6.1. eigenenergies $E_n = \hbar\omega\left(n+\frac{1}{2}\right)$ $n = 0, 1, 2 \ldots$

a) $$Q = \sum_{n=0}^{\infty} e^{-\beta E_n} = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega\left(n+\frac{1}{2}\right)}$$

$$= e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} \left(e^{-\beta\hbar\omega}\right)^n$$ geometric series

$$Q = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}}$$

b) $$E = -\frac{\partial}{\partial\beta} \ln Q = -\frac{\partial}{\partial\beta}\left(-\beta\hbar\omega/2 - \ln\left(1-e^{-\beta\hbar\omega}\right)\right)$$

$$= \frac{\hbar\omega}{2} + \frac{\hbar\omega\, e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1}$$

$$C_v = \frac{\partial E}{\partial T} = \frac{\partial E}{\partial\beta}\frac{d\beta}{dT} = \frac{\hbar\omega}{\left(e^{\beta\hbar\omega} - 1\right)^2}\,\hbar\omega e^{+\beta\hbar\omega}\,\frac{1}{k_B T^2}$$

$$= k_B\left(\frac{\hbar\omega}{k_B T}\right)^2 \frac{e^{+\beta\hbar\omega}}{\left(e^{\beta\hbar\omega} - 1\right)^2}$$

$\underline{k_B T \gg \hbar\omega}$ expand exponential

$E \approx k_B T$ $C \approx k_B$

$\underline{k_B T \ll \hbar\omega}$

$E \approx \frac{\hbar\omega}{2}$ $C \approx 0$

6.1 c)

$$A = E - TS \qquad S = \frac{1}{T}(E - A)$$

$$S = \frac{1}{T}\left(\frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\beta\hbar\omega}-1}\right) - \frac{1}{T}\left(-k_B T \ln Q\right)$$

$$= k_B\left[\cancel{\frac{\beta\hbar\omega}{2}} + \frac{\beta\hbar\omega}{e^{\beta\hbar\omega}-1} + \cancel{\left(-\frac{\beta\hbar\omega}{2}\right)} - \ln\left(1-e^{-\beta\hbar\omega}\right)\right]$$

$$= k_B\left[\frac{\beta\hbar\omega}{e^{\beta\hbar\omega}-1} - \ln\left(1-e^{-\beta\hbar\omega}\right)\right]$$

$\underline{T \to 0 \quad (\hbar\omega \gg k_B T)}$

$$S = 0$$

$T \to \infty \quad (\hbar\omega \ll k_B T)$

$$S = k_B\left[1 - \ln\left(1 - 1 + \beta\hbar\omega\right)\right]$$

$$S \approx k_B \ln k_B T/\hbar\omega \qquad \sim \quad k_B \ln T$$

6.2. a) N joints are independent $Q_N = (Q_1)^N$

$$Q_1 = 1 + 2e^{-\beta\varepsilon} \qquad Q_N = (1 + 2e^{-\beta\varepsilon})^N$$

$$A = -k_BT \ln Q_N = -Nk_BT \ln(1 + 2e^{-\beta\varepsilon})$$

b) $$\bar{E} = -\frac{\partial}{\partial\beta} \ln Q_N = -N\frac{\partial}{\partial\beta} \ln(1+2e^{-\beta\varepsilon})$$

$$\bar{E} = \frac{2N\varepsilon e^{-\beta\varepsilon}}{1+2e^{-\beta\varepsilon}} = \frac{2N\varepsilon}{e^{\beta\varepsilon}+2}$$

$$C = \frac{\partial E}{\partial T} = -\frac{1}{k_BT^2}\frac{\partial E}{\partial\beta} = \frac{2N\varepsilon^2 e^{\beta\varepsilon}}{(e^{\beta\varepsilon}+2)^2}\frac{1}{k_BT^2}$$

$$C = 2Nk_B\left(\frac{\varepsilon}{k_BT}\right)^2 \frac{1}{(e^{\beta\varepsilon}+2)^2}$$

c) $$N_{st} = Np_{st} = \frac{N}{1+2e^{-\beta\varepsilon}}$$

d) $k_BT \gg \varepsilon \qquad N_{st} \to \frac{N}{3}$

$k_BT \ll \varepsilon \qquad N_{st} \to N$

6.3 a) parallel

b) integration over 2 sets of angles, for example, orientation of S_1 and relative orientation

$$Q = 4\pi \int d\eta \, d\theta \sin\theta \; e^{\beta J \cos\theta}$$

$$= 8\pi^2 \int_{-1}^{1} d\eta \; e^{\beta J \eta} = \frac{16\pi^2}{\beta J} \sinh(\beta J)$$

$$A = -k_B T \ln\left[\frac{16\pi^2}{\beta J} \sinh(\beta J)\right]$$

c) $$E = -\frac{\partial}{\partial \beta} \ln Q = \frac{1}{\beta} - J \coth(\beta J)$$

$$C_V = \frac{\partial E}{\partial T} = k_B \left[1 + (\beta J)^2 \left(1 - \coth^2(\beta J)\right)\right]$$

d) $k_B T \ll J \Rightarrow$ angle θ small $\rightarrow$

$\sin\theta \approx \theta \;,\; \cos\theta \approx 1 - \frac{\theta^2}{2}$

$$\langle\theta\rangle = \frac{\int_0^\infty \theta \, d\theta \; \theta \; e^{-\beta J \theta^2/2}}{\int_0^\infty \theta \, d\theta \; e^{-\beta J \theta^2/2}} = \sqrt{\pi / 2\beta J}$$

$$\langle\theta^2\rangle = \frac{\int_0^\infty \theta \, d\theta \; \theta^2 \; e^{-\beta J \frac{\theta^2}{2}}}{\int_0^\infty \theta \, d\theta \; e^{-\beta J \frac{\theta^2}{2}}} = \frac{2}{\beta J}$$

$$\sigma^2 = \frac{1}{\beta J}\left(2 - \frac{\pi}{2}\right)$$

6.4. states : n links open $E_n = N\varepsilon_0 + n(\varepsilon_1 - \varepsilon_0)$

a) $$Q = \sum_{n=0}^{N} e^{-\beta N \varepsilon_0} e^{-\beta n \varepsilon} \qquad \varepsilon = \varepsilon_1 - \varepsilon_0$$

finite geometric series

$$Q = e^{-\beta N \varepsilon_0} \frac{1 - e^{-\beta\varepsilon(N+1)}}{1 - e^{-\beta\varepsilon}}$$

b) $$\langle n \rangle = -\frac{\partial}{\partial(\beta\varepsilon)} \ln Q = -\frac{\partial}{\partial(\beta\varepsilon)} \left[\ln\left(1 - e^{-\beta\varepsilon(N+1)}\right) - \ln\left(1 - e^{-\beta\varepsilon}\right) \right]$$

$$\langle n \rangle = \frac{-(N+1)\, e^{-\beta\varepsilon(N+1)}}{1 - e^{-\beta\varepsilon(N+1)}} + \frac{e^{-\beta\varepsilon}}{1 - e^{-\beta\varepsilon}}$$

$$\langle n \rangle = \frac{1}{e^{\beta\varepsilon} - 1} - \frac{N+1}{e^{\beta\varepsilon(N+1)} - 1}$$

c) $k_B T \ll \varepsilon \qquad \langle n \rangle \to 0$

$k_B T \gg \varepsilon$ expand exponentials to 2nd order

$$\langle n \rangle = \frac{1}{\beta\varepsilon + \frac{1}{2}(\beta\varepsilon)^2} - \frac{N+1}{\beta\varepsilon(N+1) + \frac{1}{2}(\beta\varepsilon(N+1))^2}$$

$$= \frac{1}{\beta\varepsilon}\left(1 - \frac{1}{2}\beta\varepsilon\right) - \frac{1}{\beta\varepsilon}\left(1 - \frac{1}{2}\beta\varepsilon(N+1)\right) = \frac{N}{2}$$