11. Propriétés générales des fonctions de réponse

1. χ''
2. Symétries
3. Conséquences de la définition ✓

$$\chi''_{\rho_q \rho_{-q}}(\omega) = -\chi''_{\rho_q \rho_{-q}}(-\omega)$$

4. Kramers-Kronig ✓
5. Représentation spectrale ←
6. " de Lehmann ←
7. Positivité de $\chi''(\omega)\omega$ et dissipation
8. Théorème de fluctuation-dissipation

$$\mathcal{H} = H + \delta\mathcal{H}(t)$$

$$\delta\mathcal{H}(t) = -\int d^3r \; A_i(\vec{r}) \, a_i(\vec{r}, t)$$

$j \cdot A$

$$U(t,0) = e^{-iHt/\hbar} \, U_I(t,0)$$

$$\delta\langle B(r)\rangle = \delta\langle U^{+}(t,t_0) \, B(r) \, U(t,t_0)\rangle$$

$$i\hbar \frac{\partial U_I}{\partial t} = \delta\mathcal{H}_I(t) \, U_I(t,0)$$

$$U_I(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt' \, \delta\mathcal{H}_I(t')$$

$$\delta\langle B(r)\rangle = \int d^3r' \int_{-\infty}^{\infty} dt' \; \boxed{\chi^{R}_{BA_i}(r,t\,;\,r',t')} \, a_i(r',t')$$

$$\chi^{R}_{BA} = 2i \boxed{\chi''_{BA}} \, \theta(t-t') \longleftarrow$$

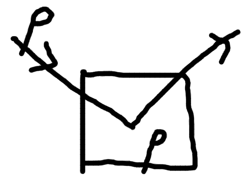
$$\chi''_{BA} = \frac{1}{2\hbar}\langle [B, A]\rangle$$

$$\delta\langle B(t)\rangle = \int dt' \; \chi^{R}_{BA}(t-t') \, a_i(t')$$

$$\delta\langle B(\omega)\rangle = \chi^{R}_{BA}(\omega) \, a(\omega)$$

$$TF\,[b(t)] = TF\left[\int dt' \; \chi(t-t') \, a(t')\right]$$
$$= [TF\,\chi]\,[TF\,a]$$

11.3 $$\boxed{\chi''_{\rho_q \rho_{-q}}(\omega) = -\chi''_{\rho_q \rho_{-q}}(-\omega)}$$



Commutateur

$$\chi''_{A_i A_j}(t) = \frac{1}{2\hbar}\langle [A_i(t), A_j(0)] \rangle$$

$$= -\chi''_{A_j A_i}(-t) \quad \Rightarrow \quad \boxed{\chi''_{A_i A_j}(\omega) = -\chi''_{A_j A_i}(-\omega)}$$

$$\langle [A_j(0), A_i(t)] \rangle$$

$$\chi''_{\underbrace{\rho_r \rho_{r'}}}(\omega) = -\chi''_{\underbrace{\rho_{r'} \rho_r}}(-\omega)$$

Hermitians:

$$\langle [A_i(t) A_j(0)] \rangle^* = \langle [A_j(0), A_i(t)] \rangle$$

$$= \mathrm{Tr}\left[\rho \left(A_i(t) A_j(0) - A_j(0) A_i(t)\right)\right]^*$$

$$= \mathrm{Tr}\left[A_j^+(0) A_i^+(t) \rho^+ - A_i^+(t) A_j^+(0) \rho^+\right]$$

$$\int dt\, e^{i\omega t} \left[\chi''^{*}_{A_i A_j}(t) = \chi''_{A_j A_i}(-t) \right]$$

$$\boxed{\chi''^{*}_{A_i A_j}(-\omega) = \chi''_{A_j A_i}(-\omega)}$$

$$\int dt\, e^{i\omega t}\, \chi^*(t) = \left[\int dt\, e^{-i\omega t}\, \chi(t)\right]^* = \chi(-\omega)^*$$

Hermitian: $\chi''_{\rho_r \rho_{r'}}(\omega)^* = \chi''_{\rho_{r'} \rho_r}(\omega)$

$$\int d^3r\, e^{-iq\cdot r} \int d^3r'\, e^{+iq\cdot r'} \qquad \boxed{\int d(r-r')\, e^{iq\cdot(r-r')}}$$

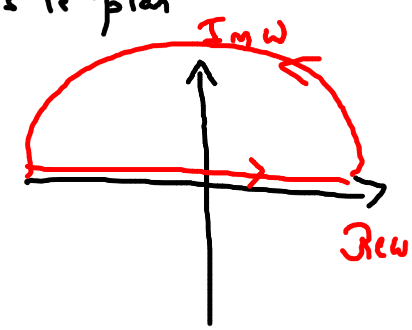
$$\left[\chi''_{\rho_{-q}\rho_q}(\omega)\right]^* = \chi''_{\rho_q \rho_{-q}}(\omega)$$

11.4 Kramers - Kronig

$$\chi^R_{ij}(t) = 2i\,\chi''_{ij}(t)\,\underbrace{\theta(t)} \rightarrow \text{causalité}$$

$\chi^R_{ij}(\omega) \rightarrow$ analytique dans le plan supérieur

$$\chi_{ij}(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t}\, \chi^R_{ij}(\omega)$$

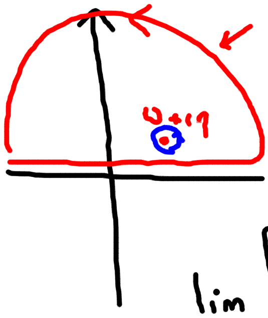


Si $\chi^R_{ij}(\omega)$ est analytique pour $\mathrm{Im}\,\omega > 0$

Si $t < 0$ $\Rightarrow$ compléter demi-plan sup.

$$\int e^{-i\omega_r t}\, \underbrace{e^{\omega_i t}} \ldots\ldots$$

$$\int \frac{d\omega'}{\pi} \frac{1}{\omega' - (\omega + i\eta)} \chi^R_{ij}(\omega') = \frac{2\cancel{\pi} i}{\cancel{\pi}} \chi^R(\omega + i\eta)$$



η infinitésimal et > 0

$\omega' = R\, e^{i\theta}$

$d\omega' = R\, i\, e^{i\theta} d\theta$

$$\lim_{\eta \to 0} \left[\frac{1}{\omega - i\eta} = \frac{\omega + i\eta}{\omega^2 + \eta^2} = \frac{\omega}{\omega^2 + \eta^2} + i \frac{\eta}{\omega^2 + \eta^2} \right]$$

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

$$\int \frac{d\omega'}{\pi}\left[\mathcal{P}\frac{1}{\omega-\omega'} + i\pi\,\delta(\omega-\omega')\right]\chi^R_{ij}(\omega')$$

$$= 2i\,\chi^R_{ij}(\omega)$$

$$\mathcal{P}\int \frac{d\omega'}{\pi}\frac{1}{\omega-\omega'}\mathrm{Re}\,\chi^R_{ij}(\omega') - \mathrm{Im}\,\chi^R_{ij}(\omega) = -2\,\mathrm{Im}\,\chi^R_{ij}(\omega)$$

$$\boxed{\begin{aligned}&\mathcal{P}\int \frac{d\omega'}{\pi}\frac{1}{\omega-\omega'}\mathrm{Re}\,\chi^R_{ij}(\omega') = -\mathrm{Im}\,\chi^R_{ij}(\omega)\\&\mathcal{P}\int \frac{d\omega'}{\pi}\frac{\mathrm{Im}\,\chi^R_{ij}(\omega')}{\omega-\omega'} = \mathrm{Re}\,\chi^R_{ij}(\omega)\end{aligned}}$$

Transformée de Hilbert

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11.5 Représentation spectrale

$\chi''(\omega)$ = fonction spectrale

poids spectral

$$\chi^R(t) = 2i\,\chi''(t)\,\theta(t)\,e^{-\eta t}$$

$$\boxed{\int e^{i(\omega+i\eta)t}\,dt}$$

$$\rightarrow \quad \chi^R(\omega) = \cancel{2i} \int \frac{d\omega'}{\cancel{2}\pi}\, \chi''(\omega')\, \theta(\underbrace{\omega+i\eta}-\omega')$$

$$\int_{-\infty}^{\infty} dt\, e^{i\omega t-\eta t}\,\theta(t) = \int_0^{\infty} dt\, e^{i\omega t-\eta t} = \left.\frac{e^{i\omega t-\eta t}}{i\omega}\right|_0^{\infty} = -\frac{1}{\cancel{i}\omega}$$

$$\boxed{\chi^R(\omega) = \int \frac{d\omega'}{\pi}\,\frac{\chi''(\omega')}{\omega'-(\omega+i\eta)}}$$

$$= \underbrace{\mathcal{P}\int \frac{d\omega'}{\pi}\,\frac{\chi''(\omega')}{\omega'-\omega}}_{\mathrm{Re}\,\chi^R(\omega)} + \underbrace{i\,\chi''(\omega)}_{\mathrm{Im}\,\chi^R(\omega)}$$

$$\mathrm{Re}\,\chi^R(\omega) = \mathcal{P}\int \frac{d\omega'}{\pi}\,\frac{\mathrm{Im}\,\chi^R(\omega')}{\omega'-\omega}$$

$$\boxed{\chi(z) = \int \frac{d\omega'}{\pi}\,\frac{\chi''(\omega')}{\omega'-z}} \qquad z = \omega + i\eta$$

$$\chi^A(\omega) = \chi(z=\omega-i\eta)$$

$$\chi^A(\omega) = \mathcal{P}\int \frac{d\omega'}{\pi}\,\frac{\chi''(\omega')}{\omega'-\omega} - i\,\chi''(\omega)$$

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11.6 Représentation de Lehmann

$$\chi''_{A_iA_j}(t) = \frac{1}{2\hbar} \mathrm{Tr}\left[\rho\left(A_i(t)\,A_j(0) - A_j(0)\,A_i(t)\right)\right]$$

$$= \frac{1}{2\hbar}\sum_{n,m} \frac{e^{-\beta E_n}}{Z}\Big[\langle n| e^{iE_nt/\hbar} A_i e^{-iE_mt/\hbar}|m\rangle\langle m| A_j |n\rangle$$

$$- \langle n| A_j |m\rangle\langle m| e^{+iE_mt/\hbar} A_i e^{-iE_nt/\hbar} |n\rangle\Big]$$

$$= \frac{1}{2\hbar}\sum_{m,n} \frac{e^{-\beta E_n} - e^{-\beta E_m}}{Z}\, e^{i(E_n-E_m)t/\hbar} \langle n|A_i|m\rangle\langle m|A_j|n\rangle$$

$$\chi''_{A_iA_j}(\omega) = \pi\sum_{n,m} \frac{e^{-\beta E_n} - e^{-\beta E_m}}{Z} \langle n|A_i|m\rangle\langle m|A_j|n\rangle\, \delta\left(\hbar\omega - (E_m - E_n)\right)$$

$T = 0 \quad \beta = \infty$

$$= \pi\sum_{m\neq 0} \overline{\langle 0|A_i|m\rangle}\,\overline{\langle m|A_j|0\rangle}\, \delta\left(\hbar\omega - (E_m - E_0)\right)$$

$$\boxed{\chi_{A_iA_j}(z) = \sum_{n,m} \frac{e^{-\beta E_n} - e^{-\beta E_m}}{Z} \frac{\langle n|A_i|m\rangle\langle m|A_j|n\rangle}{\hbar z - (E_m - E_n)}}$$

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$$\delta(a x) = \frac{1}{|a|}\delta(x)$$