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WS16/17 Condensed Matter Physics I
Exercise 2. Phonons

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Notice: *In solving the proposed exercises clearly motivate the passages to reach the result. The use of clear and compact notation is greatly encouraged, as well as the systematic use of dimensional checks of the expressions and results. When you are asked to "evaluate" something this means to provide a numerical evaluation of the expression. In this case, at times, it might be necessary to indicate a parameter whose explicit numerical value is not provided, i.e.* $\omega_c = 1.76\,H$ *(Gauss) Hertz. Otherwise specified, all the evaluations are to be given with 3 significant figures.*

2.1 Specific heat of an element (6 pts)

In figure 1 the specific heat of an unknown element is shown.

1. Explain why this data can be described satisfactorily by the Debye approximation.

2. Using the Debye model and knowing that at high temperature the specific heat is $234.4\ \mathrm{J\ Kg^{-1}K^{-1}}$ identify the element.

3. Using the plots evaluate the Debye temperature, the sound velocity, its number density (number of atoms per unit volume) and, from the result of point 1, its mass density.

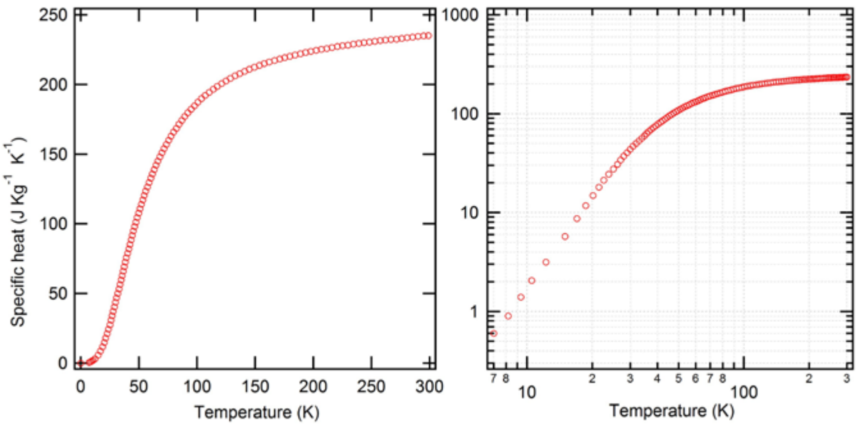

Figure 1: Specific heat of an uncknown element in linear (left) and logaritmic (right) scale.

2.2 Stability of D-dimensional crystal at T>0 (20 pts)

Consider a harmonic crystal with a single atom per cell in D dimensions. (of course we are interested in the cases D=1,2,3).

1. Show that the low-frequency phononic density of states behaves like $g(\omega) = A\omega^{D-1}$. Assume $\omega_s(\mathbf{k}) = c_s(\hat{\mathbf{k}})k$ for $\omega < \omega_c$. You should get $A = c^{-D}D\Omega_D/(2\pi)^D$ with $\Omega_D = \frac{2\pi^{D/2}}{\Gamma(D/2)}$. the D-dimensional solid angle and c an appropriate angle- and polarization- average of $c_s(\hat{\boldsymbol{k}})$. Give an expression for c.

2. Let us consider now the mean square displacement from the atomic equilibrium position
$$\overline{\mathbf{u}^2} = \frac{1}{N}\sum_{\mathrm{R}}\langle\mathbf{u}^2(\mathbf{R})\rangle,$$
with $\langle\ldots\rangle$ the thermal average at a fixed temperature. Express $\overline{\mathbf{u}^2}$ as a sum over the normal modes frequency.
[Hint: (i) express the coordinates as a sum of the normal modes $\mathbf{u}(\mathbf{R}) = \left(1/\sqrt{N}\right)\sum_{\mathbf{k},s}\mathbf{u}_s(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{R}}$, with $\mathbf{u}_s(\mathbf{k})$ the normal coordinates and $\mathbf{k}$ belonging to the FBZ; (ii) $\mathbf{u}_s(\mathbf{k}) \propto \boldsymbol{\epsilon}_s(\mathbf{k})$, and $\boldsymbol{\epsilon}_s(\mathbf{k}) \propto \boldsymbol{\epsilon}_s(-\mathbf{k})$; (iii) Because of the virial theorem, at a given temperature the average value of the potential energy of a normal mode is half the value of the average of the total energy $\hbar\omega_s(\mathbf{k})(n_s(\mathbf{k}) + 1/2)$. Remember that
$$\frac{1}{N}\sum_{\mathrm{R}} e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{R}} = \delta_{\mathbf{k}\mathbf{k}'}.$$

3. Express now $\overline{\mathbf{u}^2}$ as a frequency integral, introducing the density of states. Show that $\overline{\mathbf{u}^2} = \frac{\hbar}{2M}\int_0^{\omega_c} d\omega\,\frac{g(\omega)}{\omega}[n(\omega) + 1/2]$.

4. Specialize the formula found in the preceding point to a finite system, simply by introducing a lower cutoff frequency limiting the frequency integral to $\omega > \omega_t = 2\pi c/L$. Here $L = N^{1/D}/\rho^{1/D}$, with ρ the atomic density.

5. Evaluate now for $T > 0$ the dominant contribution to $\overline{\mathbf{u}^2}$ due to the low frequency modes ($\omega_t < \omega < \omega_c$), in the regime for which $\beta\hbar\omega \ll 1$.

6. What happens to $\overline{\mathbf{u}^2}$ for $D = 2$ when $N \to \infty$? What does that mean for the stability of the system?

7. Same question as in point 6 but with $D = 1$.

2.3 1D rare gas chain (10 pts)

Consider a 1D chain of Xenon atoms. Assume a pair interaction defined by the Lennard-Jones potential $\phi(|x|) = 4\epsilon[(\sigma/x)^{12} - (\sigma/x)^6]$. Assume atoms are evenly spaced at equilibrium (spacing $x_n^0 = na$) and that they can oscillate around equilibrium position ($x_n = x_n^0 + u_n$, with $u_n \ll a$). You can find the value of Lennard-Johnes parameters for Xenon in the Ashcroft-Mermin.

1. Calculate the energy per particle $e(a)$ for a given equilibrium spacing, as a function of ϵ and σ. [*Hint: approximating each of the sums* $\zeta(p) = \sum_{n=1}^{\infty} n^{-p}$, $p = 6,12$ *with the first 3 terms of the series we obtain* $\zeta(6) = 1.02$ *and* $\zeta(12) = 1.00$].

2. Calculate the equilibrium spacing as a function of σ and in Angrstrom.

3. Consider now a nearest-neighbor approximation. Calculate the sound velocity for the acoustic phonons.

4. Evaluate the zone boundary frequency in Hertz.