

Lattice Dynamics

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1. 1-D model of one-element crystal.

$$H = \sum_{j=1}^N \frac{m}{2} \dot{\xi}_j^2 + \sum_{j=2}^N \frac{f}{2} (\xi_j - \xi_{j-1})^2$$

equation of motion

$$m \ddot{\xi}_j = f (\xi_{j+1} + \xi_{j-1} - 2\xi_j) \quad (11-33)$$

Assume the solution is

$$\xi_j(t) = e^{i\omega t} \gamma_j \quad \gamma_j - \text{independent of } t$$

Solution is usually in the form

$$\gamma_j = A^j = (e^{i\phi})^j$$

then: $-m\omega^2 = f(e^{i\phi} + e^{-i\phi} - 2)$

$$\omega^2 = \frac{4f}{m} \sin^2\left(\frac{\phi}{2}\right)$$

$$\omega_m = \frac{4f}{m}$$

$$\omega = \omega_{\max} \left| \sin\left(\frac{\phi}{2}\right) \right|$$

$$\xi_j(t) = e^{i(\omega t + j\phi)}$$

because of lattice structure $\xi_j(t)$ repeats

for every $\Delta j = \frac{2\pi}{\phi}$

wavelength $\lambda = a \Delta j = 2\pi a / \phi$

$$\phi = \frac{2\pi a}{\lambda} = ka \quad a: \text{lattice spacing.} \quad (4)$$

$$\xi_j(t) = e^{-(jka + \omega t)}$$

$$\omega = \omega_{\max} \left| \sin\left(\frac{ka}{2}\right) \right|$$

for small ka $\lambda \gg a$

$$\omega = \omega_{\max} \frac{ka}{2} = \text{constant}$$

In general:

$$\lambda v = \frac{\omega}{k} = \frac{\omega_{\max}}{k} \left| \sin\left(\frac{ka}{2}\right) \right| = c(k)$$

$\omega(k)$: dispersion curve

$c(k)$ phase velocity

Let's try to express thermodynamic properties in terms of $[\omega(k)]$

We have periodic boundary condition

$$k = 2\pi j / Na \quad -\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$$

N : number of atoms

$$j = \pm 1, \pm 2, \dots, \pm \frac{N}{2}$$

$$E = \sum_j \frac{\hbar \omega_j}{e^{\beta \hbar \omega_j} - 1} = \frac{Na}{\pi} \int_0^{\frac{\pi}{a}} \frac{\hbar \omega(k) dk}{\exp(\beta \hbar \omega) - 1}$$

$$dk = \frac{dk}{d\omega} d\omega = \frac{2d\omega}{a(\omega_{\max} - \omega) \pm}$$

$$E = \frac{2N}{\pi} \int_0^{W_{\max}} \frac{\hbar \omega d\omega}{[\exp(\beta \hbar \omega) - 1] [W_{\max}^2 - \omega^2]^{\frac{1}{2}}} \quad (10)$$

compare to 11-9

$$g(\nu) = \frac{2N}{\pi} \frac{1}{(\nu_{\max}^2 - \nu^2)^{\frac{1}{2}}}$$

in general $g(\nu) = \frac{N\alpha}{\pi} \frac{1}{\frac{d\nu}{dk}}$

for a continuum ($\lambda \gg a$) $\frac{d\nu}{dk} = \text{const}$
 $= \text{group velocity}$

2. 1-D model of
 2-element crystal

$$H = \frac{N}{2} \left\{ \frac{m_1}{2} \dot{\rho}_{2j}^2 + \frac{m_2}{2} \dot{\rho}_{2j-1}^2 \right\} + \frac{f}{2}$$

$$\frac{N}{2} \left\{ (\rho_{2j} - \rho_{2j-1})^2 + (\rho_{2j+1} - \rho_{2j})^2 \right\}$$

$$\omega^2 = \omega_0^2 \left\{ 1 \pm \left(1 - \frac{4m_1 m_2 \sin^2 \phi}{(m_1 + m_2)^2} \right)^{\frac{1}{2}} \right\}$$

$$\omega_0^2 = \frac{f}{\mu}$$

$$\phi = m \cdot \frac{\pi}{N_1} \quad \mu \text{ is reduced mass of } (m_1, m_2)$$

see fig. 10-11

Two branches in dispersion function

high-frequency : optical branch
 low " : acoustic "

Two mass with opposite signs like NaCl ⁽¹¹⁾
vibration motion leads to an absorption
of infrared radiation.

3-D Lattice structure is much harder to
model, but the principle remains the same

Phonons

We can treat vibrating particles as
independent particles. If a crystal has
 N atoms, $3N$ normal coordinates

$$E(\{n_j\}) = \sum_{j=1}^{3N} h \nu_j (n_j + \frac{1}{2})$$

$= \sum_{j=1}^{3N} h \nu_j n_j + E_0 \rightarrow$ 0 point vibration energy
we call them "phonons"

phonons are bosons - no exclusion

From the results of ch. 4. $\lambda = e^{\frac{h\nu}{kT}}$

$$\bar{n}_j = \frac{\lambda e^{-\beta \epsilon_j}}{1 - \lambda e^{-\beta \epsilon_j}} = \frac{1}{\lambda e^{\beta \epsilon_j} - 1}$$

Further we make argument that
phonons are like photons

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$$\mu=0, \lambda=1$$

$$\bar{n}_j = \frac{1}{e^{\beta \epsilon_j} - 1}$$

$$\bar{E} = \sum_{j=1}^{3N} \bar{n}_j h\nu_j + E_0 = \sum_{j=1}^{3N} \frac{h\nu_j}{e^{\beta h\nu_j} - 1} + E_0$$

$$= E_0 + \int_0^{\infty} \frac{g(\nu) h\nu d\nu}{e^{\beta h\nu} - 1}$$

Same as equation 11-9.

So we can treat lattice vibration of
crystal as a gas of non interacting phonons

Defects in Crystals

point defect } Vacant lattice site
(Schottky defect)
Extra atom not at lattice site
(Interstitial atom)

Schottky defect: atoms are brought to
surface from the body of a crystal.

If there are n vacancies, and each take ⁽¹³⁾ an energy E_v to get to the surface, then

$$A = E - TS = nE_v - kT \ln \frac{N!}{n!(N-n)!}$$

minimize A , $\frac{\partial A}{\partial n} = 0$, $n = N e^{-E_v/kT}$

if $E_v = 1 \text{ eV}$ $T = 300 \text{ K}$ $\frac{n}{N} = 10^{-17}$
 1000 K 10^{-5}

Frenkel Defect

atoms are displaced from lattice to interstitial positions, then

$$A = nE_I - kT \ln \left\{ \frac{N!}{n!(N-n)!} \cdot \frac{N'}{n!(N'-n)!} \right\}$$

N' : available interstitial sites

minimize A : $n = (NN') e^{-E_I/2kT}$

consequences of impurity:

(1). Diffusion. flux $J = -D \frac{\partial n}{\partial x}$

diffusion constant $D = \nu a^2 e^{-E/kT}$

ν vibration frequency a : lattice spacing

(2). color in the crystal.