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)

The primitive vectors of the reciprocal lattice are given by

$$\mathbf{b}_1 = (\frac{\pi}{2a}, 0), \tag{1}$$

and

$$\mathbf{b}_2 = (\frac{2\pi}{a}, 0). \tag{2}$$

We see that they satisfy $\mathbf{a}_i.\mathbf{b}_j = 2\pi\delta_{ij}$ as expected.

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)
We found in the homework that in 2D

$$k_F = \sqrt{2\pi n}, \tag{3}$$

where the density of electrons n is given by

$$n = \frac{N}{A} = \frac{1}{4a^2}. \tag{4}$$

Notice that $N = 1$ because each atom in the primitive unit cell provides 1 electron and A is the area of the rectangular primitive unit cell, i.e. $A = 4a^2$. Then,

$$k_F = \sqrt{2\pi n} = \sqrt{\frac{2\pi}{4a^2}} = \frac{1}{a}\sqrt{\frac{\pi}{2}} = \frac{0.40\pi}{a}. \tag{5}$$

Alternative way:
We know that the FBZ can hold $2N$ electrons. Since the atoms provide N electrons this means that the system is "half-filled" and thus, the area of the Fermi sphere (circle) has to be equal to half the area of the FBZ. This means that

$$\pi k_F^2 = \frac{1}{2}\frac{2\pi}{a}\frac{\pi}{2a} = \frac{\pi^2}{2a^2}. \tag{6}$$

Then,

$$k_F = \frac{1}{a}\sqrt{\frac{\pi}{2}} = \frac{0.40\pi}{a}, \tag{7}$$

as expected.

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

e) Provide the Fermi energy, E_F for the free electrons. (5 points) The Fermi energy is given by

$$E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2(\sqrt{\frac{\pi}{2}})^2}{2ma^2} = \frac{\hbar^2\pi}{4a^2 m}. \tag{8}$$

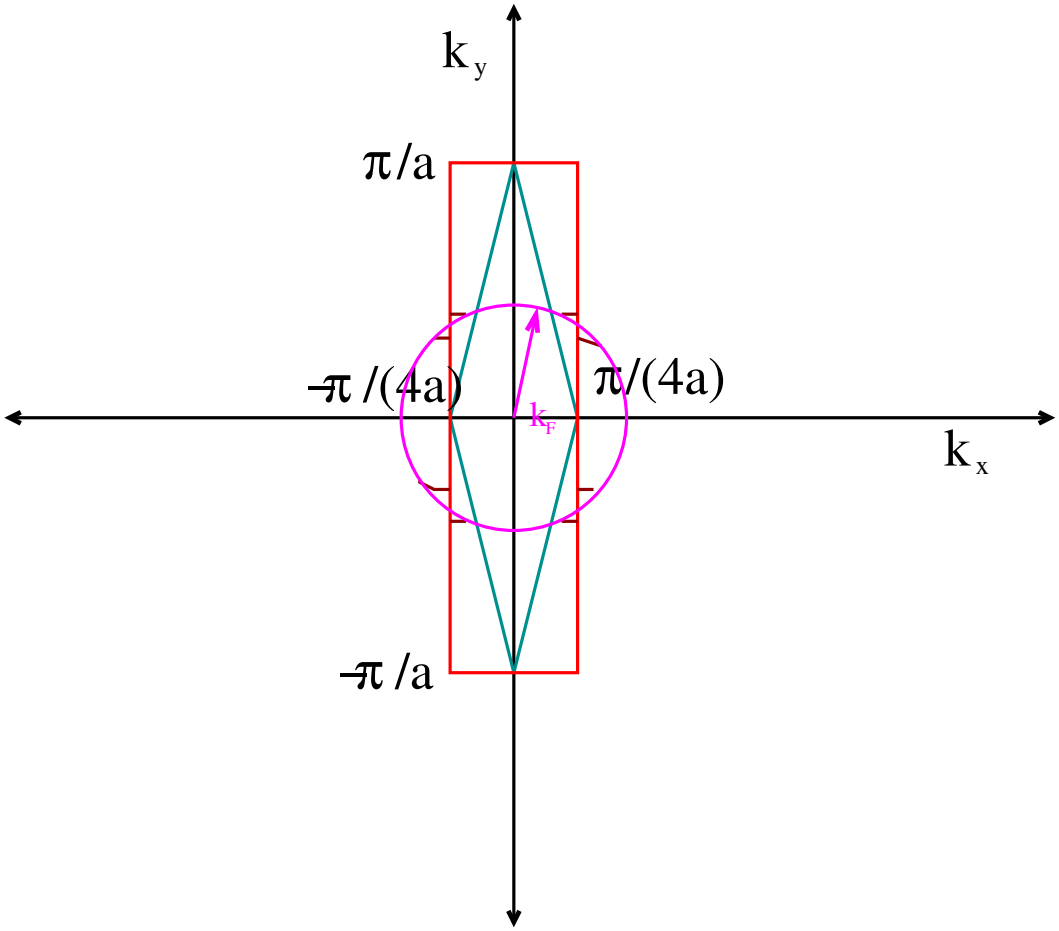

FIG. 1: The primitive unit cell is indicated in red. The FS for free electrons is indicated in purple. The Fermi momentum k_F is also indicated. The blue lines indicate the tight binding FS for a half-filled system. The brown lines indicate the distortion of the FS for free electrons due to the effects of a weak periodic potential.

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)

For free electrons the energy is given by

$$E = \frac{\hbar^2 k^2}{2m}, \tag{9}$$

which is a parabola that starts at 0 for $k = 0$ and goes up to

$$E_X = \frac{\hbar^2 k_X^2}{2m} = \frac{\hbar^2 \pi^2}{32 a^2 m}, \tag{10}$$

where we have used that $k_X = \frac{\pi}{4a}$. The parabola continues outside the FBZ, but it gets folded (or we can use the parabola centered at the first nearest neighbor site along x in the reciprocal lattice). At crystal momentum zero the actual momentum for the electron will be $\mathbf{K} + 0$ where $\mathbf{K} = (\frac{\pi}{2a}, 0)$; thus for what would become the second band we get that

$$E_\Gamma = \frac{\hbar^2 k_\Gamma^2}{2m} = \frac{\hbar^2 K^2}{2m} = \frac{\hbar^2 \pi^2}{8 a^2 m}. \tag{11}$$

The Fermi energy, found in (e) is given by

$$E_F = \frac{\hbar^2 \pi}{4a^2 m}. \tag{12}$$

We see that E_F crosses the second band as expected because the Fermi sphere ends outside the FBZ along the x axis.

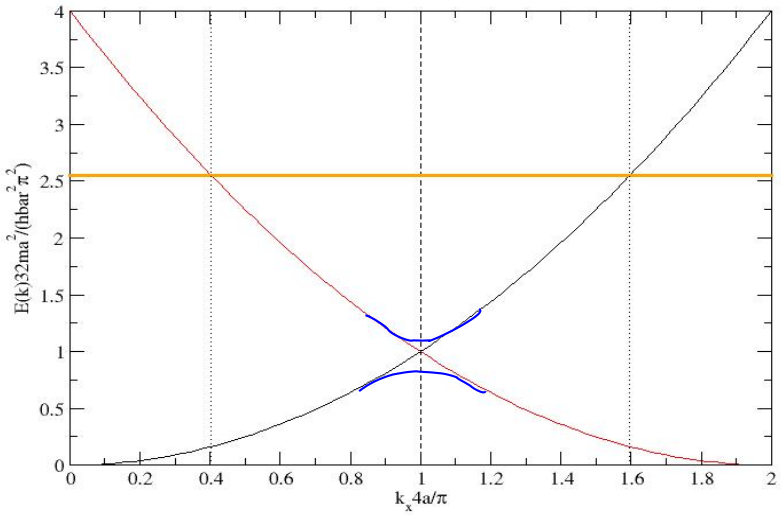

FIG. 2: The energy of the free electrons in the reduced scheme are indicated in the FBZ along the $\Gamma - X$ direction. The dotted vertical line indicates the boundary of the FBZ. The Fermi energy E_F is indicated by the orange line. The blue lines indicate the effects of the weak periodic potential. A gap opens at the boundary of the BZ and two bands appear.

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)

The weak periodic potential breaks the degeneracy of the energies at the boundary of the Brillouin zone opening a gap and producing the energy bands. In Fig. 2 we can see qualitatively how the gap opens forming two bands.

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

See the figure.

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)

The bandwidth is given by the difference between the maximum and minimum energy. We see that the minimum occurs at $\mathbf{k} = (0, 0)$ and it is $E_{min} = -4t$ while the maximum occurs when the cosines reach their minimum value, i.e. -1. This happens when $k_x = \pm\frac{\pi}{4a}$ and $k_y = \pm\frac{\pi}{a}$ with $E_{max} = 4t$. Then the bandwidth is $W = 8t$.

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

Now the Fermi energy is 0, since with N electrons half of the states are doubly occupied and since the dispersion is symmetric with respect to zero, half the available states are above zero and the other half are below zero, thus, this is where the Fermi energy has to be.

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

We need to find the values of k_x and k_y that satisfy $E(\mathbf{k}) = 0$. We can see that this is satisfied for $(k_x, k_y) = (\pm\frac{\pi}{4a}, 0)$, $(k_x, k_y) = (0, \pm\frac{\pi}{a})$, and $(k_x, k_y) = (\pm\frac{\pi}{8a}, \pm\frac{\pi}{2a})$. These points describe the indicated diamond inside the FBZ indicated in Fig. 1 with blue lines.

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)

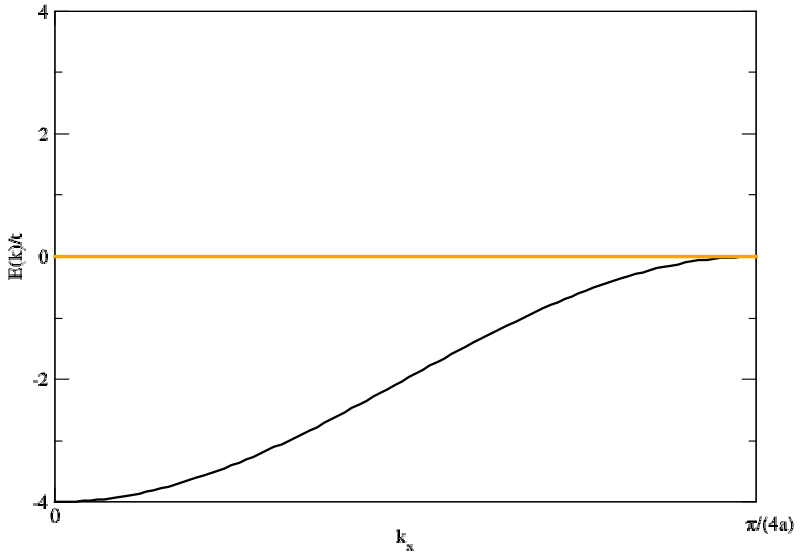

FIG. 3: The tight-binding energy in the FBZ along the $\Gamma - X$ direction. The Fermi energy E_F is indicated by the orange line.

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:

$$\begin{pmatrix} M_1\omega^2 - 2K & 2K\cos(\frac{ka}{2}) \\ 2K\cos(\frac{ka}{2}) & M_2\omega^2 - 2K \end{pmatrix} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{13}$$

Finding the eigenvalues we obtain that

$$\omega_\pm = \sqrt{K}\sqrt{\frac{(M_1 + M_2) \pm [M_1^2 + 2M_1M_2\cos(ka) + M_2^2]^{1/2}}{M_1M_2}}. \tag{14}$$

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)

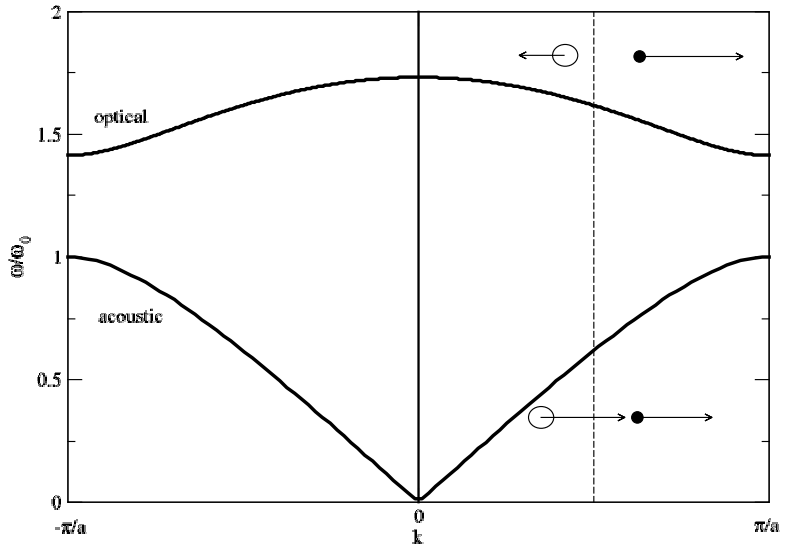

FIG. 4: Phonon dispersion relation. The acoustic and optical branches are indicated as well as the vibration modes of the atoms for $k = \frac{\pi}{2a}$.

There is an optical branch because there are two ions in the basis.

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

We need to focus on the acoustic branch and obtain ω_- for very small k. Let's replace K, M_1, and M_2 in the expression for ω_-:

$$\omega_- = \omega_0 \sqrt{\frac{3 - [4 + 4\cos(ka) + 1]^{1/2}}{2}} = \omega_0 \sqrt{\frac{3 - [5 + 4\cos(ka)]^{1/2}}{2}}. \tag{15}$$

We need to obtain the behavior for $k \to 0$ keeping the lowest order k-dependence; thus, we replace $\cos(ka) \approx 1 - \frac{k^2 a^2}{2}$. Then we obtain:

$$\omega_- \approx \omega_0 \sqrt{\frac{3 - [5 + 4(1 - \frac{(ka)^2}{2})]^{1/2}}{2}} = \omega_0 \sqrt{\frac{3 - [9 - 2(ka)^2)]^{1/2}}{2}} = \omega_0 \sqrt{\frac{3 - 3[1 - \frac{2}{9}(ka)^2)]^{1/2}}{2}}. \tag{16}$$

Now we use that $(1 + x)^{1/2} \approx 1 + \frac{x}{2}$ when $x \ll 1$ and we obtain:

$$\omega_- \approx \omega_0 \sqrt{\frac{3 - 3[1 - \frac{1}{9}(ka)^2]}{2}} = \omega_0 \sqrt{\frac{3}{9}\frac{(ka)^2}{2}} = \omega_0 \frac{ka}{\sqrt{6}} = \frac{\sqrt{6}}{6}\omega_0 ka. \tag{17}$$

The speed of sound is given by

$$c = \frac{d\omega}{dk} = \frac{\sqrt{2}}{6}\omega_0 a. \tag{18}$$

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

i) Provide the values of $\omega_\pm$ in terms of ω_0. (5 points)
For $k = \pi/2a$ we know that $\cos ka = 0$. Then:

$$\omega_\pm = \omega_0\sqrt{\frac{3 \pm [4+1]^{1/2}}{2}} = \omega_0\sqrt{\frac{3 \pm 5^{1/2}}{2}}. \tag{19}$$

Thus,

$$\omega_- = \omega_0\sqrt{\frac{3 - [4+1]^{1/2}}{2}} = \omega_0\sqrt{\frac{3 - 5^{1/2}}{2}} = 0.618\omega_0. \tag{20}$$

and

$$\omega_+ = \omega_0\sqrt{\frac{3 + [4+1]^{1/2}}{2}} = \omega_0\sqrt{\frac{3 + 5^{1/2}}{2}} = 1.618\omega_0. \tag{21}$$

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. 4. Hint: Find the eigenvectors.(5 points)
Now the matrix equations are given by

$$\begin{pmatrix} 2(\omega^2 - \omega_0^2) & \omega_0^2\sqrt{2} \\ \omega_0^2\sqrt{2} & (\omega^2 - 2\omega_0^2) \end{pmatrix} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{22}$$

Since we found ω in terms of ω_0 we can divide the equation by ω_0 and we obtain for the accoustic branch:

$$\begin{pmatrix} 2(0.618^2 - 1) & \sqrt{2} \\ \sqrt{2} & (0.618^2 - 2) \end{pmatrix} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{23}$$

$$\begin{pmatrix} -1.236 & 1.41 \\ 1.41 & -1.618 \end{pmatrix} \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{24}$$

Thus,

$$-1.236\epsilon_1 + 1.41\epsilon_2 = 0. \tag{25}$$

Then,

$$1.41\epsilon_2 = 1.236\epsilon_1, \tag{26}$$

and

$$\epsilon_2 = \frac{1.236}{1.41}\epsilon_1 = 0.8765\epsilon_1. \tag{27}$$

Since $\epsilon_1^2 + \epsilon_2^2 = 1$ we obtain that

$$1 = \epsilon_1^2 + 0.8765^2\epsilon_1^2 = 1.7684\epsilon_1^2. \tag{28}$$

Then,

$$\epsilon_1 = \frac{1}{\sqrt{1.7684}} = 0.7519 \tag{29}$$

and

$$\epsilon_2 = 0.8765\epsilon_1 = 0.65911 \tag{30}$$

We see that both atoms move in the same direction with the displacement of the heavy ion slightly larger than the one for the lighter one.

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. 4. Hint: Find the eigenvectors.(5 points)

Now the matrix equations are given by

$$\begin{pmatrix} 2(\omega^2-\omega_0^2) & \omega_0^2\sqrt{2} \\ \omega_0^2\sqrt{2} & (\omega^2-2\omega_0^2) \end{pmatrix}\begin{pmatrix}\epsilon_1\\ \epsilon_2\end{pmatrix}=\begin{pmatrix}0\\0\end{pmatrix} \tag{31}$$

Since we found ω in terms of ω_0 we can divide the equation by ω_0 and we obtain for the accoustic branch:

$$\begin{pmatrix} 2(1.618^2-1) & \sqrt{2} \\ \sqrt{2} & (1.618^2-2) \end{pmatrix}\begin{pmatrix}\epsilon_1\\ \epsilon_2\end{pmatrix}=\begin{pmatrix}0\\0\end{pmatrix} \tag{32}$$

$$\begin{pmatrix} 3.2358 & 1.41 \\ 1.41 & 1.6179 \end{pmatrix}\begin{pmatrix}\epsilon_1\\ \epsilon_2\end{pmatrix}=\begin{pmatrix}0\\0\end{pmatrix} \tag{33}$$

Thus,

$$3.2358\epsilon_1+1.41\epsilon_2=0. \tag{34}$$

Then,

$$1.41\epsilon_2=-3.2358\epsilon_1, \tag{35}$$

and

$$\epsilon_2=\frac{-3.2358}{1.41}\epsilon_1=-2.2949\epsilon_1. \tag{36}$$

Since $\epsilon_1^2+\epsilon_2^2=1$ we obtain that

$$1=\epsilon_1^2+2.2949^2\epsilon_1^2=6.2665\epsilon_1^2. \tag{37}$$

Then,

$$\epsilon_1=\frac{1}{\sqrt{6.2665}}=0.3994 \tag{38}$$

and

$$\epsilon_2=-2.294\epsilon_1=-.9163 \tag{39}$$

We see that the atoms move in opposite direction with the displacement of the heavy ion much smaller than the one for the lighter one.

Bonus: Now assume that $M=m$. Plot the resulting phonon dispersion relation and discuss the changes with respect to the dispersion shown in Fig. 4.(10 points)

Now all the atoms are the same, thus, the lattice constant becomes $a/2$ and there is no basis. This means that we will have only one acoustic branch in an extended BZ that goes from $-2\pi/a$ to $2\pi/a$. In the original reduced BZ we see that the original optical band, indicated in red, is now the folded acoustic band since there is no gap at $k=\pm\pi/a$.

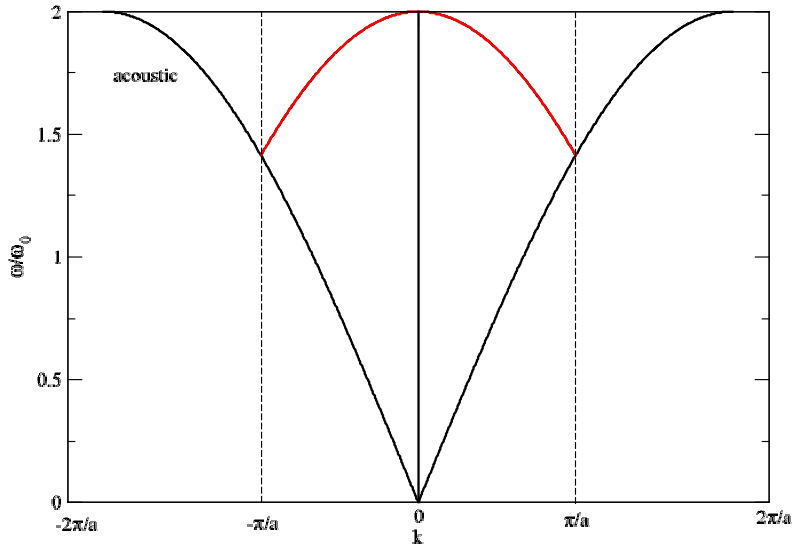

FIG. 5: Phonon dispersion relation. There is only an acoustic band, indicated in black, because all the atoms are the same. The lattice constant is now $a/2$ and thus, the FBZ has doubled in size. The red line is the folded acoustic branch.