Modèle d'Ising à une dimension

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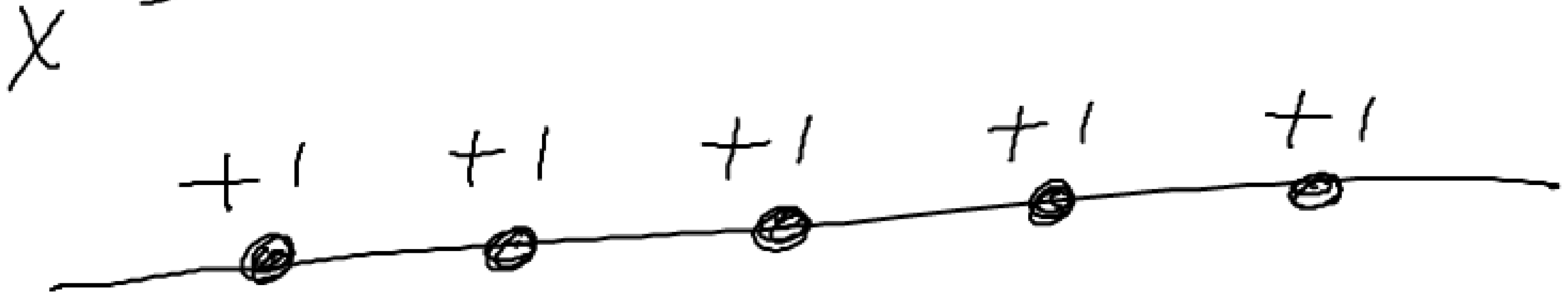
a . chaque site X a deux valeurs possible $\sigma_X = \pm 1$, et il y a N sites.

Donc il y a $\underbrace{2 \times 2 \times \cdots \times 2}_{N} = 2^N$ configurations possibles

b . Si $B = 0$, $E(\sigma) = -\sum_X \sigma_X \cdot \sigma_{X+1}$

est minimale si $\sigma_X = \sigma_{X+1}$, $\forall X$,

donc si $\sigma_X = +1 \ \forall X$:



d'énergie $E(\sigma) = -N$, aimantation $M(\sigma) = +1$

ou $\sigma_X = -1$, $\forall X$:

d'énergie $E(\sigma) = -N$, aimantation $M(\sigma) = -1$

(c)

- l'énergie est <u>maximale</u> si $-\sigma_x \sigma_{x+1} = +1, \ \forall x$,

  soit $\sigma_{x+1} = -\sigma_x$: spins alternés.

- si <u>N est pair</u>, ce sont les 2 configurations :

  $\uparrow\downarrow\uparrow\downarrow$ et $\downarrow\uparrow\downarrow\uparrow$ $(: N = 4)$

- si <u>N est impair</u>, il y a $2N$ configurations d'énergie maximale :

  ex $N = 5$: $\uparrow\downarrow\uparrow\downarrow\uparrow$, $\uparrow\uparrow\downarrow\uparrow\downarrow$, $\downarrow\uparrow\uparrow\downarrow\uparrow$, $\uparrow\downarrow\uparrow\uparrow\downarrow$, $\downarrow\uparrow\downarrow\uparrow\uparrow$

  et les opposés.

(d)

- si $B \gg 1$, alors $E(\sigma) \simeq -B \sum_{x=0}^{N-1} \sigma_x$

  est minimale pour $\sigma = \{+1, +1, \dots, +1\}$

  et maximale pour $\sigma = \{-1, -1, \dots, -1\}$

② $\langle E \rangle (T) = \sum_{\sigma \in \{-1,+1\}^\Lambda} p(\sigma)\, E(\sigma)$

$\langle M \rangle (T) = \sum_{\sigma \in \{-1,+1\}^\Lambda} p(\sigma)\, M(\sigma)$

③ On a $\sum_{\sigma} p(\sigma) = 1$

$\Leftrightarrow Z(\beta, B) = \sum_{\sigma \in \{-1,1\}^\Lambda} e^{-\beta E(\sigma)}$

donc $\frac{\partial Z}{\partial \beta} = - \sum_{\sigma} E(\sigma)\, e^{-\beta E(\sigma)}$

$\frac{\partial}{\partial \beta} \ln Z = \frac{(\partial Z/\partial \beta)}{Z} = - \sum_{\sigma} E(\sigma) \underbrace{\left(\frac{e^{-\beta E(\sigma)}}{Z}\right)}_{p(\sigma)}$

$= -\langle E \rangle$

ⓐ donc $\boxed{\langle E \rangle = - \frac{\partial}{\partial \beta} \ln Z}$

(b) Capacité calorifique :

$$C = \frac{\partial \langle E \rangle}{\partial T} = \frac{\partial \langle E \rangle}{\partial \beta} \left(\frac{\partial \beta}{\partial T} \right) = -\left(\partial_\beta^2 \ln Z \right) \left(-\frac{1}{kT^2} \right)$$

avec $\beta = \frac{1}{kT}$

donc :

$$\boxed{C = k \beta^2 \left(\partial_\beta^2 \ln Z \right)}$$

ⓒ <u>fluctuation d'énergie</u> :

$$\mathrm{Var}(E) = \langle (E - \langle E \rangle)^2 \rangle$$

$$= \langle E^2 - 2E\langle E\rangle + \langle E\rangle^2 \rangle$$

$$= \langle E^2 \rangle - 2\langle E\rangle^2 + \langle E\rangle^2$$

$$= \langle E^2\rangle - \langle E\rangle^2$$

d'après ci-dessus,

$$\frac{\partial^2 Z}{\partial \beta^2} = \sum_{b} E^2 e^{-\beta E} = Z \langle E^2 \rangle$$

donc $\langle E^2 \rangle = \frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2}$

or $\partial_\beta^2 \ln Z = \partial_\beta\left(\frac{\partial_\beta Z}{Z}\right) = \frac{(\partial_\beta^2 Z)Z - (\partial_\beta Z)^2}{Z^2}$

$$= \frac{1}{Z}(\partial_\beta^2 Z) - (\partial_\beta \ln Z)^2$$

donc

$$\langle E^2 \rangle = \partial_\beta^2 \ln Z + (\partial_\beta \ln Z)^2$$

$$\mathrm{Var}(E) = \partial_\beta^2(\ln Z) + (\partial_\beta \ln Z)^2 - (\partial_\beta \ln Z)^2$$

$$\boxed{\mathrm{Var}(E) = \partial_\beta^2(\ln Z) = \frac{1}{k\beta^2} C}$$

d) <u>Aimantation</u> :

$$\langle M \rangle = \sum_{\sigma} p(\sigma) M(\sigma)$$

avec $M(\sigma) = \frac{1}{N} \sum_{x} \sigma_x$

On observe que

$$Z = \sum_{\sigma} e^{-\beta E(\sigma)} = \sum_{\sigma} e^{\beta\left(\sum_x \sigma_x \sigma_{x+1} - B \sigma_x\right)}$$

$$= \sum_{\sigma} e^{\beta\left(\sum_x \sigma_x \sigma_{x+1}\right) - \beta B N M(\sigma)}$$

donc $$\frac{\partial Z}{\partial B} = \sum_{\sigma} \beta N M(\sigma) e^{-\beta E(\sigma)}$$

$$= \beta N Z \langle M \rangle$$

$$\Longleftrightarrow \langle M \rangle = \frac{1}{\beta N} \frac{1}{Z} (\partial_B Z)$$

$$\Longleftrightarrow \boxed{\langle M \rangle = \frac{1}{\beta N} \partial_B (\ln Z)}$$

e) Susceptibilité magnétique :

$$\boxed{\chi = \frac{\partial \langle M \rangle}{\partial B} = \frac{1}{\beta N}\left(\partial_B^2 \ln Z\right)}$$

Fluctuation de l'aimantation :

$$\frac{\partial^2 Z}{\partial B^2} = \sum_{\mathcal{C}} (\beta N M)^2 e^{-\beta E(\mathcal{C})} = Z(\beta N)^2 \langle M^2 \rangle$$

et $\mathrm{Var}(M) = \langle M^2 \rangle - \langle M^2 \rangle$

$$= \frac{1}{(\beta N)^2} \frac{1}{Z} \partial_B^2 Z - \frac{1}{(\beta N)^2} \left(\partial_Z \ln Z\right)^2$$

$$\boxed{\mathrm{Var}(M) = \frac{1}{(\beta N)^2} \partial_B^2 (\ln Z)}$$

On déduit que

$$\boxed{\mathrm{Var}(M) = \frac{1}{(\beta N)} \chi}$$

6 Entropie :

$$S = -k \sum_{\sigma} p(\sigma) \ln p(\sigma)$$

$$= -k \frac{1}{Z} \sum_{\sigma} e^{-\beta E(\sigma)} \left(-\ln Z - \beta E \right)$$

$$= k \frac{\ln Z}{Z} \underbrace{\left(\sum_{\sigma} e^{-\beta E} \right)}_{Z} + k\beta \sum_{\sigma} p(\sigma) E(\sigma)$$

$$= k \ln Z + k\beta \langle E \rangle$$

$$\boxed{S = k\left(\left(\ln Z\right) - \beta\left(\partial_\beta \ln Z\right)\right)}$$

④ Si $A = \left(A_{b_0, b_1}\right)_{b_0, b_1 \in \{-1, 1\}}$ est une matrice 2×2,

alors

$$\left(A^N\right)_{b_0, b_N} = \sum_{b_1 \in \{-1,1\}} \sum_{b_2 \in \{-1,1\}} \cdots \sum_{b_{N-1} \in \{-1,1\}} A_{b_0 b_1} A_{b_1 b_2} \cdots A_{b_{N-1} b_N}$$

$$\mathrm{Tr}\left(A^N\right) = \sum_{b_0} \sum_{b_1} \cdots \sum_{b_{N-1}} A_{b_0 b_1} A_{b_1 b_2} \cdots A_{b_{N-1} b_0}$$

$$\boxed{\mathrm{Tr}\left(A^N\right) = \sum_{b \in \{-1,1\}^N} A_{b_0 b_1} A_{b_1 b_2} \cdots A_{b_{N-1} b_0}}$$

⑤ $\sum_{\sigma} p(\sigma) = 1$

$$\Leftrightarrow Z = \sum_{\sigma \in \{-1,1\}^N} e^{-\beta E(\sigma)}$$

$$= \sum_{\sigma_0 \in \{-1,+1\}} \sum_{\sigma_1 \in \{-1,+1\}} \cdots \sum_{\sigma_{N-1} \in \{-1,+1\}} e^{\beta(\sigma_0\sigma_1 + \sigma_1\sigma_2 + \cdots + \sigma_{N-1}\sigma_0)} e^{+\beta B(\sigma_0 + \sigma_1 + \cdots + \sigma_{N-1})}$$

$$= \sum_{\sigma_0} \sum_{\sigma_1} \cdots \sum_{\sigma_{N-1}} e^{\beta(\sigma_0\sigma_1 + B\sigma_0)} e^{\beta(\sigma_1\sigma_2 + B\sigma_1)} \cdots e^{\beta(\sigma_{N-1}\sigma_0 + B\sigma_{N-1})}$$

$$= \mathrm{Tr}(A^N)$$

avec $\quad A_{\sigma_0\sigma_1} = e^{\beta(\sigma_0\sigma_1 + B\sigma_0)}$

donc
$$\boxed{A = \begin{array}{cc} & \begin{array}{cc} (\sigma_1 = -1) & (\sigma_1 = +1) \end{array} \\ \begin{array}{c} (\sigma_0 = -1) \\ (\sigma_0 = +1) \end{array} & \begin{pmatrix} e^{\beta(1-B)} & e^{\beta(-1-B)} \\ e^{\beta(-1+B)} & e^{\beta(1+B)} \end{pmatrix} \end{array}}$$

6) Soit $\lambda \in \mathbb{C}$,

$$P(\lambda) := \det(\lambda - A) \quad : \text{"polynome caractéristique"}$$

$$= \det \begin{pmatrix} \lambda - e^{\beta(1-B)} & -e^{\beta(-1-B)} \\ -e^{\beta(-1+B)} & \lambda - e^{\beta(1+B)} \end{pmatrix}$$

$$= \lambda^2 + b\lambda + c$$

avec $b = -e^{\beta}\left(e^{\beta B} + e^{-\beta B}\right) = -2e^{\beta}\,\mathrm{ch}(\beta B)$

$$c = e^{2\beta} - e^{-2\beta}$$

$$\Delta := b^2 - 4c = 4e^{2\beta}\mathrm{ch}^2(\beta B) - 4e^{2\beta} + 4e^{-2\beta}$$

$$= 4e^{2\beta}\left(\mathrm{sh}^2(\beta B) + e^{-4\beta}\right) \quad \text{car } \mathrm{ch}^2 x - \mathrm{sh}^2 x = 1$$

les zéros de $P(\lambda)$ sont

$$\lambda_{\pm} = \frac{-b \pm \sqrt{\Delta}}{2}$$

$$\boxed{\lambda_{\pm} = e^{\beta}\left[\mathrm{ch}(\beta B) \pm \left(\mathrm{sh}^2(\beta B) + e^{-4\beta}\right)^{1/2}\right]}$$

donc $\lambda_- < \lambda_+$, $\lambda_+ > 0$,

et

$$\lambda_+ + \lambda_- = \mathrm{Tr}\, A = e^{\beta(1-B)} + e^{\beta(1+B)} = 2e^{\beta} \mathrm{ch}(\beta B) \geqslant 2$$

$$\lambda_+ \lambda_- = \det A = e^{2\beta} - e^{-2\beta} = 2\, \mathrm{sh}(2\beta) \quad > 0$$

donc $\lambda_- > 0$ aussi, ainsi

$$0 < \lambda_- < \lambda_+$$

Donc $\mathrm{Tr}(A^N) = \lambda_+^N + \lambda_-^N$

$$= \lambda_+^N \left(1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N\right)$$

on a $\left(\frac{\lambda_-}{\lambda_+}\right)^N \xrightarrow[N \to \infty]{} 0$.

On a donc

$$\ln Z = \ln \mathrm{Tr}(A^N) = N \ln \lambda_+ + \ln\Big(1 + \underbrace{\left(\frac{\lambda_-}{\lambda_+}\right)^N}_{\to 0}\Big)$$

$$\boxed{\ln Z \underset{N \to \infty}{\sim} N \ln \lambda_+}$$

⑦ On a vu que

$$\langle M \rangle = \frac{1}{\beta N} \frac{\partial}{\partial B}(\ln Z)$$

$$\ln Z = N \ln \lambda_+$$

$$\lambda_+ = e^{\beta} \left[ch(\beta B) + \left(sh^2(\beta B) + e^{-4\beta} \right)^{1/2} \right]$$

donc $\langle M \rangle = \frac{1}{\beta N} \frac{\partial}{\partial B} \left(N \left(\beta + \ln [\,''\,] \right) \right)$

$$= \frac{1}{\beta} \frac{\partial}{\partial B} \ln \left[ch(\beta B) + \left(sh^2(\beta B) + e^{-4\beta} \right)^{1/2} \right]$$

$$= \frac{1}{\beta} \frac{\partial [\,''\,]}{\partial B} \frac{1}{[\,''\,]}$$

où $\frac{\partial [\,''\,]}{\partial B} = \beta\, sh(\beta B) + \frac{2\beta\, sh(\beta B) ch(\beta B)}{2 \left(sh^2(\beta B) + e^{-4\beta} \right)^{1/2}}$

$$= \beta \frac{sh(\beta B) \left[(\,''\,)^{1/2} + ch\, \beta B \right]}{(\,''\,)^{1/2}}$$

donc

$$\boxed{\langle M \rangle = \frac{sh(\beta B)}{\left(sh^2(\beta B) + e^{-4\beta} \right)^{1/2}}}$$

Pour $\beta > 0$ et $B \longrightarrow 0$, on a $sh(\beta B) \longrightarrow 0$

donc $\langle M \rangle \longrightarrow 0$,

il n'y a <u>pas d'aimantation spontanée</u>.

le système est dit "<u>paramagnétique</u>".

Alors que le modèle d'Ising en dimension 2,

à $B = 0$ manifeste une aimantation

spontanée à basse température : $T < T_c$.

(8) On a calculé : $\langle M \rangle = \dfrac{sh(\beta B)}{\left(sh^2(\beta B) + e^{-4\beta}\right)^{1/2}}$

La susceptibilité est

$$\chi = \frac{\partial \langle M \rangle}{\partial B}$$

$$= \frac{\beta\, ch(\beta B)\left(\,''\,\right)^{1/2} - sh(\beta B)\frac{1}{2}\, 2 sh(\beta B) ch(\beta B)\beta \left(\,''\,\right)^{-1/2}}{sh^2(\beta B) + e^{-4\beta}}$$

Pour $B \longrightarrow 0$,

$$\chi = \frac{\beta e^{-2\beta}}{e^{-4\beta}} = \beta e^{2\beta} = \frac{1}{kT} e^{\frac{2}{kT}}$$

$$\Longleftrightarrow \frac{1}{\chi} = kT e^{-\frac{2}{kT}}$$