Second Midterm Exam

P555
April 11, 2024

SHOW ALL YOUR WORK TO GET FULL CREDIT!

The items in blue, including the Bonus question, are the take home part of the test. Submit a pdf file with your at home work not later that April 12 at 11PM.

Problem 1: A two dimensional crystal has one atom of valency one in a simple rectangular Bravais lattice with primitive vectors $\mathbf{a_1} = (4a, 0)$ and $\mathbf{a_2} = (0, a)$.

a) Find a set of primitive vectors for the reciprocal lattice and provide their length in terms of a. (5 points)

b) In Fig. 1 the primitive unit cell in reciprocal space is shown for the given rectangular lattice. Label the boundaries of the unit cell shown along k_x and k_y in terms of a. (5 points)

c) Calculate the radius of the free fermion electron Fermi sphere (circle in 2D) at $T = 0$ in terms of a. (10 points)

d) Draw this sphere to scale if Fig. 1. (5 points)

e) Provide the Fermi energy, E_F for the free electrons. (5 points)

f) Draw the energy for the free electrons in the reduced scheme, i.e., inside the first Brillouin zone, along the k_x direction. Start at $\mathbf{k} = (0, 0)$ (which is the center of the Brillouin zone; you do not need to draw the energy for the negative values of k_x inside the BZ because by symmetry it will be the same than on the positive side) and end at $(X, 0)$ where X is the boundary of the first Brillouin zone, and indicate the Fermi energy. Hint: include as many bands as needed to indicate the place of the Fermi energy.(10 points)

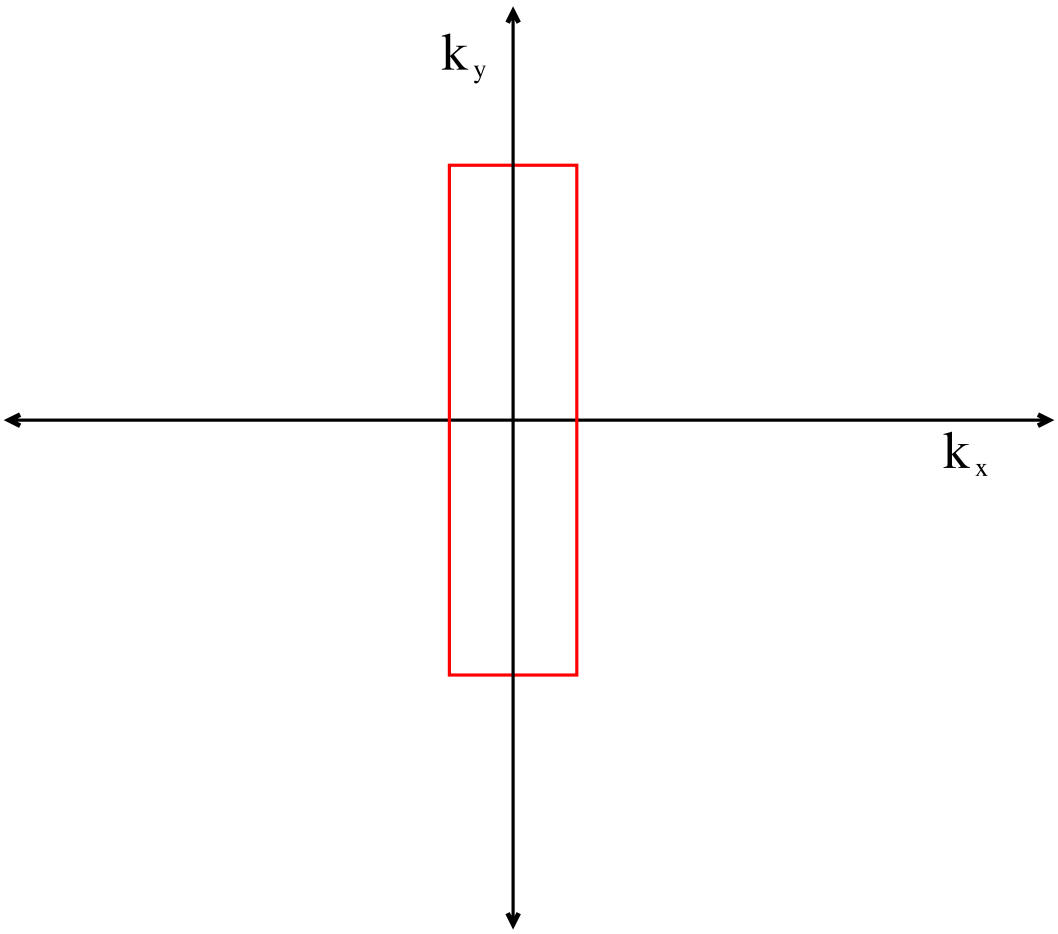

FIG. 1: The primitive unit cell is indicated in red.

g) If a weak periodic potential were applied, indicate in your previous drawing how $E(\mathbf{k})$ would be modified. You do not need to do any calculation, but explain in words the rational for your drawing, i.e., in what part of the curves the main changes occur and why.(5 points)

h) Draw the shape of the Fermi surface under the influence of the weak periodic potential in Fig. 1. (5 points)

i) Now consider the case in which the electrons are tightly bound to the atoms. In this case the energy is given by $E_{\mathbf{k}} = -2t(\cos 4k_x a + \cos k_y a)$. What is the bandwidth of this energy band? (5 points)

j) Considering that the atoms contribute one electron and the symmetry of the energy dispersion, what is the Fermi energy now?(5 points).

k) Draw the shape of the Fermi surface in Fig. 1. (5 points)

l) Draw the energy for the tight binding model inside the first Brillouin zone, along the k_x direction. Start at $\mathbf{k} = (0, 0)$ and end at $(X, 0)$ where X is the boundary of the first Brillouin zone, and indicate the Fermi energy. (5 points)

Problem 2: Consider a one-dimensional crystal with lattice constant a and a basis of two atoms. At $\mathbf{v}_1 = 0$ the atoms have mass $M = 2m$ at $\mathbf{v}_2 = a/2$ the atoms have mass m. The system has PBC. In class we found that the frequencies of oscillation as well as the displacement of the atoms are obtained from solving the following eigenvalues and eigenvectors problem:

$$\begin{pmatrix} M_1\omega^2 - 2K & 2K\cos(\frac{ka}{2}) \\ 2K\cos(\frac{ka}{2}) & M_2\omega^2 - 2K \end{pmatrix} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{1}$$

Finding the eigenvalues we obtain that

$$\omega_\pm = \sqrt{K}\sqrt{\frac{(M_1 + M_2) \pm [M_1^2 + 2M_1M_2\cos(ka) + M_2^2]^{1/2}}{M_1M_2}}. \tag{2}$$

Here M_1 and M_2 are the masses of the two atoms in the basis and you can use that the spring constant $K = m\omega_0^2$, i.e., a constant, but written in a way that will simplify the algebra.

a) In the figure you can see $\omega_\pm$ versus k. Indicate which branch is acoustic. Is there an optical branch? Why?(5 points)

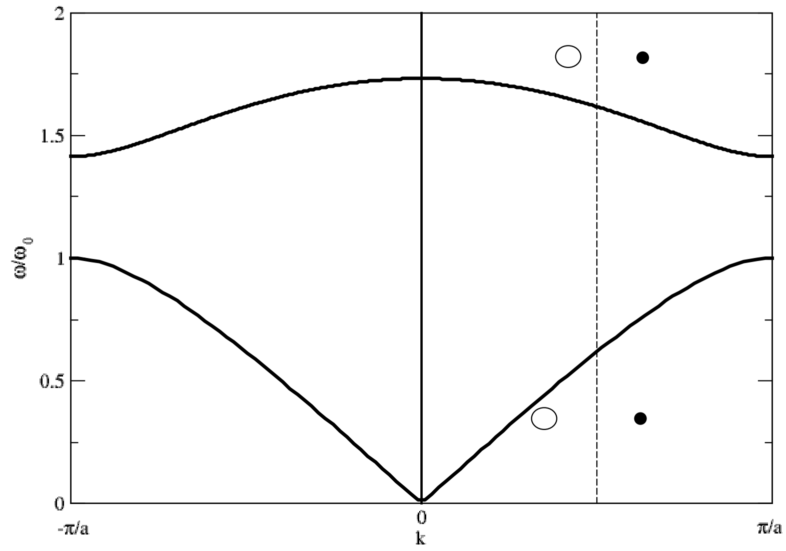

FIG. 2: Phonon dispersion relation.

b) What is the speed of sound in this system? Hint: Check your units in your final result. (10 points)

c) Now consider $k = \pi/2a$ and:

i) Provide the values of $\omega_\pm$ in terms of ω_0. (5 points)

ii) Indicate in what direction the atoms of the basis are moving in the acoustic branch and plot it by adding arrows to the ions shown in Fig. 2. Hint: Find the eigenvectors.(5 points)

iii) Indicate in what direction the atoms of the basis are moving in the optical branch and plot it by adding arrows to the ions shown in Fig. 2. Hint: Find the eigenvectors.(5 points)

Bonus: Now assume that $M = m$. Plot the resulting phonon dispersion relation and discuss the changes with respect to the dispersion shown in Fig. 2.(10 points)