Second Midterm Exam

P555

April 12, 2022

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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)

Since the atoms A and B are different there are two atoms in the primitive unit cell and the lattice constant is given by the separation between the A atoms which is $a = 2d$.

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)

A unit vector in k-space has magnitude $K = 2\pi/a = 2\pi/(2d) = \pi/d$. Then the FBZ centered at $k = 0$ goes from $-\pi/(2d)$ which is excluded, to $\pi/2d$.

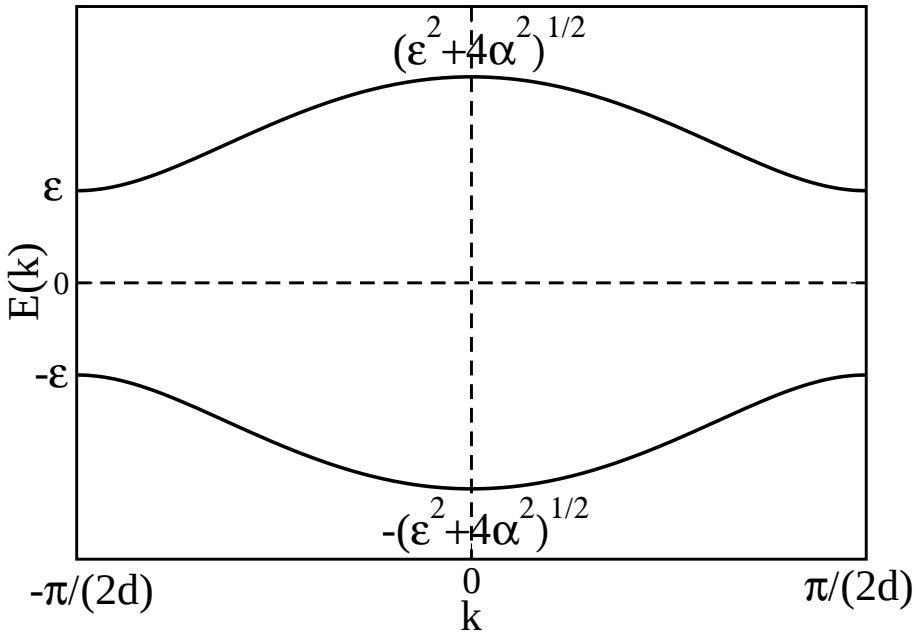

FIG. 1: The electron energy bands are plotted in the FBZ.

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

We see that at the boundary of the FBZ $E(k = \pi/(2d)) = \pm\epsilon$. Then the band gap is $\Delta = 2\epsilon$.

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)

Each band has space for $2N$ electrons where N is the number of sites in the Bravais lattice. This means that if there are $3N$ electrons the Fermi surface is in the upper electronic band since the lower band is fully occupied.

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

The bandwidth of the upper band is $W = [\epsilon^2 + 4\alpha^2 \cos^2(kd)]^{1/2} - \epsilon$. We see that the parameter that controls W is α because it multiplies the term that depends on k. The largest α^2 is, the largest W will be.

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)

Since there is one electron per primitive unit cell I do not expect to see any optical modes. Since we are in 2D I would expect to observe two acoustic branches.

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

Since there are N atoms and we are in two dimensions I expect to find $2N$ normal modes.

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)

We need to adapt the equation given in the hint to dimensions 2. We obtain

$$D(\omega) = \frac{1}{A}\sum_{\mathbf{k},\nu} \delta(\omega - \omega_{\mathbf{k},\nu}), \tag{1}$$

where A is the area of the system. In the Einstein approximation $\omega_{\mathbf{k},\nu} = \omega_E$ for all $\mathbf{k}$ and ν, then replacing in Eq. 1 we obtain:

$$D_E(\omega) = \frac{1}{A}\sum_{\nu} \delta(\omega - \omega_E) = \frac{2N}{A}\delta(\omega - \omega_E). \tag{2}$$

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)

Now we need to replace the sum over $\mathbf{k}$ in Eq. 1 by an integral and assume that $\omega_{\mathbf{k},\nu} = c_\nu(\hat{\mathbf{k}})k$, then we obtain:

$$D_D(\omega) = \int \frac{d^2k'}{(2\pi)^2}\sum_{\nu} \delta(\omega - \omega_{\mathbf{k},\nu}) = \int \frac{k'dk'd\phi}{(2\pi)^2}\sum_{\nu} \frac{\delta(k-k')}{c_\nu(\hat{\mathbf{k}})} = k\int \frac{d\phi}{(2\pi)^2}\sum_{\nu} \frac{1}{c_\nu(\hat{\mathbf{k}})} = 2\frac{\omega}{2\pi}[\frac{1}{2}\sum_{\nu}\int \frac{d\phi}{2\pi c_\nu^2(\hat{\mathbf{k}})} = \frac{\omega}{\pi c^2}, \tag{3}$$

where we have used the definition of c provided.

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)

We know that in the Debye approximation the integral of the density of modes up to the Debye frequency is equal to the total number of modes $2N$ then:

$$2N = A\int_0^{\omega_D} d\omega D_D(\omega) = A\int_0^{\omega_D} \frac{\omega}{\pi c^2}d\omega = \frac{A\omega_D^2}{2\pi c^2}. \tag{4}$$

Solving for ω_D using that $n = N/A$ we obtain

$$\omega_D = 2c\sqrt{n\pi}. \tag{5}$$