SM-2 September 2014

N oxygen molecules along Ω sites $\qquad \Omega \gg N$

$$E = \varepsilon(\sigma_1 + \sigma_2) + J\sigma_1\sigma_2$$

$\sigma_i = 1$ occupied & $\sigma_i = 0$ unoccupied

a. Evaluate partition function using canonical ensemble

Possible states:

$\sigma_1 = 0$, $\sigma_2 = 0$ $\rightarrow$ $E_{00} = 0$

$\left.\begin{matrix}\sigma_1 = 0 \\ \sigma_2 = 1 \\ \sigma_1 = 1 \\ \sigma_2 = 0\end{matrix}\right\} \rightarrow E_{01} = E_{10} = \varepsilon$

$\sigma_1 = 1$, $\sigma_2 = 1$ $\rightarrow$ $E_{11} = J + 2\varepsilon$

$$Z_1 = \sum_i e^{-\beta E_i}$$

$$= e^{-\beta E_{00}} + e^{-\beta E_{10}} + e^{-\beta E_{01}} + e^{-\beta E_{11}}$$

$$Z_1 = 1 + 2e^{-\beta\varepsilon} + e^{-\beta(J+2\varepsilon)}$$

$$Z_N = Z_1^N = \left(1 + 2e^{-\beta\varepsilon} + e^{-\beta(J+2\varepsilon)}\right)^N$$

For Ω sites:

$$Z_N = \left(1 + \Omega e^{-\beta\varepsilon} + e^{-\beta(J+\Omega\varepsilon)}\right)^N$$

b. Derive probability for 0, 1, 2. and $\langle N \rangle$

$$P_{00} = \frac{1}{Z} = \frac{1}{\left[1 + 2e^{-\beta\varepsilon} + e^{-\beta(J+2\varepsilon)}\right]}$$

$$P_{01} = P_{10} = \frac{2e^{-\beta\varepsilon}}{1 + 2e^{-\beta\varepsilon} + e^{-\beta(J+2\varepsilon)}}$$

$$P_{11} = \frac{e^{-\beta(J+2\varepsilon)}}{1 + 2e^{-\beta\varepsilon} + e^{-\beta(J+2\varepsilon)}}$$

$$\langle N \rangle = -\frac{1}{\beta}\frac{\partial}{\partial\varepsilon}\ln Z_N = -\frac{1}{\beta}\frac{\partial}{\partial\varepsilon} N \ln\left(1 + 2e^{-\beta\varepsilon} + e^{-\beta(J+2\varepsilon)}\right) = -\frac{N}{\beta}\frac{1}{Z}\left(-\beta \cdot 2e^{-\beta\varepsilon} - 2\beta e^{-\beta(J+2\varepsilon)}\right)$$

$$= \frac{2N}{Z}\left(e^{-\beta\varepsilon} + e^{-\beta(J+2\varepsilon)}\right)$$

$$\langle N \rangle = \frac{2N\left(e^{-\beta\varepsilon} + e^{-\beta(J+2\varepsilon)}\right)}{1 + 2e^{-\beta\varepsilon} + e^{-\beta(J+2\varepsilon)}}$$