2.1/ (Problem from The Oxford Solid State Basics)

a.)

i.) We calculate the partition function for the Einstein solid, where the Hamiltonian is given by

$$H = \sum_{n=1}^{N} \vec{p}_n^{\,2}/2m + \frac{1}{2} k \vec{x}_n^{\,2}$$

where $\vec{x}_n$ describes the displacement of particle n from the minimum of the harmonic potential it sits in.

$$Z = \frac{1}{N!} \frac{1}{(2\pi\hbar)^{3N}} \int \prod_{n=1}^{N} d^3x_n \, d^3p_n \, e^{-\beta \vec{p}_n^{\,2}/2m} e^{-\beta k \vec{x}_n^{\,2}/2}$$

$$= \frac{1}{N!} \frac{1}{(2\pi\hbar)^{3N}} \left(4\pi \int_{-\infty}^{\infty} p^2 e^{\beta p^2/2m} dp \right)^N \left(4\pi \int_{-\infty}^{\infty} x^2 e^{-\beta k x^2/2} dx \right)^N$$

$$= \frac{1}{N!} \frac{1}{(\cancel{2\pi}\hbar)^{3N}} \cdot \left(\frac{\cancel{2\pi} m}{\beta} \cdot \frac{\cancel{2\pi}}{k\beta} \right)^{3N/2} =$$

$$\frac{1}{N!} \left(\sqrt{\frac{m}{k}} \cdot \frac{1}{\beta\hbar} \right)^{3N} = \boxed{\frac{1}{N!} \left(\frac{1}{\hbar\omega\beta} \right)^{3N}},$$

where $\omega = \sqrt{k/m}$ is the harmonic oscillator frequency.

ii.) We now compute the heat capacity, $C_v = \partial\langle E\rangle/\partial T|_v$.

$$\langle E\rangle = -\frac{\partial}{\partial\beta}\log Z = -\frac{\partial}{\partial\beta}\left(\log\beta^{-3N} + \log \_\_\right)$$

$$= \frac{3N}{\beta} = 3Nk_BT \Rightarrow \boxed{\frac{C_v}{N} = 3k_B}$$

This is known as the Dulong-Petit law.