Phys. 807 — Statistical Mechanics

HW6 (due Tue Nov 8 at 4 p.m. in my mailbox).

Consider a two-dimensional solid with a single atom per cell of size $a \times a$. Each atom is coupled to nearest neighbours only (there are 4 of them) by springs of constant $m\omega_0^2$, where m is the atom's mass. The "volume" of the solid is $L \cdot L = L^2$, and the number of atoms is N^2.

- Write down the Hamiltonian and the equations of motion for this system.
- Look for periodic solutions and determine the eigenfrequencies $\omega_\beta(\mathbf{k})$ of the matrix $\Gamma_{\alpha\beta}(\mathbf{k})$.
- Check that the operators $A_\beta(\mathbf{k})$ defined by

$$A_\beta(\mathbf{k}) = (2\hbar\omega_\beta(\mathbf{k}))^{-1/2}(\omega_\beta(\mathbf{k})Q_\beta(\mathbf{k}) + iP_\beta(-\mathbf{k}))$$

$$A_\beta^+(\mathbf{k}) = (2\hbar\omega_\beta(-\mathbf{k}))^{-1/2}(\omega_\beta(\mathbf{k})Q_\beta(-\mathbf{k}) - iP_\beta(\mathbf{k}))$$

satisfy the commutation relations

$$[A_\beta(\mathbf{k}), A_\gamma^+(\mathbf{p})] = \delta_{\beta\gamma}\delta_{\mathbf{k},\mathbf{p}}$$

$$[A_\beta(\mathbf{k}), A_\gamma(\mathbf{p})] = [A_\beta^+(\mathbf{k}), A_\gamma^+(\mathbf{p})] = 0\,.$$

- Show that the Hamiltonian in terms of the new operators is given by the sum of Hamiltonians of quantum-mechanical oscillators corresponding to the frequences $\omega_\beta(\mathbf{k})$.
- Derive expression for the energy of this solid (similar to Debye interpolation formula) and determine the heat capacity at constant volume of this solid.

Solution

The Hamiltonian is

$$\begin{aligned}
H &= \sum_{m,n=0}^{N} \frac{\vec{p}^{\,2}_{m,n}}{2m} \\
&+ \frac{1}{2}\sum_{m,n=0}^{N} \frac{m\omega_0^2}{2}[(\vec{x}_{m+1,n}-\vec{x}_{m,n})^2 + (\vec{x}_{m-1,n}-\vec{x}_{m,n})^2 + (\vec{x}_{m,n+1}-\vec{x}_{m,n})^2 + (\vec{x}_{m,n-1}-\vec{x}_{m,n})^2]
\end{aligned}$$

where extra $\frac{1}{2}$ in the expression for potential energy is due to the fact that each spring is counted two times.

Performing rescaling $\vec{p} = \vec{\pi}\sqrt{m}$ and $\vec{x} = \frac{\vec{z}}{\sqrt{m}}$ we get

$$\begin{aligned}
H &= \sum_{m,n=0}^{N} \frac{\vec{\pi}^{\,2}_{m,n}}{2} \\
&+ \frac{\omega_0^2}{4}\sum_{m,n=0}^{N} [(\vec{z}_{m+1,n}-\vec{z}_{m,n})^2 + (\vec{z}_{m-1,n}-\vec{z}_{m,n})^2 + (\vec{z}_{m,n+1}-\vec{z}_{m,n})^2 + (\vec{z}_{m,n-1}-\vec{z}_{m,n})^2]
\end{aligned}$$

Now we rewrite the Hamiltonian in terms of the deviations from the equilibrium positions $\vec{z}_{m,n} = (am, an) + \vec{u}_{m,n}$

$$\begin{aligned}
H &= \sum_{m,n=0}^{N} \frac{\vec{\pi}^{\,2}_{m,n}}{2} + \frac{\omega_0^2}{4}\sum_{m,n=0}^{N} [(\vec{u}_{m+1,n}-\vec{u}_{m,n}+a\vec{e}_x)^2 \\
&+(\vec{u}_{m-1,n}-\vec{u}_{m,n}-a\vec{e}_x)^2 + (\vec{u}_{m,n+1}-\vec{u}_{m,n}+a\vec{e}_y)^2 + (\vec{u}_{m,n-1}-\vec{u}_{m,n}-a\vec{e}_y)^2] \\
&= \sum_{m,n=0}^{N} \Big(\frac{(\pi^x_{m,n})^2}{2} + \frac{(\pi^y_{m,n})^2}{2}\Big) \\
&+ \frac{\omega_0^2}{4}\sum_{m,n=0}^{N} [(u^x_{m+1,n}-u^x_{m,n}+a)^2 + (u^x_{m-1,n}-u^x_{m,n}-a)^2 + (u^x_{m,n+1}-u^x_{m,n})^2 + (u^x_{m,n-1}-u^x_{m,n})^2 \\
&+ \frac{\omega_0^2}{4}\sum_{m,n=0}^{N} [(u^y_{m+1,n}-u^y_{m,n})^2 + (u^y_{m-1,n}-u^y_{m,n})^2 + (u^y_{m,n+1}-u^y_{m,n}+a)^2 + (u^y_{m,n-1}-u^y_{m,n}-a)^2]
\end{aligned}$$

The terms linear in u drop because due to periodic boundary condition

$$\sum_{m=0}^{N} a(u^x_{m+1,n}-u^x_{m,n}) \;=\; a(u^x_{N,n}-u^x_{0,n}) \;=\; 0$$

and similarly for other sums linear in u's. This corresponds to the fact that $u_{m,n} = 0$ is the equilibrium position.

We get

$$
\begin{aligned}
H \;=\; & \sum_{m,n=0}^{N} \Big(\frac{(\pi^x_{m,n})^2}{2} + \frac{(\pi^y_{m,n})^2}{2} \Big) + \; \frac{\omega_0^2}{2} a^2 N^2 \\
+ \; & \frac{\omega_0^2}{4} \sum_{m,n=0}^{N} [(u^x_{m+1,n} - u^x_{m,n})^2 + (u^x_{m-1,n} - u^x_{m,n})^2 + (u^x_{m,n+1} - u^x_{m,n})^2 + (u^x_{m,n-1} - u^x_{m,n})^2 \\
+ \; & \frac{\omega_0^2}{4} \sum_{m,n=0}^{N} [(u^y_{m+1,n} - u^y_{m,n})^2 + (u^y_{m-1,n} - u^y_{m,n})^2 + (u^y_{m,n+1} - u^y_{m,n})^2 + (u^y_{m,n-1} - u^y_{m,n})^2]
\end{aligned}
$$

so the Hamiltonian is a sum of two independent Hamiltonians for propagation in x and y directions. Using

$$
\begin{aligned}
& \frac{\partial}{\partial u^x_{k,l}} \sum_{m,n=0}^{N} [(u^x_{m+1,n} - u^x_{m,n})^2 + (u^x_{m-1,n} - u^x_{m,n})^2 + (u^x_{m,n+1} - u^x_{m,n})^2 + (u^x_{m,n-1} - u^x_{m,n})^2] \\
= \; & 4u^x_{k,l} - u^x_{k+1,l} - u^x_{k-1,l} - u^x_{k,l+1} - u^x_{k,l-1}
\end{aligned}
$$

we get equations of motion in the form

$$
\begin{aligned}
\ddot{u}^x_{m,n} \;&=\; -4\omega_0^2 \Big[u^x_{m,n} - \frac{1}{4}(u^x_{m+1,n} + u^x_{m-1,n} + u^x_{m,n+1} + u^x_{m,n-1}) \Big] \\
\ddot{u}^y_{m,n} \;&=\; -4\omega_0^2 \Big[u^y_{m,n} - \frac{1}{4}(u^y_{m+1,n} + u^y_{m-1,n} + u^y_{m,n+1} + u^y_{m,n-1}) \Big] \qquad (1)
\end{aligned}
$$

Periodic ansatz

$$
\begin{aligned}
\chi^x_{m,n} \;&=\; e^{-i\omega t} a_{\vec{k}} e^{ik_x m + ik_y n} \;=\; e^{-i\omega t} a_{rs} e^{ia\frac{2\pi}{L}(mr+ns)} \\
\chi^y_{m,n} \;&=\; e^{-i\omega t} b_{\vec{l}} e^{il_x m + il_y n} \;=\; e^{-i\omega t} b_{rs} e^{ia\frac{2\pi}{L}(mr+ns)}
\end{aligned}
$$

where $\vec{k} = (k_x, k_y) = (\frac{2\pi}{L} r, \frac{2\pi}{L} s), \quad r, s \;=\; 0, 1, 2..., N.$

We get

$$
\begin{aligned}
-\ddot{\chi}^x_{m,n} \;&=\; \omega^2 \chi^x_{m,n} \;=\; 4\omega_0^2 e^{-i\omega t} e^{i\omega_0 a\frac{2\pi}{L}(mr+ns)} \Big[1 - \frac{1}{2}\big(\cos\frac{2\pi}{L} ar + \cos\frac{2\pi}{L} as \big) \Big] \\
\Rightarrow \; \omega^2 e^{-i\omega t} e^{ia\frac{2\pi}{L}(mr+ns)} \;&=\; 4\omega_0^2 e^{-i\omega t} e^{ia\frac{2\pi}{L}(mr+ns)} \Big[1 - \frac{1}{2}\big(\cos\frac{2\pi}{L} ar + \cos\omega_0 \frac{2\pi}{L} as \big) \Big] \\
\Rightarrow \; \omega_{\vec{k}} \;\equiv\; \omega_{r,s} \;&=\; 2\omega_0 \sqrt{\sin^2\frac{\pi}{L} ar + \sin^2\frac{\pi}{L} as} \;=\; 2\omega_0 \sqrt{\sin^2\frac{k_x a}{2} + \sin^2\frac{k_y a}{2}}
\end{aligned}
$$

and similarly

$$
\begin{aligned}
-\ddot{\chi}^y_{m,n} &= \omega^2\chi^y_{m,n} = 4\omega_0^2 e^{-i\omega t}e^{ia\frac{2\pi}{L}(mr+ns)}\Big[1-\frac{1}{2}\big(\cos\frac{2\pi}{L}ar+\cos\frac{2\pi}{L}as\big)\Big] \\
\Rightarrow\ \omega^2 e^{-i\omega t}e^{ia\frac{2\pi}{L}(mr+ns)} &= 4\omega_0^2 e^{-i\omega t}e^{ia\frac{2\pi}{L}(mr+ns)}\Big[1-\frac{1}{2}\big(\cos\frac{2\pi}{L}ar+\cos\omega_0\frac{2\pi}{L}as\big)\Big] \\
\Rightarrow\ \omega_{\vec{k}} \equiv \omega_{r,s} &= 2\omega_0\sqrt{\sin^2\frac{\pi}{L}ar+\sin^2\frac{\pi}{L}as} = 2\sqrt{\sin^2\frac{l_x a}{2}+\sin^2\frac{l_y a}{2}}
\end{aligned}
$$

and the general solution of Eq. (2) has the form

$$
\begin{aligned}
u^x_{m,n} &= \frac{1}{N}\sum_{r,s=0}^{N} A_{r,s}e^{-i\omega_{r,s}t}e^{ia\frac{2\pi}{L}(mr+ns)}, \qquad u^y_{m,n} = \frac{1}{N}\sum_{r,s=0}^{N} B_{r,s}e^{-i\omega_{r,s}t}e^{ia\frac{2\pi}{L}(mr+ns)} \\
\vec{u}_{m,n} &= \frac{1}{N}\sum_{r,s=0}^{N} \vec{a}_{r,s}e^{-i\omega_{r,s}t}e^{ia\frac{2\pi}{L}(mr+ns)} \quad \stackrel{a\to 0}{\to} \quad \frac{V}{(2\pi)^2 N}\int d^2k\ \vec{a}_{\vec{k}}\ e^{-i\omega_{\vec{k}}t+i\vec{k}\vec{\aleph}}
\end{aligned}
$$

(here $\vec{\aleph}\equiv(ma,na)$ and $\vec{a}_{r,s}=(A_{r,s},B_{r,s})$).

Normal modes are defined according to Eq. (8.53)

$$
Q^x_{r,s} \equiv A_{r,s}e^{-i\omega_{r,s}t}, \qquad Q^y_{r,s} \equiv B_{r,s}e^{-i\omega_{r,s}t}
$$

so that

$$
u^x_{m,n} = \frac{1}{N}\sum_{r,s=0}^{N} Q^x_{r,s}e^{ia\frac{2\pi}{L}(mr+ns)} \quad\Leftrightarrow\quad Q^x_{r,s} = \frac{1}{N}\sum_{m,n=0}^{N} u^x_{m,n}e^{-ia\frac{2\pi}{L}(mr+ns)},
$$

and

$$
\pi^x_{m,n} = \frac{1}{N}\sum_{r,s=0}^{N} P^x_{r,s}e^{-ia\frac{2\pi}{L}(mr+ns)} \quad\Leftrightarrow\quad P^x_{r,s} = \frac{1}{N}\sum_{m,n=0}^{N} \pi^x_{m,n}e^{ia\frac{2\pi}{L}(mr+ns)},
$$

(see Eqs. (8.58)-(8.61)) and similarly for y components.

At small ω's

$$
\omega_{\vec{k}} \simeq 2\omega_0\sqrt{\big(\frac{\pi}{L}ar\big)^2+\big(\frac{\pi}{L}as\big)^2} = \omega_0 ak \equiv \omega_0 a|\vec{k}|
$$

so the sound wave speed is $\omega_0 a$ (in the units after rescaling).

Similarly to Eq. (8.93) from the lecture notes we get:

$$
\begin{aligned}
E &\simeq \underbrace{\text{const}} + \sum_{\vec{k}} \frac{\hbar\frac{\omega_0 a}{2}|\vec{k}|}{e^{\beta\hbar\frac{\omega_0 a}{2}|\vec{k}|}-1} \\
&\quad \uparrow \text{independent of } T \\
&\simeq \text{const} + 2\frac{V}{(2\pi)^2}\int d\vec{k}\,\frac{\hbar\omega_0 a|\vec{k}|}{e^{\beta\hbar\omega_0 a|\vec{k}|}-1} \;=\; \text{const} + 2\frac{L^2}{2\pi}\int_0^{k_M} dk\;\frac{\hbar\omega_0 a k^2}{e^{\beta\hbar\omega_0 a|\vec{k}|}-1},
\end{aligned}
$$

where the factor 2 comes from two polarizations of the acoustical wave: longitudinal and transverse.

The maximal momentum k_M is obtained from 2-dim version of Eq. (8.95) from the lecture notes

$$
2\frac{\int_{|\vec{k}|\leq k_M} d^2\vec{k}}{\left(\frac{2\pi}{L}\right)^2} \;=\; \frac{V}{(2\pi)^2}\int_{|\vec{k}|\leq k_M} d\vec{k} \;=2N^2 \;,
$$

with N^2 being the total number of cells. In other words, we have

$$
\frac{L^2}{(2\pi)^2}\cdot\int_0^{k_M} 2\pi\, kdk = N^2 \quad\Rightarrow\quad \frac{V}{2\pi}\,\frac{k_M^2}{2} = N^2\,, \quad\Leftrightarrow\quad k_M = \left(4\pi\frac{N^2}{L^2}\right)^{1/2} = 2\sqrt{\pi n}\,,
$$

where $n \equiv \frac{N^2}{L^2}$ - area per particle.

The rest of the derivation of Debye formula repeats Eqs (8.99)-(8.102) from the lecture notes. Defining Debye temperature $\Theta_D \equiv \frac{\hbar k_M}{k_B}$ we get

$$
E \;=\; \text{const} + 4N^2 k_B\,\Theta_D\left(\frac{T}{\Theta_D}\right)^3\int_0^{\Theta_D/T} dx\,\frac{x^2}{e^x-1}
$$

and

$$
C_V \;=\; 4N^2 k_B\Big[3\Big(\frac{T}{\Theta_D}\Big)^2\int_0^{\Theta_D/T} dx\frac{x^2}{e^x-1} - \frac{\Theta_D/T}{e^{\Theta_D/T}-1}\Big]
$$

It is easy to see that as $T\to\infty$ the heat capacity coincides with the classical result $C_V = 2N^2k_B$ whereas as $T\to 0$ $C_V \sim T^2$.