\quad - \left[\Sigma'(k_F, 0) + (k - k_F) \cdot \nabla \Sigma'(k, 0) \Big|_{k_F} + \omega \frac{\partial}{\partial \omega} \Sigma'(k_F, \omega) \Big|_{\omega=0} \right] \\
 &\quad - i\Sigma''(k, \omega) + \dots \\
 &= \omega \left[1 - \frac{\partial}{\partial \omega} \Sigma'(k_F, \omega) \Big|_{\omega=0} \right] - \left[\omega_{k_F} + \Sigma'(k_F, 0) \right] \\
 &\quad - (k - k_F) \cdot \nabla [\omega_k + \Sigma'(k, 0)] \Big|_{k_F} - i\Sigma''(k, \omega) + \dots
 \end{aligned}$$

Since

$$\omega_{k_F} + \Sigma'(k_F, 0) = 0$$

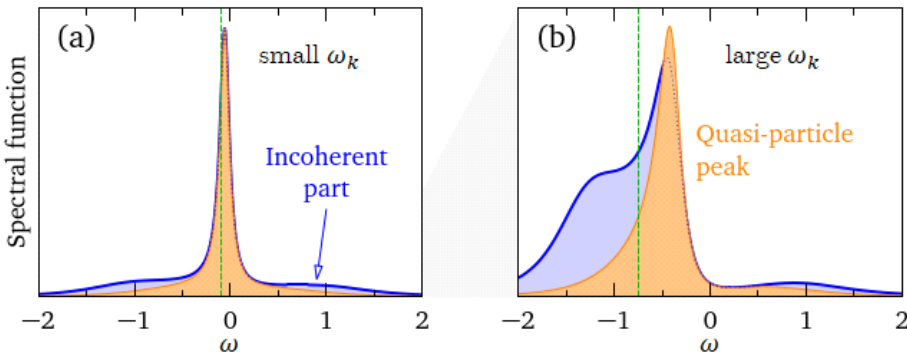
Let

$$\begin{aligned}
 \frac{1}{Z(k_F)} &= 1 - \frac{\partial}{\partial \omega} \Sigma'(k_F, \omega) \Big|_{\omega=0} \dots \text{quasiparticle residue} \\
 \omega'_k &= Z(k_F) (k - k_F) \cdot \nabla [\omega_k + \Sigma'(k, 0)]_{k_F} \dots \text{quasiparticle energy} \\
 \frac{1}{\tau(k, \omega)} &= -2Z(k_F) \Sigma''(k, \omega) \dots \text{quasiparticle life-time} \\
 \Rightarrow \frac{1}{G^R(k, \omega)} &= \frac{1}{Z(k_F)} \left[\omega - \omega'_k + \frac{i\hbar}{2\tau(k, \omega)} \right] + \dots \\
 \Rightarrow G^R(k, \omega) &= \frac{Z(k_F)}{\omega - \omega'_k + i \frac{1}{2\tau(k, \omega)}} + G_{\text{inc}}(k, \omega)
 \end{aligned}$$

The first term describes a peak with the maximum at $\omega = 0$ and a

width $\hbar/\tau$ (the so-called "coherent" quasiparticle peak). G_{inc} contains "the rest".

$$A(k,\omega) \approx \frac{-\frac{Z_k}{2\tau(k,\omega)}}{(\omega-\omega'_k)^2 + \left(\frac{1}{2\tau(k,\omega)}\right)^2} + \dots$$



5-3 Correlation Function

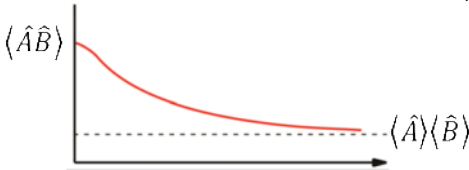
A. CORRELATION FUNCTIONS OF FLUCTUATIONS

- (1) In quantum mechanics, a correlation function gives the statistical correlation between two operators, i.e., it describes where and when a statistical relationship has vanished.
- (2) Correlation functions of two operators $\hat{A}(r, t)$ and $\hat{B}(r', t')$ for random fluctuations at thermal equilibrium are

$$C(r, t; r', t') = \langle \hat{A}(r, t) \hat{B}(r', t') \rangle$$

Properties:

1. For long time or space separations, as *fluctuations* act to randomize the system, the values of $\langle \hat{A} \hat{B} \rangle$ become uncorrelated.



2. When we observe fluctuations about an average, we often redefine the correlation function in terms of the deviation from average

$$\delta \hat{A} = \hat{A} - \langle \hat{A} \rangle$$

$$\delta \hat{B} = \hat{B} - \langle \hat{B} \rangle$$

$$\langle \delta \hat{A} \delta \hat{B} \rangle = \langle (\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle) \rangle = \langle \hat{A} \hat{B} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle$$

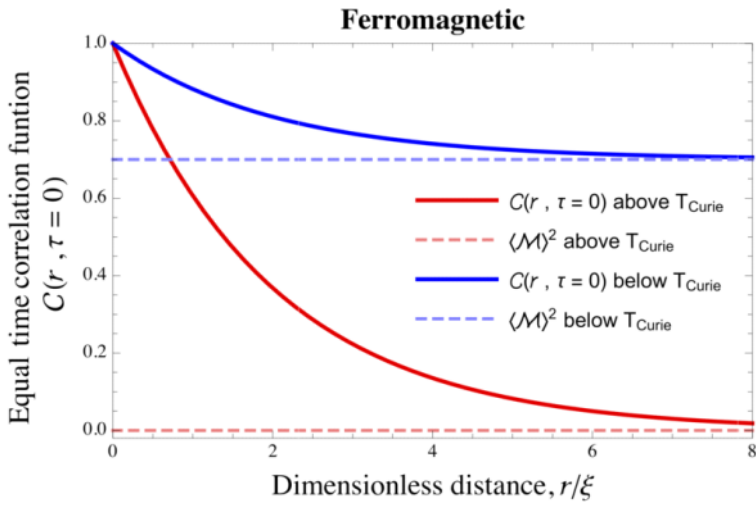
- (3) Space-correlation functions of two operators $\hat{A}(r)$ and $\hat{B}(r')$

$$C(r, r') = \langle \hat{A}(r) \hat{B}(r') \rangle$$

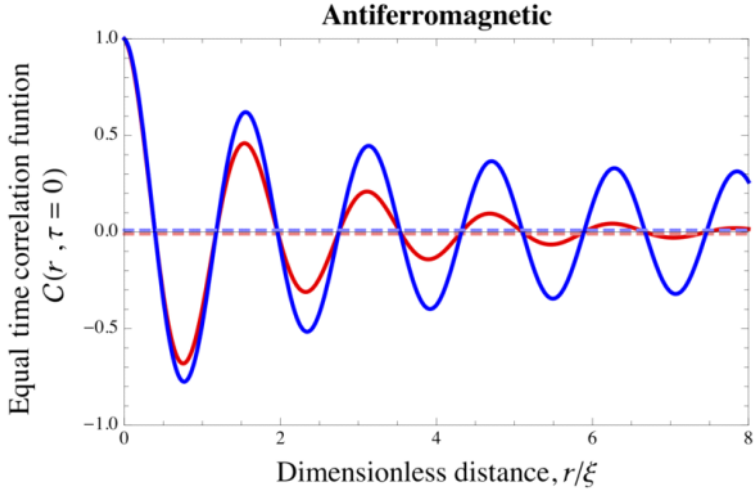
This is also called equal-time correlation function.

EXAMPLES:

1. Equal-time spin correlation functions for ferromagnetic



2. Equal-time spin correlation functions for antiferromagnetic



- (4) Time-correlation functions of two operators $\hat{A}(t)$ and $\hat{B}(t')$

$$C(t, t') = \langle \hat{A}(t) \hat{B}(t') \rangle$$

Since

$$\begin{aligned}
C(t, t') &= \langle \hat{A}(t) \hat{B}(t') \rangle \\
&= \langle \hat{U}^\dagger(t) \hat{A} \hat{U}(t) \hat{U}^\dagger(t') \hat{B} \hat{U}(t') \rangle \\
&= \langle \hat{U}(t') \hat{U}^\dagger(t) \hat{A} \hat{U}(t) \hat{U}^\dagger(t') \hat{B} \rangle \\
&= \langle \hat{U}^\dagger(t - t') \hat{A} \hat{U}(t - t') \hat{B} \rangle \\
&= \langle \hat{A}(t - t') \hat{B} \rangle \\
&= C(t - t')
\end{aligned}$$

Time-correlation function depends only on the difference of its time variables $\tau = t - t'$, i.e., $C(t, t') = C(t - t')$

Similarly, we have

$$C(t', t) = \langle \hat{B}(t') \hat{A}(t) \rangle = \langle \hat{B} \hat{A}(t - t') \rangle = \langle \hat{A}(t - t') \hat{B} \rangle^*$$

Thus, we obtain

$$C^*(t - t') = C(t' - t)$$

Time-correlation function is a complex function, i.e.,

$$C(t - t') = \underbrace{C'(t - t')}_{\text{even}} + i \underbrace{C''(t - t')}_{\text{odd}}$$

where

$C'(t - t')$ is even in time and describes the relaxation of the system to equilibrium when a force holding it away from equilibrium is released.

$C''(t - t')$ is odd in time and describes how a system is driven away from equilibrium by an external potential.

B. FLUCTUATION-DISSIPATION THEOREM

- (1) The retarded response function in Heisenberg picture at thermal equilibrium is

$$\chi(t, t') = -\frac{i}{\hbar} \Theta(t - t') \langle \hat{A}(t) \hat{O}(t') \rangle + \frac{i}{\hbar} \Theta(t - t') \langle \hat{O}(t') \hat{A}(t) \rangle$$

Let $\tau = t - t'$

$$\begin{aligned}
\chi(\tau) &= -\frac{i}{\hbar}\Theta(\tau)\langle\hat{A}(\tau)\hat{O}\rangle + \frac{i}{\hbar}\Theta(\tau)\langle\hat{O}\hat{A}(\tau)\rangle \\
&= -\frac{i}{\hbar}\Theta(\tau)\frac{1}{Z}\sum_{nm}e^{-\beta\xi_n}\langle\Psi_n|\hat{A}(\tau)|\Psi_m\rangle\langle\Psi_m|\hat{O}|\Psi_n\rangle \\
&\quad + \frac{i}{\hbar}\Theta(\tau)\frac{1}{Z}\sum_{nm}e^{-\beta\xi_n}\langle\Psi_n|\hat{O}|\Psi_m\rangle\langle\Psi_m|\hat{A}(\tau)|\Psi_n\rangle \\
&= -\frac{i}{\hbar}\Theta(\tau)\frac{1}{Z}\sum_{nm}e^{-\beta\xi_n}\langle\Psi_n|\hat{A}|\Psi_m\rangle\langle\Psi_m|\hat{O}|\Psi_n\rangle e^{-i(\xi_m-\xi_n)\tau/\hbar} \\
&\quad + \frac{i}{\hbar}\Theta(\tau)\frac{1}{Z}\sum_{nm}e^{-\beta\xi_n}\langle\Psi_n|\hat{O}|\Psi_m\rangle\langle\Psi_m|\hat{A}|\Psi_n\rangle e^{i(\xi_m-\xi_n)\tau/\hbar}
\end{aligned}$$

Fourier transform of the time-correlation function with respect to $\tau = t - t'$

$$\begin{aligned}
S^R(\omega) &= \int_{-\infty}^{\infty} \langle\hat{A}(\tau)\hat{O}\rangle e^{i\omega\tau} d\tau \\
&= \frac{1}{Z} \int_{-\infty}^{\infty} \sum_{nm} e^{-\beta\xi_n} \langle\Psi_n|\hat{A}|\Psi_m\rangle \langle\Psi_m|\hat{O}|\Psi_n\rangle e^{-i(\xi_m-\xi_n)\tau/\hbar} e^{i\omega\tau} d\tau \\
&= \frac{1}{Z} \sum_{nm} e^{-\beta\xi_n} \langle\Psi_n|\hat{A}|\Psi_m\rangle \langle\Psi_m|\hat{O}|\Psi_n\rangle 2\pi\delta(\omega - (\xi_m - \xi_n)/\hbar)
\end{aligned}$$

Similarly, we have

$$\begin{aligned}
S^A(\omega) &= \int_{-\infty}^{\infty} \langle\hat{O}\hat{A}(\tau)\rangle e^{i\omega\tau} d\tau \\
&= \frac{1}{Z} \int_{-\infty}^{\infty} \sum_{nm} e^{-\beta\xi_n} \langle\Psi_n|\hat{O}|\Psi_m\rangle \langle\Psi_m|\hat{A}|\Psi_n\rangle e^{i(\xi_m-\xi_n)\tau/\hbar} e^{i\omega\tau} d\tau \\
&= \frac{1}{Z} \sum_{nm} e^{-\beta\xi_n} \langle\Psi_n|\hat{O}|\Psi_m\rangle \langle\Psi_m|\hat{A}|\Psi_n\rangle 2\pi\delta(\omega + (\xi_m - \xi_n)/\hbar) \\
&= \frac{1}{Z} \sum_{nm} e^{-\beta\xi_m} \langle\Psi_n|\hat{A}|\Psi_m\rangle \langle\Psi_m|\hat{O}|\Psi_n\rangle 2\pi\delta(\omega - (\xi_m - \xi_n)/\hbar)
\end{aligned}$$

Suppose that $|\Psi_m\rangle = |\Psi_m^{N+1}\rangle$ and $|\Psi_n\rangle = |\Psi_n^N\rangle$.

Thus, we obtain

$$\begin{aligned}
e^{-\beta\xi_m} &= e^{-\beta(\xi_n+\hbar\omega)} \\
S^A(\omega) &= e^{-\beta\hbar\omega} S^R(\omega) \\
\chi(\tau) &= -\frac{i}{\hbar}\Theta(\tau) \int_{-\infty}^{\infty} S^R(\omega) e^{-i\omega\tau} \frac{d\omega}{2\pi} + \frac{i}{\hbar}\Theta(\tau) \int_{-\infty}^{\infty} S^A(\omega) e^{-i\omega\tau} \frac{d\omega}{2\pi}
\end{aligned}$$

(2) The Fourier transform of the retarded response function

$$\begin{aligned}
 \chi(\omega) &= -\frac{i}{\hbar} \int_0^\infty \int_{-\infty}^\infty (S^R(\omega') - S^A(\omega')) e^{-i\omega'\tau} \frac{d\omega'}{2\pi} e^{i\omega\tau} e^{-\eta\tau} d\tau \\
 &= -\frac{i}{\hbar} \int_0^\infty \int_{-\infty}^\infty (1 - e^{-\beta\hbar\omega'}) S_R(\omega') e^{-i\omega'\tau} \frac{d\omega'}{2\pi} e^{i\omega\tau} e^{-\eta\tau} d\tau \\
 &= -\frac{i}{\hbar} \int_{-\infty}^\infty (1 - e^{-\beta\hbar\omega'}) S_R(\omega') \frac{d\omega'}{2\pi} \int_0^\infty e^{i(\omega - \omega' + i\eta)\tau} d\tau \\
 &= -\frac{i}{\hbar} \int_{-\infty}^\infty (1 - e^{-\beta\hbar\omega'}) S_R(\omega') \frac{-1}{i(\omega - \omega' + i\eta)} \frac{d\omega'}{2\pi} \\
 &= \frac{1}{\hbar} \int_{-\infty}^\infty (1 - e^{-\beta\hbar\omega'}) S_R(\omega') \frac{1}{\omega - \omega' + i\eta} \frac{d\omega'}{2\pi}
 \end{aligned}$$

Since

$$\frac{1}{\omega - \omega' + i\eta} = \mathcal{P} \frac{1}{\omega - \omega'} - i\pi\delta(\omega - \omega')$$

we obtain

$$\begin{aligned}
 \text{Im} [\chi(\omega)] &= -\frac{1}{\hbar} \int_{-\infty}^\infty (1 - e^{-\beta\hbar\omega'}) S_R(\omega') \delta(\omega - \omega') \frac{d\omega'}{2} \\
 &= -\frac{1}{2\hbar} (1 - e^{-\beta\hbar\omega}) S_R(\omega) \\
 S^R(\omega) &= -\frac{2\hbar}{1 - e^{-\beta\hbar\omega}} \text{Im} [\chi(\omega)] = -2\hbar \left(1 + \frac{1}{e^{\beta\hbar\omega} - 1} \right) \text{Im} [\chi(\omega)]
 \end{aligned}$$

This is called the fluctuation-dissipation relation. The fluctuation of the time-correlation function is related to the imaginary part of the retarded response function in frequency space.

OS:

The retarded response function is a complex function

$$\chi(\tau) = -\frac{i}{\hbar} \Theta(\tau) \left[\langle \hat{A}(\tau) \hat{O} \rangle - \langle \hat{O} \hat{A}(\tau) \rangle \right] = \chi'(\tau) + i\chi''(\tau)$$

The imaginary part of the retarded response function

$$\begin{aligned}
\chi''(\tau) &= \frac{1}{2i} [\chi(\tau) - \chi^*(\tau)] \\
&= \frac{1}{2i} [\chi(\tau) - \chi(-\tau)] \\
&= -\frac{1}{2\hbar} \Theta(\tau) [\langle \hat{A}(\tau) \hat{O} \rangle - \langle \hat{O} \hat{A}(\tau) \rangle] \\
&\quad + \frac{1}{2\hbar} \Theta(-\tau) [\langle \hat{O}(-\tau) \hat{A} \rangle - \langle \hat{A} \hat{O}(-\tau) \rangle] \\
&= -\frac{1}{2\hbar} (\Theta(\tau) + \Theta(-\tau)) [\langle \hat{A}(\tau) \hat{O} \rangle - \langle \hat{O}(-\tau) \hat{A} \rangle]
\end{aligned}$$

Since $\Theta(\tau) + \Theta(-\tau) = 1$

$$\chi''(\tau) = -\frac{1}{2\hbar} [\langle \hat{A}(\tau) \hat{O} \rangle - \langle \hat{O}(-\tau) \hat{A} \rangle]$$

Since

$$\begin{aligned}
\langle \hat{O}(-\tau) \hat{A} \rangle &= \langle \hat{O} \hat{A}(\tau) \rangle \\
&= \text{Tr} [e^{-\beta \hat{H}} \hat{O} \hat{A}(\tau)] \\
&= \text{Tr} [e^{-\beta \hat{H}} e^{\beta \hat{H}} \hat{A}(\tau) e^{-\beta \hat{H}} \hat{O}] \\
&= \langle \hat{A}(\tau - i\hbar\beta) \hat{O} \rangle
\end{aligned}$$

The spectral representation of the time-correlation function

$$\begin{aligned}
S^R(\omega) &= \int_{-\infty}^{\infty} \langle \hat{A}(\tau) \hat{O} \rangle e^{i\omega\tau} d\tau \\
S^A(\omega) &= \int_{-\infty}^{\infty} \langle \hat{O}(-\tau) \hat{A} \rangle e^{i\omega\tau} d\tau \\
&= \int_{-\infty}^{\infty} \langle \hat{A}(\tau - i\hbar\beta) \hat{O} \rangle e^{i\omega\tau} d\tau \\
&= \int_{-\infty}^{\infty} \langle \hat{A}(\tau - i\hbar\beta) \hat{O} \rangle e^{i\omega(\tau - i\hbar\beta)} e^{-\beta\hbar\omega} d\tau \\
&= e^{-\beta\hbar\omega} \int_{-\infty}^{\infty} \langle \hat{A}(\tau') \hat{O} \rangle e^{i\omega\tau'} d\tau' \\
&= e^{-\beta\hbar\omega} S^R(\omega) \\
\text{Im} [\chi(\omega)] &= -\frac{1}{2\hbar} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [S^R(\omega) - S^A(\omega)] e^{-i\omega'\tau} \frac{d\omega'}{2\pi} e^{i\omega\tau} e^{-\eta\tau} d\tau \\
&= -\frac{1}{2\hbar} (1 - e^{-\beta\hbar\omega}) S_R(\omega)
\end{aligned}$$