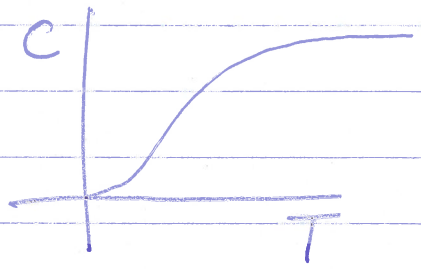
Fri. Aug. 31

- We have been discussing the "Einstein solid" which consists of independent quantum harmonic oscillators
- Classical gives Dulong-Petit law
- QHO's explain non-linear behavior of heat capacity at low temperatures
- I'd like to look at one more parameter in the fit for C
- all oscillators have one frequency ω, sometimes called "Einstein" frequency
- in the C vs. T curve: $C(T) = 3k_B (\beta\hbar\omega)^2 \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}$



- $T_E = \hbar\omega/k_B$ is a fit parameter that gives the best fit to the exp. data

$T_E \propto \omega$ or ω_E, both constants

- Example being for copper (Cu)

$$T_E = 240K \quad (-33°C)$$ *record low Flagstaff -34°C

- above T_E, we get more-or-less Dulong-Petit law

- one well known discrepancy with the classical law $C/R \simeq 3$, most materials for diamond

$$\frac{C}{R} \simeq 0.7$$ • heat capacity per mole

at room T. Why?

$$T_{E,diamond} \simeq 1320K >> room\ T$$ → so room T is "cold"

- why does it have such a value?

- due to the chemical bonds between C atoms

- the bond is strong (think of hardness of diamond) + carbon atoms are light

$$\omega = \sqrt{\frac{K}{m}}, \quad \left.\begin{array}{l} K \text{ large} \\ m \text{ small} \end{array}\right\} \begin{array}{l} \omega \text{ large} \\ \Rightarrow T_E \text{ large} \end{array}$$

- This discussion of bonds between atoms leads us directly to the idea of coupled harmonic oscillators

- let's look at a 1D "solid"

- transverse modes ↕
- long. modes ↔

- we usually use "periodic boundary conditions"

- first atom is coupled to last, etc.

- translate along solid by 'L' distance, we end up at the same place

- a wave $e^{ikr} = e^{ik(r+L)}$ (wave is same at $r + r+L$)

Note:
- We are looking at continuous medium with large L (forget atoms for moment) →

$$\Rightarrow e^{ikr} = e^{ikR} e^{ikL}$$

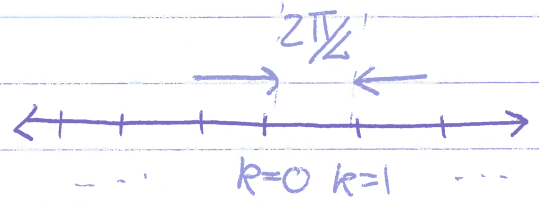
$$e^{ikL} = 1 = \cos(kL) + i\sin(kL)$$

- this is true only when $kL = 2\pi n$
- in other words only modes with wave number

$$k = \frac{2\pi n}{L}$$

are possible (recall $k = 2\pi/\lambda$)

- can be thought of as a "spatial frequency"
- in solid state, we use "k-space" a lot



1-D k-space

- each point on axis is a mode (vibration)
- for large L, $\downarrow$ separation $2\pi/L$ is small
- for solids, L is large (many atoms)

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