Thermal properties of the lattice

1. Even at absolute zero, the atoms in a crystal vibrate. This vibration is the zero point energy, or zero point motion. The origin of this motion is quantum mechanical and is best addressed by the Heisenberg uncertainty principle.

   (a) What is Heisenberg's uncertainty principle? Use your own words and include one equation.

   (b) Why would a lattice of *stationary* atoms conflict with Heisenberg's uncertainty principle?

   This is partially a review. You can find zero-point energy in most modern physics texts.

2. **Simple Harmonic Oscillator (SHO).** Following Newton's second law, the equation of motion of a simple harmonic oscillator is

$$M\frac{dx^2}{dt^2} = -\gamma x$$

   where γ is the effective spring constant.

   (a) Show, by direct substitution, that

$$x(t) = A\cos(\omega t - \delta)$$

   is a solution to the SHO equation of motion. Here, A is the amplitude, ω the angular frequency, and δ the initial phase (or phase constant).

   (b) What must be true about ω? Can ω have *any* value?

   (c) The total energy of a harmonic oscillator is

$$E = K + U = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 = \frac{1}{2}kA^2$$

   Following the equipartition theorem of statistical mechanics, the total energy at some temperature T in this case is $E = k_B T$.[1]

   Use the above to show that the amplitude

$$A = \left(\frac{2k_bT}{\gamma}\right)^2$$

   (d) Estimate ω and A for an atom in a crystal. Use $\gamma \approx Ya \approx 10$, $m \approx 10^{-27}$, and $T = 300$K.

   (following the Hofmann p47-48. 10^{13}Hz, 10^{-11}m which is a small fraction of the lattice spacing)

3. **Waves - review.** The displacement of a wave traveling on a string is given by

$$D = 3.5\sin(2.7x + 4t - \frac{\pi}{8})$$

   (a) Plot this on desmos and see what happens when you increase t. What's the shape of this wave and which way does it travel?

   Calculate this wave's (b) frequency, (c) angular frequency, (d) wavelength, (e) wave number, and (f) wave speed.

4. **Waves - review.** We often use the complex exponential to represent oscillations and waves. In this case, we use Euler's equation

$$e^{i\phi} = \cos(\phi) + i\sin(\phi)$$

   To represent the wave, the angle change over time and position $\phi(t) = kx - \omega t + \phi_0$. Provide a "proof" of this equation.

   Give a physicist's proof that captures the logic of the argument and the essence of the mathematical ideas, not a formal mathematician's proof.

5. **Infinite chain of atoms.** Following Newton's second law, the equation of motion of the nth atom in an infinite chain of atoms depends on how far it's displaced from its nearest neighbors, the $(n-1)$th and $(n+1)$th atoms

$$\begin{aligned} m\frac{du^2}{dt^2} &= -\gamma(u_n - u_{n-1}) + \gamma(u_{n+1} - u_n) \\ &= -\gamma(2u_n - u_{n-1} - u_{n+1}) \end{aligned}$$

   where u_n is the displacement of the nth atom from its equilibrium position.

   (a) Show, by direct substitution, that

$$u_n(t) = ue^{i(kan-\omega t)}$$

   is a solution to the equation of motion, as long as

$$\omega^2 = \frac{4\gamma}{m}\sin^2\left(\frac{ka}{2}\right)$$

6. **Dispersion.** The dispersion relation for an 1D infinite chain of atoms is given by

$$\omega = 2\sqrt{\frac{\gamma}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

   (a) Plot ω versus k.
   (b) Determine the periodicity of ω.

   Since this function is periodic, it makes sense to consider just one cycle. Consider the range $-\pi/a \leq k \leq \pi/a$.

   (c) Identify the long wavelength limit on the graph. Graphically determine the group velocity, $\frac{d\omega}{dk}$, in this limit.
   (d) The long wavelength limit corresponds to the propagation of sound waves. Analytically determine the group velocity, $\frac{d\omega}{dk}$, in this limit.

   (e) Identify the short wavelength limit on the graph. Graphically determine the group velocity in this limit.
   (f) The short wavelength limit corresponds to standing waves. Analytically determine the group velocity in this limit.

[1] Or to be more specific, any degree of freedom that appears squared in the Hamiltonian contributes $\frac{1}{2}k_BT$ to the energy. In this case, v^2 and x^2.