Physics 141 A
S. G. Louie

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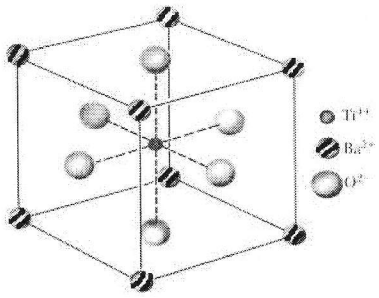
Midterm Exam #1 Solutions

1. Crystal structure, etc. (15 points)

The material barium titanate crystalizes in a structure with one molecular unit $BaTiO_3$ in each basis. The crystal structure is shown below with the Ti, O and Ba atoms occupying the body-center, face-center and corner positions of a conventional cube, respectively. This so-called perovskite structure is very important in several current research areas in condensed matter physics including ferroelectricity and high temperature superconductivity. Let us denote the nearest neightbor Ba-Ba distance by d.



(a) (4 pts.) Write down the explicit expressions (in terms of d) for a set of primitive translation vectors $\vec{a_1}$,$\vec{a_2}$ and $\vec{a_3}$ and for the corresponding set of primitive reciprocal lattice vectors $\vec{b_1}$, $\vec{b_2}$ and $\vec{b_3}$.

(b) (4pts.) What is the shape and volume of the first Brillouin zone? How many allowed $\vec{k}$-states are there in the first Brillouin zone and why?

(c) (3pts.) In addition to translations, there are 48 symmetry operations under which the above structure remains invariant. Name three distinct classes of operations that would leave the above structure the same.

(d) (4 pts.) Determine the structure factors for the first two sets of non-zero reciprocal lattice vectors assuming that the atomic form factors are of the ratios 3:2:1 for Ba:Ti:O.

Solution

(a) The primitive translation vectors are the ones connecting two adjacent Ba atoms on the edges of the cube:

$$\begin{cases} \vec{a_1} = d\hat{x} \\ \vec{a_2} = d\hat{y} \\ \vec{a_3} = d\hat{z} \end{cases}$$

The primitive vectors in reciprocal space are given by $\vec{b_1} = 2\pi \frac{\vec{a_2}\times\vec{a_3}}{|\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}|}$ and its cyclic permutations:

$$\begin{cases} \vec{b_1} = \frac{2\pi}{d}\hat{x} \\ \vec{b_2} = \frac{2\pi}{d}\hat{y} \\ \vec{b_3} = \frac{2\pi}{d}\hat{z} \end{cases}$$

(b) The first Brillouin zone is a cube with side $\frac{2\pi}{d}$, therefore its volume is $V = (\frac{2\pi}{d})^3$. The number of allowed $\vec{k}$-states in the first Brillouin zone is N, where N is the number of primitive cells in the crystal. This result is due to the application of periodic boundary conditions at the ends of the crystal. For macroscopic crystals, N is in the order of 10^{22}, which is a huge number, and that is why we see continuous curves instead of discrete points when we measure bandstructures.

(c) Symmetry operations that leave the crystal invariant are reflections through the (100) and (110) planes, rotation around the (100) axes (4-fold) or the (110) axes (2-fold) or the (111) axes (3-fold) and inversion through the atomic positions.

(d) The generic form of the reciprocal lattice vectors is $\vec{G_m} = \frac{2\pi}{d}(m_1, m_2, m_3)$ and the structure factor is given by $S_G = \sum_j f_j e^{-i\vec{G}\cdot\tau_j}$, where the sum is over all the atoms in the basis. The coordinates of the atoms in the basis are given by:

$$\begin{cases} Ba: & \vec{\tau_1} = (0,0,0) \\ Ti: & \vec{\tau_2} = (\frac{d}{2}, \frac{d}{2}, \frac{d}{2}) \\ O: & \vec{\tau_3} = (\frac{d}{2}, \frac{d}{2}, 0), \vec{\tau_4} = (\frac{d}{2}, 0, \frac{d}{2}), \vec{\tau_5} = (0, \frac{d}{2}, \frac{d}{2}) \end{cases}$$

Therefore, the structure factor is

$$\begin{aligned} S_G &= 3fe^0 + 2fe^{-i\frac{2\pi}{d}\frac{d}{2}(m_1+m_2+m_3)} + f\left[e^{-i\frac{2\pi}{d}\frac{d}{2}(m_1+m_2)} + e^{-i\frac{2\pi}{d}\frac{d}{2}(m_1+m_3)} + e^{-i\frac{2\pi}{d}\frac{d}{2}(m_2+m_3)}\right] = \\ &= 3f + 2f(-1)^{m_1+m_2+m_3} + f\left[(-1)^{m_1+m_2} + (-1)^{m_1+m_3} + (-1)^{m_2+m_3}\right] \end{aligned}$$

Two members of the first two classes of non-zero reciprocal lattice vectors are $\vec{G}_{100} = \frac{2\pi}{d}(1,0,0)$ and $\vec{G}_{110} = \frac{2\pi}{d}(1,1,0)$. For these vectors we find:

$$\begin{aligned} \vec{G}_{100} = \frac{2\pi}{d}(1,0,0) &\rightarrow S_{100} = 3f - 2f + f[-1-1+1] = 0 \\ \vec{G}_{110} = \frac{2\pi}{d}(1,1,0) &\rightarrow S_{110} = 3f + 2f + f[+1-1-1] = 4f \end{aligned}$$

2. Silicon (15 points)

Our whole electronic industry is based on the semiconductor silicon (Si). It crystallizes in the diamond structure, which is an fcc lattice with two silicon atoms per primitive unit cell and has a lattice parameter of $a = 5.43$ Ångstroms for the edge of the conventional fcc cube.

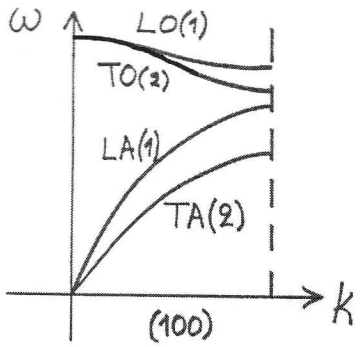
(a) (5 pts.) Make a rough sketch of the phonon dispersion curve for Si along the (100) direction in the Brillouin zone. What is the total number of phonon branches of each of the following types: longitudinal acoustical, transverse acoustical, longitudinal optical and transverse optical.

(b) (5 pts.) Estimate the maximum acoustic phonon frequency (in s^{-1}) given the above lattice constant and a measured sound velocity of 8×10^5 cm/s. Also, estimate the Debye temperature (in degrees Kelvin).

(c) (5 pts.) Sketch and label qualitatively the temperature dependence of the lattice heat capacity of Si from $T = 0K$ to near the melting point (which is $1687K$).

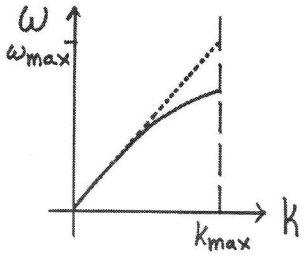
Solution

(a) The phonon dispersion curves along the (100) direction are approximately shown in the picture.



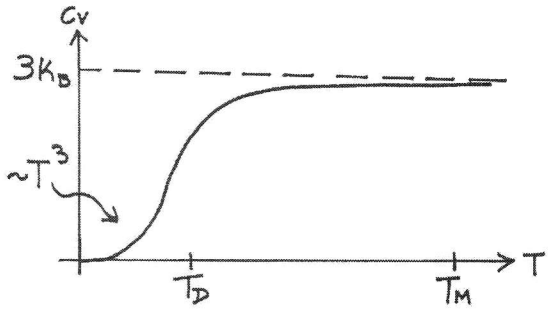
Since silicon has two atoms per unit cell and we live in three dimensions, there should be $2 \times 3 = 6$ phonon branches. These will be 3 acoustical branches (1 longitudinal and 2 transverse) and 6-3=3 optical branches (1 longitudinal and 2 transverse). Moreover, since we are looking at phonons along a high symmetry direction, we expect the transverse modes to be degenerate. Finally, we know that the acoustical modes approach $\omega = 0$ linearly as $k \to 0$.

(b) An estimate for the Debye frequency can be found if we extrapolate the linear dispersion relation for acoustical phonons $\omega = v_s k$ for all k.



At the Brillouin zone boundary, the order of magnitude for k is $k \approx \frac{\pi}{a}$ where a is the lattice constant. Therefore $\omega_{\max} \approx v_s \pi k_{\max} \approx \frac{\pi v_s}{a} = \frac{8\pi \times 10^3 m/s}{5.43 \times 10^{-10} m} = 4.62 \times 10^{13} \mathrm{s}^{-1}$. For this value of ω, $T_D = \frac{\hbar\omega}{k_B} = 352K$.

(c) The plot of the heat capacity per atom versus temperature is shown in the figure.



The qualitative features of this plot are the T^3 temperature dependence for low temperatures and the approximately constant $3k_B$ value according to Dulong-Petit law for temperatures between the Debye temperature T_D and the melting temperature T_M.

3. Density of states and heat capacity (10 points)

Let us suppose that the low-frequency phonons of a 3-dimensional crystal have a dispersion relation given by

$$\omega(\vec{k}) = Ak^2$$

(a) (5 pts.) Derive an expression for the density of states $D(\omega)$ for these phonons.

(b) (5 pts.) What is the temperature dependence for the lattive heat capacity $C_V(T)$ for such a system at low temperature and why? (You are not required to obtain the exact expression for $C_V(T)$, only its temperature dependence.)

Solution

(a) The density of states per mode is given by $D_\lambda(\omega) = \frac{V}{(2\pi)^3}\int \frac{dS_\omega}{v_g}$ where dS_ω is the infinitesimal surface element of the surface in k-space where $\omega =$ constant and $v_g = \partial\omega/\partial k$. Here $v_g = 2Ak = 2\sqrt{A\omega}$ which is constant for constant ω, and $D_\lambda(\omega) = \frac{V}{8\pi^3}\frac{1}{2\sqrt{A\omega}}\int dS_\omega = \frac{V}{8\pi^3}\frac{1}{2\sqrt{A\omega}}4\pi k^2 = \frac{V}{8\pi^3}\frac{1}{2\sqrt{A\omega}}4\pi\frac{\omega}{A} = \frac{V}{4\pi^2 A^{3/2}}\sqrt{\omega}$, because the surface of constant ω is the surface of a sphere with radius k. The total density of states is $D(\omega) = 3D_\lambda(\omega)$, since there are 3 modes of oscillation per k-point. Therefore:
$D(\omega) = \frac{dN(\omega)}{d\omega} = \frac{3}{2}\frac{V}{2\pi^2}\frac{\omega^{1/2}}{A^{3/2}}$.

(b) In analogy to the Debye frequency, there is a maximum frequency of oscillations, due to the fact that there is a finite number of normal modes (3N) in this system. By demanding $N(\omega_{\max}) = 3N$ we find $\omega_{\max} = (\frac{6\pi^2 N}{V})^{2/3}A$.

$$\begin{aligned} U &= \int_0^{\omega\max} \frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1}D(\omega)d\omega \propto \int_0^{\omega\max}\frac{\omega}{e^{\hbar\omega/k_BT}-1}\omega^{1/2}d\omega \propto \\ &\propto T^{5/2}\int_0^{x\max}\frac{x^{3/2}dx}{e^x-1} \approx T^{5/2}\int_0^{\infty}\frac{x^{3/2}dx}{e^x-1} \propto T^{5/2} \end{aligned}$$

In the calculations above, we have changed the variable in the integral $x = \frac{\hbar\omega}{k_BT}$ and have set $x_{\max} = \frac{\hbar\omega\max}{k_BT} \to \infty$ for $T \to 0$. Taking the derivative gives us

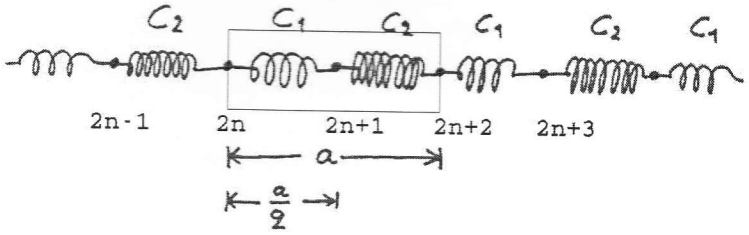
$$C_V \propto T^{3/2}$$

4. Phonons (10 points)

(a) (5 pts.) Write down the equations of motion for the atoms in a one-dimensional crystal (a linear chain) with lattice constant a and force constants between nearest-neighbor atoms that are alternatively C_1 and C_2. The atoms in the chain are of identical mass M.

(b) (5 pts.) Obtain the equations which determine the eigenfrequencies ω for lattice waves with wavevector k. Calculate the values for ω at $k = \pi/a$.

Solution



(a) The equations of motion are

$$\begin{cases} M\ddot{u}_{2n} = C_1(u_{2n+1} - u_{2n}) + C_2(u_{2n-1} - u_{2n}) \\ M\ddot{u}_{2n+1} = C_2(u_{2n+2} - u_{2n+1}) + C_1(u_{2n} - u_{2n+1}) \end{cases}$$

(b) We try a solution of the form

$$\begin{cases} u_{2n} = u_e e^{i(kna-\omega t)} \\ u_{2n+1} = u_o e^{i(kna-\omega t)} \end{cases}$$

and we find

$$\begin{cases} -M\omega^2 u_e = C_1(u_o - u_e) + C_2(u_o e^{-ika} - u_e), & i = 2n \\ -M\omega^2 u_o = C_2(u_e e^{ika} - u_o) + C_1(u_e - u_o), & i = 2n+1 \end{cases}.$$

We are only interested in the values of ω at $k = \frac{\pi}{a}$ where $e^{ika} = e^{-ika} = -1$ therefore

$$\begin{cases} -M\omega^2 u_e = C_1(u_o - u_e) - C_2(u_o + u_e) \\ -M\omega^2 u_o = -C_2(u_e + u_o) + C_1(u_e - u_o) \end{cases}.$$

We demand that the above linear system has non-trivial solution and therefore its determinant must be zero:

$$\begin{vmatrix} M\omega^2 - (C_1 + C_2) & C_1 - C_2 \\ -C_2 + C_1 & M\omega^2 - (C_1 + C_2) \end{vmatrix} = 0 \Rightarrow (M\omega^2)^2 - 2M\omega^2(C_1+C_2) + (C_1+C_2)^2 - (C_1-C_2)^2 = 0 \Rightarrow$$

$$\Rightarrow M^2\omega^4 - 2M(C_1 + C_2)\omega^2 + 4C_1C_2 = 0 \Rightarrow \omega^2 = \frac{2M(C_1 + C_2) \pm 2M|C_1 - C_2|}{2M^2} \Rightarrow$$

$$\Rightarrow \omega^2 = \frac{C_1 + C_2 \pm |C_1 - C_2|}{M} \Rightarrow \omega^2 = \begin{cases} 2C_1/M \\ 2C_2/M \end{cases}$$