1 Erreurs flagrantes du cours numéro 4:

Au bas de la page 3:

$$S_{A_j A_i}(-t) = S_{A_i A_j}(t - i\hbar\beta). \tag{1}$$

$$S_{A_j A_i}(-\omega) = e^{-\beta\hbar\omega} S_{A_i A_j}(\omega). \tag{2}$$

Au milieu de la page 5.

$$\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \omega^n \chi''_{A_i A_j}(\omega) = \left[\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left(i \frac{\partial}{\partial t} \right)^n e^{-i\omega t} 2\chi''_{A_i A_j}(\omega) \right]_{t=0} \tag{3}$$

11.5 Positivité de $\omega\chi''$ et dissipation

11.6 Th. F.-D.

11.7 Règles de somme

- T.D.
- Ordre des limites
- Moments de χ'' et $\omega \to \infty$
- Règle de somme f

12. Kubo pour σ

1 - Rappel
2 - Réponse général $(\vec{A}, \varphi)$
3 - σ cas transversal

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11.5 Positivité $a_i^* \boxed{\omega \chi''_{A_iA_j}} a_j > 0$

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

$$\int_{-T/2}^{T/2} dt \left\langle \frac{\partial \mathcal{H}(t)}{\partial t} \right\rangle = W = \int dt \left(-\langle A_i \rangle \frac{\partial a_i}{\partial t} \right)$$

$$= \int dt \, - \boxed{\langle A_i(t) \rangle} \frac{\partial a_i(t)}{\partial t}$$

$$= -\int \frac{d\omega}{2\pi} \, a_i(-\omega) \, \chi^R_{A_iA_j}(\omega) \, i\omega \, a_j(\omega)$$

$$\cos(t) = \frac{e^{i\omega t} + e^{-i\omega t}}{2}$$

11.8 F.D.

$$S_{A_iA_j}(t) = \langle \underbrace{\left(A_i(t) - \langle A_i\rangle\right)}_{\delta A_i(t)} \underbrace{\left(A_j(0) - \langle A_j(0)\rangle\right)}_{\delta A_j(0)} \rangle$$

$$\boxed{S_{A_iA_j}(\omega) = \frac{2\hbar}{1-e^{-\beta\hbar\omega}}\, \chi''_{A_iA_j}(\omega)}$$ F.D.

Preuve

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

$$= \frac{1}{2\hbar}\left[\langle \delta A_i(t)\delta A_j(0)\rangle - \langle \delta A_j(0)\delta A_i(t)\rangle\right]$$

$$\langle O \rangle = \frac{\mathrm{Tr}\left(e^{-\beta(H-\mu N)}\, O\right)}{\mathrm{Tr}\left(e^{-\beta(H-\mu N)}\right)}$$

$$e^{-\beta(H-\mu N)} \equiv e^{-\beta K}$$

$$\mathrm{Tr} \to \sum_n \langle n| \quad |n\rangle$$

$$\mathrm{Tr}\left[\rho\, \delta A_j\, \delta A_i(t)\right] = \mathrm{Tr}\left[\delta A_i(t)\, \rho\, \delta A_j(0)\right]$$

$$= \mathrm{Tr}\left[\boxed{e^{-\beta K} e^{\beta K}}\, \boxed{\delta A_i(t)}\, \frac{e^{-\beta K}}{Z}\, \delta A_j(0)\right]$$

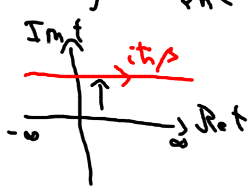
$$= \frac{1}{Z}\mathrm{Tr}\left[e^{-\beta K}\, e^{\beta K}\, e^{iKt/\hbar}\, \delta A_i\, e^{-iKt/\hbar}\, e^{-\beta K}\, \delta A_j(0)\right]$$

$$\delta A_i(t-i\hbar\beta) = e^{iK(t-i\hbar\beta)/\hbar}\, \delta A_i\, e^{-iK(t-i\hbar\beta)/\hbar}$$

$$= \langle \delta A_i(t-i\hbar\beta)\, \delta A_j\rangle = S_{A_iA_j}(t-i\hbar\beta)$$

$$\chi''_{A_iA_j}(t) = \frac{1}{2\hbar}\left(S_{A_iA_j}(t) - S_{A_iA_j}(t-i\hbar\beta)\right)$$

$$\to \chi''_{A_iA_j}(\omega) = \frac{1}{2\hbar}\left[S_{A_iA_j}(\omega) - \int dt\, e^{i\omega t}\, S_{A_iA_j}(t-i\hbar\beta)\right]$$



$$\int dt\, e^{i\omega(t+i\hbar\beta)}\, S_{A_iA_j}(t) = \boxed{e^{-\beta\hbar\omega}\, S_{A_iA_j}(\omega)}$$

$$S_{A_jA_i}(t) = S_{A_iA_j}(t-i\hbar\beta)$$

$$\boxed{S_{A_jA_i}(\omega) = e^{-\beta\hbar\omega}\, S_{A_iA_j}(\omega)}$$

11.9 Règles de somme.

- Règle de somme T. D.

$$\delta \langle A_i(\omega=0)\rangle = \chi^{R}_{A_i A_j}(\omega=0)\,\delta a_j(\omega=0)$$

$$\left(\frac{\partial n}{\partial \mu}\right)_T = \chi^{R}_{nn}(\omega=0) = \int \frac{d\omega'}{\pi}\frac{\chi''_{nn}(\omega')}{\omega' - i\eta}$$

$$= \int \frac{d\omega'}{\pi}\frac{\chi''_{nn}(\omega')}{\omega'}$$

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Cas plus général

Règles de somme $\rightarrow$ moments

$$\begin{cases} \text{Prob. } P(x) \\ \langle x^n \rangle = \int dx\, P(x)\, x^n \end{cases}$$ moments

analogue

$$\int \frac{d\omega'}{2\pi} (\omega')^n 2\chi''_{A_i A_j}(\omega') =$$

$$\int \frac{d\omega'}{2\pi} \left(i\frac{\partial}{\partial t} \right)^n \int dt'\, e^{i\omega'(t-t')} 2\chi''_{A_i A_j}(t')$$

$$= \frac{1}{\hbar} \left\langle \left[\left(i\frac{\partial}{\partial t}\right)^n A_i(t), A_j(0) \right] \right\rangle_{t=0}$$

$t \quad t' \quad t=t'$

$$i\frac{\partial}{\partial t} A(t) = i\frac{\partial}{\partial t}\left[e^{iKt/\hbar} A_i\, e^{-iKt/\hbar} \right]$$

$$= -\frac{1}{\hbar}\left[K, A_i(t) \right]$$

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Comportement haute fréquence

$$\chi^R_{A_iA_j}(\omega) = \int \frac{d\omega'}{\pi} \frac{\chi''_{A_iA_j}(\omega')}{\omega'-\omega-i\eta}$$

$\omega \gg$ domaine où $\chi''(\omega) \neq 0$

$$\chi^R_{A_iA_j}(\omega) = -\frac{1}{\omega}\int \frac{d\omega'}{\pi} \frac{\chi''_{A_iA_j}(\omega')}{1-\left(\frac{\omega'}{\omega}\right)}$$

$$= -\frac{1}{\omega}\int \frac{d\omega'}{\pi} \sum_{n=1}^{\infty}\left(\frac{\omega'}{\omega}\right)^{2n-1} \chi''_{A_iA_j}(\omega')$$

$n=1 \rightarrow \frac{1}{\omega^2}$

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Règle de somme f

$$\boxed{\int_{-\infty}^{\infty} \frac{d\omega'}{\pi}\, \omega' \chi''_{nn}(q,\omega') = \frac{n q^2}{m}}$$

indép. des interactions

$$= \left(i \frac{\partial}{\partial t} \langle [n_q(t), n_{-q}] \rangle \right)_{t=0} \frac{1}{\hbar V} =$$

$$\int d^3(r-r')\, e^{-i\vec{q}\cdot(\vec{r}-\vec{r}')} \chi_{nn}(r-r', t)$$

$$= \int \frac{d^3r\, d^3r'}{V} e^{-iq\cdot r} e^{iq\cdot r'} \frac{1}{2\hbar} \langle [n(r,t), n(r',0)] \rangle$$

$$= -\frac{1}{\hbar^2 V} \langle [[H, n_q], n_{-q}] \rangle \quad -\frac{\hbar^2}{m} N q^2 \left(-\frac{1}{\hbar^2 V}\right)$$

$$[H, n_q] = \left[H, \sum_\alpha e^{-iq\cdot r_\alpha}\right]$$

$$n_q = \int d^3r\, e^{-i\vec{q}\cdot\vec{r}} \sum_{\vec{r}_\alpha} \delta(r - \vec{r}_\alpha) = \underbrace{\sum_{r_\alpha} e^{-i\vec{q}\cdot\vec{r}_\alpha}}$$

$n(r)$

$$[H, n_q] = \left[\sum_\beta \frac{\vec{p}_\beta^{\,2}}{2m}, \sum_\alpha e^{-iq\cdot r_\alpha}\right]$$

$$[AB, C] = A[B, C] + [A, C]B$$

$$= \frac{1}{2m} \sum_{\beta, a} p_\beta^a \left[\frac{\hbar}{i}\nabla_\beta^a, e^{-iq\cdot r_\beta}\right] + \text{autre}$$

$$= \frac{\hbar}{2mi} \sum_{\beta, a} (-iq_a) e^{-iq_a r_\beta^a} p_\beta^a + \text{autre}$$

$$\langle [[H, n_q], n_{-q}] \rangle = \frac{\hbar}{2mi} \langle \sum_{\beta, a} e^{-iq_a r_\beta^a} (-iq_a) [p_\beta^a, e^{iq_a r_\beta^a}] + \text{autre} \rangle$$

$$= \frac{\hbar^2}{2mi} \sum_{\beta a} (-iq_a) q_a + \text{autre}$$

$$= -\frac{\hbar^2}{m} \sum_{\beta a} q_a^2$$

$$= -\frac{\hbar^2}{m} q^2 N$$

12. Formule de Kubo

Relie σ à χ_{jj}

$$\int d\omega \, \mathrm{Re}\, \sigma(\omega) = \frac{ne^2}{m}$$ Règle de somme f

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Rappel:

$$\vec{E} = -\frac{\partial \vec{A}}{\partial t} - \nabla\varphi \qquad \vec{B} = \vec{\nabla}\times\vec{A}$$

invariance de jauge.

$$\vec{A} \to \vec{A} + \vec{\nabla}\Lambda$$

$$\varphi \to \varphi - \frac{\partial\Lambda}{\partial t}$$

En M.Q. couplage au champ E.M.

$$\left.\begin{array}{l} \frac{\hbar}{i}\vec{\nabla} \to \frac{\hbar}{i}\vec{\nabla} - q\vec{A} \\ i\hbar\frac{\partial}{\partial t} \to i\hbar\frac{\partial}{\partial t} - q\varphi \end{array}\right) \text{Couplage minimal}$$

$$\left(i\hbar\frac{\partial}{\partial t} - q\varphi\right)\psi = \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla} - q\vec{A}\right)^2\psi + V\psi$$

$$\left(i\hbar\frac{\partial}{\partial t} - q\varphi + q\frac{\partial\Lambda}{\partial t}\right)\psi' = \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla} - q\vec{A} - q\vec{\nabla}\Lambda\right)\psi' + V\psi'$$

$$\boxed{\psi' = e^{i\Lambda q/\hbar}\,\psi}$$

$$\int d^3r\, \psi'^* \, V \, \psi'$$

$$\int d^3r\, \psi'^* \left[\frac{\hbar}{i}\vec{\nabla} - q\vec{A} - q\vec{\nabla}\Lambda\right]\psi'$$

$$= \int d^3r\, \psi^* \left[\frac{\hbar}{i}\nabla - qA\right]\psi$$

$$\boxed{\begin{array}{l} \int d^3r\, \psi'^* \frac{\hbar}{i}\vec{\nabla}\psi' \\ \neq \int d^3r\, \psi^* \frac{\hbar}{i}\vec{\nabla}\psi \end{array}}$$