Ising model of binary alloy chain

$$\begin{array}{ccccccc} A & B & B & A & A & B & (A) \\ \hline + & - & - & + & + & - & (+) \end{array} \rightarrow j$$

Periodic B.C.

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

Energies E_A E_B E_{AA} $\underbrace{E_{AB}\quad E_{BA}}_{\text{Equal unless chiral}}$ E_{BB}

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 unknows, 3 identities
$\Rightarrow$ one free variable (N_{AB})

Ising representation:

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

Total Energy

$$H = E_A N_A + E_B N_B + E_{AA} \overset{N_A - N_{AB}}{N_{AA}} + E_{AB} N_{AB} + E_{BA} N_{BA} + E_{BB} \overset{N_B - N_{BA}}{N_{BB}}$$

$$= N_A (E_A + E_{AA}) + N_B (E_B + E_{BB}) + N_{AB}(E_{AB} - E_{AA}) + N_{BA}(E_{BA} - E_{BB})$$

$$= (E_A + E_{AA}) \frac{1}{2}\sum_j (1+\sigma_j) + (E_B + E_{BB}) \frac{1}{2}\sum_j (1-\sigma_j) + (E_{AB} - E_{AA}) \frac{1}{4}\sum (1 - \sigma_j\sigma_{j+1})$$
$$+ (E_{BA} - E_{BB}) \frac{1}{4} \sum (1 - \sigma_j \sigma_{j+1})$$

$$= -J \sum_j \sigma_j \sigma_{j+1} - h \sum_j \sigma_j + C$$

$$J = \frac{1}{4}\left(\underbrace{E_{AB} + E_{BA}}_{\text{symmetric due to } N_{AB} = N_{BA}} \underbrace{- E_{AA} - E_{BB}}_{AB \,\&\, BA \Rightarrow \text{lost chances for } AA \text{ and } BB}\right)$$

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

like chemical potential

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