Homework 10
Due Thursday, April 18th

Problem 1

a) Show that in Debye theory, the energy as a function of temperature can be expressed in terms of the following integral (ignoring the ground state energy):

$$E = 9N\frac{(kT)^4}{(\hbar\omega_D)^3}\int_0^{\beta\hbar\omega_D}\frac{x^3dx}{e^x-1} \tag{1}$$

b) Show that this gives the correct limiting behavior in the high-temperature limit and low-temperature limit.

c) Compute this integral explicitly, either numerically or analytically, and compare with the Einstein formula:

$$E = \frac{3N\hbar\omega_0}{e^{\beta\hbar\omega_0}-1} \tag{2}$$

where ω_0 here is some characteristic oscillation frequency of the solid. Can we relate ω_D to ω_0? How do their heat capacities compare? Note: if you are computing the integral numerically, you want to be careful near $x = 0$ where the denominator blows up but the integrand $x^3/(e^x - 1)$ is finite. Just make sure you're doing the calculation to high accuracy and always use double-precision floating point numbers.

d) Attached is that same experimental data from that diamond we looked at a few weeks ago. Compare the data using both Einstein and Debye's formulas (you will have to take the derivative dE/dT). Which gives the better fit? Use this data to find the value of ω_D for diamond.

e) Compute ω_D as a theoretical value based on the material properties of diamond and compare to the value you found in part (d). You will have to look up some of the properties of diamond online. Keep about two significant figures (depending on how precisely you've worked out ω_D from part (d)).

Problem 2

Estimate the formula for sound speed in a material assuming a set of masses on springs characterized by mass m, spring constant κ, and an atomic spacing a. Given this estimate, show the Debye frequency ω_D is of the same order as ω_0, the characteristic oscillation frequency of a single spring-mass system.

Problem 3 (Optional – Only if you're interested)

Our model for solids seems pretty good at this point! But how about we get rid of the ad-hoc cutoff and instead sum over modes using the dispersion relation $\omega(k_x, k_y, k_z)$ we found in class (assuming a square lattice even though we know diamonds are more complicated). This will amount to a 3D integral that must be computed numerically for a given choice of temperature (there's not a lot of analytical work we can do to simplify things). Perform the integral for the energy numerically for a range of temperatures, and compute the derivative with temperature numerically as well to get the heat capacity. Check against our other methods and the diamond dataset. At this point the results will be very similar to the Debye model, but you should be able to see subtle distinctions that give a better fit to the data.