Problem 10:

a) In a two-dimensional solid the frequency of a mode is

$$\omega^2_{(l_x, l_y, i)} = c_i^2\left[\left(\frac{\pi l_x}{L_x}\right)^2 + \left(\frac{\pi l_y}{L_y}\right)^2\right]$$

The number of modes of type i with frequency less or equal to ω is

$$\Omega_i(\omega) = \frac{1}{4}\pi \frac{\omega^2}{c_i^2}\frac{L_x}{\pi}\frac{L_y}{\pi} = \frac{L_x L_y}{4\pi}\frac{1}{c_i^2}\omega^2 \qquad 2$$

~~If~~ If we add all three types of modes we get

$$\Omega(\omega) = \frac{L_x L_y}{4\pi}\left(\frac{1}{c_{t,1}^2} + \frac{1}{c_{t,2}^2} + \frac{1}{c_e^2}\right)\omega^2$$

$$\Rightarrow n(\omega) = \frac{d}{d\omega}\Omega(\omega) = \frac{L_x L_y}{2\pi}\left(\frac{1}{c_{t,1}^2} + \frac{1}{c_{t,2}^2} + \frac{1}{c_e^2}\right)\omega$$

Debye frequency given by

$$3N = \int_0^{\omega_0} d\omega\, n(\omega) = \frac{L_x L_y}{2\pi}\left(\frac{1}{c_{t,1}^2} + \frac{1}{c_{t,2}^2} + \frac{1}{c_e^2}\right)\int_0^{\omega_0} d\omega\, \omega$$

$$= \frac{L_x L_y}{4\pi}\left(\frac{1}{c_{t,1}^2} + \frac{1}{c_{t,2}^2} + \frac{1}{c_e^2}\right)\omega_D^2$$

$$\Rightarrow \omega_D = \sqrt{\frac{12\pi N}{L_x L_y\left(\frac{1}{c_{t,1}^2} + \frac{1}{c_{t,2}^2} + \frac{1}{c_e^2}\right)}} \qquad 2$$

$$\Rightarrow n(\omega) = \begin{cases} 6N\frac{\omega}{\omega_D^2} & \omega \le \omega_D \\ 0 & \omega > \omega_D \end{cases}$$

b) lecture $\rightarrow$ $C_N = \frac{1}{k_B T^2}\int_0^\infty d\omega\, n(\omega)\,(\hbar\omega)^2 \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}$

$$= \frac{6N\hbar^2}{k_B T^2 \omega_0^2}\int_0^{\omega_0} d\omega\, \omega^3 \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}$$

$$= \frac{6N\hbar^2}{k_B T^2 \omega_0^2} \frac{1}{(\beta\hbar)^4} \int_0^{T_D/T} dx\, x^3 \frac{e^{+x}}{(e^x-1)^2} = 6Nk_B \left(\frac{T}{T_D}\right)^2 \int_0^{T_D/T} dx\, x^3 \frac{e^x}{(e^x-1)^2}$$ 2

c) $T \to \infty \Rightarrow T_D/T \to 0 \Rightarrow$ we can expand the integrand

$$C_V \simeq 6Nk_B \left(\frac{T}{T_D}\right)^2 \int_0^{T_D/T} dx\, x^3 \frac{1}{x^2} = 6Nk_B \left(\frac{T}{T_D}\right)^2 \frac{1}{2} \left(\frac{T_D}{T}\right)^2 = 3Nk_B$$ 2

d) $T \to 0 \Rightarrow T_D/T \to \infty \Rightarrow$ can integrate to infinity

$$C_V \simeq 6Nk_B \left(\frac{T}{T_D}\right)^2 \int_0^{\infty} dx\, x^3 \frac{e^x}{(e^x-1)^2} = \frac{36Nk_B\zeta(3)}{T_D^2} \cdot T^2$$ 2

Problem 11:

a) $$Z_p = \sum_{L=0,2,4,\ldots} (2L+1) e^{-\frac{\beta\hbar^2}{2I} L(L+1)} = \sum_{n=0}^{\infty} (4n+1) e^{-\frac{\beta\hbar^2}{2I} 2n(2n+1)}$$ (1)

b) $$Z_o = \sum_{L=1,3,5,\ldots} 3(2L+1) e^{-\frac{\beta\hbar^2}{2I} L(L+1)} = \sum_{n=0}^{\infty} (4n+3) e^{-\frac{\beta\hbar^2}{2I} (2n+1)(2n+2)}$$ (1)

c) $$Z(T) = \frac{1}{N!} \sum_{N_p=0}^{N} \binom{N}{N_p} Z_p^{N_p} Z_o^{N-N_p} = \frac{1}{N!} (Z_p + Z_o)^N$$ (1) (1)

particles indistinguishable

$$= \frac{1}{N!} \left(\sum_{n=0}^{\infty} (4n+1) e^{-\frac{\beta\hbar^2}{2I} 2n(2n+1)} + 3\sum_{n=0}^{\infty} (4n+3) e^{-\frac{\beta\hbar^2}{2I} (2n+1)(2n+2)} \right)^N$$ (1)

d) $$\langle E_{rot} \rangle = -\frac{\partial \ln Z(T)}{\partial \beta} =$$

$$= \frac{N\hbar^2}{2I} \frac{\sum_{n=0}^{\infty} 2n(2n+1)(4n+1) e^{-\frac{\beta\hbar^2}{2I} 2n(2n+1)} + 3\sum_{n=0}^{\infty} (4n+3)(2n+1)(2n+2) e^{-\frac{\beta\hbar^2}{2I}(2n+1)(2n+2)}}{\sum_{n=0}^{\infty} (4n+1) e^{-\frac{\beta\hbar^2}{2I} 2n(2n+1)} + 3\sum_{n=0}^{\infty} (4n+3) e^{-\frac{\beta\hbar^2}{2I}(2n+1)(2n+2)}}$$ (1)

low T: $e^{-\frac{\beta\hbar^2}{2I} L(L+1)}$ vanishes very fast as L becomes larger → keep only dominant term (1)

numerator: L=0 term is exactly 0 → L=1 term dominant

denominator: L=0 term dominant

$$\langle E_{rot} \rangle \approx \frac{N\hbar^2}{2I} \frac{3 \cdot 6\, e^{-\frac{\beta\hbar^2}{2I} \cdot 2}}{1\, e^0} = \frac{9N\hbar^2}{I} e^{-\frac{\beta\hbar^2}{I}}$$ (1)

T large $\Rightarrow$ β small $\Rightarrow$ difference between $e^{-\frac{\beta\hbar^2}{2I}L(L+1)}$ and $e^{-\frac{\beta\hbar^2}{2I}(L+2)(L+3)}$ small

$\Rightarrow$ can replace sums by integrals (1)

$$N!\,Z(T) \simeq \left(\int_0^\infty (4n+1)\, e^{-\frac{\beta\hbar^2}{2I}2n(2n+1)}\, dn + 3\int_0^\infty (4n+3)\, e^{-\frac{\beta\hbar^2}{2I}(2n+1)(2n+2)}\, dn \right)^N$$

$$= \left(\int_0^\infty e^{-\frac{\beta\hbar^2}{I}u}\, du + 3\int_1^\infty e^{-\frac{\beta\hbar^2}{I}u}\, du \right)^N$$

$u = 2n^2 + n \quad du = (4n+1)\,dn \qquad u = 2n^2 + 3n + 1 \quad du = (4n+3)\,dn$

$$= \left(\frac{I}{\beta\hbar^2} + \frac{3I}{\beta\hbar^2} e^{-\frac{\beta\hbar^2}{I}} \right)^N$$

$$\langle E_{rot} \rangle = -\left(\frac{\partial \ln Z(T)}{\partial \beta} \right) \simeq N \frac{\frac{I}{\beta^2\hbar^2} + \frac{3I}{\beta^2\hbar^2} e^{-\frac{\beta\hbar^2}{I}} + \frac{3I}{\beta\hbar^2}\frac{\hbar^2}{I} e^{-\frac{\beta\hbar^2}{I}}}{\frac{I}{\beta\hbar^2} + \frac{3I}{\beta\hbar^2} e^{-\frac{\beta\hbar^2}{I}}}$$

$$= N k_B T + N \frac{3\frac{\hbar^2}{I} e^{-\beta\frac{\hbar^2}{I}}}{1 + 3\, e^{-\frac{\beta\hbar^2}{I}}} \simeq N k_B T + 3N\frac{\hbar^2}{I} \underset{T\ \text{large}}{\simeq} N k_B T \quad (1)$$

Problem 12   total for problem 11 = 8 points + 4 extra points

a)
$$Z = \sum_{\{s_i\}} e^{\beta\varepsilon_s \sum_{i=1}^{N} s_i s_{i+1} + \beta\varepsilon_0 \sum_{i=1}^{N} s_i}$$

$$= \sum_{s_1=\{0,1\}} \sum_{s_2=0}^{1} e^{\beta\varepsilon_0 s_1 + \beta\varepsilon_s s_1 s_2} \sum_{s_3=0}^{1} e^{\beta\varepsilon_0 s_2 + \beta\varepsilon_s s_2 s_3} \cdots \sum_{s_N=0}^{1} e^{\beta\varepsilon_0 s_{N-1} + \beta\varepsilon_s s_{N-1} s_N} \times e^{\beta\varepsilon_0 s_N + \beta\varepsilon_s s_N s_1}$$

$$= \operatorname{tr} \bar{T}^N \quad \text{with } \bar{T}_{ss'} = e^{\beta\varepsilon_0 s + \beta\varepsilon_s s s'}$$
(2)

$$\bar{T} = \begin{array}{c} \quad 0 \qquad s' \qquad 1 \\ \begin{pmatrix} 1 & 1 \\ e^{\beta\varepsilon_0} & e^{\beta\varepsilon_0+\beta\varepsilon_s} \end{pmatrix} \begin{array}{c} 0 \\ s \\ 1 \end{array} \end{array}$$

$$\simeq \lambda_+^N \quad \text{where } (1-\lambda_+)(e^{\beta\varepsilon_0+\beta\varepsilon_s} - \lambda_+) - e^{\beta\varepsilon_0} = 0$$

$$\Leftrightarrow \lambda_+^2 - (1+e^{\beta\varepsilon_0+\beta\varepsilon_s})\lambda_+ + e^{\beta\varepsilon_0}(e^{\beta\varepsilon_s}-1) = 0$$

$$\lambda_+ = \frac{1+e^{\beta\varepsilon_0+\beta\varepsilon_s}}{2} + \sqrt{\frac{(1+e^{\beta\varepsilon_0+\beta\varepsilon_s})^2}{4} - e^{\beta\varepsilon_0}(e^{\beta\varepsilon_s}-1)}$$ (2)

b)
$$\langle s_1 \rangle = \frac{1}{N\beta}\left(\frac{\partial}{\partial\varepsilon_0} \ln Z(T)\right) = \frac{1}{\beta}\left(\frac{\partial}{\partial\varepsilon_0} \ln \lambda_+\right)$$

$$\underset{\varepsilon_0=0}{=} \frac{1}{\beta} \frac{\beta \frac{e^{\beta\varepsilon_s}}{2} + \frac{\frac{2(1+e^{\beta\varepsilon_s})\beta e^{\beta\varepsilon_s}}{4} - \beta(e^{\beta\varepsilon_s}-1)}{2\sqrt{\frac{(1-e^{\beta\varepsilon_s})^2}{4}+1}}}{\frac{1+e^{\beta\varepsilon_s}}{2} + \sqrt{\frac{(1+e^{\beta\varepsilon_s})^2}{4} - e^{\beta\varepsilon_s} + 1}}$$

$$= \frac{e^{\beta\varepsilon_s}\sqrt{\frac{(e^{\beta\varepsilon_s}-1)^2}{4}+1} + \frac{1}{2}e^{\beta\varepsilon_s}(1+e^{\beta\varepsilon_s}) - e^{\beta\varepsilon_s} + 1}{\left(1+e^{\beta\varepsilon_s} + \sqrt{(e^{\beta\varepsilon_s}-1)^2+4}\right)\sqrt{\frac{(e^{\beta\varepsilon_s}-1)^2}{4}+1}}$$

$$= \frac{e^{\beta\varepsilon_s}\sqrt{(e^{\beta\varepsilon_s}-1)^2+4} + e^{\beta\varepsilon_s}(e^{\beta\varepsilon_s}-1) + 2}{\left(1+e^{\beta\varepsilon_s}+\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}\right)\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}}$$ (2)

c) At $\varepsilon_0 = 0$: $Z(T) = \left[\frac{1+e^{\beta\varepsilon_s}}{2} + \sqrt{\frac{(e^{\beta\varepsilon_s}-1)^2}{4}+1}\right]^N$

$$U = -\left(\frac{\partial \ln Z(T)}{\partial\beta}\right) = -N\,\frac{\varepsilon_s \frac{e^{\beta\varepsilon_s}}{2} + \frac{\frac{1}{2}(e^{\beta\varepsilon_s}-1)\,\varepsilon_s e^{\beta\varepsilon_s}}{2\sqrt{\frac{(e^{\beta\varepsilon_s}-1)^2}{4}+1}}}{\frac{1+e^{\beta\varepsilon_s}}{2} + \sqrt{\frac{(e^{\beta\varepsilon_s}-1)^2}{4}+1}}$$

$$= -N\varepsilon_s e^{\beta\varepsilon_s}\,\frac{e^{\beta\varepsilon_s}-1+\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}}{\left(1+e^{\beta\varepsilon_s}+\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}\right)\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}} \quad (2)$$

$$C = \frac{\partial U}{\partial T} = -k_B\beta^2\left(\frac{\partial U}{\partial\beta}\right)$$

$$= k_B\varepsilon_s^2\beta^2 N\Bigg[e^{\beta\varepsilon_s}\frac{e^{\beta\varepsilon_s}-1+\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}}{\left(1+e^{\beta\varepsilon_s}+\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}\right)\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}}$$

$$+e^{2\beta\varepsilon_s}\frac{\left(1+\frac{2(e^{\beta\varepsilon_s}-1)}{2\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}}\right)\left(1+e^{\beta\varepsilon_s}+\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}\right)\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}}{\left(1+e^{\beta\varepsilon_s}+\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}\right)^2\left[(e^{\beta\varepsilon_s}-1)^2+4\right]}$$

$$-e^{2\beta\varepsilon_s}\frac{\left[e^{\beta\varepsilon_s}-1+\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}\right]\left[\left(1+\frac{e^{\beta\varepsilon_s}-1}{\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}}\right)\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}+\left(1+e^{\beta\varepsilon_s}+\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}\right)\frac{e^{\beta\varepsilon_s}-1}{\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}}\right]}{\left(1+e^{\beta\varepsilon_s}+\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}\right)^2\left[(e^{\beta\varepsilon_s}-1)^2+4\right]}\Bigg]$$

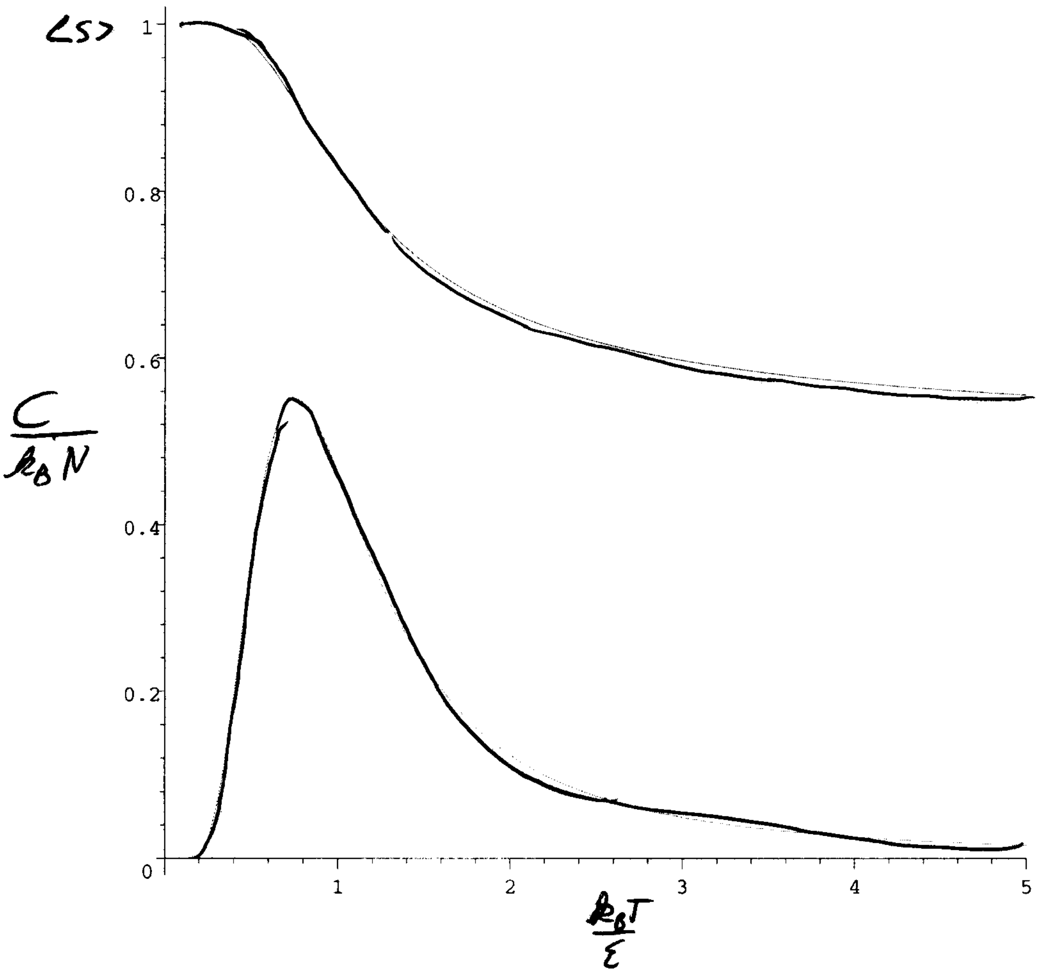
$$= 4\beta^2\varepsilon_s^2 e^{\beta\varepsilon_s} N\,\frac{2e^{2\beta\varepsilon_s}-e^{\beta\varepsilon_s}+5+2e^{\beta\varepsilon_s}\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}}{\left(1+e^{\beta\varepsilon_s}+\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}\right)^2\sqrt{(e^{\beta\varepsilon_s}-1)^2+4}^{\,3}} \quad (2)$$

maybe

make these extra points

d)

② make those extra points



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