Course overview

Crystal lattice phenomena’s

-- Crystal structures (Real and reciprocal space)
-- Scattering theory (Bragg’s law, Form Factor, Structure factor)
-- Crystal bindings (Equilibrium lattice constants, binding energies)
-- Lattice vibrations (Phonon dispersions, density of state, heat capacity)

Electronic phenomena’s

-- Free electron gas (Fermi Dirac distribution, density of states)
-- Band structure (electronic masses, Fermi surfaces)
-- Electronic measurements (Heat capacity, resistivity, Hall effect, quantum oscillations)
-- Electronic phases (metals, semi-metals, semi-conddductors, band insulators)

Exam Structure

10 min – Presentation:

Topics: (1) Crystal structures, (2) Crystal Bindings, (3) Reciprocal lattice+ scattering theory,
(4) Crystal vibrations (Phonons), (5) Heat capacity (6) Band structure
(7) Semiconductors

20 min – Discussion:

(a) Questions to the lecture material
(b) Questions to the exercises

End Exam

5 min - evaluation

5 min – Results: Passed / failed, grade will be known at a later point.

MY AVAILABILITY BEFORE EXAM:

30th-31th May
1st and 6th of June

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Exercise 5 *Sphere packings*

Calculate the ratio c/a of an ideal hexagonal dense sphere packing (hcp) and its packing density. Compare the packing density to that of an fcc lattice and explain your findings.

http://quiz.thefullwiki.org/Solid-state_physics

Question 1: Here, the electrons are modelled as a Fermi gas, a gas of particles which obey the quantum mechanical ________.
(1) Dirac delta function
(2) Fermi–Dirac statistics
(3) Boltzmann distribution
(4) Maxwell–Boltzmann distribution

Question 2: This structure can be investigated using a range of crystallographic techniques, including ________, neutron diffraction and electron diffraction.
(1) X-ray crystallography
(2) Atom
(3) Protein
(4) Protein structure

Question 5: Phonons are also necessary for understanding the lattice heat capacity of a solid, as in the Einstein model and the later ________.
(1) Copper
(2) Debye model
(3) Zinc
(4) Carbon

https://www.crcpress.com/downloads/IP662/IP662_Questions.pdf

2.5 The cohesive energy of a solid is 9 eV/atom. What does this tell you about the solid?

2.6 What types of bonding are present in a graphite crystal?

2.10 Calculate the packing fraction of the face-centered cubic structure.

4.10(a) What are alloys of copper and zinc commonly known as?

5.1(a) State the Bragg law.

5.4(a) What types of radiation other than X-rays are commonly used to obtain diffraction patterns?

6.6(a) Does the resistivity of a metal increase or decrease with temperature?

6.8(a) Which principle do electrons in a Fermi gas obey?

Today's program

Physics 481: Condensed Matter Physics - Midsemester test

Friday, March 4, 2011

Problem 1: Structure determination (70 points)

X-ray diffraction is used to study a powder specimen of a monoatomic substance that is known to crystallize in a cubic lattice structure with primitive vectors $\vec{a}_1 = (a, 0, 0)$, $\vec{a}_2 = (0, a, 0)$ and $\vec{a}_3 = (0, 0, a)$. The wavelength of the X-rays is 1.4 Å.

a) Find the primitive vectors of the reciprocal lattice. (15 points)

Problem 2: One-dimensional Morse solid (80 points points)

Consider N identical atoms of mass M whose motion is restricted to the x-axis. Nearest neighbor atoms are coupled by the so-called Morse potential

$$V_M(r) = D\left(1 - e^{-\alpha(r-r_0)}\right)^2 - D$$

where r is the distance between them and D, α, and r_0 are positive constants.

a) Calculate $V_M(0)$, $V_M(\infty)$ and qualitatively sketch the Morse potential. (10 points)

Problem 3: Phonons of a square lattice (50 points)

Consider a two-dimensional solid of identical atoms of mass M on a square lattice of lattice constant a. In this problem, we investigate vibrations perpendicular to the lattice plane. The equations of motion for the displacements $u_{j,l}$ read

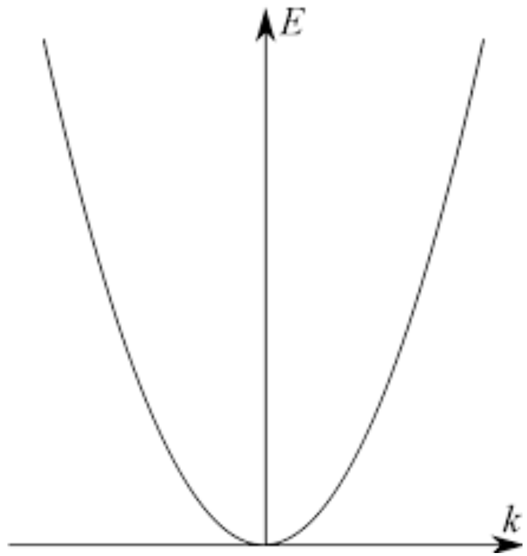
$$M\ddot{u}_{j,l} = K(u_{j+1,l} - u_{j,l}) + K(u_{j-1,l} - u_{j,l}) + K(u_{j,l+1} - u_{j,l}) + K(u_{j,l-1} - u_{j,l})$$

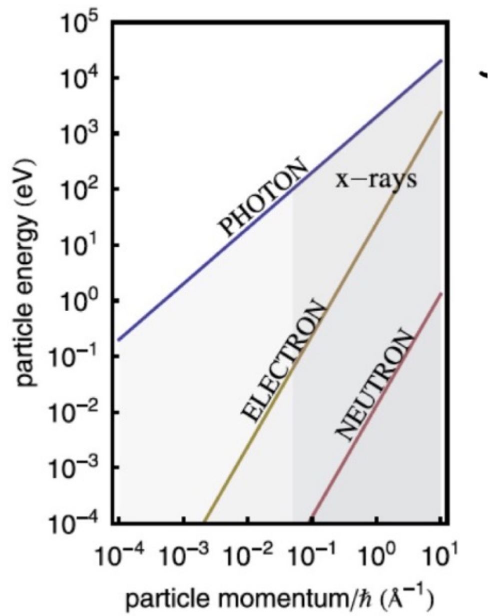
Here, j and l index the atom position in the x and y directions, respectively.

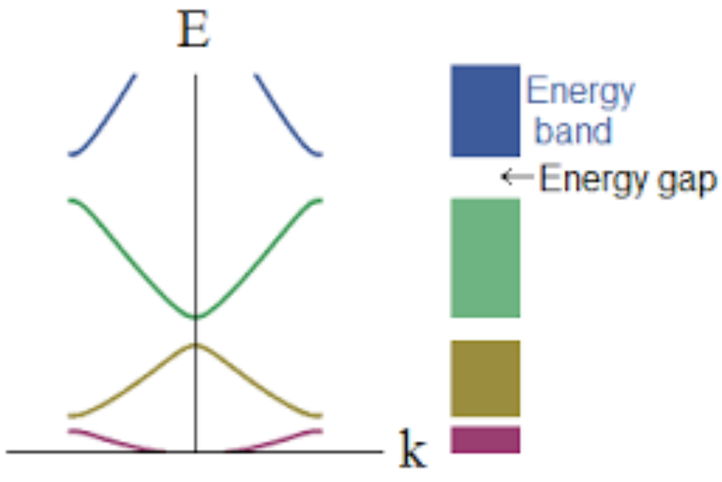
a) Determine the dispersion relation (ω as a function of $\vec{q}$) of the phonons for a wave with a wave vector $\vec{q} = (q_x, q_y)$. (30 points)

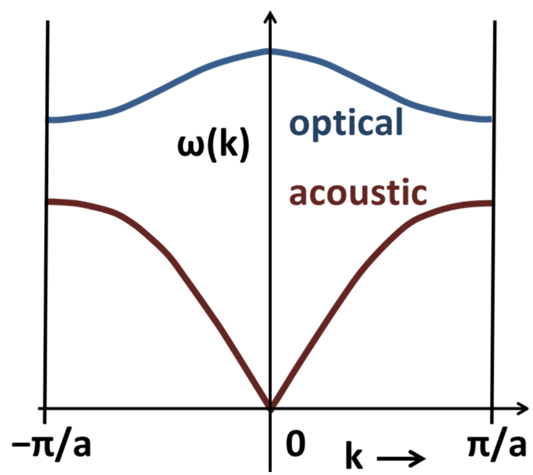
b) Calculate the speed of sound in terms of K and M. Does it depend on the direction of $\vec{q}$? (20 points).

Dispersions (Dispersion relations)

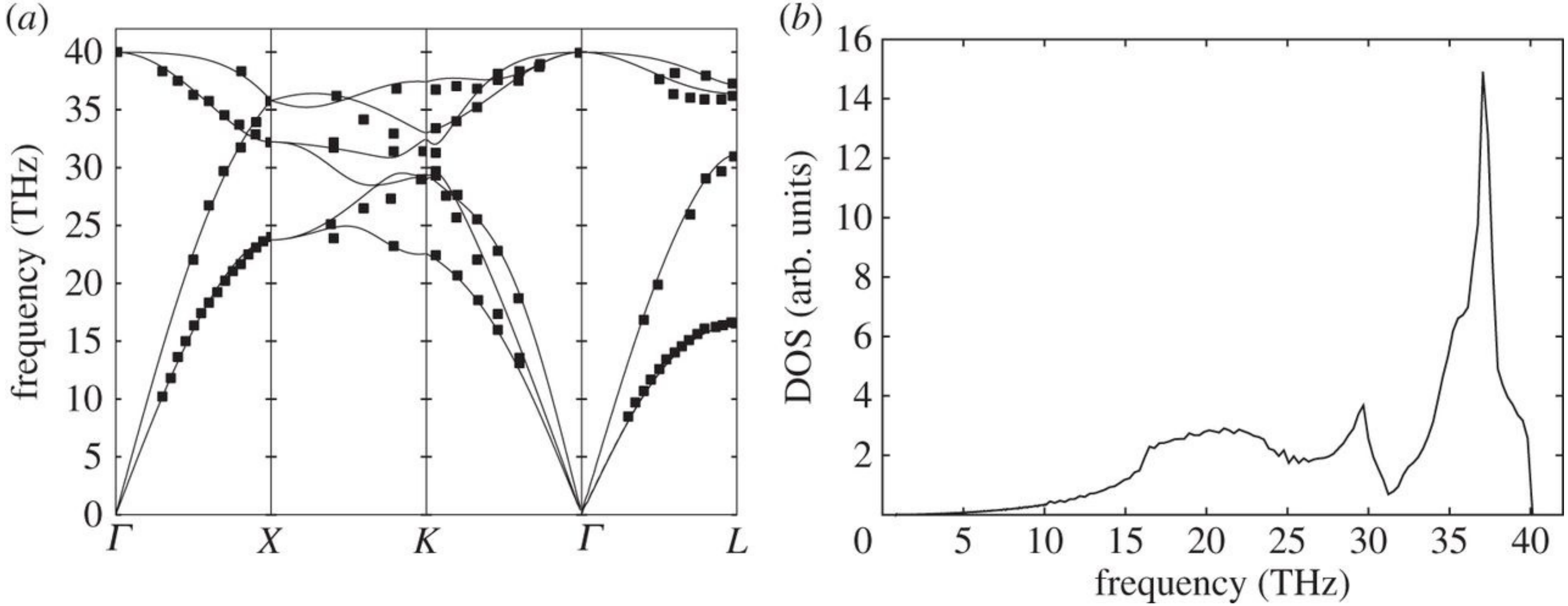








Phonon Density of States



Van Hove Singularity

Exercise 3 *Singularity in density of states*

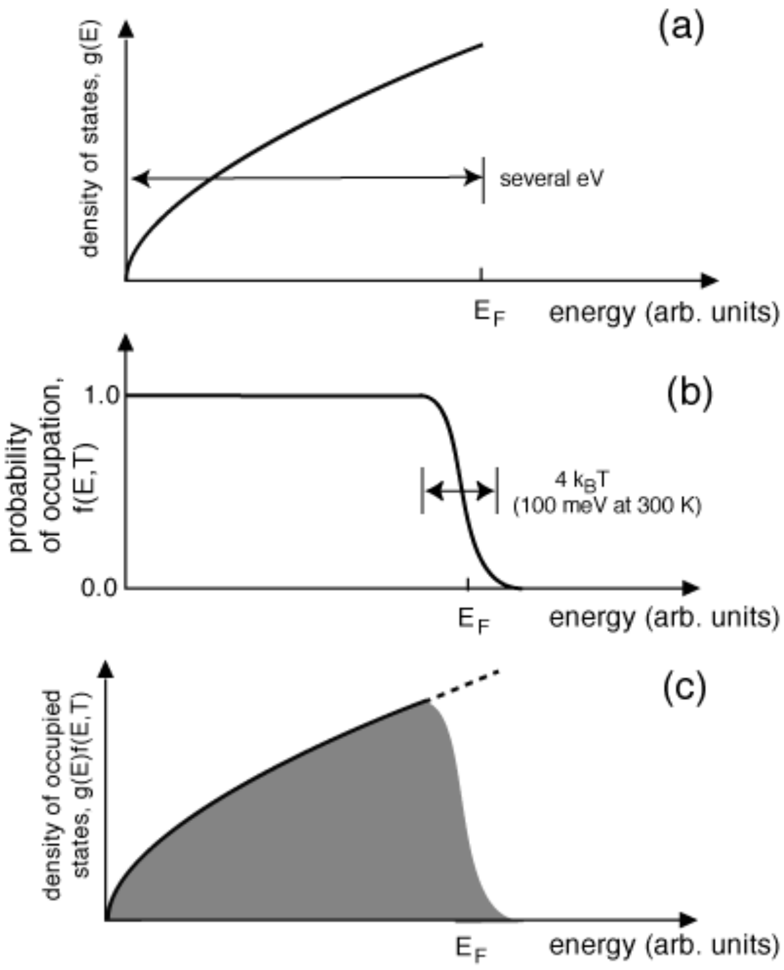
(a) From the dispersion relation derived in the lecture for a monoatomic linear lattice of N atoms with nearest neighbour interactions, show that the density of modes is

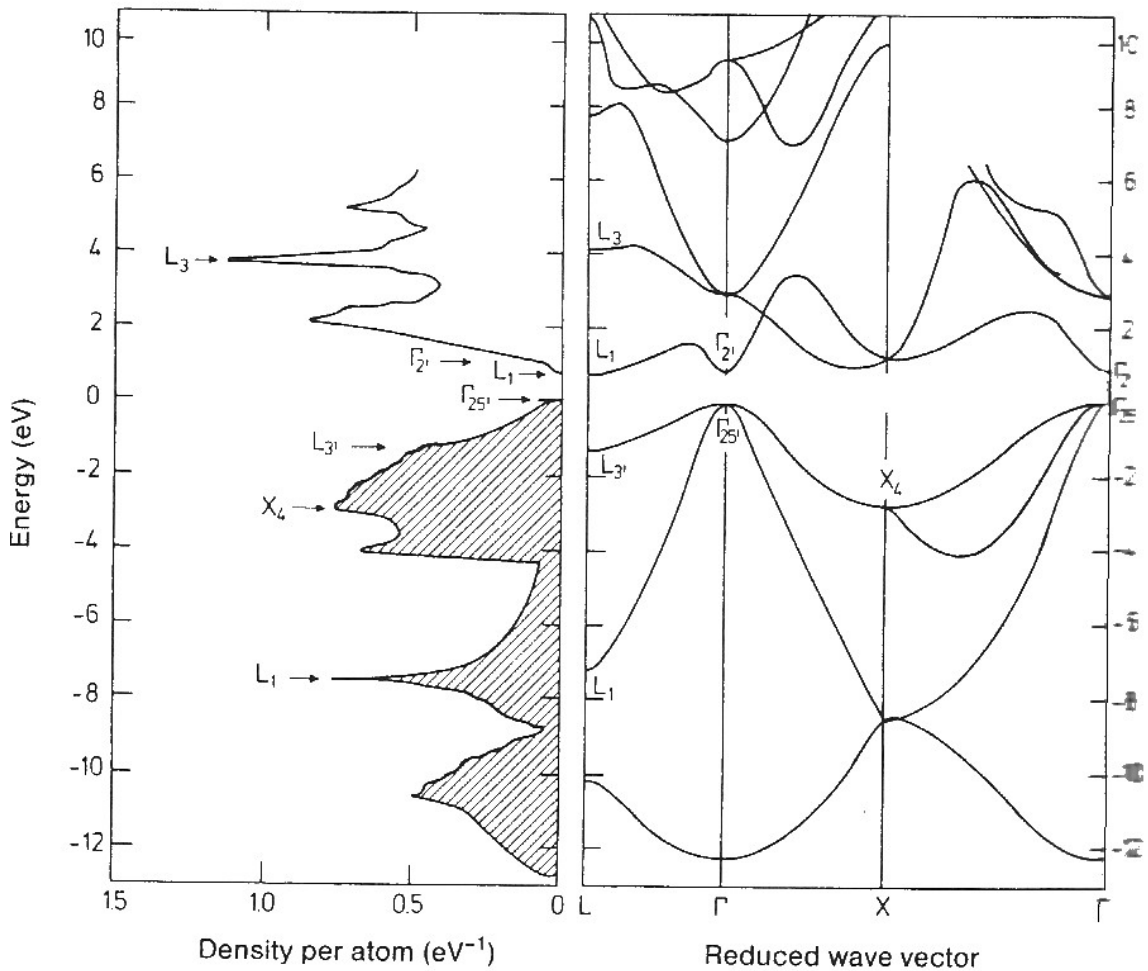
$$D(\omega) = \frac{2N}{\pi} \cdot \frac{1}{\sqrt{\omega_{\mathrm{m}}^2 - \omega^2}}, \tag{4}$$

where ω_{m} is the maximum frequency.

(b) Suppose that an optical phonon branch has the form $\omega(K) = \omega_0 - AK^2$, near $K = 0$ in three dimensions. Show that $D(\omega) = \left(\frac{L}{2\pi}\right)^3 \left(\frac{2\pi}{A^{3/2}}\right) (\omega_0 - \omega)^{\frac{1}{2}}$ for $\omega < \omega_0$ and $D(\omega) = 0$ for $\omega > \omega_0$. Here the density of modes is discontinuous.

Electronic Density of States





Physics 481: Condensed Matter Physics - Test prep homework

Problem 1: Tightly bound electrons in 1D (10 points)

Consider a one-dimensional electron system with lattice constant a in tight binding approximation. The energy-momentum relation reads

$$\epsilon(k) = -2t\cos(ka) \ .$$

a) Calculate the electronic density of states $D(\epsilon)$.

b) Does it have van-Hove singularities? If so, discuss their character!

c) Calculate the Fermi energy for 0.5, 1, and 2 electrons per unit cell.

d) For one electron per unit cell, calculate the low-temperature specific heat (per cell)!