6.730 PHYSICS FOR SOLID STATE APPLICATIONS

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PROBLEM SET 3

Issued: 2-21-96 Due: 2-28-96, at the beginning of class.

Readings:
Ashcroft and Mermin, Chapters 3, 4 and 5.
Notes from 6.730 on mathematics of periodic structures, chapter 6.

Problem 3.1 Zero-point vibration amplitudes.

(a) Consider an electron bound in a parabolic potential well such that the harmonic oscillation frequency ω_o is $4 \times 10^{15}\,\mathrm{sec}^{-1}$. Determine the width of the ground-state wavefunction.

(b) Now consider an acoustic cavity, 1 mm on a side, made of a metal of density $3\,\mathrm{g/cm}^3$. What is the root-mean-square (rms) mode amplitude due to zero-point vibrations (i.e., the ground state) for a phonon mode having the same frequency as in part (a)?

(c) Why are these numbers so different? Give a physical explanation.

Problem 3.2 Two-dimensional elastic continuum.

Consider a two-dimensional isotropic elastic continuum (with no out of plane motion).

(a) How many independent elastic constants are needed to describe this medium? Explain your answer on physical grounds.

(b) Formulate the elastic wave problem for this continuum, and determine the phonon dispersion relation. How many branches of modes (longitudinal and transverse) are there?

(c) For a square elastic cavity of length L on a side, determine the density of states for each branch (longitudinal or transverse) in frequency domain.

(d) How will the low-temperature specific heat depend on temperature?

(e) Formulate the Debye model for this problem assuming that the atoms are arranged on a square lattice with lattice spacing a. Find the Debye frequency assuming a single sound velocity v_s for both types of modes. (Different assumptions are explained in Problem 3.4.) What is the high-temperature specific heat?

Problem 3.3 Debye model details

When formulating the Debye model for an isotropic 3-D elastic continuum with different velocities for longitudinal and transverse acoustic waves, we can implement the mode limitation in the following three cases:

(1) Use a different cutoff frequency for longitudinal and transverse modes such that there are N longitudinal and $2N$ transverse modes, where N is the total number of atoms in the sample.
(2) Use a single cutoff frequency for both branches such that the total number of modes is $3N$.
(3) Use a single cutoff wavevector for both branches such that the total number of modes is $3N$.

Assume an isotropic solid with a shear modulus of $\mu = 100\,\text{GPa}$ and Poisson ratio $\gamma = 0.3$, and an average interatomic spacing of $3\,\text{Å}$ and an average atomic mass number of 27.

(a) Find the propagation velocities and densities of states for transverse and longitudinal acoustic waves, assuming periodic boundary conditions in a 3-D acoustic cavity.

(b) For each of the three ways of setting up the Debye model, use MATLAB to find the specific heat as a function of temperature. Since all curves will have the same low- and high-temperature behavior, use Case (1) as the standard, and plot C_v vs. T for that case, then plot the difference between Case (2) and Case (1), and Case (3) and Case (1).

(c) Discuss your results. Are the numerical differences large or small? Is there a computational reason for preferring one approach to the other? or is there a physical reason?