

Solutions¹ Thermische fysica 2 (NS-355b) November 9, 2010

Question 1: Energy, entropy and free energy

- a) If $\mu > 0$, it costs energy to place a particle on the lattice, so the ground states contains no particles:
 If $\mu < 0$, it gives energy to place a particle on the lattice, so the ground states contains the maximum number of particles, namely 3:

- b) If $\mu = 0$, every states has equal energy, so every state is a ground state, so

$$S = k_B \log \Omega = k_B \log 13 \quad (1)$$

where Ω is the multiplicity.

- c) If the temperature is high ($\beta\mu \approx 0$), every state is equally probable, so

$$\langle N \rangle = \frac{1}{13}(1 \times 0 + 5 \times 1 + 6 \times 2 + 1 \times 3) = \frac{20}{13} \quad (2)$$

and

$$\langle N^2 \rangle = \frac{1}{13}(1 \times 0^2 + 5 \times 1^2 + 6 \times 2^2 + 1 \times 3^2) = \frac{38}{13} \quad (3)$$

- d) Within linear response theory, $\frac{\partial \langle N \rangle}{\partial \beta\mu} = -(\langle N^2 \rangle - \langle N \rangle^2)$, so $\frac{\partial \langle N \rangle}{\partial \mu} = \frac{-1}{k_B T} \frac{94}{169}$.

Question 2: polymers

- a) In general is $R_{ee}^2 = \langle |\vec{x}_N - \vec{x}_0|^2 \rangle = \sum_{i=1}^N \sum_{j=1}^N \langle \vec{\sigma}_i \cdot \vec{\sigma}_j \rangle$. Since the orientation of connected segments is arbitrary, $\langle \vec{\sigma}_i \cdot \vec{\sigma}_j \rangle = \delta_{ij} l^2$, so $R_{ee}^2 = \sum_{i=1}^N \sum_{j=1}^N \delta_{ij} l^2 = N l^2$.
- b) The energy is minimal if $\vec{\sigma}_i \cdot \vec{\sigma}_{i+1}$ is maximal. The maximum of this inner product is l^2 , so $E_{\text{ground state}} = -\epsilon(N-1)$.
- c) The probability to find a hinge with angle θ is proportional to it's Boltzman weight;

$$P(\theta) \propto e^{-\beta E} = e^{\beta \frac{\epsilon}{l^2} \vec{\sigma}_i \cdot \vec{\sigma}_{i-1}} \quad (4)$$

$$= e^{\beta \frac{\epsilon}{l^2} l^2 \cos \theta} \quad (5)$$

$$= e^{\beta(E_{\text{ground state}} - \frac{\epsilon}{2} \theta^2)} \quad (6)$$

$$\propto e^{-\frac{\beta \epsilon}{2} \theta^2} \quad (7)$$

So θ is normally distributed with standard deviation $\sqrt{\frac{1}{\beta \epsilon}}$, so $A = 1$.

- d) Since the angle is normally distributed, you can add the angles quadratically, so $\langle \theta_{i,i+j}^2 \rangle = j \langle \theta_{i,i+1}^2 \rangle$. This means that

$$\langle \vec{\sigma}_i \cdot \vec{\sigma}_j \rangle = l^2 \langle \cos \theta_{i,i+j} \rangle = l^2 e^{-\frac{j \langle \theta_{i,i+1}^2 \rangle}{2}} \quad (8)$$

$$= l^2 e^{-j \frac{1}{2\beta \epsilon}} \quad (9)$$

¹These solutions were made with great precaution. In case of errors, the $\mathcal{TB}\mathcal{C}$ cannot be held responsible. However, she will be glad to be informed: tbc@a-eskwadraat.nl

Note that in the exam, it was abusively stated that $\langle \cos \theta \rangle \approx \exp(-\langle \theta^2 \rangle)$ instead of $\langle \cos \theta \rangle \approx \exp(-\frac{\langle \theta^2 \rangle}{2})$. You can still get full points if you used the first relation.

e) The same analysis as in (a) yields to

$$R_{ee}^2 = \sum_{i=1}^N \sum_{j=1}^N \langle \vec{\sigma}_i \cdot \vec{\sigma}_j \rangle \quad (10)$$

$$= l^2 \sum_{i=1}^N \sum_{j=1}^N e^{-|i-j|\frac{1}{2\beta\epsilon}} \quad (11)$$

This can be calculated using geometric series:

$$R_{ee}^2 = l^2 \left(N + 2 \frac{1}{1 - e^{-B}} \left(N e^{-B} - \frac{1 - e^{-(N+1)B}}{1 - e^{-B}} \right) \right) \quad (12)$$

$$\approx l^2 \left(N + 2 \frac{N e^{-B}}{1 - e^{-B}} \right) = l^2 N \frac{1 + e^{-B}}{1 - e^{-B}} \quad (13)$$