Second Midterm Exam

P555

April 13, 2023

SHOW ALL YOUR WORK TO GET FULL CREDIT!

The Bonus questions at the end are optional and you can submit them from home before midnight today.

Problem 1: Consider a tight-binding Hamiltonian that acts upon a single band of localized states in one dimension,

$$\hat{H} = \sum_j [t|j><j+1| + t|j><j-1| + t(-1)^j|j><j|], \tag{1}$$

where t is a constant. The integer j should be thought of as indexing sites along a chain of atoms separated from each other by a distance a; the state $|j>$ locates an electron on atom j.

a) i) What is the periodicity of the Hamiltonian? (5 points)

ii) What is the lattice constant of the system? (5 points)

iii) What are the boundaries of the first Brillouin zone (FBZ) centered at $k = 0$? (5 points)

b) Use Bloch's theorem to reduce the eigenvalue problem associated with the Hamiltonian given to the solution of a small finite matrix equation. Provide the basis and the resulting Hamiltonian matrix. (10 points)

c) Compute and plot the bands for k in the FBZ. In your plot clearly label the axis and indicate the value of k at the boundaries of the BZ and the energies at the top and bottom of each band. (5 points)

d) What is the band gap in the electronic band structure at the boundary of the FBZ? (5 points)

e) What is the bandwidth of the upper band? (5 points)

Problem 2: Consider a 1-dimensional system of N ions separated from each other by a distance a and with periodic boundary conditions. In this system a phonon with momentum k has a frequency given by

$$\omega_k = \omega_0 \sin(\frac{|k|a}{2}), \tag{2}$$

where ω_0 is a constant.

a) Draw the dispersion relation ω_k vs k given in Eq.(2) in the first Brillouin zone (FBZ), clearly indicating the values of k that define the FBZ and ω_0 in the ω-axis and the values of the dispersion at the boundaries of the BZ. (5 points)

b) Now using the Debye approximation in the above model, i.e., assuming that

$$\omega_k = c|k|, \tag{3}$$

where c is a constant:

i) Determine the value of c. (5 points)

ii) What physical property of the system does c represent? (5 points)

c) Draw the Debye dispersion relation ω_k vs k given in Eq.(3) in the first Brillouin zone (FBZ), in the same figure that you drew in part (a) indicating the value of the dispersion at the boundary of the BZ. (5 points)

d) From the figure you drew, in what part of the Brillouin zone is the Debye approximation good? Is this reasonable? (5 points)

Bonus:
i) Evaluate the density of phonon modes $D(\omega)$ for the model in Eq.(2) (part (a)). (5 points)
ii) Evaluate the density of phonon modes $D_D(\omega)$ for the model in the Debye approximation in Eq.(3).(5 points)
iii) Find ω_D, the Debye frequency for this system in terms of ω_0. (10 points)
iv) Plot $D(\omega)$ versus ω for each model in the same plot. (5 points)