MIDTERM EXAM, PHYSICS 285, Fall, 2013, Dr. Charles W. Myles
In Class Exam, Wednesday, October 30.

NOTE: The Exam begins at 6:00pm. Please make every effort to finish it by 8:30pm!! Thank you!!

INSTRUCTIONS:

PLEASE read all of these before doing anything else!!! Failure to follow them may lower your grade!!

1. PLEASE write on ONE SIDE of the paper only!! This wastes paper, but it makes my grading easier!
2. PLEASE do not write on the exam sheets, there will not be room! Use other paper!!

As you can see, many of the questions on this exam are Qualitative!!!

3. PLEASE answer the qualitative Questions briefly, including the "How" or the "Why" of each, not just
   the "What". Keep your answers to these short & aimed at the main ideas. A sketch with appropriate
   labels or an equation with a brief comment is often the easiest way to make a point. NOTE: The words
   "Discuss", "Define", and "Explain" below mean to write complete, grammatically correct, English
   sentences. I don't want to see a lot of equations! I want to see WORDS describing the physics!

4. PLEASE write neatly. If I cannot read or find your answer, you can't expect me to give it the credit it
   deserves and you are apt to lose credit.

5. PLEASE put the Questions in order and the pages in order before turning in this exam!

   PLEASE FOLLOW THESE SIMPLE DIRECTIONS!!!! THANK YOU!!!

NOTE: Most questions are about solids with crystal structures based on ideal 3-dimensional lattices. There
are 4 qualitative questions & 4 quantitative problems. Answer any two (2) qualitative questions plus any
three (3) quantitative problems for a total of five (5) questions required. Each is equally weighted &
worth 20 points for a total of 100 points on this exam!

Qualitative Questions! Answer ANY TWO (2) of these 4 questions!

Answer ALL PARTS briefly in a few English Sentences, with as few math symbols as possible!

1. Crystal Structure #1: In parts a to f, briefly Define or Explain:
   a. Bravais Lattice  
   b. Basis  
   c. Primitive Lattice Vectors  
   d. Wigner-Seitz Cell  
   e. Face Centered Cubic (FCC) Lattice  
   f. Body Centered Cubic (BCC) Lattice  

   g. Briefly Discuss the reasons that a periodic lattice with a five-fold symmetry axis cannot exist.  

   h. Briefly Define the Miller indices of a lattice plane.  

2. Crystal Binding #1: Crystalline solids are often considered in terms of the 4 idealized bonding categories listed in parts a to d. Yet, for each of these 4 kinds of bonding, it is the electrostatic Coulomb interaction that provides the attractive force. For each of the types of idealized bonding listed in parts a to d, and by considering only outer valence electrons of the atoms, Discuss how the Coulomb force is operating in each case. That is, Discuss the Physical Mechanisms which are primarily responsible for the bonding energy each of these kinds of solids.
   a. Ionic Bonding  
   b. Covalent Bonding  
   c. Metallic Bonding  
   d. Van der Waals Bonding  

   e. In addition to the attractive electrostatic Coulomb force responsible for the 4 kinds of bonding listed in parts a to d, it is argued in Kittel's Ch. 3 & it was discussed in class that a short ranged repulsive force must also exist between the atoms in a solid. Briefly discuss the physical reasons that such a repulsive force must exist and the physical origins of this force. 

   f. Define the Madelung Energy in ionic solids. Briefly Discuss the reasons that calculating this contribution to cohesive energies must be done carefully to avoid obtaining divergent results.
Qualitative Questions (continued)! Answer ANY TWO (2) of these 4 questions!

3. Reciprocal Lattice & Wave Diffraction #1: Briefly Define or Explain:
   a. Reciprocal Lattice  
   b. Brillouin Zone  
   c. Structure Factor  
   d. Atomic Form Factor  
   e. Bragg's Law of Diffraction  
   f. Laue Condition (Laue Equations)  
   g. Briefly Discuss the Physics underlying Bragg's Law of Diffraction.  
   h. Briefly Explain the reasons that the Bragg Law is equivalent to the Laue Condition (Laue Equations).

4. Lattice Vibrations & Lattice Dynamics #1: In parts a. - f. briefly Define or Explain:
   a. Lattice Dynamics  
   b. Harmonic Approximation  
   c. Normal Modes  
   d. Dispersion Relations  
   e. Phonon  
   f. Elastic Constants  
   g. Discuss the qualitative differences in the behavior (as a function of wave vector) of acoustic and optic phonon modes.  
   h. What characteristics must the crystal structure of a solid have in order for optic modes to exist? Is it possible for the phonon dispersion relations of a solid to contain acoustic modes only? If so, what characteristics are required for the crystal structure?

(Hopefully) Short Quantitative Problems! Answer ANY THREE (3) of these 4 problems! If any of these seems to be mathematically very messy, you've probably done something wrong!

5. Crystal Structure #2: The vectors of the primitive fcc unit cell connect a lattice point at the origin with lattice points at the center of the adjacent of cube faces.
   a. Write these vectors in standard Miller notation & calculate the angle between any two of them.
   b. Prove that the volume of the primitive cell is one quarter of the volume of the conventional cell.  

6. Crystal Binding #2:
   A quantitative model of bonding in ionic crystals was developed in the 1930's by Born and Meyer. In this model, the total potential energy of the system is assumed to have the form (in SI units):
   \[ U_{\text{tot}}(R) = N \frac{A}{R^n} - N \frac{\alpha e^2}{4\pi \epsilon_0 R} \]
   Here, \( N \) is the number of positive-negative ion pairs, \( R \) is the nearest neighbor distance in the material, \( \alpha \) is the Madelung constant for the material, \( A \) & \( n \) are adjustable empirical parameters to be fit to experimental data and \( \epsilon_0 \) is the permittivity of free space.
   a. The first term in \( U_{\text{tot}} \) is a repulsive interaction. Briefly discuss it's physical origin. The second term in \( U_{\text{tot}} \) is an attractive interaction. Briefly discuss it's physical origin.
   b. Sketch \( U_{\text{tot}} \) potential as a function of \( R \). Note: If you don't do this, you will lose points!  
   c. Calculate the equilibrium nearest-neighbor distance \( R_0 \) in terms of \( N, A, \alpha \) and \( \epsilon_0 \). The equilibrium bonding energy per ion pair in this model is simply \( U_{\text{tot}}(R_0) \). By using the \( R_0 \) you just obtained in the above equation for \( U_{\text{tot}} \) find a simple expression for the equilibrium bonding energy per ion pair. (Hint: This should be independent of the parameter \( A \).)
   d. For the ionic salt NaCl, the constant \( \alpha = 1.75 \), \( R_0 = 5.63 \text{ Å} \) and the measured bonding energy per ion pair is 7.95 eV. Use these numbers to estimate the value of the parameter \( n \) for NaCl. [Note: \((1/4\pi \epsilon_0) = 9.0 \times 10^9 \text{ Nm}^2/\text{C}^2\), 1.0 eV = 1.6 \times 10^{-19} \text{ J}, 1.0 \text{ Å} = 1.0 \times 10^{-10} \text{ m}].
Quantitative Problems (continued)!
Answer ANY THREE (3) of these 4 problems!

7. Reciprocal Lattice & Wave Diffraction #2
a. Consider a crystal with the simple cubic (SC) lattice structure. The primitive lattice vectors are \( \mathbf{a}_1 = a \mathbf{i}, \mathbf{a}_2 = a \mathbf{j}, \mathbf{a}_3 = a \mathbf{k} \), where \( a \) is the lattice constant and \( \mathbf{i}, \mathbf{j}, \mathbf{k} \) are the usual unit vectors for a Cartesian coordinate system. Prove that the reciprocal lattice is simple cubic also.
b. Find separation between closest parallel planes of the lattice which have Miller indexes \( (1,1,0) \). Compare this separation with the length of the vector \( \mathbf{K} = [1,1,0] \) in the reciprocal lattice.
c. What is orientation of the vector \( \mathbf{K} = [1,1,0] \) of the reciprocal lattice with respect to the plane \( (1,1,0) \) in the direct lattice?
d. Write two relations between the orientation and length of a general vector \([k,l,m]\) of the reciprocal lattice and the orientation and the separation of the planes with the Miller indexes \([k,l,m]\) in the direct lattice.

8. Lattice Vibrations & Lattice Dynamics #2:
Consider the model one-dimensional diatomic chain of \( 2N \) atoms, as discussed in Kittel’s Ch. 4 and as thoroughly covered in class. There are \( N \) atoms of mass \( m \) & \( N \) atoms of mass \( M \). Every mass \( m \) has two near neighbors of mass \( M \) & every mass \( M \) has two near neighbors of mass \( m \). This is a model of a solid with two atoms per unit cell. The repeat distance is \( a \), so the atoms are equally spaced with separation \( (\frac{1}{2})a \). The force constant coupling each atom to its nearest-neighbors is \( K \). As discussed in class, the normal mode vibrational frequencies have two branches \( \omega_\pm(k) \) for each wavevector \( k \). The solutions for these have the form:

\[
\omega_\pm^2 = \frac{K(m+M)}{mM} \mp \frac{K}{mM} \left( \frac{m+M}{mM} \right)^2 - \frac{4\sin^2(ka/2)}{mM} \frac{1}{\nu^2}
\]

a. Which branch is the solution for the acoustic modes and why? Which branch is the solution for the optic modes and why?
b. Derive expressions for the group velocities \( v_g \) as functions of \( k \).
c. Using the results of part b, evaluate \( v_g \) at very small values of \( k \) \((k \to 0)\). Briefly Discuss the physical significance of these low \( k \) group velocities.
d. Using the results of part b, evaluate \( v_g \) at the Brillouin Zone boundary \([k = (\pi/a)]\). Briefly Discuss the physical significance of these Brillouin Zone boundary group velocities. Specifically, what do we say about propagation of longitudinal waves in this lattice at frequencies \( \omega_\pm \) \((k = \pi/a)\)?
1. Bravais lattice: A Bravais lattice can be defined as an array of points in space. Each point is equivalent; it consists of an infinite array of discrete points arranged and oriented so that the lattice looks the same, no matter which point it is viewed from. A Bravais lattice is also invariant under translation.

2. Basis: A basis is a group of atoms that describe a crystal structure, or in other words, a set of atoms that generate a crystal structure when placed at each lattice point.

3. Primitive lattice vectors: These are vectors that make up the building blocks for crystal structure. They can be described as vectors that define a specific lattice in that the arrangement of atoms look the same when viewed from a point \( \mathbf{r} = u_1 \mathbf{a}_1 + u_2 \mathbf{a}_2 + u_3 \mathbf{a}_3 \), or a translated point \( \mathbf{r}' = \mathbf{r} + u_1 \mathbf{a}_1 + u_2 \mathbf{a}_2 + u_3 \mathbf{a}_3 \), where \( u_1, u_2, \) and \( u_3 \) are integers, and \( \mathbf{a}_1, \mathbf{a}_2, \) and \( \mathbf{a}_3 \) are the primitive lattice vectors.

4. Wigner-Seitz cell: The smallest volume in a lattice that can be repeated to fill the lattice. One finds this cell by: 1) drawing lines from a central atom to its nearest neighbors; 2) Drawing perpendicular bisectors through these lines. The enclosed volume is the Wigner-Seitz cell.

5. FCC lattice: The face centered cubic lattice is a lattice consisting of a basis with lattice points at the corners and face centers of a cube.

6. BCC lattice: The body centered cubic lattice is a lattice consisting of a basis with lattice points at the corners and body center of a cube.

7. Five-fold: The existence of n-fold symmetry depends on the ability of an n-sided shape to be able to completely fill an infinite space with no gaps between shapes. Mathematicians have proven this to be impossible with five-sided shapes (pentagons).

8. Miller Indices: Miller indices are the symbolic representations of the orientations of specific atomic planes in a crystal lattice. You find them with a 3-step process: 1) Identify the intersection of a plane and each axis in terms of lattice constants \( a, b, c \). 2) Take the reciprocals of each of these numbers. 3) Reduce these 3 reciprocals to integers.
Ionic Bonding: In ionic solids, the component atoms have gained or lost electrons in order to completely fill their outer shells. These atoms carry a permanent charge and are bound by the electrostatic force between these charges.

Covalent Bonding: In covalent bonding, the valence shells of two similarly electronegative atoms "share" electrons. It can be described as an overlapping of the atoms' respective electron clouds at the point where equilibrium is achieved.

Metallic Bonding: Electrons in the valence shell of metallic solids are very weakly bound to their atoms, causing these electrons to be mobile and form a "free-electron gas" within the solid.

Vander Waals Bonding: Vander Waals bonding occurs because of the interactions of induced dipole-dipole moments in neutral atoms. This bonding is the weakest type of bonding and is only a major factor in noble-gas solids. (also in some organic solids)

Repulsive Force: A short-ranged repulsive force must exist between atoms in a solid because the absence of a repulsive force would cause a solid to be contracted into a mathematical point. The physical origins of this force stem mainly from quantum mechanical fluctuations.

Madelung Energy: The Madelung Energy is the cohesive energy for ionic solids. It is different from standard cohesive energy because the attractive forces in ionic solids are largely electrostatic since the atoms within the solid are not electrically neutral. You calculate the Madelung Energy from: $U_{\text{tot}} = \frac{N_{\text{eq}}}{R_0} (1 - \frac{1}{R_0})$, where $(-\frac{N_{\text{eq}}}{R_0})$ is the Madelung energy. The $\alpha$ is known as the Madelung constant and is calculated by $\alpha = \frac{\pi}{\sqrt{3}} \frac{R}{Q}$, where the sign changes relative to the reference charge. If care isn't taken when computing the sum, $\alpha$ will quickly diverge, making the Madelung energy difficult to calculate.
Reciprocal Lattice & Wave Diffraction

1) Reciprocal lattice — every crystal structure has two lattices associated with it, the crystal lattice and reciprocal lattice. Reciprocal lattice is the dual of the direct lattice in $k$-space and it is represented by diffraction of a crystal.

2) Brillouin Zone — a Brillouin zone is the Wigner-Seitz primitive cell in the reciprocal space. By understanding the Brillouin zone of a material, one can understand the majority of the material relatively easily since crystals are periodic.

3) Structural Factor — Structure factor can be defined as a mathematical function that describes the amplitude and phase of a diffracted wave from a crystal lattice plane. It can be written as $S_0 = \int d\mathbf{r} n(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}}$, where $\mathbf{G}$ is the reciprocal lattice vector and $n(\mathbf{r})$ is the electron concentration. The structure factor gives insight into what types of reflections are allowed to occur within a particular type of lattice.

4) Atomic form factor — Atomic form factor can be described as a measure of scattering power of the atom in a unit cell. It can be written as $f_j = \int d\mathbf{r} n_j(\mathbf{r}) e^{-i\mathbf{p}\cdot\mathbf{r}}$, where $\mathbf{p} = \mathbf{G} - \mathbf{G}_j$ and $n_j(\mathbf{r})$ is an atomic property.

2) Bragg's Law of Diffraction — Bragg's Law of Diffraction describes the characteristic patterns of reflected x-rays that are incident on a crystalline material. Bragg's Law of Diffraction can be mathematically written as $2d\sin\theta = n\lambda$.

2) Zone Condition (Zone equations) — Zone condition or Zone equations are other ways to express the original results of diffraction theory, namely $\Delta\mathbf{k} = \mathbf{G}$. They are as below:

$$\mathbf{a}_i \cdot \mathbf{A}\mathbf{k} = 2\pi n_i \quad (i = 1, 2, 3)$$

and at a reflection, $\mathbf{A}\mathbf{k}$ must satisfy all above equations, here $\mathbf{a}_i$'s are the primitive lattice vectors in a direct lattice.
4) x-rays are incident on a crystalline material and reflected at a specific angle depending on the properties of the crystal and the wavelength of the x-ray.

\[ 2d \sin \theta = n \lambda \]

1) Lattice Dynamics is the study of lattice vibrations and their properties.

b) The harmonic approximation is that since the displacement during vibrations is much smaller than the atomic spacing, the vibrations can be approximated as harmonic oscillators. This means that they are acted upon by Hooke's law: forces with some force constant \( k \) and oscillate about an equilibrium point.

v) Normal modes are when the atoms vibrate in all directions with the same frequency.
Dispersion Relations show how a wave propagates through a material. They can be written in terms of \( k \), \( \omega \), \( \nu \), \( \gamma \), and other values.

A phonon is a quantum-mechanical quasi-particle that represents the normal modes of lattice vibration, like other particles it has energy \( E \) and momentum \( \vec{k} \), and is the carrier of propagating waves.

The elastic constants determine how much stress a material can take before it is permanently deformed.

The main differences in behaviour between optic and acoustic modes comes at small values of \( k \). At \( k = 0 \), the acoustic modes go to zero while the optic modes go to a maximum not zero. Also, the acoustic modes have a dispersion relation that is proportional to the speed of sound.

For optic modes to exist the primitive cell must contain more than one atom. On the other hand, a crystal structure must have exactly one atom in the primitive cell to have only acoustic modes which is entirely possible.
\[ \hat{\mathbf{a}}_1 = \frac{1}{a} a(\hat{x} + \hat{y}) \quad \hat{\mathbf{a}}_2 = \frac{1}{a} a(\hat{x} + \hat{z}) \quad \hat{\mathbf{a}}_3 = \frac{1}{a} a(\hat{x} + \hat{y}) \]

\[
\cos \theta = \frac{\hat{a}_1 \cdot \hat{a}_2}{|\hat{a}_1||\hat{a}_2|}, \quad \theta \text{ is the angle between } \hat{a}_1 \text{ and } \hat{a}_2
\]

\[
\hat{a}_1 \cdot \hat{a}_2 = \frac{1}{a} a(\hat{x} + \hat{y}) \cdot \frac{1}{a} a(\hat{x} + \hat{z}) = \frac{1}{a^2} a^2
\]

\[
|\hat{a}_1| = \sqrt{\hat{a}_1 \cdot \hat{a}_1} = \sqrt{\frac{1}{a^2} a^2(\hat{x} + \hat{y}) \cdot \frac{1}{a^2} a^2(\hat{x} + \hat{z})} = \frac{1}{a} a \sqrt{1 + 1} = \frac{\sqrt{2}}{a} a
\]

\[
|\hat{a}_2| = \sqrt{\hat{a}_2 \cdot \hat{a}_2} = \sqrt{\frac{1}{a^2} a^2(\hat{x} + \hat{z}) \cdot \frac{1}{a^2} a^2(\hat{x} + \hat{y})} = \frac{1}{a} a \sqrt{1 + 1} = \frac{\sqrt{2}}{a} a
\]

\[
\cos \theta = \frac{a^2}{\frac{\sqrt{2}}{a} a \cdot \frac{\sqrt{2}}{a} a} = \frac{1}{2}
\]

\[
\theta = \cos^{-1} \left( \frac{1}{2} \right)
\]

\[
\theta = 60^\circ
\]

1. Volume of conventional fcc cell: \( V_{\text{conv}} = a^3 \)

Volume of primitive cell: \( V_p = \left| \hat{a}_1 \cdot \hat{a}_2 \times \hat{a}_3 \right| \)

\[
\hat{a}_1 \times \hat{a}_2 = \begin{vmatrix}
\hat{x} & \hat{y} & \hat{z} \\
0 & 0 & a \\
a & 0 & 0
\end{vmatrix} = \hat{x}(0 \cdot a - 0 \cdot a) + \hat{y}(a \cdot 0 - 0 \cdot a) + \hat{z}(0 \cdot 0 - 0 \cdot a) = \frac{1}{a} (-a \cdot \hat{y} + \hat{z}) a^2
\]

\[
|\hat{a}_1 \times \hat{a}_2 | = \frac{1}{a} a(\hat{x} + \hat{z}) \cdot a^2 (-\hat{x} + \hat{y} + \hat{z}) = \frac{1}{8} a^3 (1 + 1) = \frac{2}{8} a^3 = \frac{1}{4} a^3
\]

\[
\frac{V_{\text{prim}}}{V_{\text{conv}}} = \frac{\frac{1}{4} a^3}{a^3} = \frac{1}{4}
\]
In a qualitative model of ionic solids, the component atoms can be thought of as spring-mass systems, and these solids, atoms of the same-sign charge repulse (hence the first term in $U_{\text{tot}}$), and atoms of opposite-sign charge attract (origin of the second term in $U_{\text{tot}}$).

Equilibrium bond length occurs when $\frac{dU_{\text{tot}}}{dR}_{R=R_0} = 0$.

$$\frac{dU}{dR} = \frac{d}{dR} \left[ N \frac{A}{R^6} - N \frac{\alpha e^2}{4 \pi \varepsilon_0 R^2} \right]$$

$$\frac{dU}{dR}|_{R=R_0} = -nN \frac{A}{R_0^{n+1}} + N \frac{\alpha e^2}{4 \pi \varepsilon_0 R_0^2} = 0$$

$$\frac{nN A}{R_0^{n+1}} = \frac{N \alpha e^2}{4 \pi \varepsilon_0 R_0^2}$$

$$\frac{n A}{R_0^{n-1}} = \frac{\alpha e^2}{4 \pi \varepsilon_0}$$

$$R_0 = \frac{4 \pi \varepsilon_0 n A}{\alpha e^2}$$

$$U_{\text{tot}}(R_0) = \frac{1}{N} \left[ \frac{A}{R_0^{n-1}} - \frac{\alpha e^2}{4 \pi \varepsilon_0} \right]$$

$$= \frac{1}{R_0} \left[ \frac{A}{4 \pi \varepsilon_0 R_0^n} - \frac{\alpha e^2}{4 \pi \varepsilon_0} \right]$$

$$= \frac{1}{R_0} \left[ \frac{\alpha e^2}{4 \pi \varepsilon_0 R_0^n} - \frac{\alpha e^2}{4 \pi \varepsilon_0} \right]$$

$$= \frac{\alpha e^2}{4 \pi \varepsilon_0 R_0} \left[ \frac{1}{n} - 1 \right]$$
\[
\frac{U_{\text{tot}}(R_0)}{N} = \frac{\alpha e^2}{4\pi \varepsilon_0 R_0 \left( \frac{1}{n} - 1 \right)}
\]

\(\alpha = 1.75, \ R_0 = 5.63 \times 10^{-10} \text{ m}, \ \frac{U_{\text{tot}}}{N} = 7.75 \text{ eV} = 1.27 \times 10^{-19} \text{ J}\)

\[
\frac{1}{4\pi \varepsilon_0} = 9 \times 10^9 \text{ N m}^2 \text{ C}^{-2}, \ e = 1.6 \times 10^{-19} \text{ C}
\]

\[
\frac{1}{n} - 1 = \left( \frac{\frac{U_{\text{tot}}(R_0)}{N}}{\frac{\alpha e^2}{\varepsilon_0 R_0}} \right)
\]

\[
n = \left[ \left( \frac{\frac{U_{\text{tot}}(R_0)}{N}}{\frac{\alpha e^2}{\varepsilon_0 R_0}} \right) + 1 \right]^{-1}
\]

\[
n = \left[ \frac{5 \times 10^5}{(9 \times 10^9)(1.75)(1.6 \times 10^{-19})} + 1 \right]^{-1}
\]

\[
n = 0.36
\]

\section*{10.2 \(\mathbf{\mathbf{z}}\)}

\[
\mathbf{\hat{a}_1} = \mathbf{\hat{x}}, \ \mathbf{\hat{a}_2} = \mathbf{\hat{y}}, \ \mathbf{\hat{a}_3} = \mathbf{\hat{z}}
\]

\[
\mathbf{b}_1 = 2\pi \frac{\mathbf{\hat{a}_x} \times \mathbf{\hat{a}_y}}{\mathbf{\hat{a}_x} \times \mathbf{\hat{a}_y} \times \mathbf{\hat{a}_z}} = \frac{2\pi}{a_z} \mathbf{\hat{a}_x}
\]

\[
\mathbf{b}_2 = 2\pi \frac{\mathbf{\hat{a}_x} \times \mathbf{\hat{a}_z}}{\mathbf{\hat{a}_x} \times \mathbf{\hat{a}_y} \times \mathbf{\hat{a}_z}} = \frac{2\pi}{a_z} \mathbf{\hat{a}_y}
\]

\[
\mathbf{b}_3 = 2\pi \frac{\mathbf{\hat{a}_y} \times \mathbf{\hat{a}_z}}{\mathbf{\hat{a}_x} \times \mathbf{\hat{a}_y} \times \mathbf{\hat{a}_z}} = \frac{2\pi}{a_z} \mathbf{\hat{a}_z}
\]

The reciprocal lattice vectors for simple cubic are

\[
\mathbf{\hat{b}_1} = \frac{2\pi}{a} \mathbf{\hat{x}}, \ \mathbf{\hat{b}_2} = \frac{2\pi}{a} \mathbf{\hat{y}}, \ \mathbf{\hat{b}_3} = \frac{2\pi}{a} \mathbf{\hat{z}}
\]

and, therefore, are also simple cubic.
b) Distance between planes in simple cubic: \( d = \frac{a}{\sqrt{h^2+k^2+l^2}} \), where \((h,k,l)\) are Miller indices.

\[
d = \frac{a}{\sqrt{h^2+k^2+l^2}} = \frac{a}{N_b}
\]

Length of vector in reciprocal lattice: \( \ell = \frac{2\pi}{\| \mathbf{b} \|} \), where \( \mathbf{b} \) is the vector \( \mathbf{b} = u_1 \mathbf{e}_1 + u_2 \mathbf{e}_2 + u_3 \mathbf{e}_3 \) where \( u_1, u_2, \) and \( u_3 \) are Miller coordinates.

\[
\| \mathbf{b} \| = \sqrt{\sum u_i^2} = \frac{2\pi}{a} \frac{\sqrt{a^2(e_1^2+e_2^2+e_3^2)}}{\sqrt{a^2}} = \frac{2\pi}{a} \sqrt{a^2+1} = \frac{2\pi}{a} N_b
\]

\[
\ell = \frac{2\pi}{\| \mathbf{b} \|} = \frac{2\pi}{\frac{2\pi}{a} N_b} = \frac{a}{N_b}
\]

The separation between planes with Miller indices \((110)\) is the same as length of vectors \( \mathbf{k} = [110,0] \) in the reciprocal lattice, \( d = \ell = \frac{a}{N_b} \).

\(\text{The vector } \mathbf{k} \text{ of the reciprocal lattice is normal to the } (110) \text{ plane in the direct lattice.}\)

Proof: \( \mathbf{a} \cdot \mathbf{b} = |\mathbf{a}| |\mathbf{b}| \cos \theta \), if \( \mathbf{a} \perp \mathbf{b} \), \( \theta = 90^\circ \), \( \mathbf{a} \cdot \mathbf{b} = 0 \)

\( \mathbf{k} \) is vector parallel to \( \mathbf{k} = \mathbf{a} + \mathbf{b} \).

A vector along the Miller plane is parallel to \( \mathbf{m} = \mathbf{a} - \mathbf{b} \).

\( \mathbf{k} \cdot \mathbf{m} = (\mathbf{a} + \mathbf{b}) \cdot (\mathbf{a} - \mathbf{b}) = 1 - 1 = 0 \)
Two relations between length and orientation of vector \([k, l, m]\) of reciprocal lattice and orientation and separation of planes with Miller indices \((k, l, m)\) in direct lattice:

1. The length of a vector \([k, l, m]\) of the reciprocal lattice is the same as the distance of separation of parallel planes with Miller indices \((k, l, m)\) in direct lattice.

2. The vector \([k, l, m]\) of the reciprocal lattice is normal to the plane with Miller indices \((k, l, m)\) of the direct lattice.
\[ W^2 = \frac{K(mM)}{mM} + K \left( \frac{m+m}{mM} \right)^2 - \frac{4 \sin^2(ka/2)}{mM} \]

(b) The first branch acoustic mode and the second branch is optic modes.

The group velocity defined by

\[ v_g = \frac{dW}{d\omega} \]

\[ W = \int \frac{K(mM)}{mM} + K \left[ \left( \frac{m+m}{mM} \right)^2 - \frac{4 \sin^2(ka/2)}{mM} \right]^{1/2} \]

Using chain rules

3. \[ v_g = \frac{dW}{d\omega} \]

\[ v_g = \frac{1}{2} \cdot \left[ \frac{K(mM)}{mM} + K \left( \frac{m+m}{mM} \right)^2 - \frac{4 \sin^2(ka/2)}{mM} \right] \cdot \frac{1}{2} \cdot K \left[ \left( \frac{m+m}{mM} \right)^2 - \frac{4 \sin^2(ka/2)}{mM} \right]^{1/2} \]

\[ \frac{a}{2} \sqrt{\frac{2K}{m} \cos \left( \frac{ka}{2} \right)} \]

... long term
\[ V_{g+} = 0 \cdot A \cdot \cos \left( \frac{ka}{2} \right) \]

A is long term above.

(2) For small value \( k \to 0 \)

\[ \cos \left( \frac{ka}{2} \right) = \cos (0) = 1 \]

So as \( k \to 0 \), group velocity will have maximum value as

\[ V_{g+} = \frac{a}{2} \cdot \sqrt{\frac{4k}{m}} \cdot \frac{1}{2} \left( \frac{k(m+M)}{mM} + k \left( \frac{m+M}{mM} \right)^2 \right)^{-\frac{1}{2}} \]

\[ = \frac{1}{2} \cdot k \left[ \left( \frac{m+M}{mM} \right)^2 \right] \]
\( k \to 0 \Rightarrow V_g \to V_{\text{maximum}} \) value

Now plug in \( k = \frac{\pi}{\alpha} \) (only cos term)

\[ \cos \left( \frac{k \alpha}{2} \right) = \cos \left( \frac{\pi \alpha}{2 \alpha} \right) = \cos \left( \frac{\pi}{2} \right) = 0 \]

\( V_{g \pm} = A \cos \left( \frac{\alpha \xi}{2} \right) \)

\[ V_{g \pm} = 0 \]

This will tell us that \( V_{g \pm} = 0 \) at boundaries that there is propagation across boundaries.