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)

The Hamiltonian has periodicity 2 because the last term is positive (negative) in even (odd) sites.

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

The lattice constant is thus $2a$.

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

The FBZ must have length $K = \frac{2\pi}{2a} = \frac{\pi}{a}$. This means that the values of k symmetric with respect to 0 in the FBZ satisfy that $\frac{\pi}{2a} < k \leq \frac{\pi}{2a}$.

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)

Due to the periodicity of the Hamiltonian we know that we will have to diagonalize a 2×2 matrix and the system will have 2 bands. We know that

$$H|\Psi>= \epsilon|\Psi>, \tag{2}$$

where $|\Psi>= |\Psi_0, \Psi_1>$ and $\Psi_j =< j|\Psi>$. Now, let's evaluate $H|\Psi_j>$ for $j = 0, 1$:

$$H|\Psi_0>= t|\Psi_{-1}> + t|\Psi_1> + t|\Psi_0> \tag{3}$$

$$H|\Psi_1>= t|\Psi_2> + t|\Psi_0> - t|\Psi_1> . \tag{4}$$

From Bloch's theorem we know that

$$\Psi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = \Psi_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}.\mathbf{R}}, \tag{5}$$

then

$$|\Psi_{-1}>= e^{-i2ka}|\Psi_1> \tag{6}$$

and

$$|\Psi_2>= e^{i2ka}|\Psi_0> . \tag{7}$$

Then

$$H|\Psi_0>=t(e^{-i2ka}+1)|\Psi_1>+t|\Psi_0>=\epsilon|\Psi_0> \tag{8}$$

$$H|\Psi_1>=t(1+e^{i2ka})|\Psi_0>-t|\Psi_1>=\epsilon|\Psi_1>. \tag{9}$$

Now we can write the Schrödinger equation in matrix form (using the notation $|j>=|\Psi_j>$):

$$\begin{pmatrix} <0|H|0> & <0|H|1> \\ <1|H|0> & <1|H|1> \end{pmatrix}\begin{pmatrix}\Psi_0\\ \Psi_1\end{pmatrix}=\begin{pmatrix} t & t(1+e^{-i2ka}) \\ t(e^{i2ka}+1) & -t\end{pmatrix}\begin{pmatrix}\Psi_0\\ \Psi_1\end{pmatrix}=\epsilon\begin{pmatrix}\Psi_0\\ \Psi_1\end{pmatrix} \tag{10}$$

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)

To find the bands we need to request that

$$\begin{vmatrix} t-\epsilon & t(1+e^{-i2ka}) \\ t(e^{i2ka}+1) & -t-\epsilon\end{vmatrix}=0. \tag{11}$$

The resultung quadratic equation is

$$\epsilon^2-t^2(1+4\cos^2(ka))=0, \tag{12}$$

which has solutions:

$$\epsilon=\pm t\sqrt{1+4\cos^2(ka)}. \tag{13}$$

The two resulting bands can be seen in Fig. 1 where ϵ/t is shown as a function of ka. The FBZ is indicated with dashed lines.

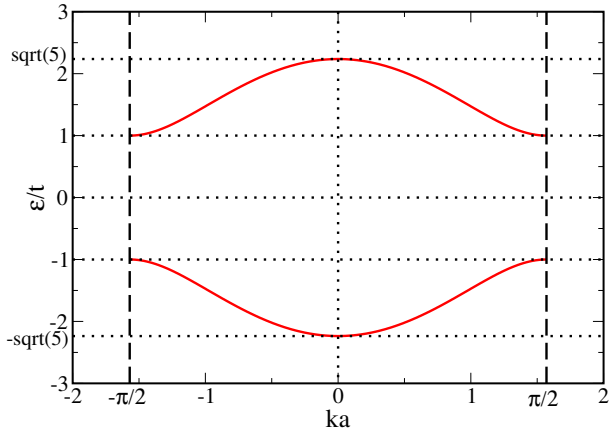

FIG. 1: Tight binding electron bands.

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

We see that at the boundary of the FBZ the two bands are separated by $E_g=2t$.

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

The bandwidth W is given by the difference between the energy ϵ_t at the top of the band and ϵ_b at the bottom of the band. Thus,

$$W=\epsilon_t-\epsilon_b=\epsilon^+(0)-\epsilon^+(\pi/2a)=\sqrt{5}t-t=(\sqrt{5}-1)t. \tag{14}$$

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

$$\omega_k = \omega_0 \sin(\frac{|k|a}{2}), \tag{15}$$

where ω_0 is a constant.

a) Draw the dispersion relation ω_k vs k given in Eq. 15 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)

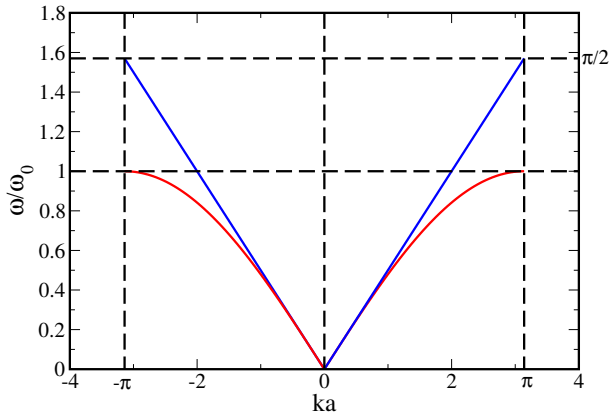

FIG. 2: The dispersion relation in Eq. 15 is indicated in red and the dispersion relation in Eq. 16 is indicated in blue.

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

$$\omega_k = c|k|, \tag{16}$$

where c is a constant:

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

The Debye approximation is the $k \to 0$ limit of the dispersion relation. In our case

$$\omega_k \approx \omega_0 \frac{|k|a}{2} = c|k|. \tag{17}$$

Then

$$c = \omega_0 \frac{a}{2}. \tag{18}$$

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

c is the sound velocity in the system since the sound velocity is given by $\frac{\partial \omega}{\partial k}$.

c) Draw the Debye dispersion relation ω_k vs k given in Eq. 16 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)

See the blue lines in Fig.2.

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

The result is reasonable because in the figure we see that both curves agree for small k and the Debye approximation is good for $k \to 0$.

Bonus:
i) Evaluate the density of phonon modes $D(\omega)$ for the model in Eq. 15 (part (a)). (5 points)

We know that in 1D the density of states for the phonons is given by

$$D(\omega) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \delta(\omega - \omega_k) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \delta(\omega - \omega_0 \sin(\frac{|k|a}{2})). \tag{19}$$

Now we change variables from k to ω using the dispersion relation so that

$$d\omega = \frac{\omega_0 a}{2} \cos(\frac{|k|a}{2}) dk. \tag{20}$$

The integral from negative values of k contributes as an integral over positive values of ω (in other words for each value of ω there are two values of k, i.e. $k = \pm k$ that have the same value of $|k|$); thus we obtain:

$$D(\omega) = 2 \int_0^{\infty} \frac{2d\omega}{2\pi\omega_0 a \cos(\frac{|k|a}{2})} \delta(\omega - \omega_0 \sin(\frac{|k|a}{2})) = \frac{2}{\pi\omega_0 a} \frac{1}{\sqrt{1 - \frac{\omega^2}{\omega_0^2}}} = \frac{2}{\pi a \sqrt{\omega_0^2 - \omega^2}}. \tag{21}$$

ii) Evaluate the density of phonon modes $D_D(\omega)$ for the model in the Debye approximation in Eq. 16.(5 points)
Now

$$D_D(\omega) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \delta(\omega - \omega_k) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \delta(\omega - c|k|). \tag{22}$$

Now we change variables from k to ω using the dispersion relation so that

$$d\omega = c dk. \tag{23}$$

The integral from negative values of k contributes as an integral over positive values of ω; thus we obtain:

$$D_D(\omega) = 2 \int_0^{\infty} \frac{2d\omega}{2\pi c} \delta(\omega - c|k|) = \frac{2}{2\pi c} = \frac{2}{\pi\omega_0 a}. \tag{24}$$

iii) Find ω_D, the Debye frequency for this system in terms of ω_0. (10 points)

We request that the total number of phonon modes N satisfies

$$N = L \int_0^{\omega_D} D_D(\omega) d\omega = \frac{L\omega_D}{\pi c}. \tag{25}$$

Then

$$\omega_D = \frac{\pi c N}{L} = \pi \frac{\omega_0 a N}{2Na} = \frac{\pi\omega_0}{2}. \tag{26}$$

iv) Plot $D(\omega)$ versus ω for each model in the same plot. (5 points)
See the curves in Fig.3. Notice that the cut frequency in the original model is ω_0 while in the Debye approximation it is $\omega_0\pi/2$.

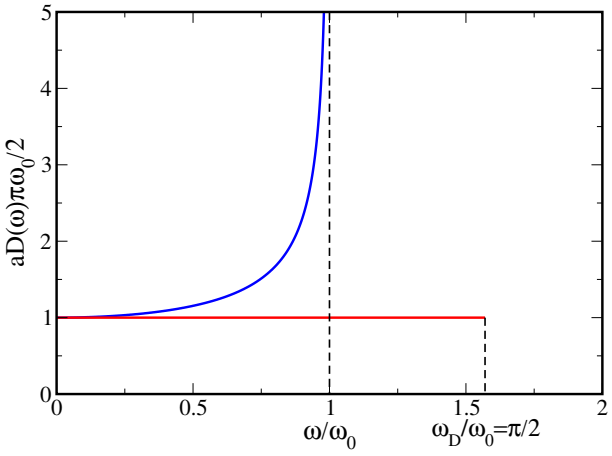

FIG. 3: Density of phonon modes for the original model in blue and in the Debye approximation in red.