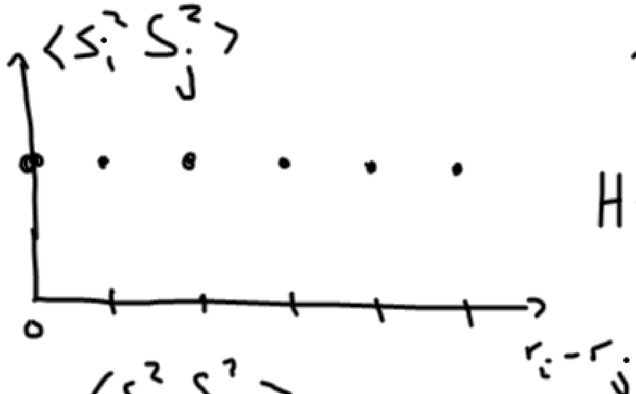
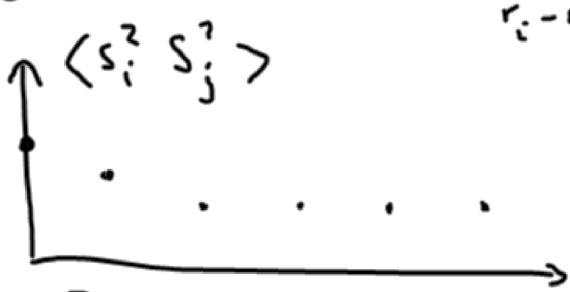


$T = 0$

$$H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$



$d = 3$

$d = 2$

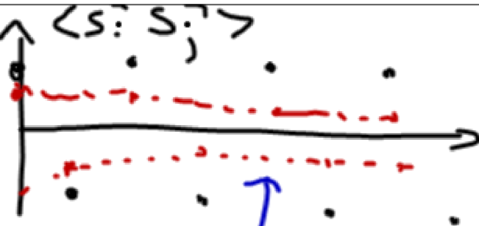
$$\langle S_i^z S_j^z \rangle = \langle S_i^z \rangle \langle S_j^z \rangle^{r_i - r_j}$$

"Émergente"

$\lim r_i - r_j \to \infty$

- Rigidité
- Excitations
- Défauts

$\langle S_i^z \rangle$ paramètre d'ordre



A.F.

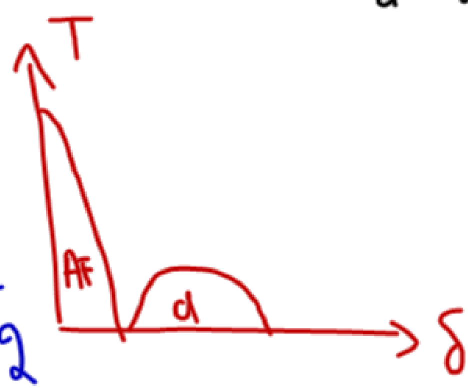
$$\mathcal{H} = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

$T = 0$

Effet des fluct. quantiques

$$\langle (-1)^i S_i^z \rangle \neq 0$$

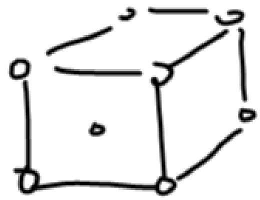
$$\langle S_Q^z \rangle \neq 0 \qquad Q = \left(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}\right)$$



∃ ordre à longue portée A.F. $d=2$

$T = 0$?

CuZn

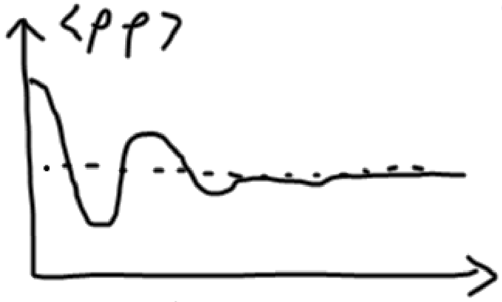


$$\sum_{r_i, r_j} \langle (\rho_{Cu}(r_i) - \rho_{Zn}(r_i)) \, e^{iQ\cdot(r_i - r_j)} \, (\rho_{Cu}(r_j) - \rho_{Zn}(r_j)) \rangle$$

$$\langle (\rho_{Cu} - \rho_{Zn})(-1)^i \rangle \neq 0$$

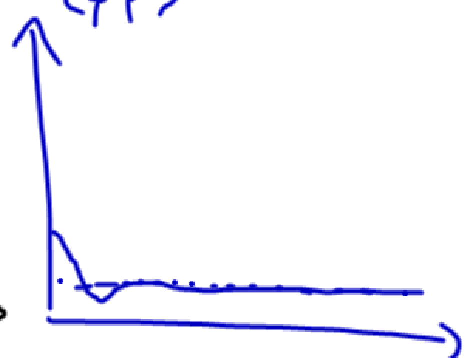
Liquide-gaz

$\langle \rho \rho \rangle$



Liquide

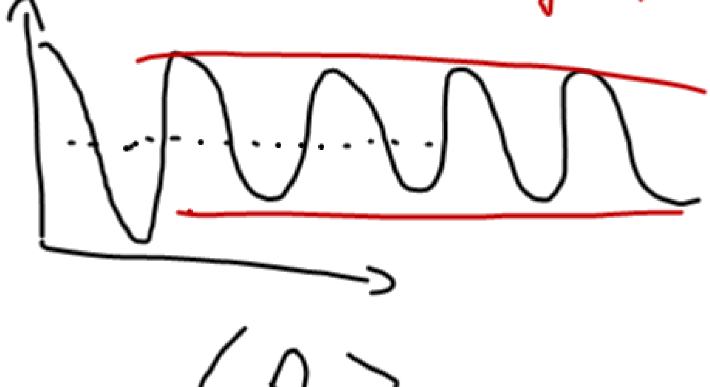
$\langle \rho \rho \rangle$



Gaz

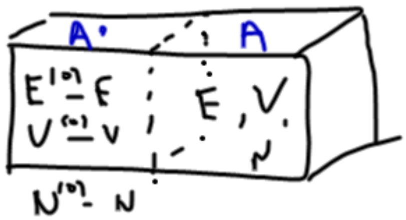
Solide

$\langle (\rho_{liquide} - \rho_{gaz}) \rangle$



$\langle \rho_G \rangle$

Rappels de T.D.



$$S_{TOT}(E^{(0)}-E, V^{(0)}-V, N^{(0)}-N, E, V, N)$$

$$= S'(E^{(0)}-E, V^{(0)}-V, N^{(0)}-N)$$

$$+ S(E, V, N)$$

$$\frac{\partial S_{TOT}}{\partial E} = 0 = \frac{\partial S'}{\partial (E^{(0)}-E)}(-1) + \frac{\partial S}{\partial E}$$

$$\frac{\partial S}{\partial E} = \frac{\partial S'(E', \dots)}{\partial E'}\Big|_{E'=E^{(0)}-E} = \frac{1}{T}$$

$$\frac{\partial S_{TOT}}{\partial V} = 0 \Rightarrow \frac{\partial S}{\partial V} = +\frac{p}{T}$$

$$\frac{\partial S_{TOT}}{\partial N} = 0 \Rightarrow \frac{\partial S}{\partial N} = -\frac{\mu}{T}$$

$$dS = \frac{1}{T}dE - \frac{\mu}{T}dN + \frac{p}{T}dV$$

$$\boxed{\begin{aligned} dE &= T\,dS - p\,dV + \mu\,dN \\ &= đQ - đW \end{aligned}}$$

Autres potentiels T.D. (Transf. de Legendre)

a) $\boxed{F = E - TS}$ $\boxed{T = \frac{\partial E}{\partial S}}$ ←

$dF = d(E - TS) = dE - TdS - SdT$

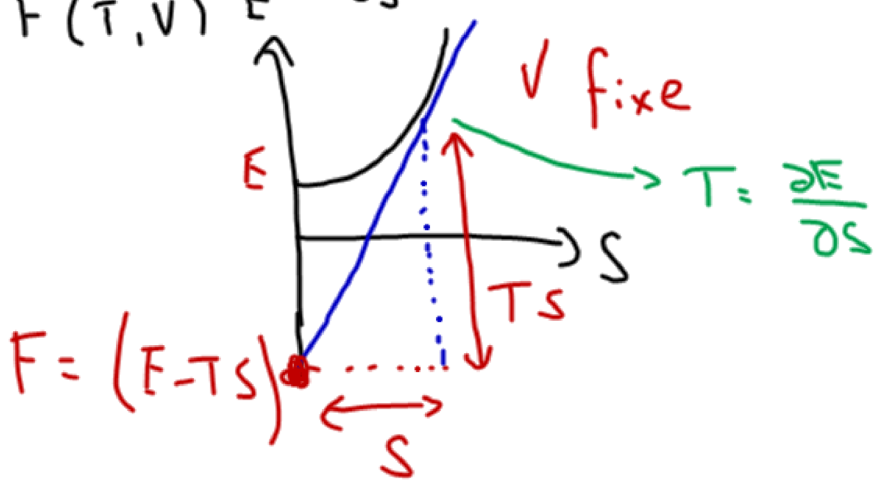
$$\boxed{dF = -SdT - pdV + \mu dN}$$

$F(T, V, N)$

b) $F(T,V) = \min_S \{E - TS\}$

$\frac{\partial E}{\partial S} = T$

c) $F(T,V)$



Physique statistique.

$$Z(\beta, p, \mu, h) = \mathrm{Tr}\left[e^{-\beta(\hat{H} - \mu\hat{N} + p\hat{V} - h\hat{M})} \right]$$

$$\boxed{-\frac{\partial \ln Z}{\partial \beta} = \langle \hat{H} - \mu\hat{N} + p\hat{V} - h\hat{M} \rangle}$$

$$= E - \mu N + pV - hM$$

$$\left\{ \frac{1}{\beta}\frac{\partial \ln Z}{\partial \mu} = \langle \hat{N} \rangle = N \qquad \frac{\partial \ln Z}{\beta\, \partial h} = \langle \hat{M} \rangle = M \right.$$

$$-\frac{1}{\beta}\frac{\partial \ln Z}{\partial p} = \langle \hat{V} \rangle = V$$

$$\Xi = -k_B T \ln Z = -\frac{1}{\beta} \ln Z(\beta,\mu,p,h)$$

$$d\Xi(T,\mu,p,h)$$

$$= \left[-k_B \ln Z - k_B T \frac{\partial \ln Z}{\partial T}\right] dT \leftarrow$$

$$-k_B T \frac{\partial \ln Z}{\partial \mu} d\mu - k_B T \frac{\partial \ln Z}{\partial p} dp - k_B T \frac{\partial \ln Z}{\partial h} dh$$

$$-\frac{\partial \ln Z}{\partial \beta} = -\frac{\partial \ln Z}{\partial T}\frac{\partial T}{\partial \beta} = +\frac{\partial \ln Z}{\partial T}\,\partial\left(\frac{1}{k_B \beta}\right)$$

$$-\left(\frac{E-\mu N+pV-hM}{T}\right) = -\frac{\partial \ln Z}{\partial T} T k_B$$

$$d\Xi = \left[\frac{\Xi}{T} - \frac{(\cancel{E}-\cancel{\mu N}+\cancel{pV}-\cancel{hM})}{T}\right] dT$$

$$-N d\mu + V dp - M dh$$

$$\boxed{\Xi = \cancel{E} - TS + \cancel{p}V - \mu \cancel{N} - M\cancel{h}}$$

$$\boxed{d\Xi = -S dT - N d\mu + V dp - M dh}$$

$$\boxed{S = -\frac{\Xi + \langle \hat{H} - \mu\hat{N} + p\hat{V} - h\hat{M} \rangle}{T}}$$

Matrice densité:

$$\boxed{\hat{D} = \frac{e^{-\beta(\hat{H}-\mu\hat{N}+p\hat{V}-h\hat{M})}}{Z}}$$

$$-k_B \mathrm{Tr}[\hat{D} \ln \hat{D}] =$$

$$-k_B \mathrm{Tr}\left[\hat{D}\left(-\ln Z - \beta(\hat{H}-\mu\hat{N}+p\hat{V}-h\hat{M})\right)\right)$$

$$\mathrm{Tr}\,\hat{D} = 1$$

$$\boxed{= +k_B \ln Z + \frac{1}{T}\langle \hat{H}-\mu\hat{N}+p\hat{V}-h\hat{M}\rangle}$$

$$= S = -k_B \mathrm{Tr}[\hat{D} \ln \hat{D}]$$

Maximiser, sujet à $\mathrm{Tr}\,\hat{D} = 1$

$\mathrm{Tr}[\hat{D}\hat{H}] = E$ etc....

Remarques sur $\hat{D}$

M.Q. valeur moyenne de $\hat{A}$
dans l'état m

$$\langle m | \hat{A} | m \rangle$$

$$\mathrm{Tr}\left[\hat{D}\hat{A}\right] \quad \text{où} \quad \hat{D} = |m\rangle\langle m|$$

$$= \sum_i \underbrace{\langle i | | m \rangle}_{\delta_{im}} \langle m | \hat{A} | i \rangle = \langle m | \hat{A} | m \rangle$$

Physique stat. "états mixtes"

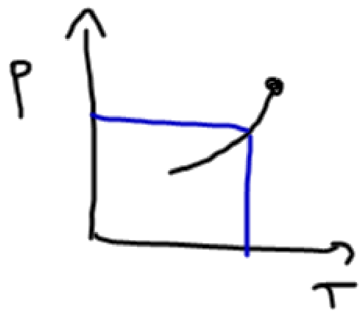
$$\hat{D} = \sum_m p_m |m\rangle\langle m|$$

$$\text{où} \sum_m p_m = 1$$

Physique stat:

$$p_m = \frac{1}{Z} e^{-\beta(E_m - \mu N_m + pV_m - hM_m)}$$

Transition 1^{er} ordre



$G(T, p, N) =$ Gibbs.

à $N =$ cte.

$$\boxed{\begin{aligned} dG &= d(E - TS + pV) \\ &= -S\,dT + V\,dp \end{aligned}}$$

$G = \mu N$

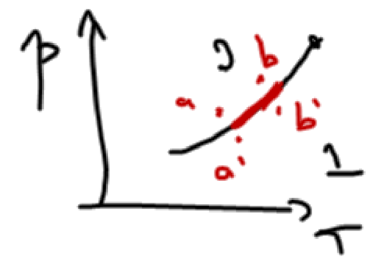
Gibbs - Duhem.

Preuve:

$$G(T, p, \lambda N) = \lambda G(T, p, N)$$

$$\left.\frac{\partial G}{\partial \lambda N}\right|_{\lambda=1} \frac{\partial(\lambda N)}{\partial \lambda} = N\mu = G$$

À la ligne de transition



Équilibre

$p_1 = p_2 \quad T_1 = T_2 \quad \mu_1 = \mu_2$

$\mu_1(T, p) = \mu_2(T, p)$ sur la ligne. $\left.\right\}$ $G_1 = G_2$ sur la ligne de coexistence.

$T_c(p_c)$

3 phases en équilibre.

$$\mu_1(T, p) = \mu_2(T, p) = \mu_3(T, p)$$

Règle des phases de Gibbs

$$dG_1 \text{ (de a à b)} = dG_2 \text{ (de a à b)}$$

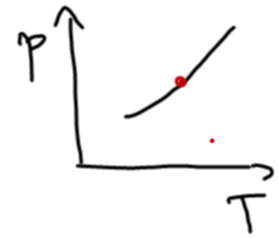
$$-S_1\,dT + V_1\,dp = -S_2\,dT + V_2\,dp$$

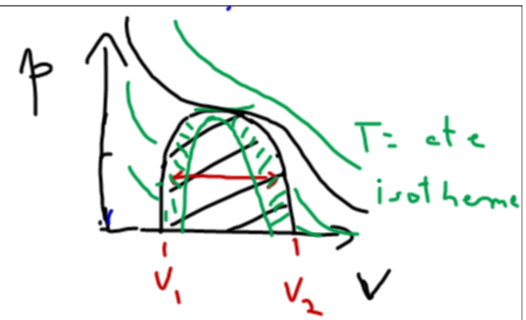
$$(S_2 - S_1)\,dT + (V_1 - V_2)\,dp = 0$$

$$\boxed{\left.\frac{dp}{dT}\right| = \frac{S_2 - S_1}{V_2 - V_1}}$$ Clausius-Clapeyron

$$\underbrace{Q}\ = T\,\underbrace{\Delta S}$$

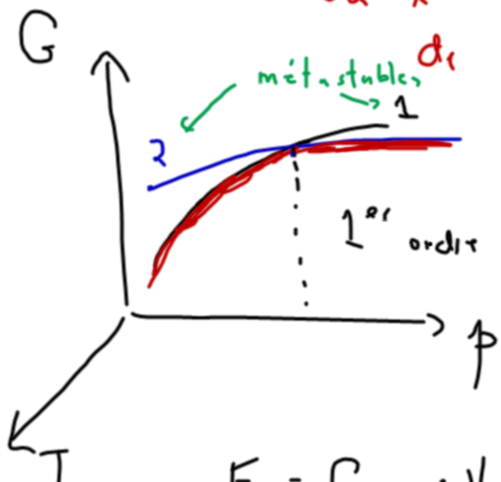
le long de la ligne de transition





$$S = xS_1 + (1-x)S_2 \; ; \; V = x(V_1) + (1-x)V_2$$

où x est la proportion de la phase 1



$$\boxed{\left(\frac{\partial G}{\partial p}\right)_T = V}$$

$$\frac{\partial V}{\partial p} < 0$$

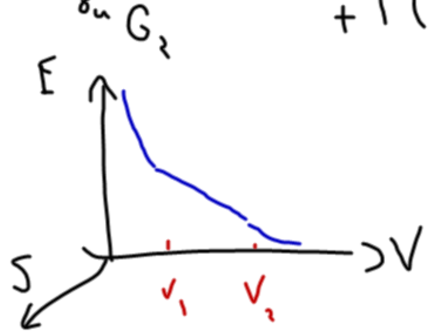
$$E_1 = G_1 - pV_1 + TS_1$$

$$E_2 = G_2 - pV_2 + TS_2$$

$$E = xE_1 + (1-x)E_2$$

$$= G_1 - p\left(xV_1 + (1-x)V_2\right)$$

ou G_2 $\quad + T\left(xS_1 + (1-x)S_2\right)$



$$\frac{\partial E}{\partial V} = -p$$

4.3 Théorie de champ moyen

- Théorie de Weiss.
- Approche variationnelle.

$$\mathcal{H} = -\sum_{ij} J_{ij}\,\vec{S}_i \cdot \vec{S}_j - g\mu_B B \sum_i S_i^z$$

Choisi B dans la direction z.

Pour simplifier $J_{ij} = 0$ si pas le premier voisin.

$J_{ij} = J$ si 1^{er} voison

$$\mathcal{H} = -Jz\sum_i \left(S_i^z \langle S^z\rangle + \langle S^z\rangle S_i^z\right) - g\mu_B B \sum_i S_i^z$$

$z \equiv$ # de premiers voisins.

$$\mathcal{H} = -A\sum_{i=1}^{N} S_i^z \quad \text{où} \quad \boxed{A \equiv 2Jz\langle S^z\rangle + g\mu_B B}$$

$$Z = \left(e^{\beta A/2} + e^{-\beta A/2}\right)^N \qquad S_i = \pm\frac{1}{2}$$

$$\mathrm{Tr}\, e^{-\beta \mathcal{H}} = \prod_{i=1}^{N} \sum_{S_i = \pm 1/2} e^{+\beta A S_i}$$

$$Z = \mathrm{Tr}\, e^{-\beta\left[-2Jz\langle S^z\rangle \sum_i S_i^z - g\mu_B B \sum_i S_i^z\right]}$$

$$\langle S_i^z\rangle = +\frac{1}{\beta}\frac{\partial \ln Z}{\partial A} = +\frac{N}{\beta}\frac{\partial \ln\left(e^{\beta A/2} + e^{-\beta A/2}\right)}{\partial A}$$

$$= +\frac{N}{\beta}\,\frac{\frac{\beta}{2}e^{\beta A/2} - \frac{\beta}{2}e^{-\beta A/2}}{e^{\frac{\beta A}{2}} + e^{-\beta\frac{A}{2}}}$$

$$= \frac{N}{2}\tanh\frac{\beta A}{2}$$

$$\boxed{N\langle S_i^z\rangle = \frac{N}{2}\tanh\frac{\beta\left[2Jz\langle S^z\rangle + g\mu_B B\right]}{2}}$$

$\beta \to 0 \quad \langle S_i^z\rangle = 0$ $\quad$ $B=0$

$\beta \to \infty \quad \langle S_i^z\rangle = \frac{1}{2}$