3.1 The madelung constant α for a linear chain is derived in the bobbe p. 64. $\alpha = 2\ln 2$

Assuming $N \gg 1$ we get

a) $U_{tot} = N\left(\frac{2A}{R} - \frac{\alpha K q^2}{R}\right)$ K is a Coulomb constant

$\frac{\partial U}{\partial R} \propto -\frac{2A}{R^2} + \frac{\alpha K q^2}{R^2}$ no minima, therefore this chain can not be stable.

b) $\frac{\partial U}{\partial R} \propto -\frac{4A}{R^3} + \frac{\alpha K q^2}{R^2} = 0 \rightarrow R_0 = \frac{4A}{\alpha K q^2}$

If compressed to $R = \frac{R_0}{2}$

$U_{tot} = N\left(\frac{2A}{\left(\frac{R_0}{2}\right)^2} - \frac{\alpha K q^2}{\frac{R_0}{2}}\right) = -\frac{N K^2 \alpha^2 q^4}{A}\left(\frac{1}{2} - \frac{1}{2}\right) = 0$

3.2 Younge modulus is defined in shear strain

$\rightarrow E = \frac{\sigma}{\varepsilon} = \frac{F/A_0}{\Delta L/L_0} = \frac{F L_0}{A_0 \Delta L}$

Poisson ratio

$\nu = \frac{\varepsilon_\perp}{\varepsilon_\parallel} = \frac{\Delta w/w_0}{\Delta L/L_0}$

3.3 Free energy $G = U - TS + PV$

Assume crystal with $N+n$ lattice points where n = # vacancies, N = # atoms.

$V = (N+n)V_0$ where V_0 is the volume for each lattice point

Configurational entropy: W = # configurationally distinct states.

Place n vacancies in a $N+n$ lattice (order do not matter)

$$W = \binom{n+N}{n} = \binom{n+N}{N} = \frac{(n+N)!}{n!\,N!}$$ using $\ln X! \approx X\ln X - X$

$$\rightarrow \frac{S}{k_B} = (n+N)(\ln(n+N) - 1) - n\ln n - N\ln N + n + N$$

$$\rightarrow \frac{\partial S}{\partial n} = k_B\left(\ln(n+N) - \frac{(n+N)}{n+N} - 1 - \ln n - 1 + 1\right) = k_B \ln\left(\frac{n+N}{n}\right)$$

Equilibrium at $\frac{\partial G}{\partial n} = 0$

$$\ln\left(\frac{n+N}{n}\right) = \ln\frac{N}{n} \quad \text{for } N \gg n$$

$$\rightarrow \frac{\partial G}{\partial n} = E_V - k_B T \ln\left(\frac{N}{n}\right) + PV_0 = 0$$

$$\rightarrow n = N e^{\frac{-PV_0 + E_V}{k_B T}}$$

3.4 Apply the derived formula.