6.730 PHYSICS FOR SOLID STATE APPLICATIONS

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PROBLEM SET 4

Issued: 2-28-96 Due: 3-6-96, at the beginning of class.

Readings:
Ashcroft and Mermin, Chapter 22.
Notes from 6.730 on Lattice Waves.

Problem 4.1 Reciprocal Lattice Vectors.

Do problem 1 in Ashcroft and Mermin, Chapter 5.

Problem 4.2 1D Monatomic lattice on Matlab.

For a 1D monatomic lattice of N atoms with a spacing a, the displacement of the n-th atom is

$$u[n,t] = \epsilon e^{i(kNa - \omega t)} .$$

Periodic boundary conditions, $u[n,t] = u[n+N,t]$, demand that

$$k = k_m = m\frac{2\pi}{Na} \qquad m = [-\frac{N}{2}, \frac{N}{2}]$$

where m is an integer. Program `onedlwb.m` generates a movie with $\epsilon = 1$ for $N = 20$, for input values of m. Program `onedlw2b.m` generates a movie of the atomic positions with $\epsilon = 0.3$ for $N = 20$, for input values of m. Use these programs to answer the following questions.

(a) How do $m = 1$, -1, 21 and -21 differ from one another? Print out the plots of $u[n,t]$ for a fixed time for each of these.

(b) How many wavelengths fit on the ring for $m = 3$, 5, and 10? Print out the plots of $u[n,t]$ for a fixed time for each of these.

(c) How do $m = 10$ and -10 differ from each other? Be sure to compare the movies from `onedlw2b.m` also.

Problem 4.3 Density of modes for a diatomic 1D lattice.

Consider a 1D ring of N atoms with $\omega_o^2 = K/M$, then (Ashcroft and Mermin, Eqn. 22.37)

$$\frac{\omega^2}{\omega_o^2} = 1 + \frac{G}{K} \pm \sqrt{1 + (G/K)^2 + 2(G/K)\cos ka}\,.$$

For each of the three cases $K/G = 1$, 2, and 5,

(a) Plot ω/ω_o versus $k = [-\pi/a, \pi/a]$.

(b) Assume $N = 2000$, numerically find the density of modes by making a histogram of ω/ω_o.

(c) For the case $K/G = 5$, model the acoustic branch as Debye model, and the optical branch as Einstein model, plot the dispersion relation, and density of modes on histogram (*hint*: you may refer to Ashcroft and Mermin, P435, for modeling).

Problem 4.4 Movies for 1D diatomic lattice.

Develop programs analogous to `onedlwb.m` and `onedlw2b.m` for a diatomic lattice with $N = 10$, $a = 1$, and $d = 0.3$. Let $\epsilon_1 = 0.1a$. Color the atoms at $x = na$ different from those at $x = na + d$. Assume $M_1 = M_2$ and $K_1 = 2K_2$.

(a) Run the program for $m = 1$ for both acoustic and opical modes. Print out the plots of $u_1[n,t]$ and $u_2[n,t]$ for a fixed time for the acoustic and optical modes respectively (attach your .m files).

(b) Repeat part (a) for $k = \pi/a$, that is $m = 5$.

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