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Exercise 1: Specific Heat of Phonons (Oral)

In classical physics, the specific heat c_v of a harmonic crystal is given by the Dulong-Petit law

$$c_v^0 = 3nk_B \,, \tag{1}$$

where n is the density of the ions. In the classical theory, the specific heat is independent of temperature while below room temperature, the specific heat of all solids starts to decline below the classical value and features a peculiar temperature dependence where the specific heat vanishes for example as T^3 for low temperatures in insulators. This temperature dependence can be explained by a quantum theory of the harmonic crystal.

a) Argue that the thermal energy density of a harmonic crystal in a quantum theory is

$$u = u^{\mathrm{eq}} + \frac{1}{2V}\sum_{\boldsymbol{k}\lambda}\hbar\omega_{\boldsymbol{k}\lambda} + \frac{1}{V}\sum_{\boldsymbol{k}\lambda}\frac{\hbar\omega_{\boldsymbol{k}\lambda}}{e^{\beta\hbar\omega_{\boldsymbol{k}\lambda}}-1}\,, \tag{2}$$

where u^{eq} is the equilibrium thermal density of the crystal.

b) Show that the leading order correction to the Dulong-Petit law for high temperatures $\hbar\omega/k_BT \ll 1$ is given by

$$\frac{\Delta c_v}{c_v^0} = -\frac{\hbar^2}{12(k_BT)^2}\frac{1}{3N}\sum_{\boldsymbol{k}\lambda}\omega_{\boldsymbol{k}\lambda}^2\,. \tag{3}$$

c) Show that in the limit of low temperatures, the specific heat is given by

$$c_v = \frac{2\pi^2}{5}k_B\left(\frac{k_BT}{\hbar c}\right)^3\,. \tag{4}$$

Hints: In the low-T regime, you may use the following simplifications:

- Only sum over the acoustic phonon branches (why?).
- Replace the dispersion relation for the acoustic branches by its long wavelength limit $\omega_{\boldsymbol{k}\lambda} = c_{\hat{\boldsymbol{k}}\lambda}k$.
- Replace the summation (integration) over the first Brillouin zone by an integral over all k-space since the integrand only gives non-negligible contributions in the vicinity of $\boldsymbol{k} = 0$.
- Define the average of the inverse third power of the long-wavelength phase velocities as

$$\frac{1}{c^3} = \frac{1}{3}\sum_{\lambda}\int\frac{d\Omega}{4\pi}\frac{1}{c_{\hat{\boldsymbol{k}}\lambda}^3}\,. \tag{5}$$

Exercise 2: Linear Chain with m-th nearest neighbour interactions (Written, 4 points)

Consider a set of N ions of mass M distributed along a line at points separated by a distance a, so that the one-dimensional Bravais lattice vectors are just $\boldsymbol{R}_n = na$ for integral n. Let s_{na} be the displacement along the line from its equilibrium position of the ion that oscillates about $\boldsymbol{R}_n$. Usually, one makes the assumption that only nearest neighbors interact in order to get the dispersion for a linear chain with a single atom in its basis. In this exercise, we relax this assumption and allow ions at all distances to interact with each other. The interaction potential (in leading order in the displacement s) is then given by

$$V = \frac{1}{2} \sum_n \sum_{m>0} K_m \left(s_{na} - s_{(n+m)a} \right)^2 \tag{6}$$

where K_m denotes the 'spring constant' between ions at lattice sites n and $n+m$.

a) Write down the equations of motion. Impose periodic boundary conditions in order to show that the dispersion relation is now given by

$$\omega = 2 \sqrt{\sum_{m>0} K_m \frac{\sin^2 \frac{1}{2} mka}{M}} \, . \tag{7}$$

b) Show that the long-wavelength limit of the dispersion relation is given by

$$\omega = a \left(\sum_{m>0} m^2 K_m / M \right)^{1/2} |k| \, , \tag{8}$$

provided the sum $\sum_{m>0} m^2 K_m$ converges.

c) Show that if $K_m = 1/m^p$ $(1 < p < 3)$, so that the sum does not converge, then in the long-wavelength limit

$$\omega \propto k^{(p-1)/2} \, . \tag{9}$$

Hint: It is no longer permissible to use the small-k expansion of the sine in (7) but one can replace the sum by an integral in the limit of small k.

d) Show that in the special case of $p = 3$,

$$\omega \sim |k| \sqrt{|\ln k|} \, . \tag{10}$$