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Midterm Exam: Solid State Physics 476
Nov. 4, 2004

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Solution guide.

1. Consider a hexagonal Bravais lattice.

   (a) What is the relationship between the lattice vectors (lengths and angles)? (2)

   Answer: If lattice vectors are $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ (I would also accept $\vec{a}$, $\vec{b}$, and $\vec{c}$) and the angle between 1 and 2 is γ, 2 and 3 is α, and 1 and 3 is β, then for a hexagonal lattice $|\vec{a}_1| = |\vec{a}_2|$, $\gamma = 120^o$, $\alpha = \beta = 90^o$.

   (b) Draw a sketch of the plane perpendicular to the 6-fold symmetry axis with the lattice points. Also sketch in the unit cell. (2)

   Answer: Just looks like a 2-D hexagonal lattice. The unit cell is a rhombus with $\vec{a}_1$ and $\vec{a}_2$ spanning the oblique angle in a right-handed coordinate system manner (if $\vec{a}_3$ is out of the page then $\vec{a}_2$ is counter-clockwise (or direction of finger on the right hand if the thumb is along $\vec{a}_3$) of $\vec{a}_1$..

   (c) What does it mean to add a "basis"? Give the basis if this is a hexagonal close packed system. (2)

   Answer: A basis is a spatial set of atoms (atom types and positions, often given in terms of the lattice units) that attaches to each lattice point. If this is a hcp then the basis that attaches to the hexagonal lattice is 000, $\frac{2}{3}\frac{1}{3}\frac{1}{2}$, both atoms the same. Although this is "standard" I mentioned a few others in class that better reflect hcp symmetry (such as $\frac{2}{3}\frac{1}{3}\frac{1}{4}$, $\frac{1}{3}\frac{2}{3}\frac{3}{4}$)

   (d) What is a screw transformation? Describe a screw transformation that transforms one of the basis points to another. (There may be a few options for this, pick whichever one you like.) Indicate the location of the screw axis on your previous diagram (4) (bonus: use the correct symbol 2)

   Answer: A screw transformation is a combination of a rotation and a translation. Put the screw axis half-way between the two basis points.

2. Consider a body-centred cubic crystal structure with a lattice constant of 5.5 Å.

   (a) Draw a diagram of the unit cell and indicate where the (110) plane is. (2)

   Answer: Consult your text for a diagram. The (110) plane intersects the cell at two of the edges and is perpendicular to the top face.

   (b) Give the length of the reciprocal lattice vector associated with the (110) plane. (hint: $\vec{G} = h\vec{A} + k\vec{B} + l\vec{C}$) Feel free to take some shortcuts if you know the values for $\vec{A}$ and $\vec{B}$. (2)

   Answer: You know that the reciprocal lattice vectors for a cubic system are in the x, y, z directions and each have length $\frac{2\pi}{a}$. Since $h = 1$ and $k = 1$ we have $|\vec{G}| = 2(\pi/a)\sqrt{h^2 + k^2} = 1.62$ Å^{-1}.

   (c) What is the Laue condition for scattering? If the magnitude of the wavevector of the incident radiation is 4 Å^{-1} Draw the appropriate scattering diagram showing initial $\vec{k}_i$, final $-\vec{k}_f$ and $\vec{G}$. Calculate the scattering angle, what we usually call 2θ. (6).

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Answer: The Laue condition for scattering is $\Delta \vec{k} = \vec{G}$, $2\vec{k}_i \cdot \vec{G} = G^2$, or $\vec{k}_i \cdot \hat{G} = \frac{1}{2}G$. In 2006, I have tried to stay consistent with the book so that $\Delta \vec{k} = \vec{k}_f - \vec{k}_i$ so it would amke more sense to draw initial $-\vec{k}_i$, final $-\vec{k}_f$ along with $\vec{G}$. It is just an isosceles triangle with sides 4, 4, and 1.62. [if $(h00)$ is depicted in the x direction of reciprocal space then $\vec{G}$ would point this way and should terminate on a reciprocal lattice point. 2θ is the angle at the apex of the triangle. Can get it from the law of cosines

$$2\theta = \cos^{-1}\left(\frac{16 + 16 - (1.62)^2}{(2)(4)(4)} \right) = 23.4^\circ \tag{1}$$

or simple construction since it is an isosceles triangle.

3. What is the Dulong-Petit law and what assumptions go into it? Briefly explain how it fails at low temperature with a sketch. What do the Einstein and Debye models say about the temperature dependence of the low temperature specific heat? (just an answer in words is fine) Which of these two models includes low energy modes? (8) (bonus: why do these modes contribute relatively little to the low temperature specific heat, two reasons, 4 points).

Answer: The Dulong-Petit law say that the molar (or per atom) heat capacity of a solid is $3k_B$ (per mole $3k_B N_A = 3R$). The assumptions that go into is that there are N atoms, each one can be treated as a 3-D harmonic oscillator meaning that there are 6 quadratic degrees of freedom. The equipartition theorem says that the thermal average energy is $\frac{1}{1}2k_B T$ per degree of freedom, per atom. So $\bar{E} = 3k_B T$. C_V is the temperature derivvative of $\bar{E}$ (in case you are wondering the ubiquitous subscript V stands for volume to distinguish this from C_P, the heat capacity at constant pressure.) I showed you a figure in class of C_V for diamond, lead, silcon, and aluminum showing how there is a rapid drop in C_V once you are below a certain temperature. The temperature seems to be related to the softness and molecular mass of the material. (soft materials with heavy atoms obey Dulong-Petit to lower temperatures). The Einstein model says that the low T specific heat falls of exponentially (form is actually a bit more complicated but this is usually what is said) and the Debye model says that is varies with T^3. Both models are referring to the lattice specific heat. It is the Debye model which includes low energy modes, which we know determines specific heat at low temperature. They contribute relatively little to the low temperature C_V because they don't actually contain much energy and they have a fairly low density of states.

4. Draw a sketch of the phonon dispersion for a one-dimensional chain of atoms each with mass m, interaction constant k (or $m\omega_0^2$), and atomic separation a. Given functional forms and quantitative descriptions of important values where possible. (8)

Consult Chapter 4, Fig. 4. We have used spring constant k in place of C. The zone edge is $K = \frac{\pi}{a}$, the frequency at the zone edge is $\omega = \sqrt{4k/m}$. The functional form of the dispersion is

$$\omega = \sqrt{\frac{4k}{m}}|\sin(\frac{1}{2}Ka)| \tag{2}$$