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): $-mA\omega^2 \sin nka = AS\{\sin(n+1)ka - 2\sin nka + \sin(n-1)ka\}$	
$= -4SA \sin nka \sin^2$ _ka.	0.6
Hence $\omega^2 = (4S/m)\sin^2$ _ka.	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 $\omega = \omega_0 \sin$ _ka,	
in which $\omega_{max} = \omega_0 = 2(S/m)^{-}$ 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: $\dfrac{\sum_{n=0}^{\infty} n\hbar\omega e^{-n\hbar\omega/k_B T}}{\sum_{n=0}^{\infty} e^{-n\hbar\omega/k_B T}} = k_B T^2 \dfrac{\partial}{\partial T} \ln \sum_{n=0}^{\infty} e^{-n\hbar\omega/k_B T}$	1.5
The sum is a geometric series and is $\{1 - e^{-\hbar\omega/k_B T}\}^{-1}$	0.5
We find $\langle E(\omega)\rangle = \dfrac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$.	
Alternatively: denominator is a geometric series = $\{1 - e^{-\hbar\omega/k_B T}\}^{-1}$	(0.5)
Numerator is $k_B T^2$(d/dT) (denominator) = $e^{-\hbar\omega/k_B T}\{1 - e^{-\hbar\omega/k_B T}\}^{-2}$ and result follows.	(1.5)

A non-calculus method:
Let $D = 1 + e^{-x} + e^{-2x} + e^{-3x} + \ldots$, where $x = \hbar\omega/k_B T$. 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)

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

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
dω/dk = _$a\omega_0$ cos _ka from part (a) & (b)

$= \frac{1}{2} a\sqrt{\omega^2_{\max} - \omega^2}$, $\omega_{\max} = \omega_0$. This second form is more convenient for integration.

The number of modes dn in the interval dω is

$$dn = (L/\pi)\Delta k = (L/\pi)\,(dk/d\omega)\,d\omega$$

0.5 for eit

$$= (L/\pi)\{\_\, a\omega_0 \cos \_\, ka\}^{-1}\, d\omega$$

This part is necessary f E_T below,

$$= \frac{L}{\pi}\,\frac{2}{a}\,\frac{1}{\sqrt{\omega^2_{\max} - \omega^2}}\,d\omega$$

but not for number of modes

$$= \frac{2(N+1)}{\pi}\,\frac{1}{\sqrt{\omega^2_{\max} - \omega^2}}\,d\omega$$

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

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

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

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

$$E_T \approx_{T\to 0} \frac{2N}{\pi}\int \hbar\omega\, e^{-\hbar\omega/k_BT} \frac{1}{\sqrt{\omega_{\max}^2 - \omega^2}} d\omega$$ 0.3

$$= \frac{2N}{\hbar\pi\omega_{\max}}(k_BT)^2 \int_0^\infty \frac{xe^{-x}}{\sqrt{1-(k_BTx/\hbar\omega_{\max})^2}}dx$$ 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

$$E_T = \frac{2N}{\pi}\sum_\omega \frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1}\frac{\Delta\omega}{\sqrt{\omega_{\max}^2-\omega^2}} \to_{T\to 0} \frac{2N}{\pi}\sum_\omega \hbar\omega e^{-\hbar\omega/k_BT}\frac{\Delta\omega}{\sqrt{\omega_{\max}^2-\omega^2}}$$

$$= \frac{2N}{\pi}\frac{(k_BT)^2}{\hbar\omega}\sum_y e^{-y} y\Delta y$$ (0.5)

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

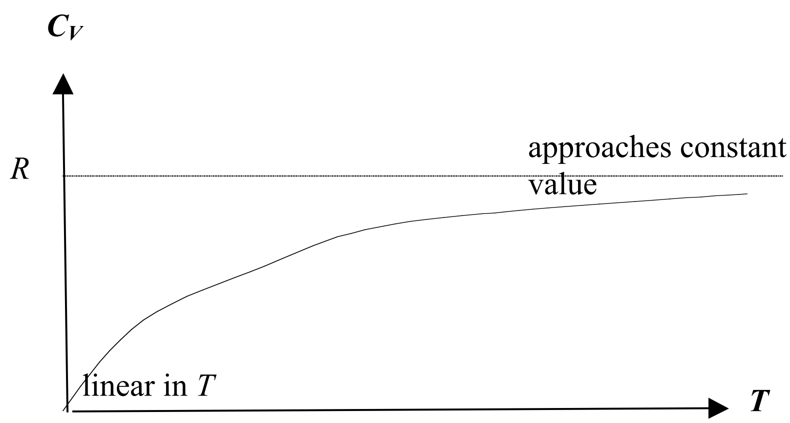
$$E_T \approx_{T\to\infty} \frac{2N}{\pi}\int_0^{\omega_{\max}} \frac{\hbar\omega}{\hbar\omega/k_BT}\frac{1}{\sqrt{\omega_{\max}^2-\omega^2}}d\omega = \frac{2N}{\pi}k_BT\frac{\pi}{2},$$ 0.1

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)

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

$$\omega^2 = (4S/m)\sin^2 \_\,ka.$$

Maximum value of ω is: $\omega_{max} = \omega_0 = 2(S/m)^{-}$

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

$$\pi/L,\ 2\pi/L,\ \ldots,\ N\pi/L.$$

How many such values of k are there? *N*

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

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

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

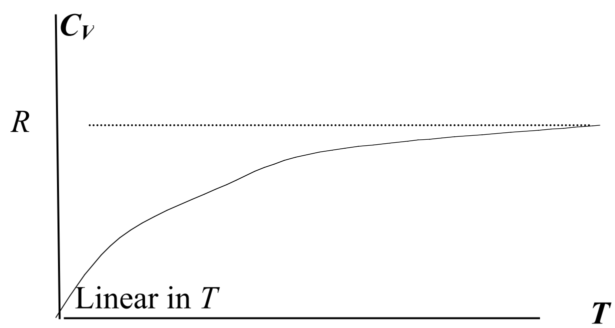
$$(L/\pi)\Delta k.$$

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

Total energy E_T of crystal is given by the formula:

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

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



For $T << 1$, 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.