Théorie de champ moyen

Approche variationnelle

Approche variationnelle (général)

$$\boxed{\underline{F(T,V)} \leq \underline{F_E(T,V) - \langle H - H_E \rangle_E}}$$

Dérivation:

$$S = -k_B \, Tr\left[\hat{D} \ln \hat{D}\right]$$

$$\rightarrow \; -Tr\left[\hat{D} \ln \hat{D}\right] \leq -Tr\left[\hat{D} \ln \hat{D}'\right]$$

$$\forall \; \hat{D}' \neq \hat{D}$$

En particulier $\boxed{Tr\,\hat{D} = Tr\,\hat{D}' = 1}$

$$\underline{-k_B Tr\left[\hat{D}_E \ln \hat{D}_E\right]} \leq -k_B Tr\left[\hat{D}_E \ln \hat{D}\right]$$

$$-TS_E \geq +T k_B Tr\left[\hat{D}_E \ln\left(\frac{e^{-\beta \hat{H}}}{Z}\right)\right]$$

$$\geq +T k_B Tr\,\hat{D}_E(-\ln Z)$$

$$+(k_B T) Tr\left[\hat{D}_E(-\beta \hat{H})\right]$$

$$\underline{\langle \hat{H}_E \rangle} - TS_E \geq -k_B T \ln Z$$

$$-\langle H \rangle_E + \underline{\langle \hat{H}_E \rangle}_E$$

$$F_E \geq F + \langle H_E - H \rangle_E$$

$$\boxed{F_E + \langle H - H_E \rangle_E \geq F}$$

Hamiltonien de départ:

$$\boxed{\mathcal{H} = -J \sum_{(ij)} S_i^z S_j^z - g\mu_B B \sum_i S_i^z}$$

Hamiltonien de Ising

$S_i^z = \pm \frac{1}{2}$ $\quad \boxed{S_i = \pm 1}$

$$\boxed{\mathcal{H} = -J' \sum_{(ij)} S_i S_j - B' \sum_i S_i}$$

$J' = \frac{J}{4} \qquad B' = g\mu_B \frac{B}{2}$

$$\boxed{\mathcal{H}_E = -\sum_i x_i S_i}$$

Paramètres variationnels

① $F_E = -k_B T \ln Z_E$

$$= -k_B T \ln \prod_i \left(\sum_{S_i = \pm 1} e^{\beta x_i S_i} \right)$$

$$= -k_B T \sum_i \ln(2\cosh \beta x_i)$$

② $\langle H_E \rangle = -\sum_i x_i \langle S_i \rangle_E = -\sum_i x_i \tanh \beta x_i$

$$\langle S_i \rangle_E = \frac{1}{Z_{E_i}} \sum_{S_i = \pm 1} S_i e^{\beta x_i S_i}$$

$$= \frac{e^{\beta x_i} - e^{-\beta x_i}}{e^{\beta x_i} + e^{-\beta x_i}}$$

$$= \tanh \beta x_i$$

③ $\langle H \rangle_E = -J' \sum_{(ij)} \langle S_i S_j \rangle_E - B' \sum_i \langle S_i \rangle_E$

?

$$= -J' \sum_{(ij)} \langle S_i \rangle_E \langle S_j \rangle_E - B' \sum_i \langle S_i \rangle_E$$

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$$F_E + \langle H - H_E \rangle_E \equiv F_{CM}(\beta, B', \{x_i\})$$

$$= -\sum_{(ij)} J'_{ij} (\tanh \beta x_i)(\tanh \beta x_j)$$

$$- \sum_i (B'_i - x_i) \tanh \beta x_i$$

$$- \beta^{-1} \sum_i \ln (2 \cosh \beta x_i)$$

$$\frac{\partial F_{CM}(\beta, B', \{x_i\})}{\partial x_i} = 0$$

Solution

$$\boxed{x_i^* = B'_i + 2\sum_j J'_{ij} \tanh \beta x_j^*}$$

On veut l'aimantation comme variable indépendante

Transformée de Legendre.

$$\boxed{\Gamma_{CM}[\beta, B', \bar{M}_i] = F_{CM}[\beta, B', \{x_i^*\}] + \sum_i B'_i \bar{M}_i}$$

$$\bar{M}_i = -\frac{dF_{CM}}{dB'_i} = -\frac{\partial F_{CM}}{\partial B'_i} - \frac{\partial F_{CM}}{\partial x_i^*}\frac{\partial x_i^*}{\partial B'_i}$$

0

$$= \tanh \beta x_i^*$$

$$x_i^* = \frac{1}{\beta} \operatorname{arctanh} \bar{M}_i = \frac{1}{2\beta} \ln\left[\frac{1+\bar{M}_i}{1-\bar{M}_i}\right]$$

$$\Gamma_{CM}[\beta, \bar{M}_i] =$$

$$- N k_B T \ln 2 - \sum_{(ij)} J_{ij} \bar{M}_i \bar{M}_j$$

$$+ \frac{1}{\beta} \sum_i \left[\frac{(1+\bar{M}_i)}{2} \ln(1+\bar{M}_i) + \frac{(1-\bar{M}_i)}{2} \ln(1-\bar{M}_i) \right]$$