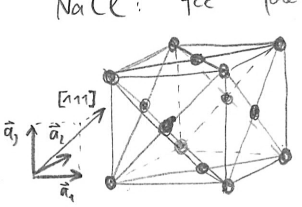
Modern Physics WS 21/22 Sören Brebaum

Problem Sheet 13

Ex. 13.1: Phonons in a linear diatomic chain and the NaCl lattice

NaCl: fcc face-centered cubic

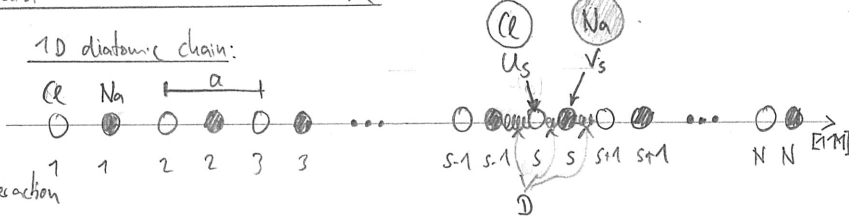


$\Rightarrow$ in [111] direction:

$\Rightarrow$ only nearest-neighbor-interaction

$\Rightarrow$ coupling constants D identical.

1D diatomic chain:



[111] = ↗

Cl: $M_1 = 35{,}5\,u$

Na: $M_2 = 23{,}0\,u$

a) eqs. of motion: $\sum_i \vec{F} = m\vec{a}$ $\quad F_D = -D\,\Delta x$

for Na: $M_1 \frac{d^2}{dt^2} u_s = -D(u_s - v_{s-1}) + D(v_s - u_s) = D(v_s + v_{s-1} - 2u_s)$ (I)

for Cl: $M_2 \frac{d^2}{dt^2} v_s = -D(v_s - u_s) + D(u_{s+1} - v_s) = D(u_{s+1} + u_s - 2v_s)$ (II)

b) Ansatz eqs. (harmonic waves)

$$\boxed{\begin{aligned} u_s &= u\, e^{i(ksa - \omega t)} \\ v_s &= v\, e^{i(ksa-\omega t)} \end{aligned}}$$

into (I) $\rightarrow$ $M_1 u \cancel{e^{i(ksa-\omega t)}}(-i\omega)^2 = D\left(v\cancel{e^{i(ksa-\omega t)}} + v e^{i(k(s-1)a - \omega t)} - 2u\cancel{e^{i(ksa-\omega t)}}\right)$

$$-\omega^2 M_1 u = D\left(v + v e^{-ika} - 2u\right) \quad \text{(III)}$$

into (II) $\rightarrow$ $M_2 v \cancel{e^{i(ksa-\omega t)}}(-i\omega)^2 = D\left(u e^{i(k(s+1)a-\omega t)} + u\cancel{e^{i(ksa-\omega t)}} - 2v\cancel{e^{i(ksa-\omega t)}}\right)$

$$-\omega^2 M_2 v = D\left(u e^{ika} + u - 2v\right) \quad \text{(IV)}$$

$\Downarrow$

$\left|\begin{matrix}\text{(III)} \\ \text{(IV)}\end{matrix}\right|$ system of coupled linear equations

$\Downarrow$ separate into u, v

$$\left|\begin{aligned} 0 &= (\omega^2 M_1 - 2D)\,u + D(1+e^{-ika})\,v \\ 0 &= D(1+e^{ika})\,u + (\omega^2 M_2 - 2D)\,v \end{aligned}\right| \;\hat{=}\; 0 = \underbrace{\begin{pmatrix} \omega^2 M_1 - 2D & D(1+e^{-ika}) \\ D(1+e^{ika}) & \omega^2 M_2 - 2D \end{pmatrix}}_{A} \cdot \underbrace{\begin{pmatrix} u \\ v \end{pmatrix}}_{\vec{x}} = 0$$

c) solutions to $A\cdot\vec{x} = 0$ only non-zero if $\det(A) = 0$

$*^1$ $\cos(x) = \frac{1}{2}\left(e^{ix} + e^{-ix}\right)$

$*^2$ $1 + \cos(x) = 2\cos^2\left(\frac{x}{2}\right)$

$$0 \overset{!}{=} \det(A) = (\omega^2 M_1 - 2D)(\omega^2 M_2 - 2D) - D^2(1+e^{-ika})(1+e^{ika})$$

$$= \omega^4 M_1 M_2 - 2\omega^2 D(M_1 + M_2) + 4D^2 - D^2\Big(1 + \underbrace{e^{-ika} + e^{ika}}_{*^1\ 2\cos(ka)} + \underbrace{\cancel{e^0}}_{+\,2}\Big) \quad = 2(1+\cos(ka)) = 4\cos^2\left(\tfrac{ka}{2}\right)$$

$*^3$ $1 - \cos^2(x) = \sin^2(x)$

$$+ 4D^2\Big(\underbrace{1 - \cos^2\left(\tfrac{ka}{2}\right)}_{*^3\ \sin^2\left(\frac{ka}{2}\right)}\Big) \quad \Big|\cdot \frac{1}{M_1 M_2}$$

$$\boxed{0 = \omega^4 - 2\omega^2 D\left(\frac{M_1 + M_2}{M_1 \cdot M_2}\right) + 4\frac{D^2}{M_1 M_2}\sin^2\left(\frac{ka}{2}\right)}$$

quadratic eq in ω^2: $\quad x^2 + px + q = 0$

$\hookrightarrow x_{1/2} = -\frac{p}{2} \pm \sqrt{\left(\frac{p}{2}\right)^2 - q}$

$p = -2D\left(\frac{1}{M_1} + \frac{1}{M_2}\right)$

$q = 4\frac{D^2}{M_1 M_2}\sin^2\left(\frac{ka}{2}\right)$

$$\omega_{1,2}^2 = D\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm \sqrt{D^2\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - 4\frac{D^2}{M_1 M_2}\sin^2\left(\frac{ka}{2}\right)}$$

$$\boxed{\omega_{1,2}^2 = D\left[\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm \sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4}{M_1 M_2}\sin^2\left(\frac{ka}{2}\right)}\right]}$$

+ optical phonon branch

− acoustical phonon branch

d) @ edge of Brillouin zone $k = \frac{\pi}{a}$: $\quad \sin\left(\frac{\pi}{2}\right) = 1$

$$\omega_{1,2}^2 \rightarrow D\left[\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm \sqrt{\left(\frac{M_1 + M_2}{M_1 M_2}\right)^2 - \frac{4}{M_1 M_2}}\right] = D\left[\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm \sqrt{\left(\frac{1}{M_2} - \frac{1}{M_1}\right)^2}\right] = D\left[\frac{1}{M_1} + \frac{1}{M_2} \pm \left(\frac{1}{M_2} - \frac{1}{M_1}\right)\right]$$

$M_2 < M_1$

$$\pm\sqrt{\frac{M_1^2 + 2M_1M_2 + M_2^2 - 4M_1M_2}{(M_1M_2)^2}} = \sqrt{\left(\frac{M_1 - M_2}{M_1 M_2}\right)^2}$$

$\omega_+ = \omega_1 = \sqrt{\frac{2D}{M_1}}$ (ac. branch)

$\omega_- = \omega_2 = \sqrt{\frac{2D}{M_2}}$ (opt. branch)

d) cont'd: ratio $\frac{\omega_1}{\omega_2} = \frac{\sqrt{\frac{2D}{M_1}}}{\sqrt{\frac{2D}{M_2}}} = \sqrt{\frac{M_2}{M_1}} \approx 80{,}5\,\% = \frac{\text{Ac.}}{\text{Opt.}}$

Cl: $M_1 = 35{,}5\,u$
Na: $M_2 = 23{,}0\,u$

$$\left.\frac{LA}{LO}\right|_{L \hat{=} k=\frac{\pi}{a}} = \frac{5{,}35\text{ THz}}{6{,}99\text{ THz}} \approx 76{,}5\,\% \qquad \left.\frac{TA}{TO}\right|_L = \frac{3{,}61\text{ THz}}{4{,}27\text{ THz}} \approx 84{,}5\,\%$$

e) ~~Longitudinal phonon branch:~~

$1u = 1{,}66 \cdot 10^{-27}\,kg$
$\omega_{LA} = 5{,}35\text{ THz}$
$\omega_{LO} = 6{,}99\text{ THz}$

$$\left.\begin{array}{ll} LA: & D = \frac{1}{2} M_1 \omega_{LA}^2 = 0{,}843\,\frac{N}{m} \\ LO: & D = \frac{1}{2} M_2 \omega_{LO}^2 = 0{,}933\,\frac{N}{m} \end{array}\right\} \langle\,\rangle = 0{,}888\,\frac{N}{m}$$

Transversal phonon branches:

$\omega_{TA} = 3{,}61\text{ THz}$
$\omega_{TO} = 4{,}27\text{ THz}$

$$\left.\begin{array}{ll} TA: & D = \frac{1}{2} M_1 \omega_{TA}^2 = 0{,}384\,\frac{N}{m} \\ TO: & D = \frac{1}{2} M_2 \omega_{TO}^2 = 0{,}348\,\frac{N}{m} \end{array}\right\} \langle\,\rangle = 0{,}366\,\frac{N}{m}$$

f) Kinetic energy of neutron has to be higher than $E_n > h \cdot \nu = 33\text{ meV}$ in order to excite an $\nu = 8\text{ THz}$ phonon.

Ex. 13.2: Phonon heat capacity – Debye model

$$(4) \quad \boxed{U = \int_0^\infty \underbrace{\frac{\hbar\omega_b(\vec{q})}{e^{\hbar\omega/k_BT}-1}}_{E_b(\vec{q})\text{ thermal energy of a phonon mode}} \underbrace{D(\omega)}_{\text{D.o.S density of phonon modes}}\,d\omega}$$

sum over all b
all $\omega_b(\vec{q})$

a)

① instead of $\int_0^\infty \ldots d\omega \rightarrow$ sum over 1st BZ, which can be approximated by integral over a sphere:

$$\hookrightarrow \sum_{\vec{q}\in 1^{st}BZ} \approx \longrightarrow \frac{1}{\frac{(2\pi)^3}{V}} \int_{q=0}^{q_{max}} 4\pi q^2\,dq$$

$\omega_D = c \cdot q_{max}$

② at low Temp. only 3 acoustic phonon modes contribute with dispersion $\omega = cq$; $dq = \frac{1}{c}d\omega$ and Deby frequency:

$$\Rightarrow \quad U = 3 \cdot \frac{V}{(2\pi)^3} \int_{q=0}^{q_{max}} 4\pi q^2\,dq \frac{\hbar\omega(q)}{e^{\hbar\omega/k_BT}-1} = 3\frac{V}{(2\pi c)^3} \int_0^{\omega_D} 4\pi\omega^2\,d\omega \frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1} = \int_0^{\omega_D} D(\omega) \frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1}\,d\omega$$

compare with (4)

③ comparing with (4):

$$\Rightarrow \boxed{D(\omega) = \frac{3}{2}\frac{V}{\pi^2 c^3}\omega^2}$$

From (5): $\int_0^{\omega_D} D(\omega)\,d\omega = 3N = \int_0^{\omega_D} \frac{3}{2}\frac{V}{\pi^2 c^3}\omega^2\,d\omega = \frac{1}{2}\frac{V}{\pi^2 c^3}\omega_D^3 = 3N$

$$\hookrightarrow \omega_D = c\sqrt[3]{6\pi^2\frac{N}{V}}$$

b)

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = \frac{\partial}{\partial T}\left(\int_0^{\omega_D} D(\omega)\frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1}\,d\omega\right) = \int_0^{\omega_D} D(\omega) \frac{\hbar\omega}{(e^{\hbar\omega/k_BT}-1)^2} \cdot e^{\hbar\omega/k_BT} \cdot \frac{\hbar\omega}{k_BT^2}\,d\omega$$

$$= \boxed{\frac{3}{2}\frac{V\hbar^2}{\pi^2 c^3 k_B T^2} \int_0^{\omega_D} \frac{\omega^4 e^{\hbar\omega/k_BT}}{(e^{\hbar\omega/k_BT}-1)^2}\,d\omega}$$

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Ex. 13.2: c) show $C_V \propto T^3$ @ low T

Hint: $\int_0^\infty \frac{x^4 e^x}{(e^x-1)^2}\,dx = \frac{4\pi^4}{15}$

substitute in (7): $x = \frac{\hbar\omega}{k_B T} \Leftrightarrow \omega = \frac{k_B T x}{\hbar}$

$d\omega = \frac{k_B T}{\hbar}\,dx$

from a) $\frac{1}{2}\frac{V}{\pi^2 c^3}\omega_D^3 = 3N$

from b) or (7): $C_V = \frac{3}{2}\frac{V\cancel{\hbar^2}}{\pi^2 c^3 \cancel{k_B}\cancel{T^2}}\left(\frac{\cancel{k_B^4 T^4}}{\cancel{\hbar^4}}\right)^{5} \int_0^{\hbar\omega_D/k_B T \to \infty} \frac{x^4 e^x}{(e^x-1)^2}\,dx$

$= 9N k_B \left(\frac{k_B T}{\hbar\omega_D}\right)^3 \cdot \frac{4\pi^4}{15} = \frac{12}{5}\pi^4 N k_B \left(\frac{k_B T}{\hbar\omega_D}\right)^3$

d) partly already done in a): From (5): $\int_0^{\omega_D} D(\omega)\,d\omega = 3N = \int_0^{\omega_D} \frac{3}{2}\frac{V}{\pi^2 c^3}\omega^2 d\omega = \frac{1}{2}\frac{V}{\pi^2 c^3}\omega_D^3$

cut-off Debye frequency: $\rightarrow \omega_D = c\sqrt[3]{6\pi^2 \frac{N}{V}} = c\sqrt[3]{6\pi^2 \frac{N_A}{V_{mol}}}$

Debye temperature $T_D = \frac{\hbar\omega_D}{k_B} = \frac{\hbar}{k_B} c\sqrt[3]{6\pi^2 \frac{N_A}{V_{mol}}}$

$$\boxed{C_V = \frac{12}{5}\pi^4 N k_B \left(\frac{T}{T_D}\right)^3} \quad \text{(I)}$$

phonon contribution to C_V for monocrystals at low T

e) $Ar_{(s)}$ @ low T

Ⓐ either plot data & fit (I) $\Rightarrow T_D = (91{,}1 \pm 0{,}1)\,K$

Ⓑ or make table

$C_V = \alpha T^3$ with $\alpha = \frac{12}{5}\pi^4 N k_B \frac{1}{T_D^3}$

$T^3\,[K^3]$					
C_V					
α					

average all five α's and calculate T_D

$\langle\alpha\rangle \approx 25\cdot 10^{-4}\,\frac{J}{K^4 mol} \Rightarrow T_D = 92\,K$

Ex 13.3: Problem Sheet 10 – "Mock Exam"

- Problem 10.3

+

- Problem 10.4