Solid state physics 2019 Final Exam

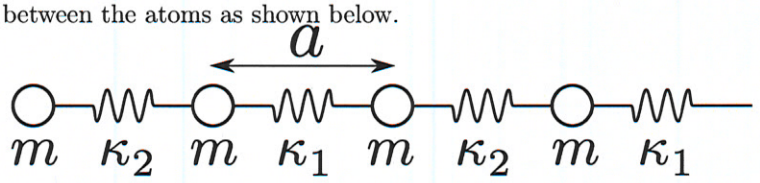
April 16th, 2019

Good luck!

- You may not use textbooks, notes, or calculators.
- When plotting, label the axes and mark the important values.
- If you need extra answer space: ask for an extra exam copy, fill in your name and continue writing the solution.

1. (35 points) **Band structure of phonons in 1D**

Consider a 1D chain of atoms of mass m connected by springs with alternating spring constants κ_1 and κ_2, and a distance a between the atoms as shown below.



(a) (5 points) Write down the equations of motion for atoms in a unit cell of this chain using the appropriate running wave ansatz.

Atom with κ_1 to the right is $x_{a,n}$, the other $x_{b,n}$ $x_{a,n} = x_a e^{2ikna}$

$$-\omega^2 m x_a = \kappa_1 (x_b - x_a) + \kappa_2 (x_b e^{-2ika} - x_a)$$
$$-\omega^2 m x_b = \kappa_2 (x_a - x_b) + \kappa_1 (x_a e^{2ika} - x_b)$$
$$-\omega^2 m \begin{pmatrix} x_a \\ x_b \end{pmatrix} = \begin{pmatrix} -\kappa_1 - \kappa_2 & \kappa_1 + \kappa_2 e^{-2ika} \\ \kappa_1 + \kappa_2 e^{2ika} & -\kappa_1 - \kappa_2 \end{pmatrix}$$

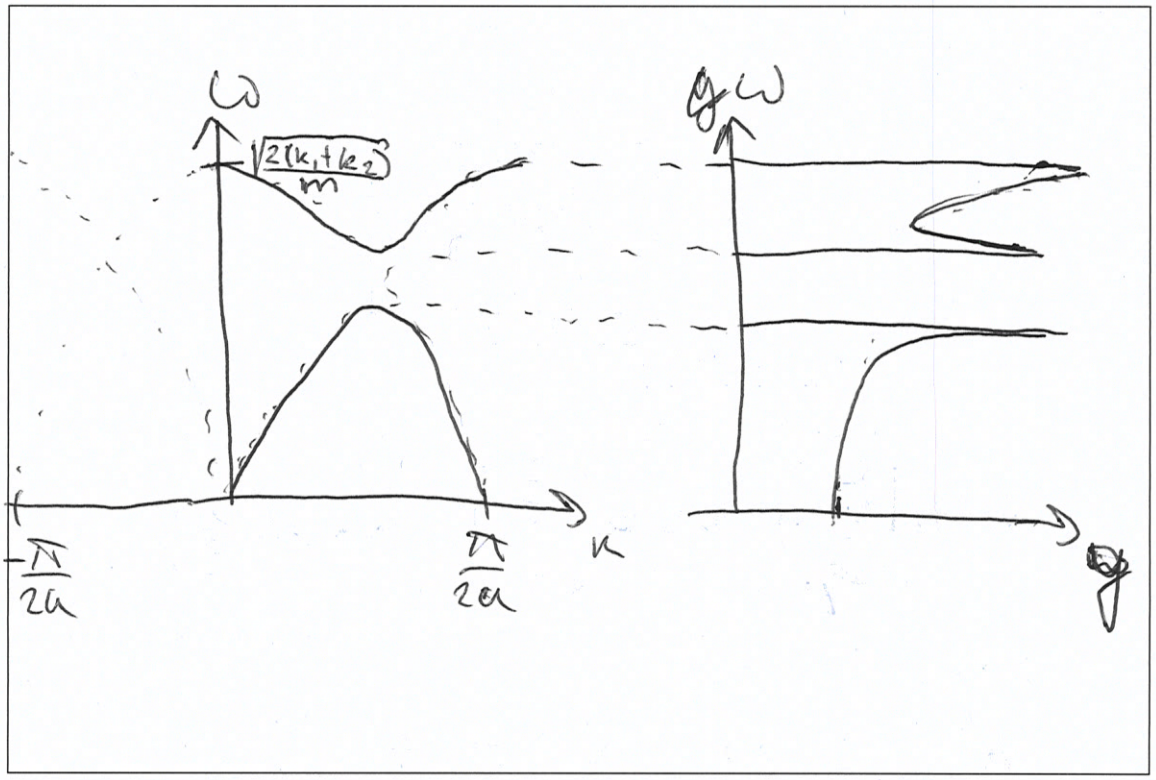
(b) (10 points) Find the dispersion relation by solving the equations of motion.

$$m\omega_\pm^2 = \kappa_1 + \kappa_2 \pm |\kappa_1 + \kappa_2 e^{2ika}|$$

(solution of the eigenproblem)

$$m\omega_\pm^2 = \kappa_1 + \kappa_2 \pm \sqrt{(\kappa_1 + \kappa_2 \cos 2ka)^2 + \kappa_2^2 \sin^2 2ka}$$

(c) (10 points) Sketch the dispersion relation $\omega(k)$ and the density of states $g(\omega)$ when $\kappa_1 \approx \kappa_2$.



(d) (10 points) Simplify the found dispersion relation of the optical and acoustic branches assuming $\kappa_1 \gg \kappa_2$. How does this approximate dispersion of the acoustic branch relate to that of a monatomic chain with only one spring constant? How can the dispersion of the optical branch be understood from the vibrational frequency spectrum of a single diatomic molecule? (If you did not derive the dispersion, try to compute what happens when $\kappa_1 \gg \kappa_2$ directly.)

$k_1 >> k_2$

Optical:

$m\omega^2 = k_1 + k_2 + |k_1 + k_2 e^{2ika}| \approx 2k_1$

$\Rightarrow \omega = \sqrt{2k_1/m}$, molecule with two atoms of mass m, and spring k_1.

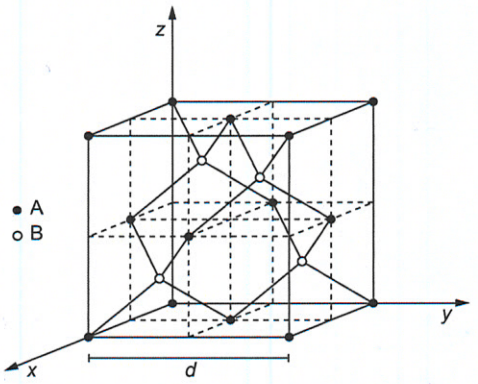
acoustic:

$m\omega^2 = k_1 + k_2 - \sqrt{k_1^2 + k_2^2 + 2k_1k_2\cos 2ka}$

$m\omega^2 \approx k_1 + k_2 - k_1 + k_2 \cos 2ka \approx k_1(1 - \cos 2ka)$

$\omega \approx \sqrt{\frac{k_1}{m}}\,|\sin ka|$: chain with mass 2m and spring constant k_2

2. (30 points) **Zinc-blende crystal structure**



(a) (5 points) Give a set of primitive lattice vectors and the corresponding basis.

$a_1 = d\begin{pmatrix}\frac{1}{2}\\ \frac{1}{2}\\ 0\end{pmatrix}$ $a_2 = d\begin{pmatrix}\frac{1}{2}\\ 0\\ \frac{1}{2}\end{pmatrix}$ $a_3 = d\begin{pmatrix}0\\ \frac{1}{2}\\ \frac{1}{2}\end{pmatrix}$

basis:

$A(0,0,0)$, $B(\frac{1}{4},\frac{1}{4},\frac{1}{4})$

(b) (10 points) Calculate the filling fraction of this crystal, assuming that the atoms have equal radii $r_A = r_B$. For what ratio of r_B/r_A do you expect the filling fraction to be maximal?

$r_a = r_b \Rightarrow 2r_a = \frac{\sqrt{3}}{4} d$

(distance between neighbors)

filled volume: $2 \times \frac{4\pi}{3} \cdot \left(\frac{\sqrt{3}}{8}\right)^3 d^3$

total volume: $d^3/4$ (FCC)

fraction: $\pi\sqrt{3}/16$

maximal density: take r_a atoms as large as possible, fill holes with atom b

$r_a = \frac{1}{2\sqrt{2}}$, $r_b = \frac{\sqrt{3}}{4} - \frac{1}{2\sqrt{2}}$

(c) (10 points) Calculate the reciprocal lattice vectors corresponding to the lattice vectors you formulated in (a). Calculate the volume of the primitive unit cell of the reciprocal lattice.

volume: $(2\pi)^3/(a^3/4)$

$b_1 = \frac{4\pi}{a}\begin{pmatrix}\frac{1}{2}\\ \frac{1}{2}\\ -\frac{1}{2}\end{pmatrix}$ $b_2 = \frac{4\pi}{a}\begin{pmatrix}\frac{1}{2}\\ -\frac{1}{2}\\ \frac{1}{2}\end{pmatrix}$ $b_3 = \frac{4\pi}{a}\begin{pmatrix}-\frac{1}{2}\\ \frac{1}{2}\\ \frac{1}{2}\end{pmatrix}$

used: bcc primitive vectors

$b_1 \cdot a_1 = 2\pi$

(d) (10 points) Compute the structure factor S corresponding to the lattice vectors found in (a). Use f_A and f_B as form factors for atoms A and B. Which diffraction peaks vanish when $f_A = f_B$?

$S = f_A + f_b e^{i\pi(h+k+\ell)/4}$

When $f_A = f_B$, $S = 0$ iff $h+k+\ell = 2 \mod 4$

3. (35 points) **A two-dimensional semiconductor**

Consider a 2D semiconductor with a band gap $E_G \gg k_B T$. The effective electron mass at the bottom of the conduction band is m_e. The effective hole mass at the top of the valence band is m_h, $m_h > m_e$. We put the zero of energy at the top of the valence band and consider the semiconductor to be in the intrinsic regime.

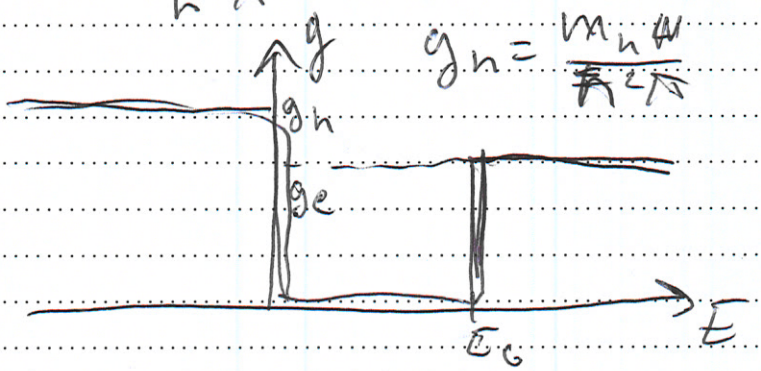
(a) (10 points) Compute and sketch the density of states of this semiconductor.

electrons:

$$g_e = 2 \times \left(\frac{L}{2\pi}\right)^2 \times \frac{dk}{dE} \times \frac{dN}{dk} =$$

$$= \left(\frac{m_e}{\hbar^2 k}\right) \times \left(2\pi k \times 2 \times \left(\frac{L}{2\pi}\right)^2\right) = \frac{m_e L^2}{\hbar^2 \pi}$$

(or $\frac{m_e}{\hbar^2 \pi}$ per unit area),



$$g_h = \frac{m_h W}{\hbar^2 \pi}$$

(b) (10 points) Calculate the concentration of holes n_h in the valence band as a function of the Fermi energy E_F, temperature T, and m_h. Also calculate the concentration of electrons n_e in the conduction band as a function of the Fermi energy E_F, temperature T, and m_e.

$$n_h \approx \int_0^\infty g_h e^{-(E+E_F)\beta} dE =$$

$$= g_h kT e^{-\beta E_F}$$

similarly

$$n_e = g_e kT e^{-\beta(E_e - E_F)}$$

(c) (10 points) Write down an expression the electron heat capacity of this semiconductor as an integral over energies.

$$C_v = \frac{d}{dT} \int_{E_c}^{\infty} E\, g_e\, e^{-(E_k - E_F)\beta}\, dE$$

$$= \int_{E_c}^{\infty} E(E_k - E_F)\, e^{-(E_k - E_F)\beta} \cdot \frac{1}{kT^2}\, dE$$

+ same for holes

(d) (5 points) Discuss whether the electron heat capacity becomes larger than the phonon heat capacity as temperature is lowered towards 0K.

electron $C_v \sim e^{-E_c\beta}$, decays exponentially.

phonon $C \sim T^2$, so

$C_{phonon} \gg C_{electron}$ as $T \to 0$

$C_{electron} / C_{phonon} \to 0$ as $T \to 0$.