M.1 Nanocrystal  A small cubic crystal has a side length $L$ of only 10 nanometers. The speed of sound in this material is 1000 meters/sec.

a) (3 points) Estimate the lowest frequency of vibration $\omega_0$ that can exist in this crystal.

b) (4 points) For temperatures below some $T_0$ the specific heat of the nanocrystal becomes much different than that of a large crystal. Estimate this $T_0$ in degrees Kelvin.

c) (1 point) Qualitatively how do the two specific heats differ for $T \ll T_0$?

Solution:

Scores: 8 8 8 8 7 7 7 6 5 | 4 4 3 3 3 2 2 1 0 0  If you were below the vertical line. You don’t understand this adequately. Several people seemed to do this problem by rote rather than looking at what was asked.

a) We saw that the lowest frequency vibrations in a crystal are the acoustic modes with wavevectors $k$ given by $\omega = c k$. In a finite crystal the allowed $k$’s are discretely spaced. The lowest frequencies correspond to the longest wavelengths $2\pi/k$. The longest wavelengths that fit in a 10 nm crystal are of the order of $10^{-8}$ meters. The corresponding frequency $\omega_0$ is thus of order $(c 2\pi/10^{-8})$. Using $c = 1000$ meters/second, we have $\omega_0 \approx 6 \times 10^{11}$/sec.

b) In general the specific heat $c_v = d/dT \int d\omega g(\omega) \hbar \omega / (\exp(\hbar \omega/k_B T) - 1)$. In a normal, large crystal the density of modes $g(\omega)$ is nonzero down to $\omega = 0$. But from part a) this nanocrystal has no oscillations below frequency $\omega_0$. If $\hbar \omega_0/(k_B T)$ is much larger than 1, these modes can’t be excited significantly, so no energy can be absorbed and the specific heat is exponentially small. The changeover happens at $T_0$ such that $1 \approx \hbar \omega_0/(k_B T_0)$, or $T_0 = \hbar \omega_0/k_B$. Recalling that one eV of energy corresponds to $T = 11611$ K and to $\omega = 1.5 \times 10^{15}$/sec we get $T_0 = 11611$ K ($\omega_0/1.5 \times 10^{15}$) or $T_0 \approx 4$ degrees Kelvin

c) As said above, the internal energy density $u$ is exponentially small for temperatures below $T_0$ in the nanocrystal. Its specific heat is thus much smaller than that of a normal-sized crystal.
Identical atoms of mass \( m \) are arranged on a triangular lattice of spacing \( a \). The horizontal direction or x direction is a nearest-neighbor direction. Normal modes in this lattice have displacement \( u_{\hat{k}}(\vec{R}) \) of the form \( u_{\hat{k}}(\vec{R}) = Ae^{i\hat{k} \cdot \vec{R}} \).

a) (4 points) Give the x and y co-ordinates of some wavevector \( \hat{k} \) such that \( u_{\hat{k}}(\vec{R}) \) is the same mode as \( u_{-\hat{k}}(\vec{R}) \).

b) (2 points) sketch and describe the displacement of the atoms in this mode.

**Solution:**

Scores: 6 6 6 6 5 4 4 4 4 4 | 3 3 3 3 2 2 2 2 1 1  | Many students found modes that were uniform translations of the lattice. Such modes aren’t really vibrations and this answer was not given full credit.

a) The book and lecture pointed out that not all \( k \)'s give distinct modes. Indeed, a mode with \( k + K \) is the same mode as \( k \) for any reciprocal lattice vector \( K \). This question tests your knowledge of this point. We are given that \( u_k(R) = u_{-k}(R) \) for all lattice vectors \( R \) since the two modes are the same. Thus \( e^{ik \cdot R} = e^{-ik \cdot R} \), or \( e^{2k \cdot R} = 1 \). This is the condition for \( 2k \) to be a reciprocal lattice vector. We may thus satisfy the condition by finding any convenient reciprocal lattice vector. We may take one that is perpendicular to \( a_1 \), i.e., vertical. The smallest one satisfies \( K \cdot a_2 = 2\pi \). Now, \( K \cdot a_2 = K(\sqrt{3}/2)a \). so \( |K| = 2\pi(2/\sqrt{3}a) \). Thus the desired \( k \) is given by

\[
\frac{1}{2}K = \hat{y} \frac{2\pi}{(\sqrt{3}a)}
\]

b) \( u(r) = \text{const} \exp(iR \cdot \hat{y}(2\pi)/(\sqrt{3}a)) \). Evidently \( u \) depends only on the vertical component of \( R \), so it is constant along horizontal lines. From one horizontal lattice line to the next, \( R \cdot \hat{y} \) changes by \( \sqrt{3}a/2 \), so the argument of the exp changes by \( \pi \); thus the sign of \( u \) is reversed. This property of zone-boundary modes was noted in the text in one dimension. To indicate this oscillation, one can put an arrow in any direction on a lattice site and copy that same arrow for the whole horizontal line. For the lines above and below, the arrow should be reversed. Equivalent lines of constant \( u \) are the lattice lines at \( \pm 60 \) degrees to the horizontal.

**M.3 Anomalous modes**

A certain solid of unusual construction has vibrational modes with a density of vibrational frequencies given by \( g(\omega) = A \omega^{3/2} \) for low frequencies. Recall that \( g(\omega)d\omega \) is the number of vibrational modes between \( \omega \) and \( \omega + d\omega \) per unit volume of the crystal.

a) (5 points) From this information, find the specific heat \( c_v \) as a function of temperature \( T \) when the temperature is sufficiently low. You may leave numerical factors undetermined.
Solution:

Most people correctly wrote the basic equation. Many could use this equation to get the correct answer.

a) The internal energy energy per unit volume $u$ at temperature $T = \beta/k_B$ is given by $u = \int d\omega(h\omega)g(\omega)[1/(e^{\beta h\omega} - 1)]$, where the $[\ldots]$ factor is the average number of phonons in a mode of frequency $\omega$. To find the temperature dependence of this integral we use a rescaled variable $x \equiv \beta h\omega$. Then the $(h\omega)$ factor is $x/\beta$ and $d\omega = dx/(\beta h)$. $g(\omega) = A\omega^{3/2} = Ax^{3/2}/(\beta h)^{3/2}$ The integral becomes

$$u = 1/\beta 1/(\beta h) A/(\beta h)^{3/2} \int dx \ x^{3/2}[1/(e^x - 1)].$$

or

$$u = A(k_B T)^{7/2} h^{-5/2} \int dx \ x^{3/2}[1/(e^x - 1)].$$

The integral is a numerical factor which we are allowed to ignore. Thus

$$c_v = \partial u/\partial T \simeq A(k_B T/h)^{5/2} k_B.$$

M.4 Energy flow In a certain crystal the vibrational energy $u$ varies in space and time according to $\partial u/\partial t = D_u \nabla^2 u$. The constant $D_u$ is called the thermal diffusivity, as told in class. A square slab this material of width $L$, thickness $h$ and specific heat $c_v$ is placed between two reservoirs at slightly different temperatures $T$ and $T - \Delta T$. Energy flows through the crystal from the hotter to the cooler reservoir at a rate $dE/dt$.

a) (5 points) Find $dE/dt$ in terms of the quantities given.

Solution:

People were confused by the geometry. Some people supposed that energy was building up in the slab rather than flowing through it. But most people had a basic understanding.

a) The energy passing through the slab from the hotter region on the left to the colder region on the right per unit time is the integral of the energy current density $j_u$, ie $dE/dt = L^2 j_u$. From the definition of thermal conductivity $\kappa$, $j_u = \kappa \nabla T$. The given thermal diffusivity is related to $\kappa$ by $j_u = D_u \nabla u = D_u c_v \nabla T$, so that $\kappa = D_u c_v$. (Thus $\partial u/\partial t = \nabla \cdot j_u = D_u \nabla^2 u$, confirming the formula for $D_u$ given in the problem.) Then the desired $dE/dt = L^2 D_u c_v \nabla T$. The $\nabla T$ is given by the temperature drop across the slab: $\nabla T = \Delta T/h$. Thus $dE/dt = D_u c_v \Delta T/h$. 

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