

1 Theoretical background

The partition function of the system is given,

$$Z = \sum e^{-\beta E[\{\sigma_i\}]} = \sum e^{-\beta(J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i)}$$

Expectation value of the energy is

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z = \sum E[\{\sigma_i\}] \frac{1}{Z} e^{-\beta E[\{\sigma_i\}]}$$

Specific heat can be obtained by differentiating $\langle E \rangle$ by temperature.

$$\begin{aligned} c_V &= \frac{1}{N} \frac{\partial}{\partial T} \langle E \rangle = \frac{\partial \beta}{\partial T} \left(-\frac{\partial^2}{\partial \beta^2} \ln Z \right) \\ &= \frac{1}{NT^2} \sum E[\{\sigma_i\}]^2 \frac{1}{Z} e^{-\beta E[\{\sigma_i\}]} - \frac{1}{NT^2} \sum E[\{\sigma_i\}] \frac{1}{Z} e^{-\beta E[\{\sigma_i\}]} \sum E[\{\sigma_i\}] \frac{1}{Z} e^{-\beta E[\{\sigma_i\}]} \\ &= \frac{1}{NT^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) = \frac{N}{T^2} \left(\langle (E/N)^2 \rangle - \langle E/N \rangle^2 \right) \\ &= \frac{N}{T^2} \text{Var}(E/N) \end{aligned}$$

Magnetization and magnetic susceptibility can be calculated in a similar manner.

$$\frac{\partial}{\partial h} \ln Z = \sum \beta \left(\sum_i \sigma_i \right) \frac{1}{Z} e^{-\beta(J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i)} = \frac{1}{T} \langle M \rangle$$

$$\begin{aligned} \chi &= \frac{1}{N} \frac{\partial}{\partial h} \langle M \rangle = \frac{\partial}{\partial h} \left(T \frac{\partial}{\partial h} \ln Z \right) \\ &= \frac{1}{NT} \sum \beta^2 \left(\sum_i \sigma_i \right)^2 \frac{1}{Z} e^{-\beta(J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i)} \\ &\quad - \frac{1}{NT} \sum \beta \left(\sum_i \sigma_i \right) \frac{1}{Z} e^{-\beta(J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i)} \sum \beta \left(\sum_i \sigma_i \right) \frac{1}{Z} e^{-\beta(J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i)} \\ &= \frac{1}{NT} \left(\langle M^2 \rangle - \langle M \rangle^2 \right) = \frac{N}{T} \left(\langle m^2 \rangle - \langle m \rangle^2 \right) \\ &= \frac{N}{T} \text{Var}(m) \end{aligned}$$