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Effect of $1/\tau(\xi)$ on spectral function

$$n_{\bar p}(t) = e^{-t/\tau(\xi_p)} \qquad \text{(occup. decays with rate } 1/\tau(\xi_p)\text{)}$$

$$\downarrow$$

$$\langle \Psi_0 | a_p^+(t)\, a_p(t) | \Psi_0 \rangle \quad \text{with} \quad |\Psi_0\rangle = a_p^+(0)|G\rangle$$

(the init. state contains occup. state $\bar p$)

$$\langle \Psi_0 | a_p^+(t)\, a_p(t) | \Psi_0 \rangle = \langle G | a_p(0)\, a_p^+(t)\, a_p(t)\, a_p^+(0) | G \rangle$$

$$= \sum_n \langle G | a_p(0)\, a_{\bar p}^+(t) | n \rangle \langle n | a_p(t)\, a_p^+(0) | G \rangle \cong \left| \langle G | a_p(t)\, a_p^+(0) | G \rangle \right|^2$$

At weak int. the largest element is with $|n\rangle = |G\rangle$ (all others vanish at $V(q) \to 0$)

$$\left| \langle G | a_p(t)\, a_p^+(0) | G \rangle \right|^2 = e^{-t/\tau(\xi_{\bar p})}$$

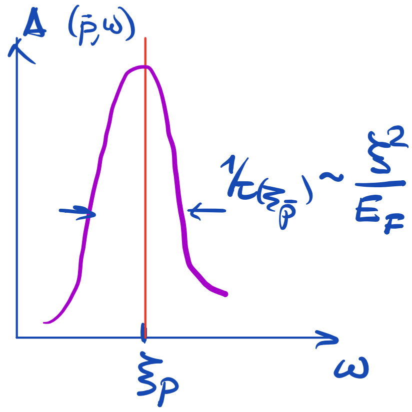
$$\langle G | a_p(t)\, a_p^+(0) | G \rangle = e^{-i\xi_{\bar p} t - t/2\tau(\xi_{\bar p})}$$

Similar consideration for holes.

Combining p and h parts of $A(\bar{p},\omega)$:

$$\boxed{A(\bar{p},\omega) = \operatorname{Im} \frac{1}{\omega - \xi_{\vec{p}} - i/2\tau(\xi_{\vec{p}})}}$$

$(\hbar = 1)$



5. Linear response, FDT, and the dynamic structure factor

5.1. General linear response theory (Kubo, 1956)

$$\langle A \rangle = \operatorname{Tr}(\hat{\rho}\hat{A})$$

Consider a time-independent variable $\hat{A}$ (in Schrödinger rep.) and a Hamiltonian of the form:

$$\hat{\mathcal{H}} = \underbrace{\hat{\mathcal{H}}_0}_{\text{system}} + \underbrace{\hat{\mathcal{H}}_1}_{\text{perturbation}} = \hat{\mathcal{H}}_0 + \underbrace{e^{0\cdot t}\hat{V}(t)}_{\mathcal{H}_1}, \qquad t \le 0$$

How $\langle A \rangle$ responds to a small $\hat{\mathcal{H}}_1$?

$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\hat{\mathcal{H}}_0, \hat{\rho}] + [\hat{\mathcal{H}}_1, \hat{\rho}]$$

First-order perturbation theory in $\hat{\mathcal{H}}_1$: $\quad \hat{\rho} = \hat{\rho}_0 + \hat{\rho}_1$

$\hat{\rho}_0 \to \frac{1}{Z} e^{-\beta\hat{\mathcal{H}}_0}$, $\quad \hat{\rho}_1 \propto \mathcal{H}_1$

$$i\hbar \frac{\partial \hat{\rho}_1}{\partial t} - [\hat{\mathcal{H}}_0, \hat{\rho}_1] = [\hat{\mathcal{H}}_1, \hat{\rho}_0]$$

Define ρ_1 in the interaction rep.:

$$\hat{\rho}_1 = e^{-i\mathcal{H}_0 t/\hbar}\, \hat{\rho}_1^I\, e^{i\mathcal{H}_0 t/\hbar}$$

$$i\hbar \frac{\partial \hat{\rho}_1^I}{\partial t} = [\hat{\mathcal{H}}_1^I, \hat{\rho}_0], \quad \text{where} \quad \hat{\mathcal{H}}_1^I = e^{\frac{i\mathcal{H}_0 t}{\hbar}} \hat{\mathcal{H}}_1 e^{-\frac{i\mathcal{H}_0 t}{\hbar}}$$

$$\rho_1^I(t) = \frac{1}{i\hbar}\int_{-\infty}^{t} dt_1 \,[\mathcal{H}_1^I(t_1), \hat{\rho}_0]$$

$$\hat{\rho}_1(t) = \frac{1}{i\hbar}\int_{-\infty}^{t} dt_1 \; e^{-\frac{i\mathcal{H}_0 t}{\hbar}} [\mathcal{H}_1^I(t_1), \hat{\rho}_0]\, e^{\frac{i\mathcal{H}_0 t}{\hbar}}$$

To the first order in $\mathcal{H}_1$:

$$\langle \hat{A} \rangle = \underbrace{Tr(\hat{\rho}_0 \hat{A})}_{\langle A \rangle_0} + Tr(\hat{\rho}_1(t)\hat{A})$$

$$\langle A \rangle - \langle A \rangle_0 = \int_{-\infty}^{t} dt_1 \, Tr\left\{ \frac{1}{i\hbar} e^{-\frac{i\mathcal{H}_0 t}{\hbar}} [\mathcal{H}_1^I(t_1), \rho_0]\, \underbrace{e^{\frac{i\mathcal{H}_0 t}{\hbar}} \hat{A}} \right\}$$

$$= \frac{1}{i\hbar}\int_{-\infty}^{t} dt_1 \, Tr\left\{ \hat{A}^I(t)\, [\mathcal{H}_1^I(t_1), \hat{\rho}_0] \right\}; \qquad \hat{A}^I(t) = e^{\frac{i\mathcal{H}_0 t}{\hbar}} \hat{A}\, e^{-\frac{i\mathcal{H}_0 t}{\hbar}}$$

$$\langle A \rangle - \langle A \rangle_0 = \frac{1}{i\hbar}\int_{-\infty}^{t} dt_1 \, Tr\left\{ \hat{\rho}_0 [\hat{A}^I(t), \mathcal{H}_1^I(t_1)] \right\};$$

Now recall that $\mathcal{H}_1 = e^{0 \cdot t}\, \hat{V}(t)$ and take $\hat{V}(t) = f(t) \cdot \hat{B}$ (the field $f(t)$ couples to the variable $\hat{B}$ of the system).

$$\mathcal{H}_1^I(t) = f(t) \cdot \hat{B}^I(t)$$

$$\langle A \rangle - \langle A \rangle_0 = \frac{1}{i\hbar}\int_{-\infty}^{t} dt_1 \, Tr\left\{ \rho_0 [A^I(t), B^I(t_1)] \right\} f(t_1) \cdot e^{0 \cdot t_1}$$

$$\langle A\rangle - \langle A\rangle_0 = \frac{1}{i\hbar}\int_{-\infty}^{t} dt_1 \, \langle [A^I(t), B^I(t_1)]\rangle_0 \, f(t_1)$$

$$\hat{A}^I(t) = e^{i\frac{\mathcal{H}_0 t}{\hbar}} \hat{A} \, e^{-i\frac{\mathcal{H}_0 t}{\hbar}}, \qquad \hat{B}^I(t) = e^{i\frac{\mathcal{H}_0 t}{\hbar}} \hat{B} \, e^{-i\frac{\mathcal{H}_0 t}{\hbar}}$$

(we included $e^{0 \cdot t_1}$ into $f(t_1)$) Kubo, 1956

Invariance wrt translation in time:

$$\langle [A^I(t), B^I(t_1)]\rangle_0 = \langle [A^I(t-t_1), B^I(0)]\rangle_0$$

$$\langle A\rangle - \langle A\rangle_0 = \frac{1}{i\hbar}\int_{-\infty}^{t} dt_1 \, \langle [A^I(t-t_1), B^I(0)]\rangle_0 \, f(t_1)$$

Re-write it as:

$$\langle A\rangle - \langle A\rangle_0 = \int_{-\infty}^{\infty} dt_1 \, \Pi_R^{AB}(t-t_1) \, f(t_1)$$ (Kubo, 1956)

where

$$\Pi_R^{AB}(t) = -\frac{i}{\hbar}\theta(t) \langle [A^I(t), B^I(0)]\rangle_0$$

is the retarded response function (retarded correlation function)

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In the special case of $\hat{A} = \hat{B}$:

$$\Pi_R(t) = -\frac{i}{\hbar}\theta(t) \langle [A^I(t), A^I(0)]\rangle_0$$

The Fourier transform:

$$\Pi_R(\omega + i\delta) = \int_{-\infty}^{\infty} dt \, e^{i\omega t} e^{-\delta t} \, \Pi_R(t), \qquad \delta \to +0$$

def. of $\Pi_R(\omega)$

$\Pi_R(\omega)$ is analytical at $\mathrm{Im}\,\omega > 0$, because $\Pi_R(t<0) = 0$

5.2. Fluctuation-dissipation theorem (FDT)

$$\Pi_R(\omega) = -\frac{i}{\hbar}\int_0^\infty dt\, e^{i\omega t} \langle [\hat{A}^I(t), \hat{A}^I(0)] \rangle_0 = -\frac{i}{\hbar}\int_0^\infty dt\, e^{i\omega t} \sum_{nm} \frac{1}{Z} e^{-\beta E_n} \Big(e^{i\omega_n t}$$

$$\times A_{nm} e^{-i\omega_m t} A_{mn} - A_{nm} e^{i\omega_m t} A_{mn} e^{-i\omega_n t} \Big), \qquad \omega_{n,m} = \frac{E_{n,m}}{\hbar}$$

$$\Pi_R(\omega^+) = -\frac{1}{\hbar}\sum_{nm}\frac{1}{Z} e^{-\beta E_n} A_{nm}A_{mn} \left(i\int_0^\infty dt\, e^{i(\omega^+ + \omega_n - \omega_m)t} - i\int_0^\infty dt\, e^{i(\omega^+ + \omega_m - \omega_n)t} \right)$$

$\mathrm{Im}\,\omega^+ > 0$ (the real-ω limit: $\omega^+ = \omega + i\delta$, $\delta \to +0$)

$$\Pi_R(\omega^+) = -\frac{1}{\hbar}\cdot\frac{1}{Z}\sum_{nm} e^{-\beta E_n} |A_{nm}|^2 \left(\frac{-1}{\omega + \omega_n - \omega_m + i\delta} - \frac{-1}{\omega + \omega_m - \omega_n + i\delta} \right)$$

used $\hat{A} = \hat{A}^+$

(real ω) $\delta \to +0$

$$\mathrm{Im}\,\Pi_R(\omega) = -\frac{1}{\hbar}\cdot\frac{\pi}{Z}\sum_{nm} e^{-\beta E_n} |A_{nm}|^2 \underbrace{\Big(\delta(\omega + \omega_n - \omega_m) - \delta(\omega + \omega_m - \omega_n) \Big)}$$

$\mathrm{Im}\,\Pi(\omega)$ is an odd function of ω!

Using the properties of δ-functions and $\hat{A} = \hat{A}^+$, we may re-write

$$\mathrm{Im}\,\Pi_R(\omega) = -\frac{1}{\hbar}\cdot\frac{\pi}{Z}\sum_{nm} e^{-\beta E_n} |A_{nm}|^2 \Big(\delta(\omega + \omega_n - \omega_m) - \delta(\omega + \omega_m - \omega_n) \Big)$$

$$= -\frac{1}{\hbar}\cdot\frac{\pi}{Z}\sum_{nm}\Big(\underbrace{e^{-\beta E_n} |A_{nm}|^2 \delta(\omega + \omega_n - \omega_m)}_{\text{perform } m \rightleftarrows n} - e^{-\beta E_n} |A_{nm}|^2 \delta(\omega + \omega_m - \omega_n) \Big)$$

$$\mathrm{Im}\,\Pi_R(\omega) = \frac{1}{\hbar}\frac{\pi}{Z}\sum_{mn} \delta(\omega + \omega_m - \omega_n) |A_{mn}|^2 \left(e^{-\beta E_n} - e^{-\beta E_m} \right)$$

$|A_{mn}|^2 = |A_{nm}|^2$

$$= \frac{\pi}{\hbar}\left(e^{-\beta\hbar\omega} - 1 \right) \sum_{mn} \frac{e^{-\beta E_m}}{Z} |A_{mn}|^2 \delta(\omega + \omega_m - \omega_n)$$

Now consider, in parallel, the symmetrized corr. function:

$$\int_{-\infty}^{\infty} dt\, \frac{1}{2} \langle \hat{A}(0)\hat{A}(t) + \hat{A}(t)\hat{A}(0) \rangle_0\, e^{i\omega t - 0 \cdot |t|} \equiv \langle A^2 \rangle_\omega$$

(Spectral density of fluctuations)

(We assume $\langle A \rangle_0 = 0$, generalization is trivial)

$$\int_{-\infty}^{\infty} dt\, \frac{1}{2} \langle \hat{A}(0)\hat{A}(t) + \hat{A}(t)\hat{A}(0) \rangle_0\, e^{i\omega t}$$

$$= \frac{1}{2} \sum_{nm} \frac{e^{-\beta E_n}}{Z} A_{nm} A_{mn} \int_{-\infty}^{\infty} dt \left(e^{i(\omega_m - \omega_n + \omega)t} + e^{i(\omega_n - \omega_m + \omega)t} \right) e^{-0 \cdot |t|}$$

$$= \sum_{nm} \frac{e^{-\beta E_n}}{Z} A_{nm} A_{mn} \int_{-\infty}^{\infty} dt\, e^{i\omega t} \underbrace{\cos(\omega_m - \omega_n)t}_{\text{no Im part}} \cdot e^{-0 \cdot |t|}$$

$$= \pi \sum_{n,m} \frac{e^{-\beta E_n}}{Z} A_{nm} A_{mn} \left(\delta(\omega + \omega_m - \omega_n) + \delta(\omega + \omega_n - \omega_m) \right)$$

$$\langle A^2 \rangle_\omega = \pi \left(1 + e^{-\beta \hbar \omega}\right) \sum_{mn} \frac{e^{-\beta E_m}}{Z} |A_{nm}|^2 \delta(\omega + \omega_m - \omega_n)$$

Comparing with $\mathrm{Im}\,\Pi_R(\omega)$, we find:

$$\boxed{\langle A^2 \rangle_\omega = -\coth\left(\frac{\hbar\omega}{2k_B T}\right) \cdot \hbar \cdot \mathrm{Im}\,\Pi_R(\omega)}$$

(Callen, Welton, 1951)

$$\boxed{\langle A^2 \rangle_0 = -\hbar \int_0^{\infty} \frac{d\omega}{\pi} \coth\left(\tfrac{1}{2}\beta\hbar\omega\right) \mathrm{Im}\,\Pi_R(\omega)}$$

we used here $\mathrm{Im}\,\Pi_R(\omega) = -\mathrm{Im}\,\Pi_R(-\omega)$

5.3. Absorption power

Consider a perturbation $\hat{V}(t) = f(t)\hat{A} \equiv \underbrace{V_0 \cos\omega t}_{f(t)} \cdot \hat{A}$

$$\mathcal{H} = \mathcal{H}_0 + \hat{V}$$

$$\frac{d\mathcal{H}}{dt} = \frac{\partial \mathcal{H}}{\partial t} \underset{\uparrow}{=} \frac{\partial \hat{V}}{\partial t} = -V_0 \omega \sin\omega t \, \hat{A} \, ; \quad \overline{\langle \frac{d\mathcal{H}}{dt} \rangle}^{t} = -V_0 \omega \, \overline{\sin\omega t \langle A \rangle}^{t}$$

average over time

($\mathcal{H}_0$ independent of time)

$$= -\omega V_0^2 \, \overline{\sin\omega t \int_{-\infty}^{\infty} dt_1 \cos\omega t_1 \, \Pi_R(t-t_1)}^{t}$$

$\Pi_R(t-t_1) \propto \Theta(t-t_1)$

$t_2 = t_1 - t$

$$= -\omega V_0^2 \, \overline{\sin\omega t \int_{-\infty}^{0} dt_2 \left(\cos\omega t \cos\omega t_2 - \sin\omega t \sin\omega t_2\right) \Pi_R(-t_2)}^{t}$$

$$= \omega V_0^2 \cdot \frac{1}{2} \int_{-\infty}^{0} dt_2 \sin\omega t_2 \, \Pi_R(-t_2) = -\omega V_0^2 \cdot \frac{1}{2} \int_{0}^{\infty} dt_2 \sin\omega t_2 \, \Pi_R(t_2)$$

$$= -\frac{1}{2}\omega V_0^2 \, \mathrm{Im}\, \Pi_R(\omega)$$

Absorption power: $W \equiv \overline{\frac{d\mathcal{H}}{dt}}^{t} = -\frac{1}{2}\omega V_0^2 \, \mathrm{Im}\, \Pi_R(\omega)$

even function of ω!