Solid State Physics Homework 4

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Problem 1

Solution From [1], it can be seen the frequencies of optical phonons in NaCl are around $\sim 6\,\text{THz} \sim 0.06\,\text{eV}$. The lattice constant is $0.563\,\text{nm}$, which is also the magnitude of the "wave length" of phonons. The magnitude of wave lengths in the visible light spectrum is $\sim 500\,\text{nm}$, which is much longer than the wave length of phonons, so its momentum is much smaller than the momentum of phonons.

TODO

Problem 2

Solution

(a) The EOM is

$$M\ddot{x}_n = C(x_{n-1} + x_{n+1} - 2x_n). \tag{1}$$

At the edge of the Brillouin zone, we have

$$x_n = A\mathrm{e}^{\mathrm{i}kan - \mathrm{i}\omega t}, \quad k = \frac{\pi}{a}. \tag{2}$$

The wave vector $k = -\pi/a$ is also possible, but the difference between it and π/a is a reciprocal lattice vector, so we can just work with $k = \pi/a$. Thus at the edge of the Brillouin zone, we have

$$\begin{gathered} -M\omega^2 A = C(\mathrm{e}^{-\mathrm{i}ka} + \mathrm{e}^{\mathrm{i}ka} - 2)A = -4CA, \\ \omega = \sqrt{\frac{4C}{M}}. \end{gathered} \tag{3}$$

(b) Again we take the ansatz (2), and we have

$$-M\omega^2 A = C(\mathrm{e}^{-\mathrm{i}ka} + \mathrm{e}^{\mathrm{i}ka} - 2)A = CA(2\cos ka - 2) \approx -CA(ka)^2,$$

so

$$\omega = \sqrt{\frac{C}{M}} ka, \tag{4}$$

and

$$v_{\text{sound}} = \frac{\omega}{k} = \sqrt{\frac{C}{M}} a. \tag{5}$$

(c) In Case B, the EOMs are

$$\begin{aligned} M_1 \ddot{x}_{2n} &= C(x_{2n-1} + x_{2n+1} - 2x_{2n}), \\ M_2 \ddot{x}_{2n+1} &= C(x_{2n+2} + x_{2n} - 2x_{2n+1}). \end{aligned} \tag{6}$$

The ansatz is

$$\begin{aligned} x_{2n} &= A_1 \mathrm{e}^{2\mathrm{i}kan - \mathrm{i}\omega t}, \\ x_{2n+1} &= A_2 \mathrm{e}^{\mathrm{i}ka(2n+1) - \mathrm{i}\omega t}, \end{aligned} \tag{7}$$

and (6) becomes

$$\begin{aligned} -M_1\omega^2 A_1 \mathrm{e}^{2\mathrm{i}kan} &= C(A_2\mathrm{e}^{\mathrm{i}ka(2n-1)} + A_2\mathrm{e}^{\mathrm{i}ka(2n+1)} - 2A_1\mathrm{e}^{2\mathrm{i}kan}), \\ -M_2\omega^2 A_2 \mathrm{e}^{\mathrm{i}ka(2n+1)} &= C(A_1\mathrm{e}^{\mathrm{i}ka(2n+2)} + A_1\mathrm{e}^{2\mathrm{i}kan} - 2A_2\mathrm{e}^{\mathrm{i}ka(2n+1)}), \end{aligned}$$

$$\begin{pmatrix} 2C - M_1\omega^2 & C(\mathrm{e}^{-\mathrm{i}ka} + \mathrm{e}^{\mathrm{i}ka}) \\ C(\mathrm{e}^{\mathrm{i}ka} + \mathrm{e}^{-\mathrm{i}ka}) & 2C - M_2\omega^2 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = 0. \tag{8}$$

So we have

$$(2C - M_1\omega^2)(2C - M_2\omega^2) - 4C^2\cos^2 ka = 0, \tag{9}$$

and therefore

$$\omega^2 = \frac{M_1 + M_2 \pm \sqrt{(M_1+M_2)^2 - 4M_1M_2(1-\cos^2 ka)}}{M_1M_2}C. \tag{10}$$

The positive and negative branches correspond to the acoustic and optical phonons, respectively.

When $M_1 = M_2$, we get

$$\omega^2 = \frac{2M \pm 2M\cos ka}{M^2}C = \frac{2C}{M}(1 \pm \cos ka). \tag{11}$$

In the $k \to 0$ limit, we have

$$\frac{2C}{M}(1+\cos ka) \approx \frac{4C}{M}, \quad \frac{2C}{M}(1-\cos ka) \approx \frac{C}{M}(ka)^2,$$

so

$$\omega_{\text{acoustic}} \approx \sqrt{\frac{C}{M}}ka, \quad \omega_{\text{optical}} \approx \sqrt{\frac{4C}{M}}. \tag{12}$$

So the sound speed is also (5).

(d) The frequency of the optical phonon near $k = 0$ is the same as (3). We notice that the first equation is the same as (4), and the second equation is the same as (3). That's to say, when Δ is small enough, the acoustic phonon spectrum of case B near the Γ point is the same as the phonon spectrum of case A near the Γ point, while the optical phonon spectrum of case B near the Γ point is the same as the phonon spectrum of case A near the boundary of the Brillouin zone.

Problem 3
Solution

(a) We can wait until one wave crest of the black wave is at one of the atoms, and then it's clear that half of the wave length of the black wave is a, so the total wavelength is $2a$ and thus $k = 2\pi/(2a) = \pi/a$; it's positive because the black wave is heading right. Similarly, for the red wave, 2.5 times of the total wavelength is a, so the wavelength is $a/2.5$, and $k = -2\pi/(a/2.5) = -5\pi/a$.

Since the two waves are describing the same lattice motion, ω's are the same.

(b) In the animation, each atom is moving as if it's a harmonic oscillator away from anything else, so there is no transmission of energy here: the speed of energy transmission is zero.

Problem 4
Solution There are 12 curves in the first figure, so there are $12/3 = 4$ atoms in each primitive unit cell. The only crystal that may satisfy this requirement is Ni_3Ti.

There are 30 curves in the left part of the second figure, and 20 curves in the right part. This difference is likely to be a result of degeneracy, so we pick up $30/3 = 10$ as the expected number of atoms per primitive unit cell. Among the possible crystals, only $LiNbO_3$ has a total atom number that divides 10, so we can expect the second figure gives the phonon spectrum of $LiNbO_3$, and just like the case of graphene, there are two Li atoms, two Nb atoms, and six O atoms in one primitive unit cell; the two Li atoms have different surroundings.

References

[1] IS Messaoudi, A Zaoui, and M Ferhat. Band-gap and phonon distribution in alkali halides. *physica status solidi (b)*, 252(3):490–495, 2015.