Fluctuation-Dissipation Theorem

Linear response $\propto$ equilibrium fluctuation

Let us consider the Ising Hamiltonian for N spins:

$$V(s^N) = -J \sum_{(k,l)\in\{\text{nearest neighbor}\}} s_k s_l - H \underbrace{\sum_k s_k}_{M(s^N):\ \text{magnetization}} .$$

Specific Heat

The expectation value of the energy is

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

and the specific heat is defined as

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

Now

$$\frac{d\langle V \rangle}{d\beta} = \frac{d}{d\beta}\frac{\sum V e^{-\beta V}}{\sum e^{-\beta V}} = \frac{\sum V(-V)e^{-\beta V}}{\sum e^{-\beta V}} + \sum V e^{-\beta V} \times (-1)\frac{\sum (-V)\,e^{-\beta V}}{(\sum e^{-\beta V})^2}$$

$$= -\frac{\sum V^2 e^{-\beta V}}{\sum e^{-\beta V}} + \left(\frac{\sum V e^{-\beta V}}{\sum e^{-\beta V}}\right)^2 = -\langle V^2 \rangle + \langle V \rangle^2 = -\langle (\delta V)^2 \rangle \quad (\delta V = V - \langle V \rangle),$$

and thus

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

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

Magnetic Susceptibility

Note

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

The magnetic susceptibility is

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

$$= \beta\langle M^2 \rangle - \beta\langle M \rangle^2 = \beta\langle (\delta M)^2 \rangle \quad (\delta M = M - \langle M \rangle)$$