

Exercise 1. Complex wavenumbers in a diatomic chain

Consider the diatomic chain shown in Fig. 1. From the lecture we know its dynamical matrix

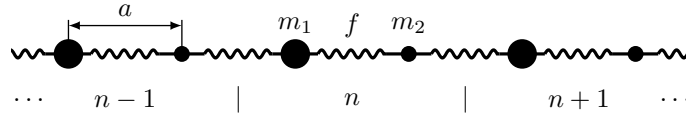


Figure 1: A diatomic chain.

in k -space is given by

$$D(k) = \frac{f}{m} \begin{pmatrix} \omega_0^2 + 2r & -(1 + e^{i2ka}) \\ -(1 + e^{-i2ka}) & \omega_0^2 + \frac{2}{r} \end{pmatrix}, \quad m = \sqrt{m_1 m_2}, \quad r = \sqrt{\frac{m_2}{m_1}}, \quad (1)$$

where we added an offset ω_0^2 .

- (a) Find the eigenvalues of $D(k)$ for a generic $k \in \mathbb{C}$.

Hint: Complex k values render the $D(k)$ matrix non-hermitian.

Solution. By solving

$$\det(\nu - D(k)) = 0, \quad (S.1)$$

we find the eigenvalues of $D(k)$ [Eq. (1)] are

$$\nu_{1,2} = \frac{f}{m} \left(\omega_0^2 + \frac{1}{r} \left[1 + r^2 \pm \sqrt{1 + 2r^2 \cos(2ak) + r^4} \right] \right), \quad (S.2)$$

and the corresponding eigenvectors are

$$\xi_{1,2} = \begin{pmatrix} \frac{f}{mr} \left[-1 + r^2 \pm \sqrt{1 + 2r^2 \cos(2ak) + r^4} \right] \\ -(1 + e^{-i2ka}) \end{pmatrix}. \quad (S.3)$$

- (b) Use the above result, to solve the equation of motion

$$\omega^2 u_k = D(k) u_k, \quad \omega \in \mathbb{R}. \quad (2)$$

Which $k \in \mathbb{C}$ remain valid, given that the frequencies ω are real-valued?

Hint: The condition on k depends on the frequency regime we are looking at.

Solution. To simplify notation, we write

$$k = q + i \frac{1}{\xi}, \quad q, \xi \in \mathbb{R}. \quad (S.4)$$

The eigenvalues $\nu_{1,2}$ are real valued if and only if

$$1 + 2r^2 \cos(2aq + i2a/\xi) + r^4 > 0. \quad (S.5)$$

There are two ways to make the expression real:

- (i) $2a/\xi \rightarrow 0$ and q arbitrary, or

(ii) $2aq \in \{0, \pi\}$ and ξ bound by some value to be determined.

In case (i) we directly have

$$1 + 2r^2 \cos(2aq + i^{2a}/\xi) + r^4 = 1 + 2r^2 \cos(2aq) + r^4 > 1 - 2r^2 + r^4 = (1 - r^2)^2 > 0. \quad (\text{S.6})$$

In case (ii) we distinguish two more cases. The first one is $aq = 0$ in which

$$1 + 2r^2 \cos(2aq + i^{2a}/\xi) + r^4 = 1 + 2r^2 \cos(i^{2a}/\xi) + r^4 = 1 + 2r^2 \cosh(2a/\xi) + r^4 > 0, \quad (\text{S.7})$$

as all the summands are greater than zero.

In the second case we have $2aq = \pi$ and therefore

$$1 + 2r^2 \cos(2aq + i^{2a}/\xi) + r^4 = 1 + 2r^2 \cos(i^{2a}/\xi) + r^4 = 1 - 2r^2 \cosh(2a/\xi) + r^4. \quad (\text{S.8})$$

In this second case we need

$$\cosh(2a/\xi) < \frac{1 + r^4}{2r^2} \Leftrightarrow \xi < \frac{2a}{\operatorname{arccosh}\left(\frac{1+r^4}{2r^2}\right)}. \quad (\text{S.9})$$

In all of these cases we have

$$\omega^2 = \nu_{1,2} \in \mathbb{R}, \quad (\text{S.10})$$

with the eigenvectors given in Eq. (S.3).

Note that we never needed to restrict ξ to positive values. Indeed we can have ξ positive or negative with the exact same formulas, giving rise to exponentially growing / decaying solutions. The eigenvectors of the exponentially growing / decaying solutions are different however as we can see from Eq. (S.3).

(c) Draw the dispersion relation $\omega(k) \in \mathbb{R}$ for $k \in \mathbb{C}$.

Solution. From part (b) we already know the valid solutions $\omega(k) = \pm\sqrt{\nu_{1,2}} \in \mathbb{R}$, which are plotted in Fig. 2. We only plotted solutions with $\xi > 0$, but we could also plot solutions with $\xi < 0$.

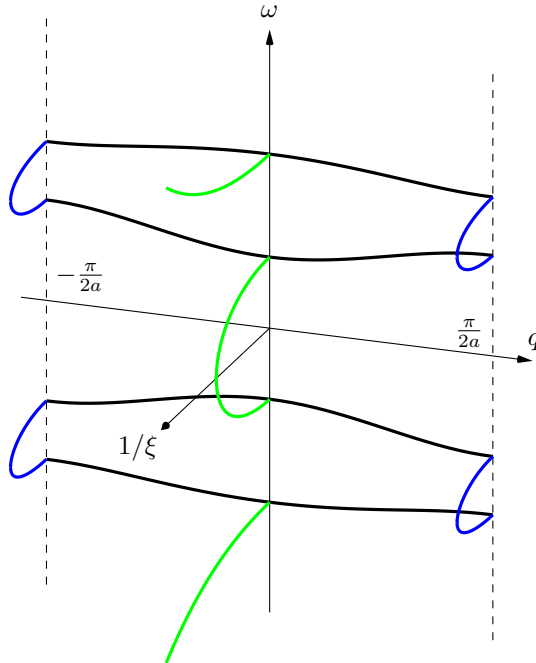


Figure 2: Dispersion relation of the diatomic chain. The two bands arising from the eigensolutions are shown in black. In blue and green are the two cases of complex k leading to real frequencies $\omega(k)$.

- (d) Some of the solutions are exponentially growing / decaying and therefore not well-defined on an infinite or periodic chain. Assume for these solutions that the chain is semi-infinite. What boundary condition would you need at the cut of the system for the solution to still be valid on the remainder of the system?

Solution. Let's assume that we cut the system between site 0 and site 1, such that only the sites $n > 0$ are part of the system. The exponential growing solutions are energetically not possible and we focus on the exponential decaying ones. To excite such an evanescent wave, we need to make sure that the boundary condition exactly fits the solution of the remaining differential equation: the boundary has to make the same movement as if it was part of the evanescent wave. Therefore we need that the motion of the boundary fits exactly the eigensolution of the evanescent wave,

$$u_0 = \xi_{1,2} e^{-i\omega_{1,2}t}. \quad (\text{S.11})$$

Exercise 2. Number of bands of a generic discrete model

We have seen that the number of bands a discrete system provides changes with the number of sites in the unit cell.

- (a) Consider a one-dimensional chain of atoms, in which three atoms form one unit cell. Assume that only nearest neighbors of atoms are coupled with each others. Make a sketch and write down its generic dynamical matrix in k -space. How many bands would you find upon diagonalization?

Solution. A sketch of the triatomic chain is given in Fig. 3. Its equation of motion is

$$\begin{pmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \end{pmatrix} \begin{pmatrix} \ddot{u}_{1,n} \\ \ddot{u}_{2,n} \\ \ddot{u}_{3,n} \end{pmatrix} = \begin{pmatrix} \alpha_1 & f_{12} & 0 \\ f_{12} & \alpha_2 & f_{23} \\ 0 & f_{23} & \alpha_3 \end{pmatrix} \begin{pmatrix} u_{1,n} \\ u_{2,n} \\ u_{3,n} \end{pmatrix} + \begin{pmatrix} 0 & 0 & f_{13} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} u_{1,n-1} \\ u_{2,n-1} \\ u_{3,n-1} \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ f_{13} & 0 & 0 \end{pmatrix} \begin{pmatrix} u_{1,n+1} \\ u_{2,n+1} \\ u_{3,n+1} \end{pmatrix}. \quad (\text{S.12})$$

Therefore, after Fourier transform we find

$$\begin{pmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \end{pmatrix} \begin{pmatrix} \ddot{u}_{1,k} \\ \ddot{u}_{2,k} \\ \ddot{u}_{3,k} \end{pmatrix} = \begin{pmatrix} \alpha_1 & f_{12} & f_{13}e^{ik} \\ f_{12} & \alpha_2 & f_{23} \\ f_{13}e^{-ik} & f_{23} & \alpha_3 \end{pmatrix} \begin{pmatrix} u_{1,k} \\ u_{2,k} \\ u_{3,k} \end{pmatrix}. \quad (\text{S.13})$$

To arrive at an eigenvalue problem we then write

$$\begin{pmatrix} \ddot{u}_{1,k} \\ \ddot{u}_{2,k} \\ \ddot{u}_{3,k} \end{pmatrix} = \begin{pmatrix} \frac{\alpha_1}{m_1} & \frac{f_{12}}{\sqrt{m_1 m_2}} & \frac{f_{13}e^{ik}}{\sqrt{m_1 m_3}} \\ \frac{f_{12}}{\sqrt{m_1 m_2}} & \frac{\alpha_2}{m_2} & \frac{f_{23}}{m_2 m_3} \\ \frac{f_{13}e^{-ik}}{\sqrt{m_1 m_3}} & \frac{f_{23}}{\sqrt{m_2 m_3}} & \frac{\alpha_3}{m_3} \end{pmatrix} \begin{pmatrix} \tilde{u}_{1,k} \\ \tilde{u}_{2,k} \\ \tilde{u}_{3,k} \end{pmatrix}, \quad (\text{S.14})$$

where we defined $\tilde{u}_{i,k} = \sqrt{m_i} u_{i,k}$.

As we deal with a 3×3 matrix we obtain three eigenvalues $\omega_i(k)^2$ for every k value leading to three bands (six bands if we count $\pm\omega_i(k)$ instead).

- (b) How many bands would you find in case the system in (a) would have next nearest neighbor interactions as well?

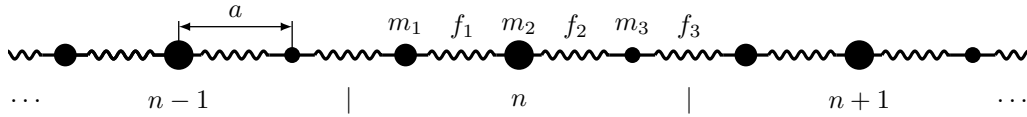


Figure 3: One-dimensional crystal with lattice constant a .

Solution. Adding next nearest neighbor couplings would add further terms to Eq. (S.12). However, after taking the Fourier transform we still have to deal with a 3×3 matrix. Diagonalizing this matrix then still results in 3 bands.

- (c) Assume you have n sites per unit cell. How many distinct bands do you expect? How do the number of bands change if we consider a three-dimensional system instead of a one-dimensional one?

Solution. Based on the above considerations, we see that the dimension of the dynamical matrix in k space only depends upon the number of degrees of freedom per unit cell. In case of n sites per unit cell we obtain a $n \times n$ matrix resulting in n bands. So far we had in mind a one-dimensional system, but the statement holds for higher dimensional systems as well (assuming that each site has one degree of freedom).