Solution 1

(a) $m\ddot{X}_n = S(X_{n+1} - X_n) - S(X_n - X_{n-1})$. 0.7

(b) Let $X_n = A \sin nka \cos(\omega t + \alpha)$, which has a harmonic time dependence. By analogy with the spring, the acceleration is $\ddot{X}_n = -\omega^2 X_n$.

Substitute into (a): $-mA\omega^2 \sin nka = AS\{\sin(n+1)ka - 2\sin nka + \sin(n-1)ka\}$

$$= -4SA \sin nka \, \sin^2 \frac{ka}{2}.$$

0.6

Hence $\omega^2 = \dfrac{4S}{m} \sin^2 \dfrac{ka}{2}$. 0.2

To determine the allowed values of k, use the boundary condition $\sin(N+1)ka = \sin kL = 0$. 0.7

The allowed wave numbers are given by $kL = \pi,\ 2\pi,\ 3\pi,\ \ldots,\ N\pi$ (N in all), 0.3

and their corresponding frequencies can be computed from $\omega = \omega_0 \sin \dfrac{ka}{2}$,

in which $\omega_{\max} = \omega_0 = 2\sqrt{S/m}$ is the maximum allowed frequency. 0.4

(c) $\langle E(\omega) \rangle = \dfrac{\sum_{p=0}^{\infty} p\hbar\omega \, P_p(\omega)}{\sum_{p=0}^{\infty} P_p(\omega)}$

First method:

$$\frac{\sum_{n=0}^{\infty} n\hbar\omega \, e^{-n\hbar\omega/k_BT}}{\sum_{n=0}^{\infty} e^{-n\hbar\omega/k_BT}} = k_BT^2 \frac{\partial}{\partial T} \ln \sum_{n=0}^{\infty} e^{-n\hbar\omega/k_BT}$$

1.5

The sum is a geometric series and is $\{1 - e^{-\hbar\omega/k_BT}\}^{-1}$. 0.5

We find $\langle E(\omega) \rangle = \dfrac{\hbar\omega}{e^{\hbar\omega/k_BT} - 1}$.

Alternatively: denominator is a geometric series $= \{1 - e^{-\hbar\omega/k_BT}\}^{-1}$. (0.5)

Numerator is $k_BT^2 \, (d/dT)$(denominator) $= e^{-\hbar\omega/k_BT}\{1 - e^{-\hbar\omega/k_BT}\}^{-2}$ and result follows. (1.5)

A non-calculus method: Let $D = 1 + e^{-x} + e^{-2x} + e^{-3x} + \ldots$, where $x = \hbar\omega/k_BT$. This is a geometric series and equals $D = 1/(1 - e^{-x})$. Let $N = e^{-x} + 2e^{-2x} + 3e^{-3x} + \ldots$. The result we want is N/D. Observe (2.0)

$$\begin{aligned} D - 1 &= e^{-x} + e^{-2x} + e^{-3x} + e^{-4x} + e^{-5x} + \ldots \\ (D-1)e^{-x} &= e^{-2x} + e^{-3x} + e^{-4x} + e^{-5x} + \ldots \\ (D-1)e^{-2x} &= e^{-3x} + e^{-4x} + e^{-5x} + \ldots \end{aligned}$$

Hence $N = (D-1)D$ or $N/D = D - 1 = \dfrac{e^{-x}}{1 - e^{-x}} = \dfrac{1}{e^x - 1}$.

(d) From part (b), the allowed k values are $\pi/L,\ 2\pi/L,\ \ldots,\ N\pi/L$.

Hence the spacing between allowed k values is π/L, so there are $(L/\pi)\Delta k$ allowed modes in the wave-number interval Δk (assuming $\Delta k \gg \pi/L$). 1.0

(e) Since the allowed k are $\pi/L, \ldots, N\pi/L$, there are N modes. 0.5

Follow the problem: 0.5

$$\frac{d\omega}{dk} = \frac{a\omega_0}{2} \cos \frac{ka}{2} \quad \text{from part (a) \& (b)}$$

$$= \frac{1}{2}\, a\sqrt{\omega_{\max}^2 - \omega^2}, \quad \omega_{\max} = \omega_0.$$

This second form is more convenient for integration.

The number of modes dn in the interval $d\omega$ is

$$\begin{aligned} dn &= (L/\pi)\Delta k = (L/\pi)\left(\frac{dk}{d\omega}\right) d\omega \\ &= \frac{L}{\pi}\left\{\frac{a\omega_0}{2}\cos\frac{ka}{2}\right\}^{-1} d\omega \\ &= \frac{L}{\pi}\,\frac{2}{a}\,\frac{1}{\sqrt{\omega_{\max}^2 - \omega^2}}\, d\omega \\ &= \frac{2(N+1)}{\pi}\,\frac{1}{\sqrt{\omega_{\max}^2 - \omega^2}}\, d\omega \end{aligned}$$

0.5 for either

This part is necessary for E_T below, but not for number of modes.

Total number of modes $= \int dn = \int_0^{\omega_{\max}} \frac{2(N+1)}{\pi}\,\frac{d\omega}{\sqrt{\omega_{\max}^2-\omega^2}} = N+1 \approx N$ for large N. (0.5)

Total crystal energy from (c) and dn of part (e) is given by

$$E_T = \frac{2N}{\pi}\int_0^{\omega_{\max}} \frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1}\,\frac{d\omega}{\sqrt{\omega_{\max}^2-\omega^2}}.$$

0.7

(f) Observe first from the last formula that E_T increases monotonically with temperature since
$\{e^{\hbar\omega/kT}-1\}^{-1}$ is increasing with T. 0.2

When $T \to 0$, the term -1 in the last result may be neglected in the denominator so 0.2

$$\begin{aligned} E_T &\approx_{T\to 0} \frac{2N}{\pi}\int \hbar\omega\, e^{-\hbar\omega/k_BT}\,\frac{1}{\sqrt{\omega_{\max}^2-\omega^2}}\, d\omega \\ &= \frac{2N}{\hbar\pi\omega_{\max}}(k_BT)^2\int_0^\infty \frac{xe^{-x}}{\sqrt{1-(k_BTx/\hbar\omega_{\max})^2}}\, dx \end{aligned}$$

0.3 0.2

which is quadratic in T (denominator in integral is effectively unity) hence C_V is linear in T near absolute zero. 0.2

Alternatively, if the summation is retained, we have (0.5)

$$\begin{aligned} E_T &= \frac{2N}{\pi}\sum_\omega \frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1}\,\frac{\Delta\omega}{\sqrt{\omega_{\max}^2-\omega^2}} \xrightarrow{T\to 0} \frac{2N}{\pi}\sum_\omega \hbar\omega\, e^{-\hbar\omega/k_BT}\,\frac{\Delta\omega}{\sqrt{\omega_{\max}^2-\omega^2}} \\ &= \frac{2N}{\pi}\frac{(k_BT)^2}{\hbar\omega}\sum_y e^{-y}\, y\,\Delta y \end{aligned}$$

When $T \to \infty$, use $e^x \approx 1+x$ in the denominator, 0.2

$$E_T \approx_{T\to\infty} \frac{2N}{\pi}\int_0^{\omega_{\max}} \frac{\hbar\omega}{\hbar\omega/k_BT}\,\frac{1}{\sqrt{\omega_{\max}^2-\omega^2}}\, d\omega = \frac{2N}{\pi}\, k_BT\,\frac{\pi}{2},$$

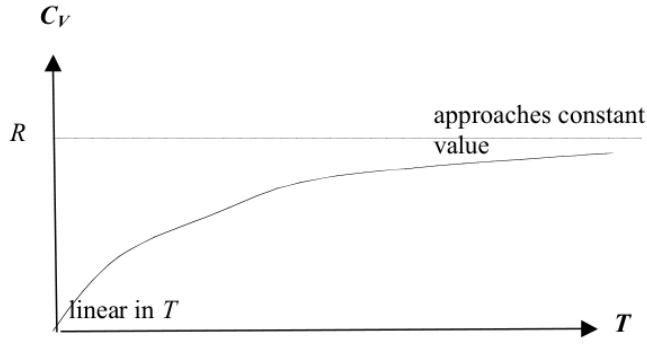
0.1

which is linear; hence $C_V \to Nk_B = R$, the universal gas constant. This is the Dulong-Petit rule.

Alternatively, if the summation is retained, write denominator as $e^{\hbar\omega/k_BT} - 1 \approx \hbar\omega/k_BT$ and (0.2)

$$E_T \xrightarrow{T\to\infty} \frac{2N}{\pi} k_BT \sum_{\omega} \frac{\Delta\omega}{\sqrt{\omega_{\max}^2 - \omega^2}} \qquad \text{which is linear in } T\text{, so } C_V \text{ is constant.}$$

Sketch of C_V versus T: 0.5



Answer sheet: Question 1

(a) Equation of motion of the n^{th} mass is:

$$m\ddot{X}_n = S(X_{n+1} - X_n) - S(X_n - X_{n-1}).$$

(b) Angular frequencies ω of the chain's vibration modes are given by the equation:

$$\omega^2 = \frac{4S}{m} \sin^2 \frac{ka}{2}.$$

Maximum value of ω is: $\omega_{\max} = \omega_0 = 2\sqrt{S/m}$.

The allowed values of the wave number k are given by:

$$\frac{\pi}{L}, \frac{2\pi}{L}, \ldots, \frac{N\pi}{L}.$$

How many such values of k are there? N

(f) The average energy per frequency mode ω of the crystal is given by:

$$\langle E(\omega)\rangle = \frac{\hbar\omega}{e^{\hbar\omega/k_BT} - 1}.$$

(g) There are how many allowed modes in a wave number interval Δk?

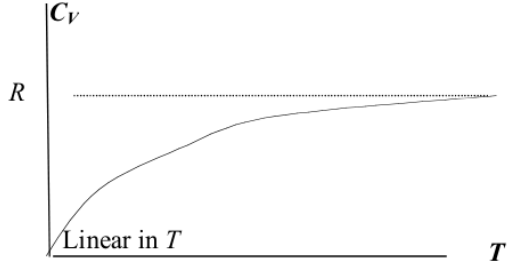
$$(L/\pi)\Delta k.$$

(e) The total number of modes in the lattice is: N

Total energy E_T of crystal is given by the formula:

$$E_T = \frac{2N}{\pi} \int_0^{\omega_{\max}} \frac{\hbar\omega}{e^{\hbar\omega/k_BT} - 1} \frac{d\omega}{\sqrt{\omega_{\max}^2 - \omega^2}}.$$

(h) A sketch (graph) of C_V versus absolute temperature T is shown below.



For $T \ll 1$, C_V displays the following behaviour: C_V is linear in T.

As $T \to \infty$, C_V displays the following behaviour: $C_V \to Nk_B = R$, the universal gas constant.