P555

April 12, 2022

SHOW ALL YOUR WORK TO GET FULL CREDIT!

Problem 1: Consider a linear array of A and B atoms of the form (...ABABAB...) with equal spacing d between each atom. The energies of the electrons in the system are given by $E_k = \pm[\epsilon^2 + 4\alpha^2 \cos^2(kd)]^{1/2}$ where ϵ and α are constants and k is the wavevector of the electron state.

a) What is the lattice constant of the crystal? Why? (5 points)

b) Draw the energy of the electrons in the first Brillouin zone (FBZ) clearly indicating the values of k and E_k at the zone boundaries. (10 points)

c) What is the band gap in the electronic band structure for the system? (10 points)

d) If there are 3 electrons per site of the Bravais lattice in what electronic band is the Fermi surface of the system? (5 points)

e) What is the bandwidth of the upper band? What parameter in E_k controls the bandwith? Why? (10 points)

Problem 2: Consider a solid in 2 dimensions made of N atoms with one atom at each point of the Bravais lattice.

a) How many acoustic and/or optical branches you expect to find for the phonon frequencies? Why? (5 points)

b) How many normal modes due to the ionic oscillations will be present? Why? (5 points)

c) Calculate the phonon density of states $D(\omega)$ in the Einstein approximation. Hint: remember that in 3D $D(\omega) = \frac{1}{V}\sum_{\mathbf{k},\nu}\delta(\omega - \omega_{\mathbf{k},\nu})$. (10 points)

d) Calculate the phonon density of states $D(\omega)$ in the Debye approximation. Hint: the average speed of sound in 2D is defined as $c^{-2} = \frac{1}{2}\sum_\nu \int \frac{d\phi}{2\pi c_\nu^2(\hat{\mathbf{k}})}$. (10 points)

e) Provide an expression for the Debye frequency ω_D in terms of the density of electrons in the system and the average speed of sound c.(10 points)