4.7 3 théorèmes généraux

1. Wick
2. Graphs connexes
3. Principe variationnel

Résumé:

$$G^R(k,\omega) = \frac{1}{\omega - \xi_k - \Sigma^R(k,\omega)}$$

$$A(k,\omega) = -2\,\mathrm{Im}\,G^R(k,\omega)$$

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

$$\Sigma''(k,\omega) = -\gamma\omega^2$$

$$\Sigma^R(k,\omega) - \Sigma^R(k,\infty) = \int\frac{d\omega'}{\pi}\,\frac{\Sigma''(k,\omega')}{\omega'-\omega}$$

$$\Sigma'(k,\omega) = c - \gamma\omega$$

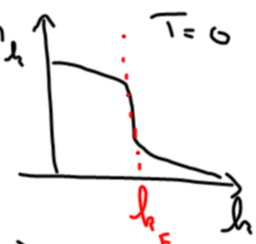
$$\omega - \xi_k - \Sigma^R(k,\omega)\Big|_{\omega=E_k-\mu} = 0$$

$$\omega-\xi_k-\Sigma' = (\omega - E_k+\mu)\underbrace{\left(1-\frac{\partial\Sigma'}{\partial\omega}\right)}_{Z^{-1}}$$

$$A(k,\omega) = Z_k\,2\pi\left[\frac{1}{\pi}\,\frac{\Gamma_k}{(\omega-E_k+\mu)^2+\Gamma_k^2}\right] + \mathrm{Inc.}$$

$$\boxed{\Gamma_k = Z_k\,\mathrm{Im}\,\Sigma^R}$$

$$n_k = \int\frac{d\omega}{2\pi}\,f(\omega)\,A(k,\omega) \underset{T=0}{\Longrightarrow}$$



$$\chi(q=0,\omega=0) \propto N(0) \quad \text{à } T=0$$

$$\frac{m}{m^*} = Z\left(1+\frac{\partial\Sigma'}{\partial\xi_k}\right)$$

$\frac{k^2}{2m}$

$$\chi \propto N^*(0)\Big/(1+F_0^s)$$

$$\frac{\partial n}{\partial\mu} \propto N^*(0)\Big/(1+F_0^a)$$

1. Théorème de Wick:

$$\boxed{K_0 = \sum_\alpha \xi_\alpha a^+_\alpha a_\alpha}$$

Base propre:

$\langle a_\alpha a^+_\alpha a_\beta a^+_\beta \rangle_0$ où $\alpha \neq \beta$

$$= \langle a_\alpha a^+_\alpha \rangle_0 \langle a_\beta a^+_\beta \rangle_0$$

$$(1 + a^+_1)(1 + a^+_2)(1 + a^+_3) \ldots |0\rangle$$

$$\langle a_i(\tau_i)\, a_j(\tau_j)\, a^+_h(\tau_h)\, a^+_l(\tau_l) \rangle$$

$$\boxed{a_i(\tau_i) = \langle i|\alpha\rangle a_\alpha e^{-\xi_\alpha \tau_i}}$$

$$= e^{-\xi_\alpha \tau_i} e^{-\xi_\beta \tau_j} e^{\xi_\gamma \tau_h} e^{\xi_\delta \tau_l}$$

$$\langle i|\alpha\rangle \langle j|\beta\rangle \langle a_\alpha a_\beta a^+_\gamma a^+_\delta \rangle \langle \gamma|h\rangle \langle \delta|l\rangle$$

$$\langle a_\alpha a_\beta a^+_\gamma a^+_\delta \rangle = \langle a_\alpha a^+_\delta \rangle \langle a_\beta a^+_\gamma \rangle \delta_{\alpha\delta} \delta_{\beta\gamma}$$

$$\langle a_\alpha a_\beta a^+_\gamma a^+_\delta \rangle = -\langle a_\alpha a^+_\gamma \rangle \langle a_\beta a^+_\delta \rangle \delta_{\alpha\gamma} \delta_{\beta\delta}$$

$$\langle a_\alpha a_\beta a^+_\gamma a^+_\delta \rangle =$$

$$\langle a_\alpha a^+_\delta \rangle \langle a_\beta a^+_\gamma \rangle - \langle a_\alpha a^+_\gamma \rangle \langle a_\beta a^+_\delta \rangle$$

$$\langle T_\tau [a_i(\tau_i)\, a_j(\tau_j)\, a^+_h(\tau_h)\, a^+_l(\tau_l)] \rangle$$

$$= \langle T_\tau [a_i(\tau_i)\, a^+_l(\tau_l)] \rangle \langle T_\tau [a_j(\tau_j)\, a^+_h(\tau_h)] \rangle$$

$$- \langle T_\tau [a_i(\tau_i)\, a^+_h(\tau_h)] \rangle \langle T_\tau [a_j(\tau_j)\, a^+_l(\tau_l)] \rangle$$

1 2 3 4

$$- \langle a_j(\tau_j)\, a_i(\tau_i)\, a^+_h(\tau_h)\, a^+_l(\tau_l) \rangle$$

$$= -\langle a_i(\tau_i)\, a^+_h(\tau_h) \rangle \langle a_j(\tau_j)\, a^+_l(\tau_l) \rangle$$

3 4

$$+ \langle a_j(\tau_j)\, a^+_h(\tau_h) \rangle \langle a_i(\tau_i)\, a^+_l(\tau_l) \rangle$$

2 1

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$\tau_i > \tau_k > \tau_j > \tau_l$

$$= -\langle a_i\, a_k^{+}\, a_j\, a_l^{+} \rangle$$

$$= -\langle a_i a_l^{+} \rangle \langle a_k^{+} a_j \rangle$$

$$- \langle a_i a_k^{+} \rangle \langle a_j a_l^{+} \rangle$$

$$= \langle T_\tau [a_i a_l^{+}] \rangle \langle T_\tau [a_j a_k^{+}] \rangle$$

$$- \langle T_\tau [a_i a_k^{+}] \rangle \langle T_\tau [a_j a_l^{+}] \rangle$$

$$\langle a_\alpha^{+} a_\alpha \rangle \neq -\langle a_\alpha a_\alpha^{+} \rangle$$

$$\langle T_\tau [a_\alpha a_\beta^{+}] \rangle = -\langle T_\tau [a_\beta^{+} a_\alpha] \rangle$$

$$\langle a_\alpha a_\beta^{+} \rangle \Theta(\tau_\alpha - \tau_\beta) \qquad - \langle a_\beta^{+} a_\alpha \rangle \Theta(\tau_\beta - \tau_\alpha)$$

$$- \langle a_\beta^{+} a_\alpha \rangle \Theta(\tau_\beta - \tau_\alpha) \qquad + \langle a_\alpha a_\beta^{+} \rangle \Theta(\tau_\alpha - \tau_\beta)$$

9. Théorème des graphes connexes

$\uparrow$ moyennes.

→ Moyenne "connectée"

→ Cumulant

<u>Motivation:</u>

$$P(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2}$$

$$\langle x^2 \rangle = \sigma^2$$

$$\langle x^4 \rangle = 3(\sigma^2)^2 = \langle x\, x\, x\, x \rangle$$

$$\langle x^6 \rangle = X(\sigma^2)^3$$

$$\boxed{\langle x^2 \rangle - \langle x \rangle^2 \equiv \langle x^2 \rangle_c}$$

Cumulant, connexe.

$$\langle x^4 \rangle = \langle x^4 \rangle_c + 3\langle x^2 \rangle^2$$
$$+ a\langle x \rangle^4 + b\langle x^2 \rangle\langle x \rangle^2$$
$$+ c\langle x^3 \rangle\langle x \rangle + \ldots$$

Green: $\dfrac{\langle T_\tau \, e^{-\int \underline{v(\tau)} d\tau} \psi^+ \psi \rangle}{\langle T_\tau \, e^{-\int v(\tau) d\tau} \rangle}$

<u>Cas général:</u>

à prouver $\boxed{\dfrac{\langle e^{-f(x)} A(x) \rangle}{\langle e^{-f(x)} \rangle} = \langle e^{-f(x)} A(x) \rangle_c}$

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Preuve:

Développer num. en puissances de f:

$$\sum_{n=0}^{\infty} \frac{1}{n!} \langle (-f(x))^n A(x) \rangle$$

$$= \cancel{\sum_{n=0}^{\infty}} \frac{1}{\cancel{n!}} \sum_{l,m} \cancel{\delta_{n,m+l}} \frac{\cancel{n!}}{m!\, l!} \langle (-f)^l A \rangle_c \langle (-f)^m \rangle$$

$$\langle f \; f \; f \dots f \; A \rangle$$

$$= \langle e^{-f(x)} \rangle \langle e^{-f(x)} A \rangle_c$$

À prouver :

$$\boxed{\ln \langle e^{-f(x)} \rangle = \langle e^{-f(x)} \rangle_c - 1}$$

$$\frac{\partial}{\partial \lambda} \langle e^{-\lambda f(x)} \rangle = - \langle e^{-\lambda f(x)} f(x) \rangle$$

Remarque $\frac{\partial}{\partial \lambda} T_\tau e^{-\lambda \int V(\tau) d\tau}$

$= T_\tau \left[\left(- \int V(\tau) d\tau \right) e^{-\lambda \int V(\tau) d\tau} \right]$

$$= - \langle e^{-\lambda f(x)} f(x) \rangle_c \langle e^{-\lambda f(x)} \rangle$$

$$\frac{\partial}{\partial \lambda} \ln \langle e^{-\lambda f(x)} \rangle = - \langle e^{-\lambda f(x)} f(x) \rangle_c$$

$$= \langle \frac{\partial}{\partial \lambda} e^{-\lambda f(x)} \rangle_c$$

$$\ln \langle e^{-\lambda f(x)} \rangle \Big|_0^1 = \langle e^{-\lambda f(x)} \rangle_c \Big|_0^1$$

$$\boxed{\ln \langle e^{-f(x)} \rangle = \langle e^{-f(x)} \rangle_c - 1}$$

$C_k = \langle e^{+kx} \rangle$ = fonction génératrice des moments

$$\left. \frac{\partial^n C_k}{\partial k^n} \right|_{k=0} = \langle x^n \rangle$$

$C_k' = \ln \langle e^{kx} \rangle$ = fonction génératrice des cumulants

$$\left. \frac{\partial^n C_k'}{\partial k} \right|_{k=0} = \langle x^n \rangle_c$$

exemple :

$$\ln \langle e^x \rangle = \langle e^x \rangle_c - 1$$

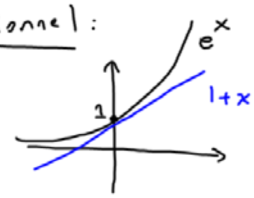
$$\ln \left\langle \left(1 + x + \frac{x^2}{2} + \dots \right) \right\rangle \qquad \boxed{\ln(1+y) = y - \frac{y^2}{2}}$$

$$= \ln \left(1 + \langle x \rangle + \frac{\langle x^2 \rangle}{2} + \dots \right)$$

$$= \left(\langle x \rangle + \frac{\langle x^2 \rangle}{2} + \dots \right) - \frac{\langle x \rangle^2}{2} = \langle x \rangle_c + \frac{\langle x^2 \rangle_c}{2}$$

3. Principe variationnel:

$$\boxed{e^x \geq 1+x}$$



Convexité:

$$\frac{\partial^2 e^x}{\partial x^2} > 0 \quad \forall x$$

Classique:

$$H = H_0 + V \quad \text{et} \quad [H_0, V] = 0$$

$$Z = \mathrm{Tr}\, e^{-\beta H}$$

$$Z_0 = \mathrm{Tr}\, e^{-\beta \tilde{H}_0}$$ où $\tilde{H}_0$ est quadratique "soluble"

$$\begin{aligned}
F &= -T \ln Z \\
&= -T \ln \mathrm{Tr}\, e^{-\beta \tilde{H}_0 - \beta(H - \tilde{H}_0)} \\
&= -T \ln \left[\frac{\mathrm{Tr}\, e^{-\beta \tilde{H}_0} e^{-\beta(H - \tilde{H}_0)}}{\mathrm{Tr}\, e^{-\beta \tilde{H}_0}} \right] - T \ln \left[\mathrm{Tr}\, e^{-\beta \tilde{H}_0} \right] \\
&= -T \ln Z_{\tilde{0}} - T \ln \langle e^{-\beta(H - \tilde{H}_0)} \rangle_{\tilde{0}} \\
&= -T \ln \tilde{Z}_0 - \cancel{T} \underbrace{\left[\langle e^{-\beta(H - \tilde{H}_0)} \rangle_c - 1 \right]}_{\geq \langle -\cancel{\beta}(H - H_{\tilde{0}}) \rangle_c}
\end{aligned}$$

$$\boxed{-T \ln Z \leq -T \ln \tilde{Z}_0 + \langle H - \tilde{H}_0 \rangle_{c\,\tilde{0}}}$$

Physique:

$$\longrightarrow \rho_{\tilde{0}} = \frac{e^{-\beta(H_{\tilde{0}} - \mu N)}}{\tilde{Z}_0} \quad \text{matrice densité}$$

$$F = -T \ln Z \leq \mathrm{Tr}\left[\rho_0 (H - \mu N)\right] + T\, \mathrm{Tr}\left[\rho_0 \ln \rho_0\right]$$

$$\langle E - \mu N \rangle + TS$$

$$\mathrm{Tr}\left[\rho_0 \ln \rho_0\right]$$

$$= \mathrm{Tr}\left[\frac{e^{-\beta(\tilde{H}_0 - \mu N)}}{\tilde{Z}_0}\left(-\ln \tilde{Z}_0 + \left(-\beta(\tilde{H}_0 - \mu N)\right)\right)\right]$$

$$= -\ln \tilde{Z}_0 - \beta \langle \tilde{H}_0 - \mu N \rangle$$

$$-T \ln Z \leq \langle H - \mu N \rangle + T\left(-\ln Z_0\right) - \langle \tilde{H}_0 - \mu N \rangle$$

$$\leq -T \ln Z_0 + \langle H - \tilde{H}_0 \rangle \quad \longleftarrow$$

Hartree Fock

$$\tilde{H}_0 = -\int d^d r \; \psi^\dagger(r) \, \frac{\nabla^2}{2m} \, \psi(r)$$

$$\psi^\dagger(r) = \sum_\alpha |\alpha\rangle \underbrace{\langle\alpha|r\rangle}_{\varphi^*_\alpha(r)} c^\dagger_\alpha$$

Motivation:

Gaz de Coulomb:

$$= -\frac{\langle T_\tau \hat{U}(\beta,\tau)\hat{\Psi}(\tau)\hat{U}(\tau,\tau')\hat{\Psi}^+(\tau')\hat{U}(\tau',0)]}{\langle \hat{U}(\beta,0)\rangle}$$

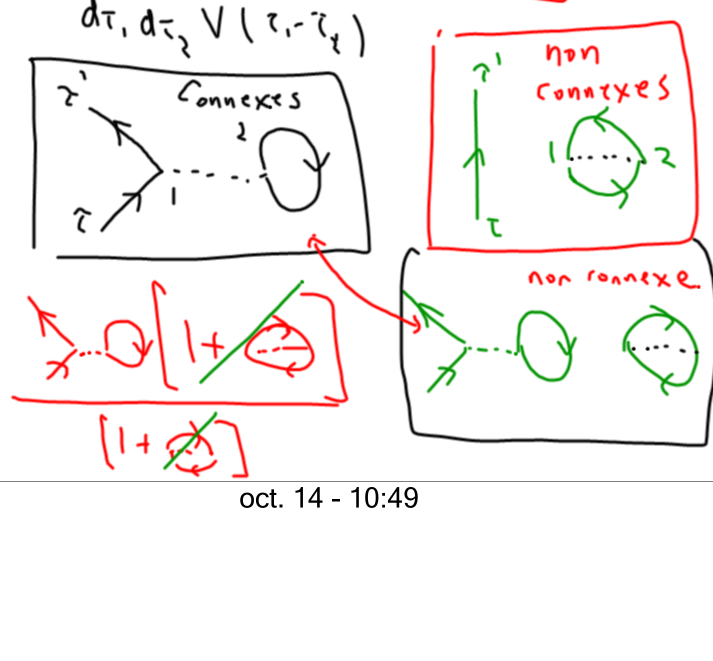
$$H = H_0 + V$$

$$= -\frac{\langle T_\tau \hat{U}(\beta,0)\hat{\Psi}(\tau)\hat{\Psi}^+(\tau')\rangle}{\langle T_\tau \hat{U}(\beta,0)\rangle}$$

$$= -\frac{\langle T_\tau\left[e^{-\int_0^\beta d\bar{\tau}\,\hat{V}(\bar{\tau})}\hat{\Psi}(\tau)\hat{\Psi}^+(\tau')\right]\rangle}{\langle T_\tau\left[e^{-\int_0^\beta d\bar{\tau}\,V(\bar{\tau})}\right]\rangle} \leftarrow$$

$$= -\langle T_\tau e^{-\int_0^\beta V(\bar{\tau})d\bar{\tau}}\hat{\Psi}(\tau)\hat{\Psi}^+(\tau')]\rangle_c$$

$$-\int \langle T_\tau \Psi^+(1)\Psi(2)\Psi^+(2)\Psi(1)\Psi(\tau)\Psi^+(\tau')\rangle_c \, d\tau_1 d\tau_2 V(\tau_1-\tau_2)$$



$$\langle \dot{j}^{R} \rangle = \langle G^{R} G^{A} \rangle$$

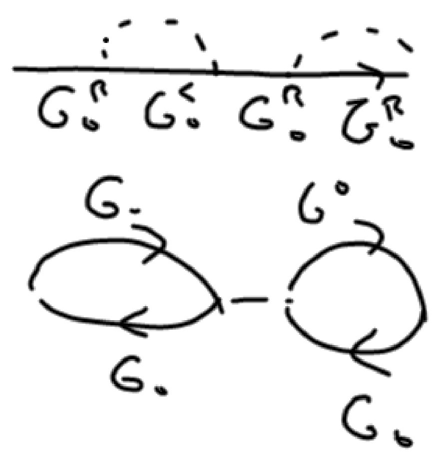
$$-\langle T_{\tau}\, \psi(\tau)\, \psi^{\dagger}(\tau') \rangle = \mathcal{G}(\tau - \tau')$$

$$\underset{\tau}{\longrightarrow}\ \tau'$$

$$\psi^{(\tau)}\, \psi^{\dagger} |0\rangle \qquad 0 \longrightarrow \tau$$

$$\psi^{\dagger}_{(0)}\, \psi_{(\tau)} |0\rangle \qquad 0 \longleftarrow \tau$$

$$G = G_0 G_0 G_0$$



$G^< \quad G^>$

G^R