Théorie de champ moyen
Approche variationnelle

Approche variationnelle (général)

\[ F(T, \nu) \leq F_E(T, \nu) - \langle H - H_E \rangle_E \]

Dérivation:

\[ S = -\hbar g \text{Tr} [\hat{D} \ln \hat{D}] \]

\[ \rightarrow -\text{Tr} [\hat{D} \ln \hat{D}] \leq -\text{Tr} [\hat{D} \ln \hat{D}'] \]

\[ \forall \hat{D}' + \hat{D} \]

\[ \text{Tr} \hat{D} = \text{Tr} \hat{D}' = 1 \]

En particulier

\[ -\hbar g \text{Tr} [\hat{D}_E \ln \hat{D}_E] \leq -\hbar g \text{Tr} [\hat{D}_E \ln \hat{D}] \]

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

\[ > + T\hbar \text{Tr} \hat{D}_E (-\ln Z) \]

\[ + (\hbar g T) \text{Tr} [\hat{D}_E (-\beta \hat{H})] \]

\[ \langle H_E \rangle - TS_E \geq -\hbar g T \ln Z \]

\[ - \langle H \rangle_E + \langle \hat{H}_E \rangle_E \]

\[ F_E \geq F + \langle H - H_E \rangle_E \]

\[ F_E + \langle H - H_E \rangle_E \geq F \]
Hamiltonien de départ:

\[ H = - J \sum_{<ij>} S_i S_j - g m_B B \sum_i S_i^2 \]

Hamiltonien de Ising:

\[ S_i^2 = \pm \frac{1}{2} \quad S_i = \pm 1 \]

\[ H = - J' \sum_{<ij>} S_i S_j - B' \sum_i S_i \]

\[ J' = \frac{J}{4} \quad B' = g m_B B \frac{3}{2} \]
\[ H_E = - \sum_i x_i S_i \]

Variationnels

1. \[ F_E = -k_B T \ln Z_E \]
   \[ = -k_B T \ln \prod_i \left( \sum_{S_i = \pm 1} e^{\beta x_i S_i} \right) \]
   \[ = -k_B T \sum_i \ln \left( 2 \cosh \beta x_i \right) \]

2. \[ \langle H_E \rangle = - \sum_i x_i \langle S_i \rangle_E - \sum_i \frac{x_i \tanh \beta x_i}{\beta x_i} \]
   \[ \langle S_i \rangle_E = \frac{1}{Z_{E_i}} \sum_{S_i = \pm 1} S_i e^{\beta x_i S_i} \]
   \[ = \frac{e^{\beta x_i} - e^{-\beta x_i}}{e^{\beta x_i} + e^{-\beta x_i}} \]

3. \[ \langle H \rangle_E = -J' \sum_{(ij)} \langle S_i S_j \rangle_E - B' \sum_i \langle S_i \rangle_E \]
   \[ = -J' \sum_{(ij)} \langle S_i \rangle \langle S_j \rangle_E - B' \sum_i \langle S_i \rangle _E \]
\[ F_E + \langle H - H_E \rangle_E \equiv \mathcal{F}_{CM}(\beta, B', \{x_i\}) \]
\[ = -\sum_{i,j} J_{i,j}(\tanh/\beta x_i)(\tanh/\beta x_j) \]
\[ - \sum_i (B'_i - x_i)\tanh/\beta x_i \]
\[ - \beta^{-1} \sum_i \ln(2\cosh/\beta x_i) \]
\[ \frac{\partial \mathcal{F}_{CM}(\beta, B', \{x_i\})}{\partial x_i} = 0 \]
On veut l'ajoutation comme variable indépendante

Transformée de Legendre.

\[
\Gamma_{cm} [\beta, \beta', \vec{M}_i] = F_{cm} [\beta, \beta', \{x_i^*\}] + \sum_i \beta' \vec{M}_i
\]

\[
\vec{M}_i = - \frac{\partial F_{cm}}{\partial \beta'} = - \frac{\partial F_{cm}}{\partial \beta'}
\]

\[
= \tanh \beta x_i^*
\]

\[
x_i^* = \frac{1}{\beta} \arctan \tanh \vec{M}_i = \frac{1}{2\beta} \ln \left[ \frac{1 + \vec{M}_i}{1 - \vec{M}_i} \right]
\]
\[ \Gamma_{cm}[\beta, \bar{M}_i] = \]
\[ - N k_b T \ln \Omega - \sum_{(i,j)} j_{ij} \bar{M}_i \bar{M}_j \]
\[ + \frac{1}{\beta} \sum_i \left[ \frac{(1+\bar{M}_i)}{2} \ln \left( \frac{1+\bar{M}_i}{2} \right) \right. \]
\[ + \left( \frac{1-\bar{M}_i}{2} \right) \ln \left( \frac{1-\bar{M}_i}{2} \right) \]