6.730 PHYSICS FOR SOLID STATE APPLICATIONS

Department of Electrical Engineering and Computer Science
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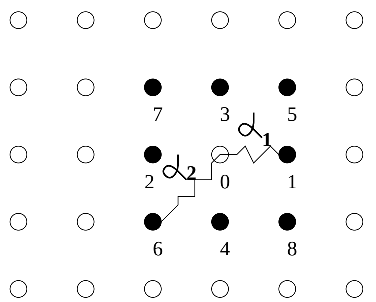
PROBLEM SET 5

Issued: 3-6-96 Due: 3-13-96, at the beginning of class.

Readings:
Ashcroft and Mermin, Chapter 22 and Chapter 23.
Acoustic and Optical Phonons, 6.730 notes.

Problem 5.1 2D Monatomic square lattice.

Atoms of mass M on a 2D monatomic square lattice with lattice spacing a are modeled as being connected by springs with spring constant α_1 to nearest neighbor atoms and with spring constant α_2 to next-nearest neighbor atoms. For example, in the figure the atom at 0 is connected by α_1 to atoms 1, 2, 3, and 4 and by α_2 to atoms 5, 6, 7, and 8.



(a) Find the equations of motion for for $u_x(x, y, t)$ and for $u_y(x, y, t)$.

(b) For a 2D monatomic square lattice of N atoms with a spacing a, the displacement of the n-th atom is

$$\begin{pmatrix} u_x[n,t] \\ u_y[n,t] \end{pmatrix} = \begin{pmatrix} \epsilon_x \\ \epsilon_y \end{pmatrix} e^{i(\mathbf{k} \cdot \mathbf{R} - \omega t)} .$$

The polarization vector ϵ is a solution of

$$M\omega^2 \begin{pmatrix} \epsilon_x \\ \epsilon_y \end{pmatrix} = \begin{pmatrix} D_{xx} & D_{xy} \\ D_{yx} & D_{yy} \end{pmatrix} \begin{pmatrix} \epsilon_x \\ \epsilon_y \end{pmatrix} .$$

Hence, both the polarization vector ϵ and the propagation vector are needed to specify a mode.

Show that the dynamical matrix $\mathbf{D}(\mathbf{k})$ is

$$\mathbf{D}(\mathbf{k}) = \begin{pmatrix} 2\alpha_1(1-\cos k_x a) + 2\alpha_2(1-\cos k_x a\cos k_y a) & 2\alpha_2 \sin k_x a \sin k_y a \\ 2\alpha_2 \sin k_x a \sin k_y a & 2\alpha_1(1-\cos k_y a) + 2\alpha_2(1-\cos k_x a\cos k_y a) \end{pmatrix}$$

Problem 5.2 2D Continuum Modeling.

(a) Assume the two-dimensional equivalence of "plane strain", by applying a uniform x-directed load to this 2D continuum, determine the elastic modulus and the in-plane Poisson ratio in terms of the Lame's constants μ and λ. (*hint*: similar to the definitions of Young's modulus and Poisson ratio in 3D isotropic continuum, start from the strain-stress relation.)

(b) Recall from Problem Set 3.3 that $c_L = \sqrt{(\lambda+2\mu)/\rho}$ and $c_T = \sqrt{\mu/\rho}$ for the two sound velocities for 2D elastic continuum, we now wish to relate the elastic constant and Poisson ratio you get in part (a) to those of the 2D monatomic lattice in Problem 5.1. Find μ and λ in terms of the microscopic parameters α_1, α_2, a, and M. (*hint*: Choose $[k_x, k_y]$ along $[1,0]$ direction and you will get two sound velocities from the dynamical matrix $\mathbf{D}(\mathbf{k})$. The "long wavelength limit ($ka \ll 1$)" should then model the continuum.)

Problem 5.3 2D Monatomic square lattice on Matlab.

For a 2D monatomic square lattice of N atoms with a spacing a, the dispersion relation and polarization vectors are solved by finding the eigen values and eigen vectors of the Dynamical matrix in problem 5.1 by using the program `lw2dcu.m`, (lattice waves 2D cubic).

Use the program `lw2d.m` to do the following. (Using the command `help lw2dcu` will tell you what the variables are.)

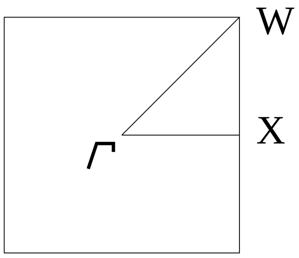
(a) Run the program and plot out the two resulting plots for the 3D dispersion relations and the contour plots.

(b) Plot the density of modes for the lower modes and upper modes separately, and then for both modes together.

(c) Make a plot of ω/ω_o versus k_x and k_y in the first Brillouin zone along the following directions. (You will need to understand what the command `meshdom` does. For example, if $N = 50$ then the origin is at $[mk_x(26,26), mk_y(26,26)]$.)

- Γ to X

- Γ to W
- X to W



(d) Check you answers with the analytical expressions at the points of high symmetry X and W for both modes.

Problem 5.4 Demo of lattice motion for 2D square lattice.

Program `twolwcu.m` generates a movie for a square lattice with nearest neighbor interactions for the atomic positions of an 8×8 array with lattice constant $a = 1$ and $M = 1$. When a value of the propagation vector (k_x, k_y) is input, then the values are given for the two eigen frequencies (in units of $\sqrt{(2\alpha_1/M)}$) and the corresponding polarization vectors. Two movies for the lower modes and the higher modes follow.

Use the program to answer the following questions. (Again `help twolwcu` gives you information about the program.) You are to describe the motion for each of the **k**-values given by printing out the final two figures for each of the propagation values given and drawing what the motion is like. Furthermore, be sure to determine if the modes are transverse modes, longitudinal modes, or neither.

(a) Let $[k_x, k_y] = [1, 0]$, that is along the Γ to X direction.

(b) Let $[k_x, k_y] = [1, 1]$, that is along the Γ to W direction.

(c) Let $[k_x, k_y] = [\pi/a, 1]$, that is along the X to W direction.

(d) Let $[k_x, k_y] = [\pi/a, 0]$, that is at the point X on the Brillouin zone edge.

(e) Let $[k_x, k_y] = [\pi/a, \pi/a]$, that is at the point W on the Brillouin zone edge.

(f) Let $[k_x, k_y] = [1, \sqrt{2}]$, that is at the point not along a symmetry axis.

Quiz 1 is on Friday, March 8, 1996 from 1—3pm in class.