Fluctuation-Dissipation Theorem

Linear response \propto equilibrium fluctuation

Let us consider the Ising Hamiltonian for *N* spins:

$$V(s^{N}) = -J \sum_{(k,l) \in \{\text{nearest neighbor}\}} s_{k}s_{l} - H \sum_{\substack{k \\ M(s^{N}): \text{ magnetization}}} s_{k}s_{l} - H$$

Specific Heat

The expectation value of the energy is

$$\langle V \rangle = \sum_{s^N} V(s^N) P(s^N) = \frac{\sum_{s^N} V(s^N) e^{-\beta V(s^N)}}{\sum_{s^N} e^{-\beta V(s^N)}} \quad \left(\beta = \frac{1}{k_{\rm B}T}\right),$$

and the specific heat is defined as

$$C = \frac{d\langle V \rangle}{dT} = \frac{d\beta}{dT} \frac{d\langle V \rangle}{d\beta} = -\frac{1}{k_{\rm B}T^2} \frac{d\langle V \rangle}{d\beta}.$$

Now

$$\begin{aligned} \frac{d\langle V \rangle}{d\beta} &= \frac{d}{d\beta} \frac{\sum V e^{-\beta V}}{\sum e^{-\beta V}} = \frac{\sum V (-V) e^{-\beta V}}{\sum e^{-\beta V}} + \sum V e^{-\beta V} \times (-1) \frac{\sum (-V) e^{-\beta V}}{(\sum e^{-\beta V})^2} \\ &= -\frac{\sum V^2 e^{-\beta V}}{\sum e^{-\beta V}} + \left(\frac{\sum V e^{-\beta V}}{\sum e^{-\beta V}}\right)^2 = -\langle V^2 \rangle + \langle V \rangle^2 = -\langle (\delta V)^2 \rangle \quad (\delta V = V - \langle V \rangle), \end{aligned}$$

and thus

$$C = \frac{1}{k_{\rm B}T^2} \langle (\delta V)^2 \rangle.$$

(Note) Both the specific heat and energy fluctuation diverge at the phase-transition (or Curie) temperature, T_c .

Magnetic Susceptibility

Note

$$\frac{\partial V}{\partial H} = \frac{\partial}{\partial H} \left[-J \sum_{(k,l)} s_k s_l - HM(s^N) \right] = -M(s^N).$$

The magnetic susceptibility is

$$\chi \equiv \frac{d\langle M \rangle}{dH} = \frac{d}{dH} \frac{\sum M e^{-\beta V}}{\sum e^{-\beta V}} = \frac{\sum M(\beta M) e^{-\beta V}}{\sum e^{-\beta V}} + \sum M e^{-\beta V} \times (-1) \frac{\sum (\beta M) e^{-\beta V}}{(\sum e^{-\beta V})^2}$$
$$= \beta \langle M^2 \rangle - \beta \langle M \rangle^2 = \beta \langle (\delta M)^2 \rangle \quad (\delta M = M - \langle M \rangle)$$