Sheet 1

Ex 3

a) detailed balance: $P_i \omega_{ij} = P_j \omega_{ji} \quad \forall i,j$

Metropolis criterion (canonical ensemble): $\begin{cases} \omega_{ij} = e^{-\beta \Delta E} & \text{if } \Delta E > 0 \\ \omega_{ij} = 1 & \text{if } \Delta E < 0 \end{cases}$ $\quad \Delta E = E_j - E_i$

if $\Delta E > 0 \Rightarrow \omega_{ij} = e^{-\beta \Delta E} \Rightarrow \omega_{ji} = 1$

$\Rightarrow P_i e^{-\beta \Delta E} = P_j \rightarrow \frac{P_i}{P_j} = e^{\beta \Delta E} \Leftrightarrow \frac{P_j}{P_i} = e^{-\beta \Delta E}$

if $\Delta E < 0 \Rightarrow \omega_{ij} = 1$ and $\omega_{ji} = e^{-\beta \Delta E}$

$\Rightarrow P_i = e^{-\beta \Delta E} P_j \Rightarrow \frac{P_i}{P_j} = e^{-\beta \Delta E}$

b) $\omega_{ij} = \frac{e^{-\beta \Delta E}}{e^{-\beta \Delta E} + 1} \Rightarrow \omega_{ji}$

$\frac{\omega_{ij}}{\omega_{ji}} = e^{-\beta \Delta E} \Leftarrow \omega_{ij} = \omega_{ji} e^{-\beta \Delta E} = \frac{e^{-\beta \Delta E}}{e^{-\beta \Delta E} + 1}$

$\Leftrightarrow \omega_{ji} = e^{\beta \Delta E} \left(\frac{e^{-\beta \Delta E}}{e^{-\beta \Delta E} + 1} \right) = \frac{1}{e^{-\beta \Delta E} + 1}$

Exercise 4)

a) What happens at low temperatures?

- large areas of the same orientation,

What happens at high temperatures?

- noise, no discernable areas of a specific orientation

At which temperature does the phase transition occur?

- at around 2 K

Metropolis-algo is appropriate for: $< 2K$

Wolff-algo is appropriate for: $> 2K$