

## Thermal properties of the lattice - recap

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1. We consider lattice vibrations even at absolute zero. Why? Refer to the Heisenberg uncertainty principle in your response. Use both words and equations.
2. We often use the simple harmonic oscillator to model lattice vibrations. Why? Provide text, a diagram and equations. Is this always a valid model?
3. The simplest model of lattice vibrations uses  $3N$  *independent* oscillators. The mass is the ion mass  $m$  and we approximate the spring constant  $\gamma \approx Ya$ , the Young's modulus times the lattice spacing.
  - (a) Sketch a diagram of this model.
  - (b) What's predicted for the frequency of oscillations? How do we get this expression?
  - (c) What's predicted for the amplitude of the oscillations? How do we get this expression?
4. A more realistic model of lattice vibrations is an *infinite* chain of atoms, which couples atoms to each other. We use a spring constant of  $\gamma$  to represent the interaction between neighboring atoms, and  $m$  as the mass of the atom.
  - (a) Sketch a diagram of this model.
  - (b) What's predicted for the frequency of oscillations? How do we get this expression?
  - (c) How does  $\omega(k)$  differ from the independent oscillator model?

We can extend this model to two different atoms.

- (d) Sketch a diagram of this model
  - (e) Here,  $\omega(k)$  is said to have an optical and acoustic branch. What are those? How are they physically different motions/behavior?
5. The solutions to the equations of motion for the chain of atoms above uses a wave-like motion<sup>1</sup>
    - (a) We often use the wavenumber and the frequency to describe the wave. What physical properties do these two values describe?
    - (b) What is the long wavelength region, in terms of wavenumber? How about the short wavelength region? Which region corresponds to sound waves?
    - (c) How fast does the wave travel through the chain? Do they all travel at the same speed?
  6. We improve our model by using a *finite* chain.
    - (a) One way to address the ends is to impose *periodic boundary conditions*. What does this mean? Use words, a diagram, and an equation.

- (b) What effect does this have on the lattice vibrations?
7. The above<sup>2</sup> uses a classical treatment of oscillations. A QM treatment of the SHO results in energy quantization.
    - (a) What are the allowed energies of the SHO? Give an equation and explain how this shows quantization.
    - (b) What's a *phonon*? What is its energy and momentum?
  8. What is heat capacity?
    - (a) Give an explanation using words and an equation.
    - (b) What is the experimentally observed behavior of a solid's heat capacity? Consider, for example, diamond. Describe this in terms of words, diagrams, and equations.
    - (c) How is heat capacity calculated from energy?
  9. What is the classical model of heat capacity?
    - (a) What are the assumptions of this model?
    - (b) How is the energy of the system calculated?
    - (c) What is the heat capacity according to this model? What are the successes and failures of this model?
  10. What is the Einstein model of heat capacity?
    - (a) What are the assumptions of this model?
    - (b) How is the energy of the system calculated?
    - (c) What is the heat capacity according to this model? What are the successes and failures of this model?
  11. What is the Debye model of heat capacity?
    - (a) What are the assumptions of this model?
    - (b) How is the energy of the system calculated?
    - (c) What is the heat capacity according to this model? What are the successes and failures of this model?
  12. (a) What is thermal conductivity? Use words, a diagram and an equation.
    - (b) Give a microscopic explanation of thermal conductivity. Use words, a diagram and an equation. Include phonons and mean free path in your answer.
  13. (a) What is thermal expansion? Use words, a diagram and an equation.
    - (b) Give a microscopic explanation of thermal expansion. Use words, a diagram and an equation. Include the idea of *anharmonic effects* in your answer.

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<sup>1</sup>This is a wave that only exists at the lattice sites, as opposed to a wave in a continuous medium.

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<sup>2</sup>Well, except for (1) which deals with absolute zero and the Heisenberg uncertainty principle.