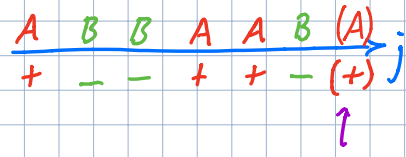


Ising model of binary alloy chain



Species A $\Rightarrow \sigma = +$ Species B $\Rightarrow \sigma = -$

Energies E_A E_B E_{AA} E_{AB} E_{BA} E_{BB}
 Equal unless Chiral

Known: $N_A, N_B, N = N_A + N_B$ Unknown: $N_{AA}, N_{AB}, N_{BA}, N_{BB}$

Identities:
 ① $N = N_{AA} + N_{AB} + N_{BA} + N_{BB}$ (PBC)
 ② $N_{AB} = N_{BA}$ (PBC)
 ③ $N_A = N_{AA} + N_{AB}$
 ④ $N_B = N_{BA} + N_{BB}$
 note: ④ follows from ① & ③
 \therefore 4 unknowns, 3 identities
 \Rightarrow one free variable (N_{AB})

Ising representation:

$$N_A = \sum_j \left(\frac{1+\sigma_j}{2} \right) \quad N_B = \sum_j \left(\frac{1-\sigma_j}{2} \right) \quad N_{AB} = N_{BA} = \frac{1}{2} \sum_j \left(\frac{1-\sigma_j \sigma_{j+1}}{2} \right)$$

Total Energy

$$\begin{aligned} H &= E_A N_A + E_B N_B + E_{AA} N_{AA} + E_{AB} N_{AB} + E_{BA} N_{BA} + E_{BB} N_{BB} \\ &= N_A (E_A + E_{AA}) + N_B (E_B + E_{BB}) + N_{AB} (E_{AB} - E_{AA}) + N_{BA} (E_{BA} - E_{BB}) \\ &= (E_A + E_{AA}) \frac{1}{2} \sum_j (1 + \sigma_j) + (E_B + E_{BB}) \frac{1}{2} \sum_j (1 - \sigma_j) + (E_{AB} - E_{AA}) \frac{1}{4} \sum_j (1 - \sigma_j \sigma_{j+1}) \\ &\quad + (E_{BA} - E_{BB}) \frac{1}{4} \sum_j (1 - \sigma_j \sigma_{j+1}) \\ &= -J \sum_j \sigma_j \sigma_{j+1} - h \sum_j \sigma_j + G \end{aligned}$$

$$J = \frac{1}{4} (E_{AB} + E_{BA} - E_{AA} - E_{BB})$$

Symmetric due to $N_{AB} = N_{BA}$
 $AB + BA \Rightarrow$ lost chances for AA and BB

$$h = \frac{1}{2} (E_B - E_A)$$

like chemical potential

$$G = \frac{1}{2} (E_A + E_B) + \frac{1}{4} (E_{AA} + E_{AB} + E_{BA} + E_{BB})$$