Einstein Model of Solid

a) There are 3N oscillators, i.e. N atoms which can move in 3-directions. Each Harmonic oscillator has two quadratic forms

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega_0^2 x^2$$

So each oscillator has two dof leading to

$$E = 3N \cdot 2 \times \frac{1}{2} k_B T = 3N k_B T$$

b) The partion fcn of the oscillator is

average energy of each

$$Z = \frac{1}{1 - e^{-\beta \hbar \omega_0}} \qquad \langle \varepsilon_0 \rangle = \frac{1}{Z} \frac{-\partial Z}{\partial \beta} = -\frac{\partial}{\partial \beta} \ln Z$$

$$= \frac{e^{-\beta \hbar \omega_0}}{1 - e^{-\beta \hbar \omega_0}} \hbar \omega_0$$

So the total energy is

$$\bar{E} = 3N \hbar \omega_0 \frac{e^{-\beta \hbar \omega_0}}{1 - e^{-\beta \hbar \omega_0}} = 3N \hbar \omega \frac{1}{e^{\beta \hbar \omega_0} - 1}$$

c) Now using $\partial X / \partial T = \partial X / \partial \beta \, (\partial \beta / \partial T) = -k_B \beta^2 \, \partial X / \partial \beta$

$$C_V = \frac{\partial \bar{E}}{\partial T} = -k_B \beta^2 \frac{\partial E}{\partial \beta} \quad \leftarrow \text{now differentiate}$$

So

$$C_V = 3Nk_B\beta^2\left(\frac{-\partial}{\partial\beta}\right)\frac{\hbar\omega_0}{e^{\beta\hbar\omega_0}-1}$$

$$C_V = 3Nk_B\beta^2\frac{e^{\beta\hbar\omega_0}}{(e^{\beta\hbar\omega_0}-1)^2}(\hbar\omega_0)^2$$

or for one mole $N = N_A$ and $N_A k_B = R$ we have

$$\underline{C_V = 3R\,(\beta\hbar\omega_0)^2\frac{e^{\beta\hbar\omega_0}}{(e^{\beta\hbar\omega_0}-1)^2}}$$

This equals the form given in the problem after multiplying numerator and denominator by $(e^{-\beta\hbar\omega_0})^2$.

d) See attatched plot

e) $Z = \dfrac{1}{1-e^{-\beta\hbar\omega_0}}$ and $F = -k_BT\ln Z$

So $F = k_BT\ln(1-e^{-\beta\hbar\omega_0}) = \underline{E-TS}$

Now

$$S = \frac{E-F}{T} = k_B\beta(E-F)$$ (using $\langle\varepsilon\rangle$ and $\beta k_BT = 1$

$$= k_B\left[\frac{\beta\hbar\omega_0}{e^{\beta\hbar\omega_0}-1} - \ln(1-e^{-\beta\hbar\omega_0})\right]$$

We have computed the entropy for one oscillator. For $3N_A$ oscillators we just multiply by $3N_A$

$$S_{TOT} = 3N_A k_B \left[\frac{\beta \hbar \omega_0}{e^{\beta\hbar\omega_0} - 1} - \log\left(1 - e^{-\beta\hbar\omega_0}\right) \right]$$

f) We have

$$\bar{n} = \frac{1}{e^{\beta\hbar\omega_0} - 1}$$

We need to solve for β in terms of $\bar{n}$

$$\frac{1}{\bar{n}} = e^{\beta\hbar\omega_0} - 1 \implies \frac{1+\bar{n}}{\bar{n}} = e^{\beta\hbar\omega_0} \quad (1)$$

So $$\beta = \frac{1}{\hbar\omega_0} \ln\left(\frac{1+\bar{n}}{\bar{n}}\right) \quad (2)$$

Expressing S in terms of $\bar{n}$ we have using (1) and (2)

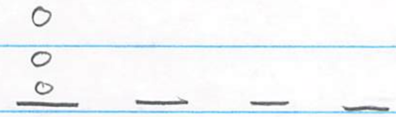
$$S = 3N_A k_B \left[\bar{n} \ln\left(\frac{1+\bar{n}}{\bar{n}}\right) - \log\left(1 - \frac{\bar{n}}{1+\bar{n}}\right) \right]$$

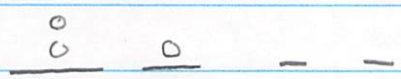
algebra

$$= 3N_A k_B \left[(1+\bar{n}) \ln(1+\bar{n}) - n \ln \bar{n} \right]$$

Ways to partition energy amongst N SHO

a)

 4 configs like this

 12 configs like this

 4 configs like this

b) There are $\frac{4}{20}$ configs with one partice having all the energy

c) The $(N+q-1)$ objects we choose q of them to be balls $N-1$ to be dividers. The combinatorics of choosing says there are

$$ {}_{N+q-1}C_q = \frac{(N+q-1)!}{q!\,(N-1)!} \quad \text{ways to do this} $$

d) Using the stirling approximation for Large N and large q but $\bar{n} = \frac{q}{\ }$ fixed we have (dropping the 1) and using that N $N! \doteq (N/e)^N$

$$ \Omega(q) = \left(\frac{N+q}{e}\right)^{N+q} \frac{1}{\left(\frac{q}{e}\right)^q} \frac{1}{\left(\frac{N}{e}\right)^N} = \frac{N^{N+q}}{N^{N+q}} \frac{(1+\bar{n})^{N+q}}{\bar{n}^q} $$

So

$$\Omega(q) = e^{(N+q)\ln(1+\bar{n}) - q\ln\bar{n}}$$

Pulling out a factor of N

$$\boxed{\Omega(q) = e^{N[(1+\bar{n})\ln(1+\bar{n}) - \bar{n}\ln\bar{n}]}}$$

So

$$\ln \Omega(q) = N\left[(1+\bar{n})\ln(1+\bar{n}) - \bar{n}\ln\bar{n}\right]$$

For $q = \frac{1}{2}$, $\bar{n} = \frac{1}{2}$, and then

$$\ln\Omega(q) = N\,2\ln 2$$

and $$\boxed{\Omega(q) \simeq e^{N\,2\ln 2} \simeq 10^{240}}$$

e) See above

f) The entopy is

$$\frac{S}{k_B} = \ln\Omega(q) = N\left[(1+\bar{n})\ln(1+\bar{n}) - \bar{n}\ln\bar{n}\right]$$

The energy of the system is $E = q\hbar\omega_0 = N\hbar\omega_0\bar{n}$

Then

$$\boxed{\frac{\partial S}{\partial E} = \frac{1}{T}}$$

And since $E \propto \bar{n}$ up to a constant $\bar{n} = E/N\hbar\omega_0$

$$\frac{\partial S}{\partial E} = \frac{\partial S}{\partial \bar{n}} \frac{\partial \bar{n}}{\partial E} = \frac{1}{N\hbar\omega_0} \frac{\partial S}{\partial \bar{n}}$$

Differentiating

$$\frac{1}{N\hbar\omega_0} \frac{\partial S}{\partial \bar{n}} = \frac{k_B}{\hbar\omega_0} \frac{\partial}{\partial \bar{n}} \left[(1+\bar{n}) \ln (1+\bar{n}) - \bar{n} \ln \bar{n} \right]$$

$$= \frac{k_B}{\hbar\omega_0} \left[\ln (1+n) + 1 - (\ln \bar{n} + 1) \right]$$

$$\boxed{\frac{1}{T} = \frac{k_B}{\hbar\omega_0} \ln \left(\frac{1+\bar{n}}{\bar{n}} \right)}$$

this gives the temperature in terms of $\bar{n}$