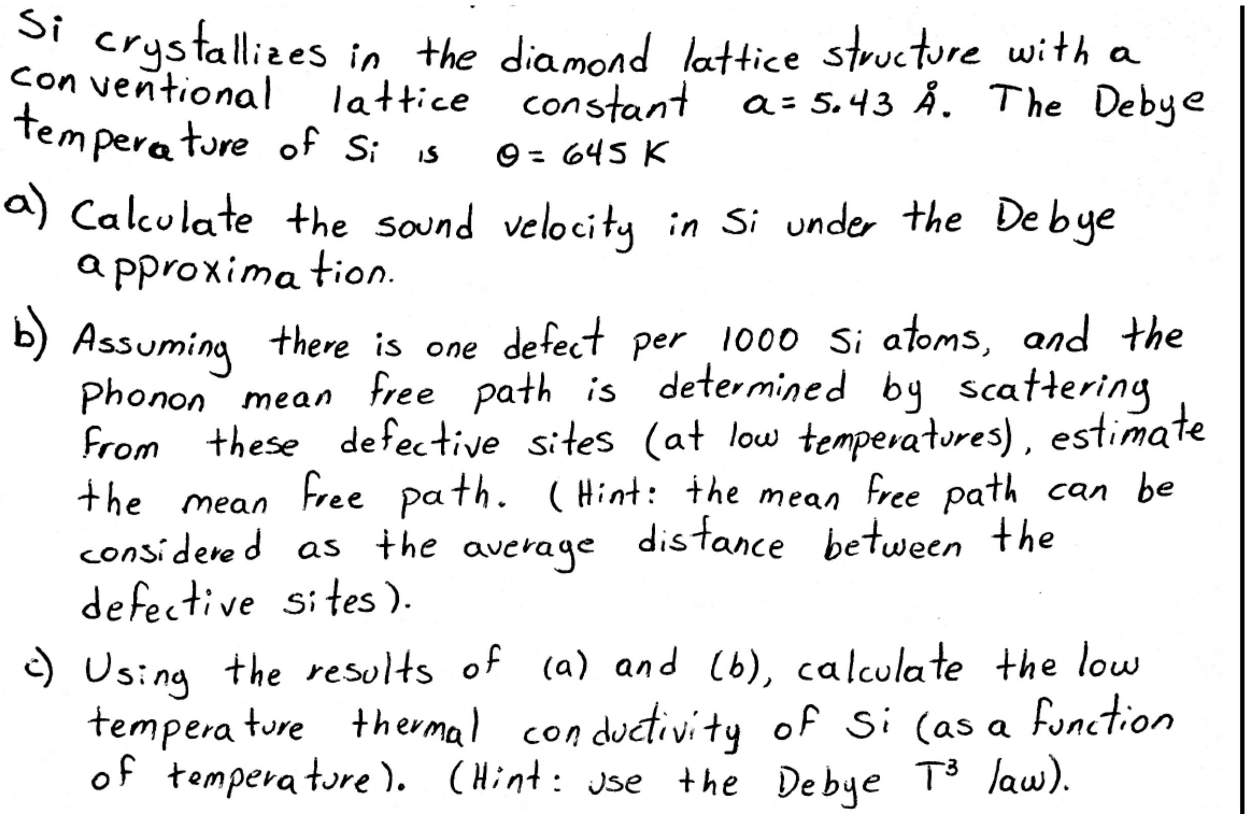
These questions were constructed by the students that took Solid State Physics, i.e. PHYS5320, in spring 2015. Special thanks to Parisa Jalili, Roberto Lopez, Vicente Estrada Carpeter, Eric Welch, Fidel Twagirayezu, Ahad Talukder, Rony Saha, Jung-Yong Lee, Elizabeth Leblanc, and Yubo Cui.

1. Explain the phenomenon heat capacity in terms of elastic waves in a crystal. Address also on how heat is transported in solid materials. Use in your answer the following terminology: Einstein model, Debye model, heat capacity, phonons.

As we can see photons as an interaction of electromagnetic field, we can see phonons as a collection of particles which propagate through crystals. In order to explain the heat capacity of a solid, Einstein thought that each atom in a crystal acts like an harmonic oscillator independently. His theory was well consistent with experimental results at high temperature, but it was not at low temperature. On the contrary, Debye thought that atoms in a crystal were affected by other atoms' motion, and he succeeded in explaining the heat capacity of a solid. To be specific, the vibration of atoms which is generated in a center of a certain lattice point in a crystal is an interaction of atoms, therefore vibration cannot stay at one atom, but it propagates as waves in a crystal. This is a sound wave in a crystal. As a result, we have to follow the rule of quantum mechanics to explain the motion of an atom exactly. And if we quantize the sound wave, it represents the features of particles. A phonon is a sound wave which has features of particles.

2.



Si crystallizes in the diamond lattice structure with a conventional lattice constant $a = 5.43$ Å. The Debye temperature of Si is $\Theta = 645$ K

a) Calculate the sound velocity in Si under the Debye approximation.

b) Assuming there is one defect per 1000 Si atoms, and the phonon mean free path is determined by scattering from these defective sites (at low temperatures), estimate the mean free path. (Hint: the mean free path can be considered as the average distance between the defective sites).

c) Using the results of (a) and (b), calculate the low temperature thermal conductivity of Si (as a function of temperature). (Hint: use the Debye T^3 law).

a) From Kittel pg. 112 Eq. 28

$$\theta = \frac{\hbar v}{K_B}\left(\frac{6\pi^2 N}{V}\right)^{\frac{1}{3}} \longrightarrow v = \frac{K_B\,\theta}{\hbar}\left(\frac{V}{6\pi^2 N}\right)^{\frac{1}{3}}$$

For a diamond lattice we have 8 atoms per unit cell

$$\frac{V}{N} = \frac{a^3}{8\text{ atoms}} = \frac{(5.43\times10^{-10}m)^3}{8\text{ atoms}} = 2\times10^{-29}\,m^3$$

$$v = \frac{K_B\,\theta}{\hbar}\left(\frac{V}{6\pi^2 N}\right)^{\frac{1}{3}} = \frac{(1.38\times10^{-23}\,JK^{-1})\,(645\,K)}{1.05\times10^{-34}\,Js}\left(\frac{2\times10^{-29}\,m^3}{6\pi^2}\right)^{\frac{1}{3}}$$

$$\boxed{v \approx 5903.5\ m/s}$$

b) If we have 8 atoms per unit cell, then on 1000 atoms we have $\frac{1000}{8} = 125$ unit cells. If we form a cube with those 125 unit cells, then the volume is going to be $125\,a^3$, so we know that each side is going to have a length of $(125)^{\frac{1}{3}}a = 5a$, and the mean free path can be considered as the average distance between the defective sites, wich is

$\ell = 5a = 27.15\ \text{Å}$

c) From Eq. 42 on page 122

$K = \frac{1}{3} C v \ell$

we already know v and ℓ, and C is the heat capacity per unit volume, so $C = \frac{C_V}{V}$

From Eq. 32 on page 114

$C_V = 234 \, N k_B \left(\frac{T}{\theta}\right)^3$

$C = \frac{C_V}{V} = 234 \, \frac{N k_B}{V} \left(\frac{T}{\theta}\right)^3$

$C = 234 \left[\frac{(8)(1.38 \times 10^{-23} \, J \, K^{-1})}{(5.43 \times 10^{-10} \, m)^3}\right] \left(\frac{T}{645 \, K}\right)^3$

$C = 0.601 \, T^3$

$K = \frac{1}{3} (0.601 \, T^3)(5903.5)(27.15 \times 10^{-10})$

$\boxed{K = 3.21 \times 10^{-6} \, T^3}$

3. A 1-d line of atoms with length L=4, has periodic boundary conditions such that the atom at n=0 is identical to the atom at n=4. Notice that this system contains 4 different atoms.

a. Draw the lattice in real space, label each atom with its numerical position.

b. How many phonon modes does this system has. Draw them and label them with the appropriate k-vector.

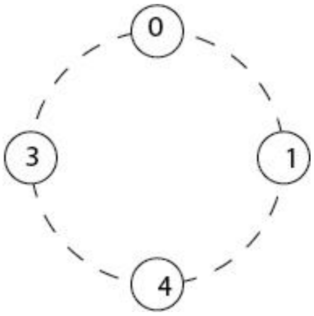
c. We derived in class the dispersion relation for such system (see page 92 in Kittel) it is plotted in Fig. 4. For very large N-case. Note that this plot is actually a series of delta functions. Draw the dispersion relation for this particular case.

d. Draw the density of states function for this system.

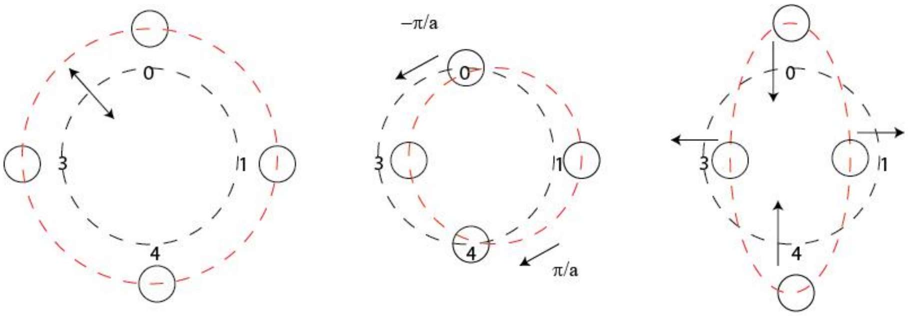
e. Write down an expression for internal energy of this system. It is not necessary to convert the summation in an integral as the number of states is so low.

Note that we could use the U to calculate C_V by taking the derivative towards T. We won't do that here as it will only show our Calculus talents.

Key: a. I draw them in a circle as we are considering periodic boundary conditions.



b. The modes are given below. I call K=0 the heart beat mode, K=π/a the CW traveling wave, K=-π/a the CCW traveling wave, and K=2π/a the "squeezy" standing wave if that were a word. Note that K=-2π/a will result in exactly the same type of standing wave as K=2π/a, so they are similar modes.

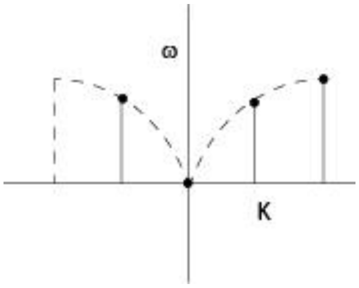


K=0 K=+/-π/a K=2π/a

c. We have only four modes so there are four different non-zero values in our graph. See graph below. Notice that even figure 4 of chapter 4 is not a continuous function but consists of a series of points separated by 2π/L.

The dashed line is a guide to the eye and is described by the root of equation 7 of chapter 4, i.e.

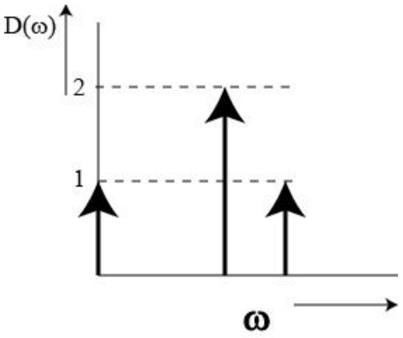
$$\omega = \sqrt{\frac{4C}{M}}\sin\left(\frac{Ka}{2}\right)$$



d. Using above dispersion equation we can calculate the w for the allowed K-values of the different modes:

$$\omega = 0,\ \frac{1}{\sqrt{2}}\sqrt{\frac{4C}{M}}, \sqrt{\frac{4C}{M}}$$

Note that both the positive and negative K values have the same frequency.



e. Since this is a 1D problem we have only 1 mode, i.e. the longitudinal mode, at least if we assume that we live a 1D and there is only 1 direction in space.

$$U = \sum_P \sum_K \frac{\hbar\omega_{P,K}}{e^{\hbar\omega_{P,K}/\tau} - 1} = \sum_K \frac{\hbar\omega_{P,K}}{e^{\hbar\omega_{P,K}/\tau} - 1} = \left[0 + 2\frac{\hbar\frac{1}{\sqrt{2}}\sqrt{\frac{4C}{M}}}{e^{\hbar\frac{1}{\sqrt{2}}\sqrt{\frac{4C}{M}}/\tau} - 1} + \frac{\hbar\sqrt{\frac{4C}{M}}}{e^{\hbar\sqrt{\frac{4C}{M}}/\tau} - 1} \right]$$

Note that real 1D system do not exists, even a straight polymer is situated in our 3D world. So in addition to the longitudinal mode, atoms can also vibrate perpendicular to the axis of the molecule. A lot of the polymers are not straight but have some type of “zig-zag” which means that the elastic compliance constants in the x and y-directions (perpendicular to the polymer axis) might be different, resulting in two transverse modes and one longitudinal mode.

4. Consider a linear chain in which alternate ions have mass M_1 and M_2, and only nearest neighbors interact.

a. Set up the system of difference equations for such system and determine the characteristic equation.

b. Assume that the dispersion relation and the nature of the normal model is given by the following equation:

$$\omega^2 = \frac{C}{M_1 M_2}\left(M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 \cos(Ka)} \right)$$

Discuss the form of the dispersion relation and the nature of the normal modes when $M_1 >> M_2$ (i.e. calculate and draw the normal modes).

c. Compare the dispersion relation with that of the monatomic linear chain when M_1 is approximately equal to M_2.

Key problem 4: a. is worked out in Kittel on pages 97 and 98. The characteristic equation is given by equation (22). b. Using the abc equation we can rewrite (22) so it looks the same as the equation provided above. $\omega^2 = \frac{C}{M_2}\left(1+\frac{M_2}{M_1} \pm \sqrt{1+\frac{M_2^2}{M_1^2}+2\frac{M_2}{M_1}\cos(Ka)}\right)$

For the optical branch, i.e. the plus sign, and the assumption that $M_1 >> M_2$ we find that the dispersion relation will be:

$$\omega^2 \approx 2\frac{C}{M_2}$$

Note that this is consistent with equation (23) in Kittel as for M1>>M2 the sum of the reciprocal masses equals the reciprocal mass of the lighter atom, i.e. (1/M1+1/M2) is approximately 1/M2.

For the acoustic branch near small K value I have to include the K-dependence in the square root. I can do a Taylor approximation for the square root: $\sqrt{1+x} \approx 1+\frac{1}{2}x$. I believe that it is still ok to ignore the M2/M1 terms as they are offsets that shift the whole dispersion curve of the acoustic branch.

$$\omega^2 = \frac{C}{M_2}\left(1+\frac{M_2}{M_1} \pm \sqrt{1+\frac{M_2^2}{M_1^2}+2\frac{M_2}{M_1}\cos(Ka)}\right) \approx \frac{C}{M_2}\left(1+\frac{M_2}{M_1}-1-\frac{1}{2}\frac{M_2^2}{M_1^2}-\frac{M_2}{M_1}\cos(Ka)\right)$$

Note that the cosine will vary slowly for small K so a series will give a K^2 term, i.e.

$$\omega^2 = \frac{C}{M_2}\left(1+\frac{M_2}{M_1} \pm \sqrt{1+\frac{M_2^2}{M_1^2}+2\frac{M_2}{M_1}\cos(Ka)}\right) \approx \frac{C}{M_2}\left(1+\frac{M_2}{M_1}-1-\frac{M_2}{M_1}\cos(Ka)\right)$$

$$= \frac{C}{M_2}\left(\frac{M_2}{M_1}-\frac{M_2}{M_1}+\frac{1}{2}\left(\frac{M_2}{M_1}\right)(Ka)^2\right) \approx \frac{C}{2}\frac{1}{M_1}K^2a^2$$

Which is similar to equation (24) in Kittel. Note that both do not tell us a lot about the motion. In order to learn more about the motion we need to plug the w values into the difference equations. First for the optical branch, i.e. using

$$\omega = \sqrt{\frac{2C}{M_2}}$$

Plugging into difference equations gives (equation (24) in Kittel):

$$-\frac{2C}{M_2}M_1u_o = Cv_o\left[1+e^{-iKa}\right]-2Cu_o$$
$$-\frac{2C}{M_2}M_2v_o = Cu_o\left[e^{iKa}+1\right]-2Cv_o$$

We can write those equations as a matrix to find u_o and v_o:

$$\begin{pmatrix} -2C+\frac{2CM_1}{M_2} & C\left(1+e^{-iKa}\right) \\ C\left(e^{iKa}+1\right) & -2C+\frac{2CM_1}{M_2} \end{pmatrix}\begin{pmatrix} u_o \\ v_0 \end{pmatrix}=0$$

For u_o over v_o I find now:

$$\frac{u_o}{v_o}=-\frac{M_2}{M_1}$$

So for the optical branch the amplitude of vibration of the mass 1, i.e u, is much larger than the amplitude of vibration of mass 2. In other words the vibration amplitude of the lightest atom is the largest.

For the acoustic branch, we have the following dispersion relation (note K dependence):

$$\omega=\sqrt{\frac{C}{2M_1}}Ka$$

So we find for the difference equations (plugging in equation (20) of Kittel:

$$-\frac{C}{2M_1}K^2a^2M_1u_o = Cv_o\left[1+e^{-iKa}\right]-2Cu_o$$
$$-\frac{C}{2M_1}K^2a^2M_2v_o = Cu_o\left[e^{iKa}+1\right]-2Cv_o$$

Assuming that K is very small, the left sides will go to zero while the exponential term becomes 1. So then we find for the ratio of uo and vo 1, so they both have the same amplitude.

Note that for values away from the center of the Brillouin zone the ratio of u0 and vo in general is complex. This means that both atoms oscillate out of phase. In general the phase difference is somewhere between 0 and π.

c. When M1=M2 the dispersion relation is similar to that of a mono-atomic linear chain, at least it should be. Let see, for a monatomic linear chain we would only have one branch. Let us plug in M1=M2=M into the given dispersion relation:

$$\omega^2 = \frac{C}{MM}\left(M + M \pm \sqrt{M^2 + M^2 + 2M^2\cos(Ka)}\right) = \frac{C}{M}\left(2 \pm \sqrt{2 + 2\cos(Ka)}\right)$$
$$= \frac{C}{M}\left(2 \pm \sqrt{2 + 4\cos^2\left(\frac{Ka}{2}\right) - 2}\right) = \frac{C}{M}\left(2 \pm 2\cos\left(\frac{Ka}{2}\right)\right)$$

Which is indeed the normal dispersion relation for a mono-atomic linear branch. So there is only one branch, which makes sense.

For those of you who have time left, you might want to consider to repeat problem (b) but now not for the center of the Brillouin zone but near the edges of the Brillouin zone, so assume k=π/a and determine ω from the dispersion equation provided under question b. Then use this ω to calculate the u_o and the v_o from equation (20) in Kittel. Note that you have two different ωs, one for the optical branch and one for the acoustical branch. For the optical branch you will find that only v is time dependent and u is actually independent of the time. For the acoustical branch you will find the opposite.

5a. Find N, the total number of phonon modes in 4D. Assume that the volume of a sphere in 4D is equal to:

$$V = \frac{1}{2}\pi^2 r^4$$

b. Determine the density of states in 4D. Assume that the speed of elastic waves is constant and given by the following dispersion relation: $\omega = vK$

c. Determine the total thermal energy in 4D.

d. Find the heat capacity of the lattice in 4D.

Key Problem 5:

a. For periodic boundary conditions I expect the following traveling waves to be eigenfunctions of the 4D system. The wave-vector has now four components and I expect the following modes in a material that is LxLxLxL:

   K_x, K_y, K_z, K_γ = 0, +/-2π/L, +/-4π/L, +/-6π/L, …….

   So states are separated by 2π/L in all four directions resulting in one state per 4d-volume of $(2\pi/L)^4$. Or the density of states in k-space is $(L/2\pi)^4$ per 4d-volume unit. So the total number of states with a K-vector smaller than K_m is equal to the volume of the 4d-sphere times the density in K-space, i.e.

$$\frac{1}{2}\pi^2 K_m^4 \left(\frac{L}{2\pi}\right)^4$$

b. I can find the density of states by taking the derivative towards ω, i.e.

$$D(\omega)=\frac{\partial N}{\partial \omega}=\frac{\partial N}{\partial K}\frac{\partial K}{\partial \omega}=\left(\frac{L}{2\pi}\right)^4\frac{1}{2}\pi^2 4K^3\frac{\partial K}{\partial \omega}$$

Now I use the provided dispersion relation:

$$D(\omega)=\frac{V_{4D}\omega^3}{8\pi^2 v^4}$$

Where V_{4D} is the four dimensional volume and v is the speed of sound.

c. I can find the total thermal energy by assuming that I can still use Planck's distribution function in 4D, i.e.

$$U=\sum_p\int_0^\infty\frac{V_{4D}\omega^3}{8\pi^2 v^4}\frac{\hbar\omega}{e^{\hbar\omega/(k_BT)}-1}d\omega$$

Now substitute $\hbar\omega/(k_BT)=\hbar\omega/\tau \Leftrightarrow \omega=\frac{\tau x}{\hbar}$ and $\mathrm{d}\omega=\frac{\tau}{\hbar}dx$

$$U=4\frac{V_{4D}}{8\pi^2 v^4}\int_0^\infty\frac{\tau^3x^3}{\hbar^3}\frac{\tau^2 x}{\hbar}\frac{1}{e^x-1}dx=4\frac{V_{4D}k_B^5T^5}{8\pi^2v^4\hbar^4}\int_0^\infty\frac{x^4}{e^x-1}dx\approx\frac{25k_B^5T^5}{8\pi^2v^4\hbar^4}$$

Note that we assumed four different polarizations, i.e. one longitudinal and 3 transverse polarizations.

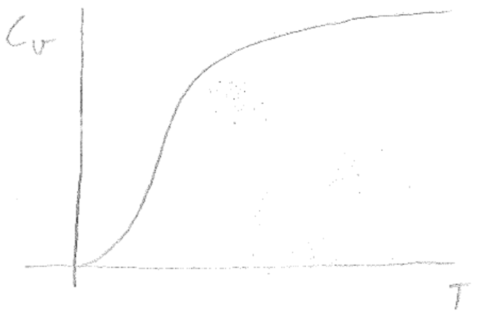
d. I find the heat capacity by taking the derivative of the internal energy towards T, i.e.

$$C_V=\frac{\partial U}{\partial T}=\frac{125Vk_B^5T^4}{8\pi^2v^4\hbar^4}$$

Possible Exam Question w/ Solution

Sketch the experimental behavior of the heat capacity of crystalline solids. Discuss which models should be used in the different temperature regimes. Show calculations to support your discussion. Include in your discussion which density of state model you are using.

Solution:



In the low temperature regime $\left(x = \frac{\hbar\omega}{k_B T} \gg 1 \right)$ we can use the Debye model approximation.

First we need to start with the Debye model for density of states. Recall that $D(\omega) = \frac{dN}{d\omega}$ where N is the number of modes below $\vec{K}_{max}$. N can be found using the relation:

$$N = \left(\frac{\text{\# of modes}}{\text{Volume in K-space}} \right) \left(\begin{matrix} \text{Volume of sphere} \\ \text{w/ radius} = K_{max} \end{matrix} \right).$$

In 3D, the unit volume in K-space is given by $\left(\frac{2\pi}{L}\right)^3$, so then

$$N = \left(\frac{L}{2\pi}\right)^3 \left(\frac{4}{3} \pi K_{max}^3\right)$$

we can convert this to $N(\omega)$ using the dispersion relation

$\omega = v K$ so then we get $N(\omega) = \left(\frac{L}{2\pi}\right)^3 \frac{4}{3} \pi \left(\frac{\omega}{v}\right)^3$

Solution continued

Now taking a derivative, we get

$$D(\omega) = \frac{V}{2\pi^2}\frac{\omega^2}{v^3}$$

with this we can now find the total internal energy of the crystal using

$$U = \int D(\omega)\langle n(\omega)\rangle \hbar\omega \, d\omega$$

Recall that $\langle n(\omega)\rangle$ is given by Planck's distribution:

$$\langle n(\omega)\rangle = \frac{1}{\exp\left(\frac{\hbar\omega}{k_bT}\right)-1}$$

so then our integral becomes

$$U = \int_0^{\omega_D}\left(\frac{V\omega^2}{2\pi^2 v^3}\right)\frac{\hbar\omega}{\exp\left(\frac{\hbar\omega}{k_bT}\right)-1}\, d\omega$$

for each polarization

In 3D, there are 3 polarizations so then

$$U = \frac{3V}{2\pi^2 v^3}\int_0^{\omega_D}\omega^2\frac{\hbar\omega}{\exp\left(\frac{\hbar\omega}{k_bT}\right)-1}\, d\omega$$

Now lets make a change of variable

Let $x \equiv \frac{\hbar\omega}{k_bT}$; $\hbar\omega = k_bTx$; $\omega = x\frac{k_bT}{\hbar}$; $\omega^2 = \frac{x^2(k_bT)^2}{\hbar^2}$

and $d\omega = \frac{k_bT}{\hbar}dx$

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Because we are working in the low temperature limit,

$x_D = \frac{\hbar \omega_D}{k_b T} >> 1$, we can let $x_D \to \infty$, with this we get

$$U = \frac{3V}{2\pi^2 v^3 \hbar^3} (k_b T)^4 \int_0^\infty \frac{x^3}{\exp(x) - 1} \, dx$$

Recall that

$$\zeta(n)\Gamma(n) = \int_0^\infty \frac{u^{n-1}}{\exp(u) - 1} \, du$$ so then

$$U = \frac{3V}{2\pi^2 v^3 \hbar^3} (k_b T)^4 \zeta(4)\Gamma(4) \qquad \zeta(4)\Gamma(4) = \frac{\pi^4}{15}$$

$$U = \frac{3V}{2\pi^2 v^3 \hbar^3} (k_b T)^4 \frac{\pi^4}{15}$$ and finally $C_v = \left(\frac{\partial U}{\partial T}\right)_V$

$$C_v = \frac{3V}{2\pi^2 v^3 \hbar^3} \frac{\pi^4}{15} k_b^4 \cdot 4T^3$$ this explains the curvature of the C_v vs T graph in the low temperature limit

Now lets look at the high temperature limit. We see from the curve that as T → ∞ C_v approaches a constant value. For this, $\left(x = \frac{\hbar\omega}{k_b T} << 1\right)$ we can use the Einstein model. Once again, we need to start with the density of states. According to the Einstein model,

$D(\omega) = N\delta(\omega - \omega_0)$ so then the total energy is given by $U = \int_0^{\omega_D} \langle n(\omega)\rangle \hbar\omega N \delta(\omega-\omega_0)\, d\omega$

$$U = \int_0^{\omega_D} \frac{\hbar\omega}{\exp\left(\frac{\hbar\omega}{k_b T}\right) - 1} N\delta(\omega - \omega_0)\, d\omega$$

$$U = \frac{\hbar\omega_0 N}{\exp\left(\frac{\hbar\omega_0}{k_b T}\right) - 1}$$

with this we can find the heat capacity using $C_v = \left(\frac{\partial U}{\partial T}\right)_V$

$$C_v = \frac{dU}{dT} = N\hbar\omega_0 \frac{d}{dT}\left(\frac{1}{\exp\left(\frac{\hbar\omega_0}{k_b T}\right) - 1}\right)$$

$$= N\hbar\omega_0 \left[-\left(\exp\left(\frac{\hbar\omega_0}{k_b T}\right) - 1\right)^{-2} \cdot \exp\left(\frac{\hbar\omega_0}{k_b T}\right) \cdot \left(-\frac{\hbar\omega_0}{k_b} T^{-2}\right)\right]$$

$$C_v = N\left(\frac{\hbar\omega_0}{k_b T}\right)^2 k_b \cdot \frac{\exp\left(\frac{\hbar\omega_0}{k_b T}\right)}{\left(\exp\left(\frac{\hbar\omega_0}{k_b T}\right)-1\right)^2}$$

For the high temperature limit, $x = \frac{\hbar\omega_0}{k_b T} << 1$, meaning that we can approximate the exponential terms as $e^x \simeq 1 + x$. So then we get

$$C_v \simeq N\left(\frac{\hbar\omega_0}{k_b T}\right)^2 k_b \cdot \left[\frac{1+\frac{\hbar\omega_0}{k_b T}}{\left(1+\frac{\hbar\omega_0}{k_b T}-1\right)^2}\right]$$

$$C_v \simeq N \cancel{\left(\frac{\hbar\omega_0}{k_b T}\right)^2} k_b \left[1+\frac{\hbar\omega_0}{k_b T}\right] \cancel{\left[\frac{\hbar\omega_0}{k_b T}\right]^{-2}}$$

$$C_v \simeq N k_b \left[1+\frac{\hbar\omega}{k_b T}\right]$$

But $x = \frac{\hbar\omega_0}{k_b T} << 1$, so then this can be approximated as

$C_v \simeq N k_b$ for 1D. For 3D, there are 3 polarization, so then we need to include a leading factor of 3:

$C_v \simeq 3Nk_b$ which agrees with the nearly constant behavior of the heat capacity in the high temperature limit

7. Derive an expression for the specific heat of a one-dimensional diatomic lattice. Make the Debye approximation for the acoustic branch and assume that the optical branch is flat. Investigate the high and low temperature limits. Assume that the speed of the elastic waves is constant and equal to v.

Solution: The density of states in 1D is given by:

$$D(\omega)=\frac{L}{\pi}\left(\frac{\partial\omega}{\partial K}\right)^{-1}=\frac{L}{\pi v}$$

In the Debye approximation the number of allowed modes in the acoustic branch is:

$$\int_0^{\omega_D} D(\omega)d\omega = N$$

So we get for ω_D:

$$\omega_D=\frac{N\pi v}{L}\Leftrightarrow D(\omega)=\frac{N}{\omega_D}$$

So we find now for the heat capacity at constant volume:

$$C_V^{acoustic}=\frac{dU}{dT}$$

After differentiation, change to the dimensionless variable $x=\hbar\omega/(k_BT)$ and by defining the Debye temperature θ_D as $k_B\theta_D=\hbar\omega_D$ we get:

$$C_V^{acoustic}=\frac{RT}{\theta_D}\int_0^{\theta_D/T}\frac{x^2e^x}{\left(e^x-1\right)^2}dx$$

At low temperature, T<<qD, so the upper limit of the integral approaches infinity and we get

$$C_V^{acoustic}=R\frac{T}{\theta_D}\frac{\pi^2}{3}$$

Or the heat capacity is linear proportional to T. Note that at low temperature I do not expect that optical phonon modes are occupied.

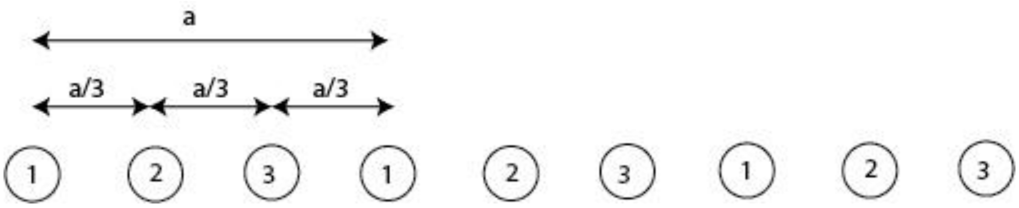
At high temperatures however these optical phonons need to be included in the model. Note that since we assume that the optical branch is flat I can use the Einstein model for the optical branch heat capacity (only one oscillator). So we get:

$$C_V^{tot} = C_V^{acoustic} + C_V^{optical} = \frac{RT}{\theta_D}\int_0^{\theta_D/T} \frac{x^2 e^x}{\left(e^x - 1\right)^2} dx + R\left(\frac{\hbar\omega_E}{k_B T}\right)^2 \frac{e^{\hbar\omega/(k_B T)}}{\left(e^{\hbar\omega/(k_B T)} - 1\right)^2}$$

Where we use a similar approach as Kittel did on pages 114-117. For $T \gg \theta_D$ and $k_B T \gg \hbar\omega_E$ we get:

$$C_V^{total} = 2R$$

8. For the 1D lattice shown below find the characteristic equation assuming that the force constant between atoms 1 and 2 is C, between atoms 2 and 3 is 2C and between atoms 3 and 1 is 2C. Furthermore consider only nearest neighbor interaction. The masses of the atoms are as follows: $M_1=M$, $M_2=M_3=2M$.



<u>Key Problem 8:</u> I first determine the difference equations following the description above. I name the displacement of atoms 1, u, the displacement of atoms 2, v, and the displacement of atom 3, x:

$$M\frac{\partial^2 u_{s,t}}{\partial t^2} = C\left[v_{s,t} - u_{s,t}\right] + 2C\left[x_{s-1,t} - u_{s,t}\right]$$
$$2M\frac{\partial^2 v_{s,t}}{\partial t^2} = 2C\left[x_{s,t} - v_{s,t}\right] + C\left[u_{s,t} - v_{s,t}\right]$$
$$2M\frac{\partial^2 x_{s,t}}{\partial t^2} = 2C\left[u_{s+1,t} - x_{s,t}\right] + 2C\left[v_{s,t} - x_{s,t}\right]$$

Now I use appropriate trial solutions for this set of difference equations to get rid of the time dependence. Mathematically this is the same as separation of variables (assume that $u_{s,t}=u_s f(t)$). For trial solutions I choose:

$$u_{s,t} = u_o e^{-i\omega t} e^{isKa}$$
$$v_{s,t} = v_o e^{-i\omega t} e^{isKa}$$
$$x_{s,t} = x_o e^{-i\omega t} e^{isKa}$$

Plugging in gives:

$$
\begin{aligned}
-M\omega^2 u_o &= C[v_o - u_0] + 2C[x_o e^{-iKa} - u_o] \\
-2M\omega^2 v_o &= 2C[x_o - v_o] + C[u_o - v_o] \\
-2M\omega^2 x_o &= 2C[u_o e^{iKa} - x_o] + 2C[v_o - x_o]
\end{aligned}
$$

Reworking:

$$
\begin{aligned}
0 &= M\omega^2 u_o - 3Cu_o + Cv_o + 2Cx_o e^{-iKa} \\
0 &= Cu_o + 2M\omega^2 v_o - 3Cv_o + 2Cx_o \\
0 &= 2Cu_o e^{iKa} + 2Cv_o + 2M\omega^2 x_o - 4Cx_o
\end{aligned}
$$

Or in matrix form:

$$
\begin{bmatrix} M\omega^2 - 3C & C & 2Ce^{-iKa} \\ C & 2M\omega^2 - 3C & 2C \\ 2Ce^{iKa} & 2C & 2M\omega^2 - 4C \end{bmatrix} \begin{bmatrix} u_o \\ v_o \\ x_o \end{bmatrix} = 0
$$

For non-trivial solutions this determinant needs to be zero so:

$$
\begin{vmatrix} M\omega^2 - 3C & C & 2Ce^{-iKa} \\ C & 2M\omega^2 - 3C & 2C \\ 2Ce^{iKa} & 2C & 2M\omega^2 - 4C \end{vmatrix} = 0
$$

Which gives:

$$
\begin{aligned}
&0 = (M\omega^2 - 3C)(2M\omega^2 - 3C)(2M\omega_2 - 4C) - (4C^2M\omega^2 - 12c^3) - (2C^2M\omega^2 - 4C^3) + 4C^3e^{iKa} + \\
&4C^3e^{-iKa} - (8C^2M\omega^2 - 12C^3) \Leftrightarrow \\
&0 = (M\omega^2 - 3C)(2M\omega^2 - 3C)(2M\omega_2 - 4C) - (14C^2M\omega^2 - 28c^3) + 8C^3\cos(Ka)
\end{aligned}
$$

Note that this polynomial has six solutions so I expect three different branches for each displacement direction. So if I only allow motions of the molecules parallel to the chain I will find 3 different longitudinal branches. If I also allow motions perpendicular to the chain I could get up to 6 additional modes, for two different transverse directions. Some of those modes might have the same dispersion relation depending on the geometry. The spring constants for motions parallel to the chain and perpendicular to chain are in generally not the same. Check the end of chapter 3: shear elastic stiffness constants are different from the normal elastic stiffness constants even for a cubic material.

9. We know that atoms in a solid are vibrating from their equilibrium positions at all temperature above zero. If we consider such oscillators to be harmonic, their energy is quantized and given by the following expression:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

So the material can only absorb energy packages equal to $\hbar\omega$. We say that for a certain phonon mode, i.e. read a certain ω, the material contains n phonons. The number of phonons will have a major impact on the conduction of materials, since phonons act as scatter-centre for conduction electrons. As the number of phonons increases with temperature, the electrical resistivity increase with temperature. Consider a single diatomic crystal of CsCl (M_{Cs}=132.905451 amu, M_{Cl}=35.446 amu, so $M_{Cs}>M_{Cl}$).

a. For which frequency range do stationary phonon states not exist in the crystal.
b. For which wave-vectors do the lattice vibrations have a much longer wavelength than the lattice constant?
c. Assume that you can describe the CsCl by a 1D diatomic lattice. Use the dispersion relation to determine the speed of sound. Use the results of Kittel on page 98 or start from the following dispersion relation:

$$\omega^2 = C\frac{M_{Cl}+M_{Cs}}{M_{Cs}M_{Cl}}\left[1 \pm \sqrt{1 - 4\frac{M_{Cl}M_{Cs}}{M_{Cl}+M_{Cs}}\sin^2\left(\frac{Ka}{2}\right)}\right]$$

Where C is the spring constant.

Key: a. I do not expect stationary states with frequencies between $(2C/M_1)^{0.5}$ and $(2C/M_2)^{0.5}$. See also the dispersion graph on page 96 of Kittel. So elastic waves with those frequencies can still exist in the material but they will not be stationary states. This means that if I create an elastic wave in the material with a frequency in that particular range by for example an actuator on top of the material, if I stop the actuator the elastic wave will reduce in amplitude in time and its energy will go to other phonon modes. After a while the forced elastic wave is no longer there.

b. K is inversely proportional to the wavelength, so small K-vector means long waves. The smallest K-vector of course is the K-vector for which one wavelength fits in the material (for standing wave case, i.e. fixed atoms on both surfaces of the material) or the situation where all atoms move in phase and K=0 (for traveling wave with periodic boundary conditions; to be honest this is not really a traveling wave as you move your whole block of material back and forward). In all case however small K means long wavelength.

d). given dispersion relation.

$$\omega^2 = \frac{c(m_{cl} + m_{cs})}{m_{cl}\, m_{cs}} \left[1 \pm \sqrt{1 - \frac{4 m_{cl} m_{cs}}{(m_{cl} + m_{cs})^2} \sin^2 \frac{ka}{2}} \right]$$

$\lambda >> a$, sin

$ka << 1$

Then $\sin \frac{ka}{2} \Rightarrow \frac{ka}{2}$

$$= \frac{c(m_{cl} + m_{cs})}{m_{cl}\, m_{cs}} \left[1 - \sqrt{1 - \frac{4 m_{cl} m_{cs}}{(m_{cl} + m_{cs})^2} \frac{k^2 a^2}{2}} \right]$$

$$= \frac{c(m_{cl} + m_{cs})}{m_{cl}\, m_{cs}} \left[1 - \left(1 - \frac{\frac{4 m_{cl} m_{cs} k^2 a^2}{4 \cdot (m_{cl} + m_{cs})^2}}{2} \right) \right]$$

$$\left[(1-x)^{1/2} = 1 - \frac{x}{2} \cdots \right]$$

=

$$w^2 = \frac{C(m_a + m_{cs})}{m_a m_{cs}} \left[1 - 1 + \frac{2 m_a m_{cs} k^2 a^2}{(m_a + m_{cs})} \right]$$

$$w^2 = \frac{2c\, k^2 a^2}{(m_a + m_{cs})^2}$$

$$w = \sqrt{\frac{2c\, a^2}{(m_a + m_{cs})^2}} \cdot k$$

Group velocity $\quad v_g = \frac{dw}{dk}$

$$v_g = \frac{d}{dk} \sqrt{\left(\frac{2c\, a^2}{(m_a + m_{cs})^2}\right.} \cdot k$$

$$= \sqrt{\frac{2c\, a^2}{(m_a + m_{cs})^2}}$$

which is speed of sound

10. You have a monatomic cubic lattice of lattice spacing a, and sound velocity v. Say you want to do a lattice heat-capacity experiment in the fully quantum mechanical regime (i.e. most of the acoustic modes have ”frozen out”). Your apparatus is capable of reaching a temperature, 4 K. How small does your sample have to be? Give the answer in unitcells.

[Hint: For a finite sample, the allowed wavevectors are discrete. You are looking for the smallest, non-zero wavevector, as this will give you the lowest energy excitation of the crystal. Relate this energy to the thermal energy to solve the problem.]

Key: At extremely low temperature where even acoustic modes have frozen out, the discretized nature of energy levels becomes important due to different phonon modes, i.e. the possible values of the K vector. For a crystal of length L, the phonon modes with the following wave-vectors are allowed:

Since $K = 2\pi n/L$, where $n = 0,1,2,3,\ldots\ldots\ldots\ldots\ldots,$

The smaller the wave-vector of a phonon mode the smaller the energy of the phonon in that mode and the smaller the energy difference between the first excited state and the ground state. So we need to look to the energy of phonons with the longest wavelength and compare that to k_BT. The wave-vector of the first excited phonon mode $K = 2\pi/L$. To observe physics in this regime, the thermal energy k_BT should be comparable with the energy difference between ground state and first excited state,

$\hbar\omega = \hbar vk = \hbar v 2\pi/\lambda$

i.e., $k_BT < \hbar v 2\pi/\lambda = \hbar v 2\pi/L$

$L < \hbar v 2\pi/(k_BT)$

which gives: $L/a < 2\pi\hbar v/(k_BTa)$ so the size of the sample should be about $(2\pi\hbar v/(k_BTa))$ atoms, with v the speed of sound.

Note1 that at very small dimensions the lattice parameter might be significantly different from the bulk lattice parameters. This will change the coupling between the atoms and thus the speed of the elastic wave. In the next chapter we will see that the size of the system will also change electron density through our material. For small particles this electron density can significantly differ from the bulk electron density distribution. The electron density distribution will influence the elastic properties.

Note2: the speed of sound in copper is 4600 m/s and the lattice parameter of copper is 3.6A, so plugging in the numbers gives: 145 lattice spacings, i.e. 52 nm. Of course at higher temperatures, phonon related finite size effects are only showing up for much smaller systems.