PROBLEM SET 3   Due Friday November 8

Physics 240A– FALL 2019

[**1.**] Consider a one-dimensional chain of identical atoms. The springs between them alternate in strength between values K_1 and K_2.
a) Find the vibrational frequencies as a function of wave number q. Study the low q limit and find the sound velocity.
b) Discuss the physical meaning of the two branches. Sketch the way the atoms move in both cases.
c) Discuss the dispersion and the normal modes for $K_1 \gg K_2$.
d) Discuss the limit $K_1 \approx K_2$ and compare with the homogeneous chain where all springs are identical (see class).

[**2.**] Consider a one-dimensional chain of identical atoms of mass M. The springs are not only between nearest neighbors but between all pairs of atoms. Thus, the elastic energy reads

$$E_{\text{el}} = \frac{1}{2} \sum_n \sum_{m>0} K_m \left(x_n - x_{n+m} \right)^2$$

where x_n is the displacement of atom n.
a) Find the dispersion relation, i.e. the vibrational frequency ω as a function of wave number q.
b) Assume $K_m = K_0/m^p$ with $p > 1$ a parameter controlling how rapidly the interaction drops of with distance. Study the long-wavelength limit of the dispersion relation for $p > 3$. Determine the sound velocity.
c) Investigate the long-wavelength limit of the dispersion relation for $1 < p < 3$. Show that one gets "anomalous sound", i.e., the frequency is not proportional to the wavenumber. (Hint: You may want to approximate the m-sum by an integral.)

[**3.**] The specific heat C of a two level system goes to zero at high T, but the specific heat of a classical (or quantum) oscillator remains finite no matter how high T gets. What property of the energy levels of a system determines whether C vanishes at high T or not? Interpret your answer in terms of the formula $dE = C\, dT$.

[**4.**] The specific heat C of a two level system goes to zero exponentially at low T. How does the specific heat C of a quantum oscillator of frequency ω_0 go to zero at low T? In class we saw that a 3D set of oscillators with a linear dispersion relation $\omega(q) = vq$ has a low T specific heat which vanishes as a power law $C(T) = AT^3$. What property of the energy levels of a system determines whether $C(T)$ is exponentially small at low T vs some less rapidly decaying function like T^α?

Note: The last two problems are *numeric*. For the first, you will need to be able to do integrals numerically. For the second you will need to be able to diagonalize a matrix by calling some appropriate mathematical library. I will post a way to do both of these using C programs on the course website, but feel free to use whatever software/language you like. Talk to me or Ben if you need help.

[**5.**] We showed in class that the specific heat of a 1D classical harmonic oscillator with energy $E(x,p) = kx^2/2 + p^2/2m$ is $C(T) = k_{\rm B}$. Compute and plot the specific heat of an *anharmonic* oscillator $E(x,p) = kx^2/2 + \gamma x^4/4 + p^2/2m$. Choose $k = 0.7$ and $\gamma = 0.0, 0.1, 0.2, 0.5$. Comment on your results. Does γ increase or decrease C? What happens to C at low and high T? Is there any way to have predicted some of these answers?

One approach is to solving this problem is to use the fluctuation form for the specific heat

$$
\begin{aligned}
C &= \beta^2 \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \\
\langle E \rangle &= \frac{1}{Z} \int dxdp \, E(x,p) \, \exp[-E(x,p)/k_{\rm B}T\,] \\
\langle E^2 \rangle &= \frac{1}{Z} \int dxdp \, E(x,p)^2 \, \exp[-E(x,p)\,/k_{\rm B}T\,] \\
Z &= \int dxdp \, \exp[-E(x,p)\,/k_{\rm B}T\,]
\end{aligned}
$$

Then do the integrals numerically. Can the integrals be done analytically?

[**6.**] Consider a linear (1D) mass-spring system in which one of the springs (a "defect") has a value k_* which is different from all the others, which have value k. Assume all masses m are equal. As in the isotropic case, the normal mode frequencies ω^2 are determined by writing down Newtson's equations $F = ma$ for all the masses. If you assume, as usual, $x_n(t) = a_n e^{i\omega t}$, write down the matrix which, when diagonalized, has eigenvalues which are the squares ω^2 of the normal mode frequencies. Now diagonalize the matrix (numerically). Choose number of masses $N = 64$, spring constant $k = 1.9$, mass $m = 1.1$, and defect spring $k_* = 5.2$.

What do you notice about the eigenvalues?

Compute the participation ratios (see below) of the 64 eigenvectors. What do you notice? Interpret your result physically.

This is actually a really important problem which arises in many contexts. If you have time, play around with your code a bit further. What happens as $k_* \to k$? What happens if $k_* < k$? Think about why $k_* < k$ might be different from $k_* > k$.

Definition: Given a normalized vector $\vec{v}$ with components v_n, $n = 1, 2, \cdots N$, the participation ratio

$$
\mathcal{P} = \Big(\sum_n v_n^4 \Big)^{-1}
$$

provides an estimate of the number of components of $\vec{v}$ which are of significant size. (See class discussion.)