

PHYS 353 SOLID STATE PHYSICS STUDY GUIDE FOR PART 2

Lattice Vibrations and Phonons

OUTLINE:

- A. Vibrations of crystals
 - 1. monatomic basis
 - 2. two atoms per primitive basis
 - 3. phonons
 - a) energy
 - b) momentum
 - c) scattering
- B. Heat Capacity
 - 1. 1-dimensional
 - 2. 3-dimensional
 - 3. Einstein model
 - 4. Debye model
- C. Thermal expansion
- D. Thermal conductivity

STUDY QUESTIONS: (for 2nd test - **not** for collected homework assignment)

1. Starting with $\Sigma \mathbf{F} = m \mathbf{a}$, get the dispersion relation for a monatomic 1-D and 2-D square lattice.
2. Explain why $K_x > G_x$ is not physically or mathematically different than $(K_x - 2G_x)$.
3. Starting from $\Sigma \mathbf{F} = m \mathbf{a}$, get the dispersion relation for a diatomic lattice assuming each plane interacts only with its nearest-neighbor planes and that the force constants are identical between all pairs of nearest-neighbor planes
4. From the dispersion relation from #3 above, show the existence of 2 modes (acoustical and optical) and by looking at the limiting cases distinguish the acoustical from the optical.
5. Describe C_V with an equation and with words.

6. Show the derivation of the Planck Distribution: $\langle n \rangle = 1/[e^{\hbar\omega/kT} - 1]$

To do this, consider the following:

- State the Boltzmann probability distribution:
- Explain where the Boltzmann distribution came from (what is the basis for this distribution).
- Show the steps in the derivation of the Planck distribution, starting with the Boltzmann distribution.
- State the expression for the Planck distribution.
- Tell in words what it says.
- What does this distribution reduce to for high temperature ($k_B T \gg \hbar\omega$) ?
- What does this distribution reduce to for low temperature ($k_B T \ll \hbar\omega$) ?

7. List the assumptions in the Einstein model of C_V , show the derivation, and look at the low T and high T limits.

8. Discuss a better derivation of C_V including enumeration of modes and derive $D(\Omega)$ in 1-D.

9. Starting from the results of #8 above, derive U and C_V for the Debye model and list the assumptions.

10. Starting from the results of #9 above, consider high T and low T limits.

11. Show that $\langle x \rangle \propto T$, relate this to thermal expansion, and discuss the assumptions involved. Be able to explain this graphically.

12. Define thermal conductivity (K_{th}) and relate to thermal resistivity. Show that $K_{th} = \frac{1}{3}CvL$, and define C, v, and L.

COLLECTED HOMEWORK ASSIGNMENTS:

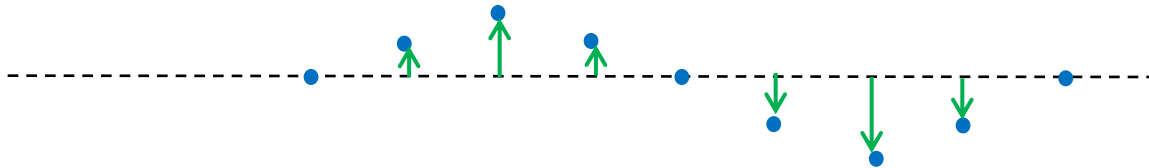
9. Demonstrate that $(-\pi \leq K_x a \leq \pi)$ covers all possible values of oscillations of atoms separated by "a" by showing one case where

$$K'_x = K_x + b_x \text{ [where } b_x = 2\pi/a_x, \text{ i.e., } b_x \text{ is the reciprocal lattice vector]}$$

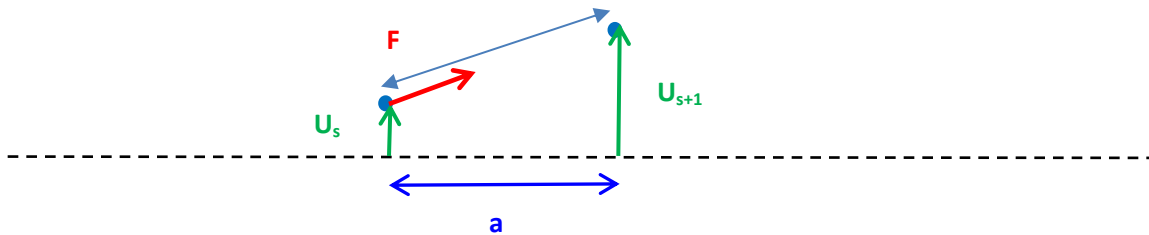
and both K'_x and K_x give the same oscillation pattern for the atoms. Do this by drawing the positions of several atoms, and drawing the wave pattern for both K_x and K'_x and showing that the atom's positions fall on both wave patterns. Indicate also the wavelength for each of the unprimed and primed waves. [Hint: recall $K = 2\pi/\lambda$, so draw two waves, one of $\lambda > a$, and one of λ' where you can solve for λ' from $K' = K + 2\pi/a$. See the excel spreadsheet on B-zone oscillations.]

For problems 10 and 11: Vibrations of a square lattice: Consider transverse vibrations of a planar square lattice of rows and columns of identical atoms, and let $u_{L,N}$ denote the displacement normal to the plane of the lattice of the atom in the L th column and N th row. The mass of each atom is M , and C is the force constant for nearest neighbor atoms.

First consider a 1-D line of atoms, the blue dots, in the x direction that undergo displacements in the y direction (perpendicular to the line of atoms), the green arrows. We'll assume that the atoms are connected by "springs", and we'll use u_s to indicate the amount of displacement up or down from the equilibrium position of atom s ; u_{s-1} , the displacement of the atom to the immediate left of atom s ; and u_{s+1} , the displacement of the atom to the immediate right of atom s .



If atom $s+1$ is above atom s , then $(u_{s+1} - u_s)$ is positive and assuming the atoms are not significantly displaced in the x direction, then there will be a y component of the spring force pulling atom s up and pulling atom $s+1$ down. The direction of that push will be along the line connecting the two atoms. Below is a magnified view of the situation:



If we assume that the u 's are small compared to the lattice spacing, a , then L doesn't change much as the u 's change and so the magnitude of the spring force doesn't change much. However, the direction of the spring force will change. The y component of the spring force will be $F_{sy} = CL\sin(\theta)$ where $\sin(\theta) = \{u_{s+1} - u_s\}/L$. Thus the y component of the spring force will be $F_{sy} = C \{u_{s+1} - u_s\}$. There will be a similar force on atom s due to atom $s-1$.

Now we consider having a 2-D plane of atoms with a row in the x direction as above and a column of atoms in the z direction (in and out of the page). There will be similar forces due to the atoms in the z direction due to displacements, u_s , in the y direction also.

10. a) Show that the equation of motion ($\Sigma F=ma$) for the transverse direction is:

$$M(d^2u_{L,N}/dt^2) = C[(u_{L+1,N} + u_{L-1,N} - 2u_{L,N}) + (u_{L,N+1} + u_{L,N-1} - 2u_{L,N})].$$

(further parts of this problem are on the next page)

b) Then assume solutions of the form:

$$u_{L,N} = u_0 \exp[i(LK_x a + NK_y a - \Omega t)], \quad u_{L+1,N} = u_0 \exp[i\{(L+1)K_x a + NK_y a - \Omega t\}], \text{ ect.}$$

where a is the spacing between nearest-neighbor atoms, and show that the equation of motion is satisfied if:

$$\Omega^2 M = 2C[2 - \cos(K_x a) - \cos(K_y a)].$$

This is the **dispersion relation** for the problem. Compare this result to the dispersion relation for longitudinal waves in the notes.

11. a) Show that the region of \mathbf{K} space for which independent solutions exist for the dispersion relation in problem 10 above may be taken as a square of side $2\pi/a$.

[HINT: see problem #9 above.] This is the first Brillouin zone of the square lattice.

b) Graph Ω verses K for $K = K_x$ (with $K_y = 0$) from $K_x = -\pi/a$ to $K_x = +2\pi/a$.

Note how Ω at some wavevector $K > \pi/a$ gives the same value for Ω at the wavevector $(K - 2\pi/a)$.

In drawing the graph, you can either specify values for C , M , and a ; or label the axis in terms of the symbols C , M , and a .

c) Graph Ω verses K for $K_x = K_y$ [recall $K = \sqrt{K_x^2 + K_y^2}$, so that when $K_x = \pi/a$, $K = \sqrt{2} * \pi/a$] on the same graph as part b.

d) Expand $\cos(K_x a)$ in a Taylor series and show the first five terms.

e) Then for $K_x a \ll 1$ (and $K_y a \ll 1$), show that:

$$\Omega = \sqrt{[Ca^2/M]} * \sqrt{[K_x^2 + K_y^2]} = \sqrt{[Ca^2/M]} * K,$$

so that in this limit the phase velocity ($v_{\text{phase}} = \Omega/K$) is constant.

f) In part e above, which terms in the Taylor series were used and which were neglected since we assumed $Ka \ll 1$?

12. Given that the speed of sound (v_{phase}) in aluminum is 5,100 m/s and that the spacing of atoms, a , is 2.5×10^{-10} m (based on density of aluminum is 2.7 gm/cm^3 and atomic mass of aluminum is 27 gm/mole):

a) find Ω for $K = 0.1 * \pi/a$; HINT: remember how wavelength, frequency, and wave speed are related

b) since an aluminum atom has a mass of about 27 amu (27 grams per mole), where $1 \text{ amu} = 1.66 \times 10^{-27} \text{ kg}$, calculate an approximate value for C per volume for aluminum using the results of part a and the previous problem.

13. Monatomic linear lattice: Consider a **longitudinal** wave: $u_s = u_0 \cos(\Omega t - sKa)$ which propagates in a monatomic linear lattice of atoms of mass M , spacing a , and nearest-neighbor interaction C .

a) Show that the total energy of each atom (or plane of atoms) is

$$E_{\text{one atom}} = \frac{1}{2}M(\frac{du_s}{dt})^2 + \frac{1}{2}C(u_s - u_{s-1})^2 + \frac{1}{2}C(u_s - u_{s+1})^2.$$

Specifically, identify each term in the above expression.

b) Show that the total energy of the wave is:

$$E = \frac{1}{2} M [\sum_s (\frac{du_s}{dt})^2] + \frac{1}{2} C [\sum_s (u_s - u_{s+1})^2],$$

where \sum_s runs over all atoms. In particular, explain why the term $\frac{1}{2}C[\sum(u_s - u_{s-1})^2]$ is NOT included.

c) By substitution of u_s in this expression, show that the time-average total energy per atom is:

$$\langle E \rangle = \frac{1}{4} M \Omega^2 \langle u_0^2 \rangle + \frac{1}{2} C [1 - \cos(Ka)] \langle u_0^2 \rangle = \frac{1}{2} M \Omega^2 \langle u_0^2 \rangle,$$

where in the last step we have used the dispersion relation (assuming nearest-neighbor interactions only for this problem: $\Omega^2 = (2/m) C [1 - \cos(Ka)]$). This shows $\langle E \rangle \propto \Omega^2$ and $\langle E \rangle \propto \text{ampl}^2$ as in all waves! HINT: use trig identity $\cos(a+b) = \cos(a)\cos(b) - \sin(a)\sin(b)$ where $a = (\Omega t - sKa)$ and $b = Ka$ so $\cos(\Omega t - [s+1]Ka) = \cos(\Omega t - sKa - Ka) = \cos(\Omega t - sKa)\cos(Ka) + \sin(\Omega t - sKa)\sin(Ka)$; and recall that $\langle \cos(\Omega t - sKa) \rangle = 0 = \langle \sin(\Omega t - sKa) \rangle$, $\langle \cos(\Omega t - sKa)\sin(\Omega t - sKa) \rangle = 0$, and $\langle \cos^2(\Omega t - sKa) \rangle = \frac{1}{2}$.

d) Assuming $\langle E \rangle$ is on the order of the thermal energy, $\langle E \rangle \approx (3/2)k_B T$, and using the results of the previous problem for Ω , calculate an approximate value for $u_{0-\text{rms}} = \sqrt{\langle u_0^2 \rangle}$ for aluminum at room temperature, and compare this value to the value of the spacing of atoms, a , that we assumed in the previous problem.

14. Optical and Acoustical Modes

a) Starting with the following equations of motion ($\Sigma \mathbf{F} = m\mathbf{a}$):

$$(2C - M_1\Omega^2) u_o - C v_o (1 + e^{-iKa}) = 0$$

$$(2C - M_2\Omega^2) v_o - C u_o (e^{iKa} + 1) = 0$$

get the dispersion relation:

$$\Omega^2 = \{2C(M_1 + M_2) \pm \sqrt{4C^2(M_1 + M_2)^2 - 4M_1M_2(2C^2)(1 - \cos(Ka))}\} / 2M_1M_2$$

Then consider the limiting cases:

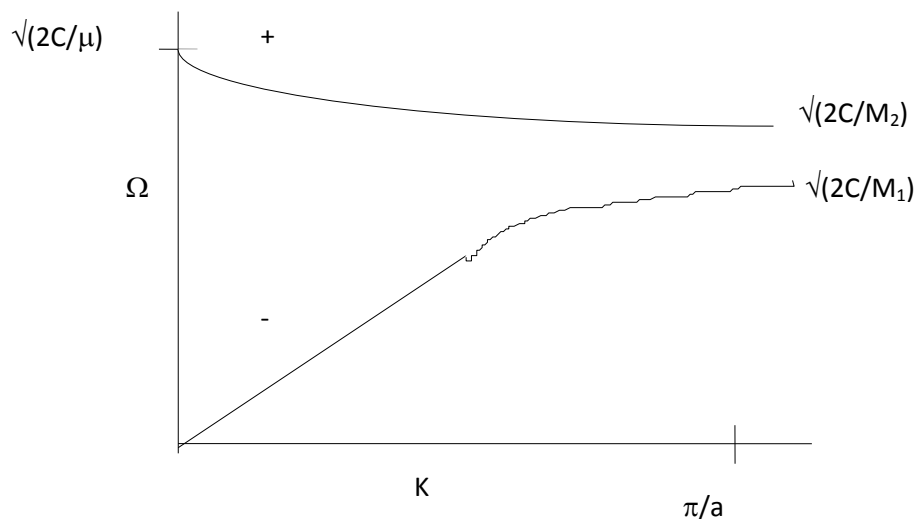
b) $Ka \ll \pi$

$$\{\text{show: } \Omega_-^2 = CK^2a^2 / (2[M_1 + M_2]) \quad \text{AND} \quad \Omega_+^2 = 2C[(1/M_1) + (1/M_2)]\}$$

(for this and the next case below be sure to indicate which Taylor series approximations you used and which terms you kept and which you neglected)

c) $Ka \approx \pi$ {show: $\Omega_-^2 = 2C/M_1$ AND $\Omega_+^2 = 2C/M_2$ } .

Below we show what the graph of Ω vs K for this case (diatomic lattice) looks like:



where $1/\mu = [(1/M_1) + (1/M_2)]$.

15. a) Compare the **momentum** of a **photon** of angular frequency, ω , where ω has the value for Ω from problem 12 above, with the momentum of a **phonon** of angular frequency, Ω , where Ω has the value of Ω from problem 12. (We are now using ω to refer to angular frequency of photons and Ω to refer to the angular frequency of phonons). This compares the momenta of photons and phonons that have the same energy (same frequency).

b) Compare the **energy** of a **photon** with $k = 0.1 * \pi/a$ with the energy of the **phonon** of part a above with $K = 0.1 * \pi/a$. Recall that the wavevector is related to the momentum, so if the photon and the phonon have the same wavevector, they would have the same momentum. (We are now using k to refer to the wavevector of photons and K to refer to the wavevector of phonons.) This compares the energy of photons and phonons that have the same momenta (same wavevector).

16. a) Calculate n_{avg} (Planck distribution) for $\epsilon = \hbar\Omega$ using the Ω from problem 12 at the following temperatures: $T = 3K$ (space), $30K$, $300K$ (earth), and $6000 K$ (sun).

b) How many phonons of energy $\hbar\Omega$ (using the Ω from problem 12) are needed to reach the thermal energy, $k_B T$, at the above four temperatures? Use $n = k_B T / \hbar\Omega$. Compare these answers to the results of the Planck distribution for n_{avg} . [Note that the Planck distribution includes the fact of lower probabilities for higher energies.] See the excel spreadsheet on [Thermal Energies](#).

17. Show by calculating the first 20 terms that : $6 \sum [1/s^4] = \pi^4 / 15$.

18. a) Calculate the Debye temperature, Θ , given $v_{phase} = v_{group} = 5,100$ m/s and $a \approx 0.25$ nm as we have used in previous problems. HINT: first calculate Ω_D using $v = \Omega_D / K_{max}$, then Θ using Ω_D .

b) Calculate the Debye frequency, $\Omega_D = \Omega_{max}$ using a Θ (Debye Temperature) for Aluminum of $428K$. Compare this frequency to the Ω calculated in problem 12.

c) For Aluminum with the Θ above, calculate the speed, v , and compare to our assumed value of $5,100$ m/s used in problem 12. HINT: use density of Al = 2.7 gm/cm³ and atomic mass of Al = 27 gm/mole to get N/V for AL, and relate Ω_D from above to $\Omega_D = [6\pi^2 v^3 N/V]^{1/3}$.

19. C_V for a monatomic 1-D lattice

Show that C_V for a monatomic lattice in 1-D in the Debye approximation is proportional to T/Θ for low temperatures [$T \ll \Theta$], where $\Theta = \hbar \Omega_M / k_B$, where $\Omega_M = \pi v_g/a$. [Note: values for Θ , the Debye temperature, range from $38K$ for Cs to $2,230K$ for C.]

20. Thermal Expansion under the "harmonic approximation"

Recall that the "harmonic approximation" means that $U(x)$ is expanded in a Taylor series and only terms through x^2 are kept.

a) Justify why the zero and first order terms in the expansion for $U(x)$ are not important leaving only the second order (x^2) term if we neglect higher order terms.

b) Show that thermal expansion in crystals is impossible under the "harmonic approximation", i.e., show that $\langle x \rangle$ is independent of T for $U(x) = \frac{1}{2} C x^2$.