Dispersion relations for spring-mass lattices

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Abstract

This document present some results pertaining the dispersion in lattices made with springs and masses. The main idea is to study the bulk behavior of the *materials* made with these lattices. We present prototypical systems in the study of phononic crystals, and its relative simplicity allow for analytical solutions in some cases. What is not commonly possible in the continuum counterpart.

1 Simple mass-spring lattice

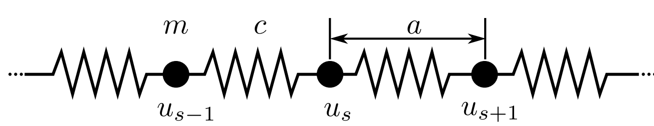


Figure 1. Simple mass-spring lattice.

1.1 Direct formulation

The force in the plane s cause by the displacement of the plane $s+p$ is proportional to the difference $u_{s+p} - u_s$ of the displacements. For brevity we will consider only nearest-neighbor interactions, so $p = \pm 1$. The total force on s comes from planes $s = \pm 1$:

$$F_s = c(u_{s+1} - u_s) + c(u_{s-1} - u_s). \tag{1}$$

The constant c is the stiffness between nearest-neighbour planes and will differ for longitudinal and transverse waves.

The equation of motion of the plane s is

$$m\ddot{u} = c(u_{s+1} + u_{s-1} - 2u_s),$$

assuming a harmonic time dependence $\exp(-i\omega t)$

$$-m\omega^2 u_s = c(u_{s+1} + u_{s-1} - 2u_s) \ . \tag{2}$$

Due to the Bloch-periodicity condition

$$u_{s\pm 1} = u_s e^{\pm ika}.$$

So (2) is now

$$-m\omega^2 u_s = c(u_s \exp(ika) + u_s \exp(-ika) - 2u_s)$$

and canceling u_s from both sides, we have

$$\omega^2 m = -c[\exp(ika) + \exp(-ika) - 2] \ .$$

Using the identity $2\cos ka = \exp(ika) + \exp(-ika)$, and taking $\Omega^2 = \omega^2/\omega_0^2 = \omega^2 m/c$, we have the dispersion relation

$$\Omega^2 = 2(1 - \cos ka) \ . \tag{3}$$

The boundary of the first Brillouin zone lies at $k = \pm\pi/a$. We show from (3) that the slope of Ω versus ka is zero at the zone boundary

$$\frac{d\Omega^2}{d\,ka} = 2\sin ka = 0$$

at $ka = \pm\pi$, $\sin ka = 0$.

By a trigonometric identity (2) may be written as

$$\Omega^2 = 4\sin^2\frac{1}{2}ka, \qquad \Omega = 2\left|\sin\frac{1}{2}ka\right| \ . \tag{4}$$

1.2 Unit cell formulation

This problem could also be solved taking a single cell and imposing the Bloch conditions after the assemblage process for the matrices. The force balance (in frequency domain) is

$$\begin{aligned} c(u_2 - u_1) &= -\frac{m}{2}\omega^2 u_1 \ , \\ c(u_1 - u_2) &= -\frac{m}{2}\omega^2 u_2 \ , \end{aligned}$$

we should take care since the total amount of mass in the cell should be consistent. That is why we choose each particle to have $m/2$. And this system could be expressed as

$$c\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}\{\mathbf{u}\} = -\frac{m\omega^2}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\{\mathbf{u}\} \ , \tag{5}$$

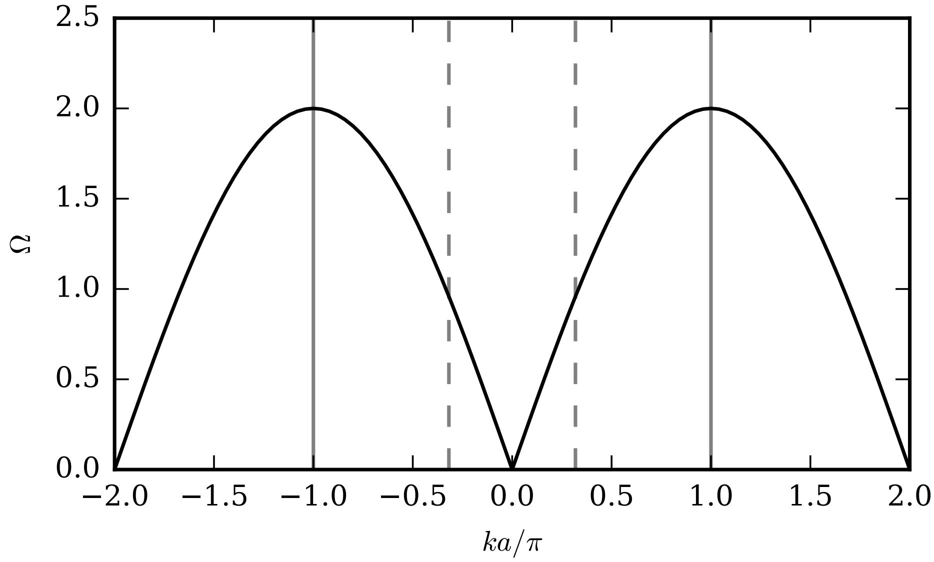


Figure 2. Plot of Ω versus ka. The region of $ka << 1$ or $\lambda/a >> 1$ corresponds to the continuum approximation; where Ω is directly proportional to ka (and is enclosed between the dashed lines). The First Brillouin Zone is placed between -1 and 1.

or, using $\Omega^2 = \omega^2 m/c$ multiplying the second row by $\exp(-ika)$ and the second column by its complex conjugate $\exp(ika)$ we get

$$\begin{bmatrix} -1 & e^{ika} \\ e^{-ika} & -1 \end{bmatrix} \{\mathbf{u}\} = -\frac{\Omega^2}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \{\mathbf{u}\} \quad ,$$

adding the second row to first one, and then adding the second column to first one yields

$$\begin{bmatrix} e^{ika} + e^{-ika} - 2 & e^{ika} - 1 \\ e^{-ika} - 1 & -1 \end{bmatrix} \{\mathbf{u}\} = -\frac{\Omega^2}{2} \begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix} \{\mathbf{u}\} \quad .$$

Now, were interested just in the reduced system, we delete the second row and column and get

$$\left[e^{ika} + e^{-ika} - 2\right] = -\Omega^2 \quad , \tag{6}$$

and this could be rewritten as

$$\Omega = 2\left|\sin\frac{1}{2}ka\right| \quad , \tag{7}$$

which is the same result obtained before.

The phase speed is

$$v_p = \frac{\Omega}{ka} = \frac{2}{ka}\left|\sin\frac{1}{2}ka\right| \quad ,$$

and the group speed

$$v_g \equiv \nabla_{ka}\Omega = \frac{d\Omega}{d\,ka} = \cos\left(\frac{1}{2}ka\right)\,\mathrm{sign}\left[\sin\frac{1}{2}ka\right]$$

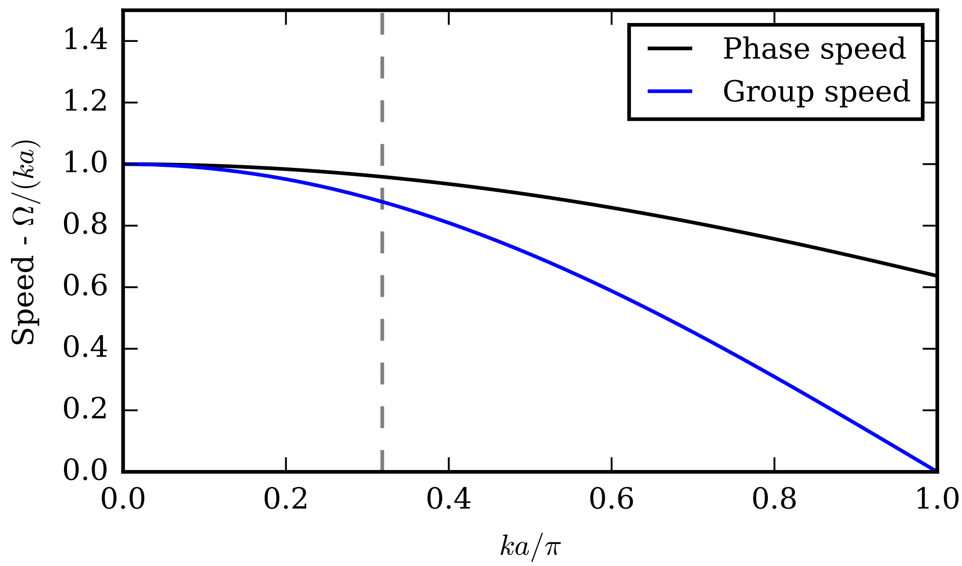


Figure 3. Plot of speed versus ka. The initial value is 1 and the approximation around 0 is constant speed.

1.3 Finite case

In practice, we cannot have infinite (periodic) repetition of unit cells, and, at some point, we need to truncate them to make them finite (Figure 4). When the number of unit cells increase, the behavior should get closer to the infinite case, and the presence of bandgaps could be inferred from the analysis of the response in frequency.

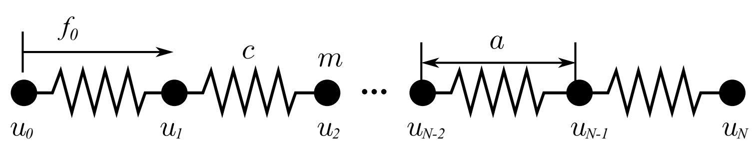


Figure 4. Finite simple mass-spring lattice.

If we start from a single unit cell the equations of motion for harmonic force of frequency ω are given by

$$\begin{aligned} &-c(u_0 - u_1) + f_0 = -\omega^2 m u_0 \\ &-c(u_1 - u_0) = -\omega^2 m u_1 \ , \end{aligned}$$

or

$$\begin{bmatrix} -1+\Omega^2 & 1 \\ 1 & -1+\Omega^2 \end{bmatrix} \begin{Bmatrix} u_0 \\ u_1 \end{Bmatrix} = \begin{Bmatrix} -\hat{f}_0 \\ 0 \end{Bmatrix} \quad , \tag{8}$$

where we normalized the equation. $\Omega^2 = \omega^2/\omega_0^2 = \omega^2 m/c$ and $\hat{f}_0 = f_0/c$. And the solutions for this system of equations is

$$\begin{aligned} u_0 &= \frac{\hat{f}_0(1-\Omega^2)}{\Omega^2(\Omega^2-2)} \\ u_1 &= \frac{\hat{f}_0}{\Omega^2(\Omega^2-2)} \quad . \end{aligned}$$

We are interested in the response of the last mass with respect to the force impinged in the first one, i.e.

$$\frac{u_1}{\hat{f}_0} = \frac{1}{\Omega^2(\Omega^2-2)} \quad . \tag{9}$$

For the case of two unit cells the (dimensionless) system of equations read

$$\begin{bmatrix} -1 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{bmatrix} \begin{Bmatrix} u_0 \\ u_1 \\ u_2 \end{Bmatrix} + \Omega^2 \begin{Bmatrix} u_0 \\ u_1 \\ u_2 \end{Bmatrix} = \begin{Bmatrix} -\hat{f}_0 \\ 0 \\ 0 \end{Bmatrix} \quad , \tag{10}$$

where the solutions are

$$\begin{aligned} u_0 &= \frac{\hat{f}_0(\Omega^2-\Omega-1)(\Omega^2+\Omega-1)}{\Omega^2(\Omega-1)(\Omega+1)(\Omega^2-3)} \\ u_1 &= \frac{-\hat{f}_0}{\Omega^2(\Omega^2-3)} \\ u_2 &= \frac{\hat{f}_0}{\Omega^2(\Omega-1)(\Omega+1)(\Omega^2-3)} \quad . \end{aligned}$$

And the response in this case is given by

$$\frac{u_2}{\hat{f}_0} = \frac{1}{\Omega^2(\Omega-1)(\Omega+1)(\Omega^2-3)} \quad . \tag{11}$$

In the case of N unit cells the system of equations is

$$\begin{bmatrix} -1+\Omega^2 & 1 & \cdots & 0 & 0 \\ 1 & -2+\Omega^2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -2+\Omega^2 & 1 \\ 0 & 0 & \cdots & 1 & -1+\Omega^2 \end{bmatrix} \begin{Bmatrix} u_0 \\ u_1 \\ \vdots \\ u_{N-1} \\ u_N \end{Bmatrix} = \begin{Bmatrix} -\hat{f}_0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{Bmatrix} \quad . \tag{12}$$

Given the structure of the matrix it is possible that the system has a closed solution. Here, we solved the system numerically and plotted the ratio $u_N/\hat{f}_0$ for different N values (Figure 5).

We can see that for N big enough there is not propagation for frequencies larger than $\Omega = 2$, what was expected based on the Bloch analysis and the dispersion curves presented in Figure 2.

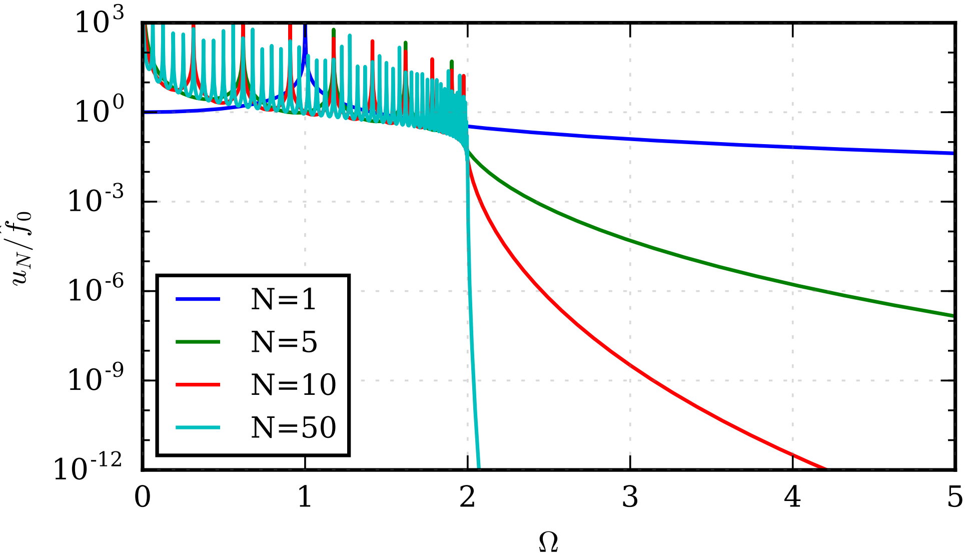


Figure 5. Frequency response for a finite mass-spring lattice.

2 Diatomic crystal

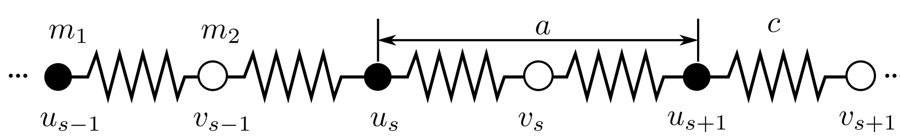


Figure 6. Lattice made with spring and two species of masses.

We write the equations of motion under the assumption that each plane interacts only with its nearest-neighbour planes and that the force constants are identical between all pairs of nearest-neighbour planes.

$$m_1 \frac{d^2 u_s}{dt^2} = c(v_s + v_{s-1} - 2u_s); \tag{13a}$$

$$m_2 \frac{d^2 v_s}{dt^2} = c(u_{s+1} + u_s - 2v_s). \tag{13b}$$

We look for a solution in the form of a traveling wave, now with different amplitudes u, v on alternate phases:

$$u_s = u \exp(ika) \exp(-i\omega t); \tag{14a}$$

$$v_s = v \exp(ika) \exp(-i\omega t). \tag{14b}$$

Replacing (14) in (13) we have

$$-\omega^2 m_1 u = cv[1 + \exp(-ika)] - 2cu;$$
$$-\omega^2 m_2 v = cu[1 + \exp(ika)] - 2cv.$$

It has no trivial solution only if the determinant vanishes, i.e.

$$\begin{vmatrix} 2c - m_1\omega^2 & -c[1+\exp(-ika)] \\ -c[1+\exp(ika)] & 2c - m_2\omega^2 \end{vmatrix} = 0,$$

or

$$m_1 m_2 \omega^4 - 2c(m_1+m_2)\omega^2 + 2c^2(1-\cos ka) = 0 \ . \tag{15}$$

Solving this biquadratic equation and doing some algebraic manipulations, we get

$$\omega^2 = \frac{c}{m_1 m_2}\left[m_1 + m_2 \pm \sqrt{(m_1+m_2)^2 - 2m_1 m_2(1-\cos ka)}\right] \ . \tag{16}$$

Let's examine the limiting cases $ka << 1$ and $ka = \pm\pi$ at the boundary zone.

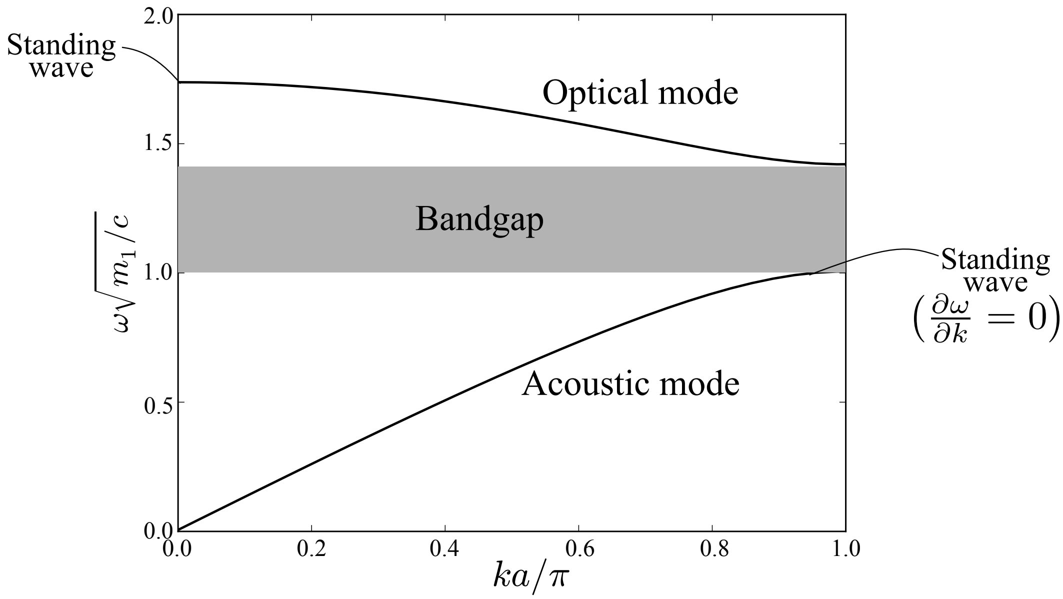


Figure 7. Optical and acoustical branches of the dispersion relation for a diatomic linear lattice. The values are computed for a ratio $m_2/m_1 = 2$.

For small ka we have $\cos ka \approx 1 - \frac{1}{2}k^2a^2 + \cdots$, and the two roots are

$$\omega^2 \approx 2c\left(\frac{1}{m_1} + \frac{1}{m_2}\right) \quad \text{(optical branch)} \tag{17}$$

$$\omega^2 \approx \frac{\frac{1}{2}c}{m_1+m_2}k^2a^2 \quad \text{(acoustical branch)} \ . \tag{18}$$

At $k_{max} = \pm\pi/a$ the roots are

$$\omega^2 = 2c/m_1, \quad \omega^2 = 2c/m_2 \ .$$

2.1 Finite case

Let's consider now the finite case, depicted in Figure 8.

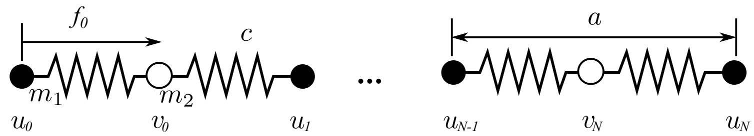


Figure 8. Finite *lattice* made with spring and two species of masses.

For the case of a single unit cell the system of equation read

$$
\begin{aligned}
&-c(u_0 - v_0) + f_0 = -\omega^2 m_1 u_0 \\
&-c(v_0 - u_0) - c(v_0 - u_1) = -\omega^2 m_2 v_0 \\
&-c(u_1 - v_0) = -\omega^2 m_1 u_1 \ ,
\end{aligned}
$$

or

$$
c \begin{bmatrix} -1 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{bmatrix} \begin{Bmatrix} u_0 \\ v_0 \\ u_1 \end{Bmatrix} + m_1\omega^2 \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{m_2}{m_1} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} u_0 \\ v_0 \\ u_1 \end{Bmatrix} = \begin{Bmatrix} -f_0 \\ 0 \\ 0 \end{Bmatrix} \ ,
$$

making $\hat{f}_0 = f_0/c$, $\Omega^2 = \omega^2/\omega_0^2$, $\omega_0^2 = c/m_1$, $\mu = m_2/m_1$ we obtain

$$
\begin{bmatrix} -1+\Omega^2 & 1 & 0 \\ 1 & -2+\mu\Omega^2 & 1 \\ 0 & 1 & -1+\Omega^2 \end{bmatrix} \begin{Bmatrix} u_0 \\ v_0 \\ u_1 \end{Bmatrix} = \begin{Bmatrix} -\hat{f}_0 \\ 0 \\ 0 \end{Bmatrix} \ . \tag{19}
$$

The solution of this system is given by

$$
\begin{aligned}
u_0 &= \frac{-\hat{f}_0(\mu\Omega^4 - \mu\Omega^2 - 2\Omega^2 + 1)}{\Omega^2(\Omega-1)(\Omega+1)(\mu\Omega^2 - \mu - 2)} \\
v_0 &= \frac{\hat{f}_0}{\Omega^2(\mu\Omega^2 - \mu - 2)} \\
u_1 &= \frac{-\hat{f}_0}{\Omega^2(\Omega-1)(\Omega+1)(\mu\Omega^2 - \mu - 2)} \ ,
\end{aligned}
$$

thus, the response is given by

$$
\frac{u_1}{\hat{f}_0} = \frac{-1}{\Omega^2(\Omega-1)(\Omega+1)(\mu\Omega^2 - \mu - 2)} \ . \tag{20}
$$

For the case of two unit cells the system of (dimensionless) equations is written as

$$
\begin{bmatrix} -1+\Omega^2 & 1 & 0 & 0 & 0 \\ 1 & -2+\mu\Omega^2 & 1 & 0 & 0 \\ 0 & 1 & -2+\Omega^2 & 1 & 0 \\ 0 & 0 & 1 & -2+\mu\Omega^2 & 1 \\ 0 & 0 & 0 & 1 & -1+\Omega^2 \end{bmatrix} \begin{Bmatrix} u_0 \\ v_0 \\ u_1 \\ v_1 \\ u_2 \end{Bmatrix} = \begin{Bmatrix} -\hat{f}_0 \\ 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix} \ , \tag{21}
$$

with solutions

$$
\begin{aligned}
u_0 &= \frac{-\hat{f}_0(\mu^2\Omega^8 - 3\mu^2\Omega^6 - 4\mu\Omega^6 + 2\mu^2\Omega^4 + 9\mu\Omega^4 + 4\Omega^4 - 4\mu\Omega^2 - 6\Omega^2 + 1)}{\Omega^2(\mu\Omega^4 - 3\mu\Omega^2 - 2\Omega^2 + 2\mu + 3)(\mu\Omega^4 - \mu\Omega^2 - 2\Omega^2 + 1)} \\
v_0 &= \frac{\hat{f}_0(\mu\Omega^6 - 3\mu\Omega^4 - 2\Omega^4 + 2\mu\Omega^2 + 4\Omega^2 - 1)}{\Omega^2(\mu\Omega^4 - 3\mu\Omega^2 - 2\Omega^2 + 2\mu + 3)(\mu\Omega^4 - \mu\Omega^2 - 2\Omega^2 + 1)} \\
u_1 &= \frac{-\hat{f}_0}{\Omega^2(\mu\Omega^4 - 3\mu\Omega^2 - 2\Omega^2 + 2\mu + 3)} \\
v_1 &= \frac{\hat{f}_0(\Omega - 1)(\Omega + 1)}{\Omega^2(\mu\Omega^4 - 3\mu\Omega^2 - 2\Omega^2 + 2\mu + 3)(\mu\Omega^4 - \mu\Omega^2 - 2\Omega^2 + 1)} \\
u_2 &= \frac{-\hat{f}_0}{\Omega^2(\mu\Omega^4 - 3\mu\Omega^2 - 2\Omega^2 + 2\mu + 3)(\mu\Omega^4 - \mu\Omega^2 - 2\Omega^2 + 1)} \ ,
\end{aligned}
$$

then, the response is

$$
\frac{u_2}{\hat{f}_0} = \frac{-1}{\Omega^2(\mu\Omega^4 - 3\mu\Omega^2 - 2\Omega^2 + 2\mu + 3)(\mu\Omega^4 - \mu\Omega^2 - 2\Omega^2 + 1)} \ . \tag{22}
$$

For N unit cells the (dimensionless) system of equation is of the form

$$
\mathbb{A}\begin{Bmatrix} u_0 \\ v_0 \\ u_1 \\ \vdots \\ u_{N-1} \\ v_{N-1} \\ u_N \end{Bmatrix} = \begin{Bmatrix} -\hat{f}_0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix} \tag{23}
$$

with

$$
\mathbb{A} = \begin{bmatrix}
-1+\Omega^2 & 1 & 0 & \cdots & 0 & 0 & 0 \\
1 & -2+\mu\Omega^2 & 1 & \cdots & 0 & 0 & 0 \\
0 & 1 & -2+\Omega^2 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -2+\Omega^2 & 1 & 0 \\
0 & 0 & 0 & \cdots & 1 & -2+\mu\Omega^2 & 1 \\
0 & 0 & 0 & \cdots & 0 & 1 & -1+\Omega^2
\end{bmatrix}
$$

One more time, the matrix present a structure and it might be possible that the system has a closed solution. Here, we solved the system numerically and plotted the ratio $u_N/\hat{f}_0$ for different N values and a mass ratio $\mu = m_2/m_1 = 2$ (Figure 9).

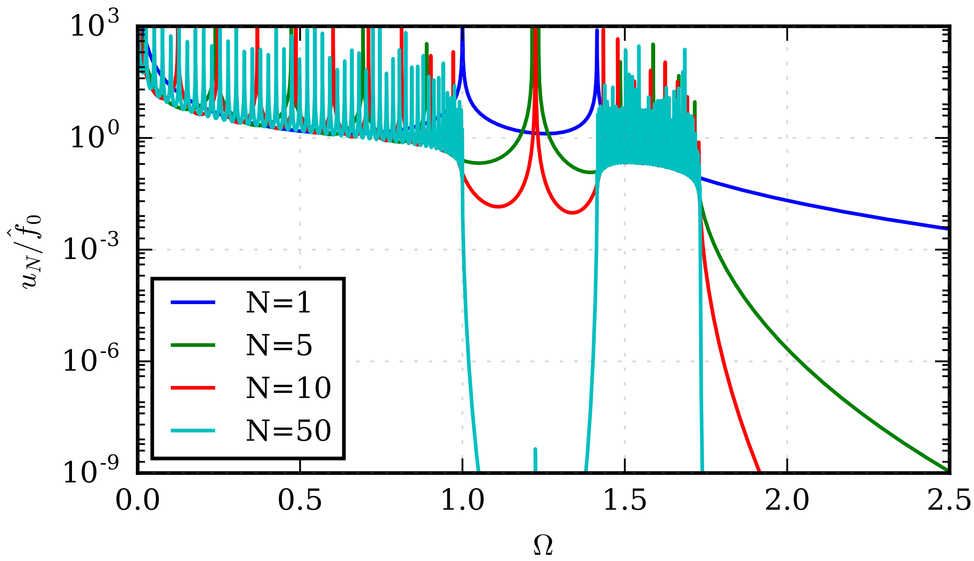


Figure 9. Frequency response for a finite mass-spring lattice for unit cell composed of two different masses.

We can see that for N big enough there is not propagation for frequencies in the interval $\Omega \in [\sqrt{2/\mu}, \sqrt{2/\mu}]$, and for $\Omega > \sqrt{\frac{2}{\mu}(1+\mu)}$, what was expected based on the Bloch analysis and the dispersion curves presented in Figure 7. The mass ratio used was $\mu = 2$, what gives as interval $\Omega \in [1, \sqrt{2}]$ and a cut frequency of $\Omega = \sqrt{3}$, that are clearly depicted in Figure 7.

3 Three masses lattice

The equations are

$$m_1 \frac{d^2 u_s}{dt^2} = c(v_s + w_{s-1} - 2u_s); \tag{24a}$$

$$m_2 \frac{d^2 v_s}{dt^2} = c(w_s + u_s - 2v_s); \tag{24b}$$

$$m_3 \frac{d^2 w_s}{dt^2} = c(u_{s+1} + v_s - 2w_s). \tag{24c}$$

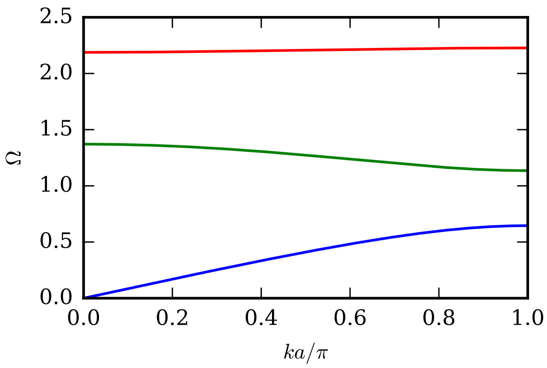
After assumin an harmonic solution and apply Bloch conditions the following system is found

$$\begin{bmatrix} -2 & 1 & \exp(-ika) \\ 1 & -2 & 1 \\ \exp(ika) & 1 & -2 \end{bmatrix} \begin{Bmatrix} u \\ v \\ w \end{Bmatrix} = -\frac{\omega^2}{\omega_0^2} \begin{bmatrix} 1 & 0 & 0 \\ 0 & \mu_1 & 0 \\ 0 & 0 & \mu_2 \end{bmatrix} \begin{Bmatrix} u \\ v \\ w \end{Bmatrix} , \tag{25}$$

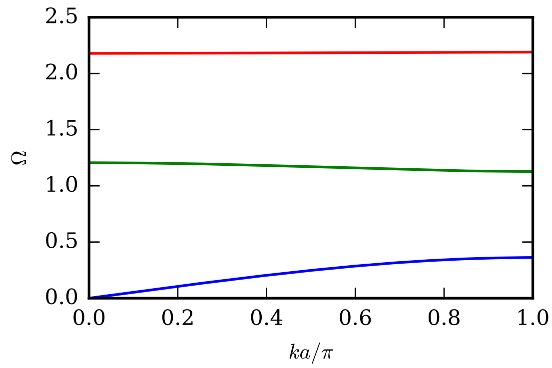
where $\omega_0^2 = c/m_1$, $\mu_1 = m_2/m_1$ and $\mu_2 = m_3/m_1$. The characteristic polynomial for this system is

$$\mu_1\mu_2 x^3 - 2[\mu_1\mu_2 - \mu_1 - \mu_2]x^2 + 3[\mu_1 + \mu_2 + 1]x + 2[\cos ka - 1] = 0 \ . \qquad (26)$$

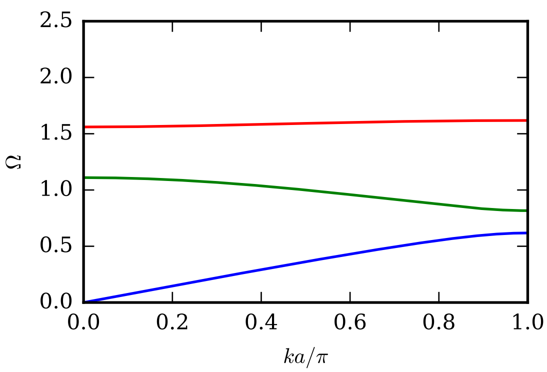
Figure 10 presents some dispersion curves for different mass ratios.



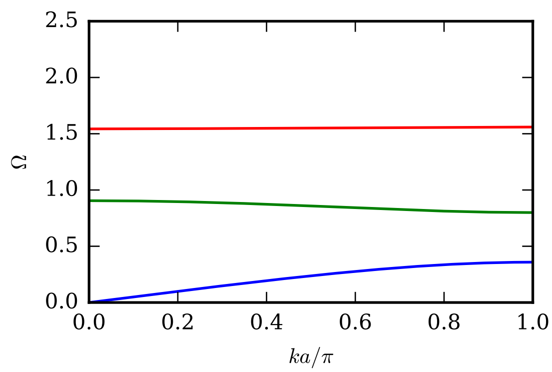
(a) $\mu_1 = 1/2$, $\mu_2 = 3$.



(b) $\mu_1 = 1/2$, $\mu_2 = 10$.



(c) $\mu_1 = 2$, $\mu_2 = 3$.



(d) $\mu_1 = 2$, $\mu_2 = 10$.

Figure 10. Dispersion curves for different values of mass ratios μ_1, μ_2.

3.1 Finite case

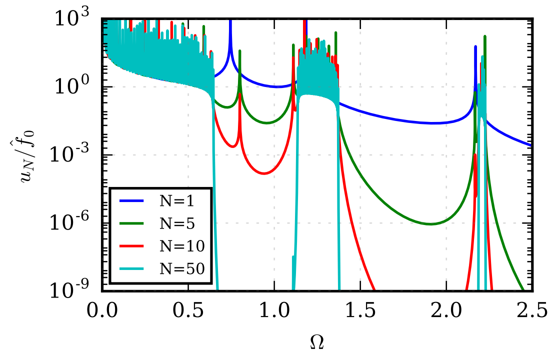
We can repeat the analysis done for one-mass and two-masses unit cells for the case of three-masses unit cell. In this case, the closed solution for one and two unit cells is not shown since the expression are large compared with the other two cases. Nevertheless, we present the equation form for the N cells case

$$
[\mathbb{A} - 2\mathbb{I}] \begin{Bmatrix} u_0 \\ v_0 \\ w_0 \\ u_1 \\ \vdots \\ u_{N-1} \\ v_{N-1} \\ w_{N-1} \\ u_N \end{Bmatrix} = \begin{Bmatrix} -\hat{f}_0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix} , \tag{27}
$$

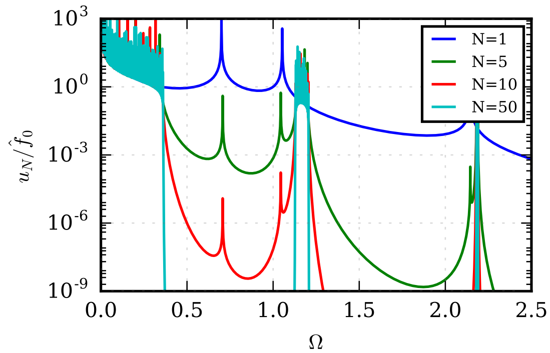
with

$$
\mathbb{A} = \begin{bmatrix}
\Omega^2+1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & \mu_1\Omega^2 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 \\
0 & 1 & \mu_2\Omega^2 & 1 & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & \Omega^2 & \cdots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & \Omega^2 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & \cdots & 1 & \mu_1\Omega^2 & 0 & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 1 & \mu_2\Omega^2 & 1 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & \Omega^2+1
\end{bmatrix}
$$

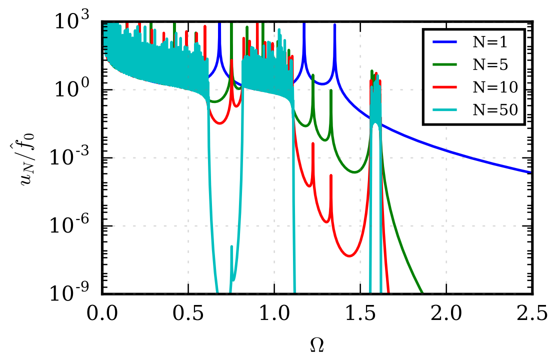
Figure 11 presents the frequency response for this case (computed numerically) for different mass ratios μ_1 and μ_2.



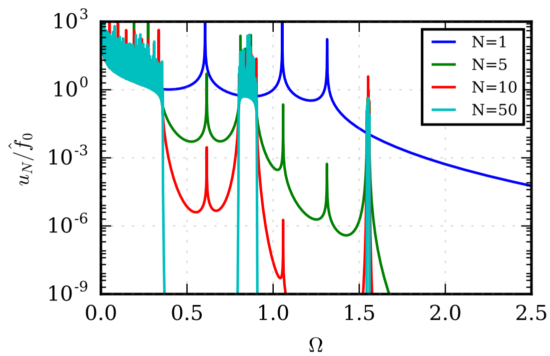
(a) $\mu_1 = 1/2$, $\mu_2 = 3$.



(b) $\mu_1 = 1/2$, $\mu_2 = 10$.



(c) $\mu_1 = 2$, $\mu_2 = 3$.



(d) $\mu_1 = 2$, $\mu_2 = 10$.

Figure 11. Frequency response for a finite mass-spring lattice for unit cell composed of three different masses for different mass ratios.

The bandgap regions and cut frequencies are (essentially) the same as those presented in the dispersion relations, Figure 10.

4 2D square lattice

For the simple cases shown before is easy to formulate the complete balance of forces taking into account the first neighbours. In general is easier to take the unit cell for the lattice and find the resulting system through row and column operations, just as exemplified before.

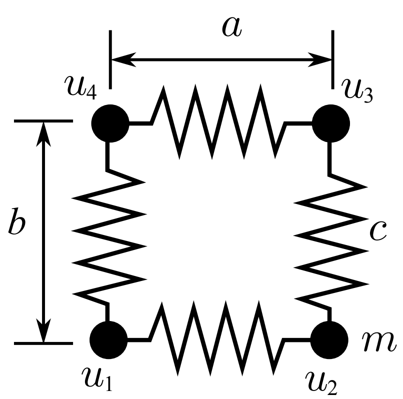


Figure 12. Unit cell for a two dimensional square lattice with a unique species.

The system of equation in frequency domain is

$$c\begin{bmatrix}-1 & 0 & 1 & 0 & 0 & 0 & 0 & 0\\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1\\ 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & -1 & 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0\\ 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0\\ 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0\\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1\end{bmatrix}\begin{Bmatrix}u_1\\ v_1\\ u_2\\ v_2\\ u_3\\ v_3\\ u_4\\ v_4\end{Bmatrix} = -\frac{\omega}{4}m\mathbb{I}_8\begin{Bmatrix}u_1\\ v_1\\ u_2\\ v_2\\ u_3\\ v_3\\ u_4\\ v_4\end{Bmatrix}\,, \tag{28}$$

and after applying the row operations for the Bloch-conditions imposition, we get

$$\frac{4c}{m}\begin{bmatrix}1-\cos(k_x a) & 0\\ 0 & 1-\cos(k_y b)\end{bmatrix}\begin{Bmatrix}u_1\\ v_1\end{Bmatrix} = \omega^2\begin{Bmatrix}u_1\\ v_1\end{Bmatrix}. \tag{29}$$

Or, equivalently

$$\omega_x^2 = \frac{8c}{m}\left(\sin\frac{1}{2}k_x a\right)^2, \qquad \omega_y^2 = \frac{8c}{m}\left(\sin\frac{1}{2}k_y b\right)^2 \,. \tag{30}$$

Figure 13 shows the dispersion relation for this problem.

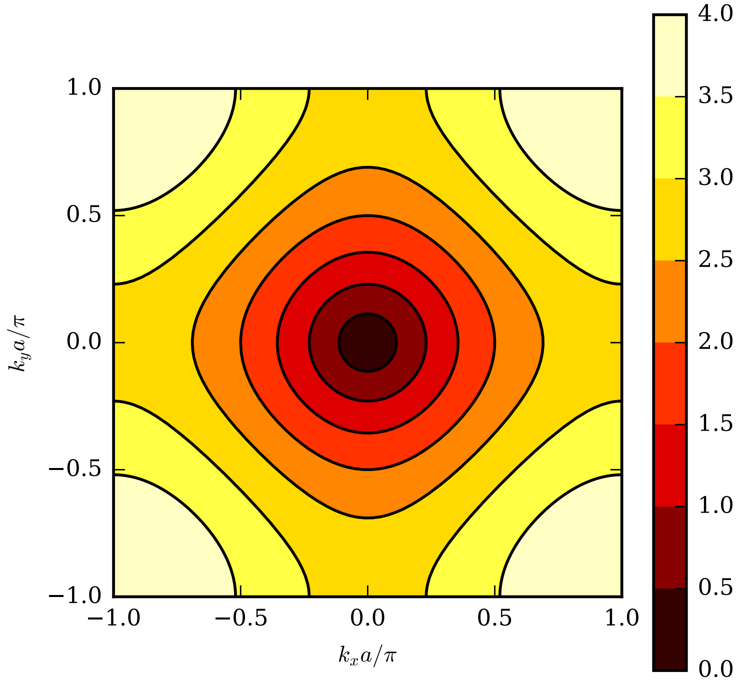


Figure 13. Dispersion relations–shown as isofrequency contours for the 2D square lattice.

It is customary to plot the dispersion relations over the irreducible Brillouin zone, this is depicted in Figure 14 for the square lattice.

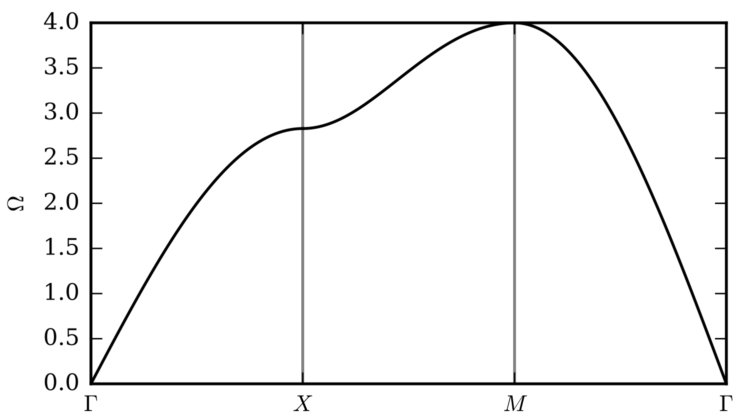


Figure 14. Dispersion relations over the irreducible Brillouin zone for the 2D square lattice.

5 2D rectangular lattice with diagonal springs

In this case we have a rectangular cell with springs with constant c in the sides. We added diagonal springs with constants c_d (see Figure 15). It should be noted that the value c_d is the *effective* spring in the x and y directions –they are the same for a square lattice, in the case of $a \neq b$ the constants should vary.

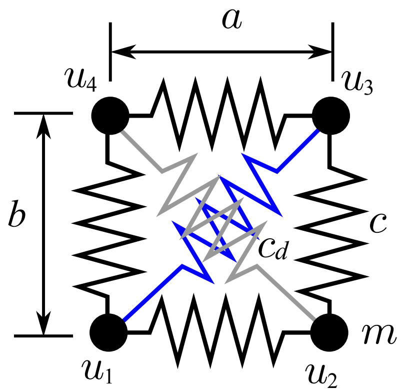


Figure 15. Unit cell for a two dimensional square lattice with a unique species and diagonal springs.

The system of equation in frequency domain is

$$\mathbb{K}\begin{Bmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \\ u_3 \\ v_3 \\ u_4 \\ v_4 \end{Bmatrix} = -\frac{\omega^2}{4} m \mathbb{I}_8 \begin{Bmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \\ u_3 \\ v_3 \\ u_4 \\ v_4 \end{Bmatrix} \tag{31}$$

with

$$\mathbb{K} = \begin{bmatrix} -c_d - c_1 & 0 & c_1 & 0 & c_d & 0 & 0 & 0 \\ 0 & -c_d - c_2 & 0 & 0 & 0 & c_d & 0 & c_2 \\ c_1 & 0 & -c_d - c_1 & 0 & 0 & 0 & c_d & 0 \\ 0 & 0 & 0 & -c_d - c_2 & 0 & c_2 & 0 & c_d \\ c_d & 0 & 0 & 0 & -c_d - c_1 & 0 & c_1 & 0 \\ 0 & c_d & 0 & c_2 & 0 & -c_d - c_2 & 0 & 0 \\ 0 & 0 & c_d & 0 & c_1 & 0 & -c_d - c_1 & 0 \\ 0 & c_2 & 0 & c_d & 0 & 0 & 0 & -c_d - c_2 \end{bmatrix}$$

And the solutions are

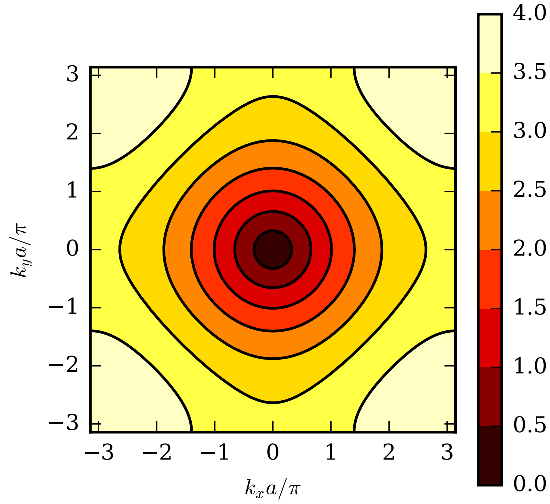
$$
\begin{aligned}
\omega_1^2 &= \frac{4c_1}{m}\left[1-\cos k_x a\right] + \frac{4c_d}{m}\left[1-\cos k_x a \cos k_y b\right] \\
\omega_2^2 &= \frac{4c_2}{m}\left[1-\cos k_y a\right] + \frac{4c_d}{m}\left[1-\cos k_x a \cos k_y b\right] \quad .
\end{aligned}
$$

equivalently (after some manipulations)

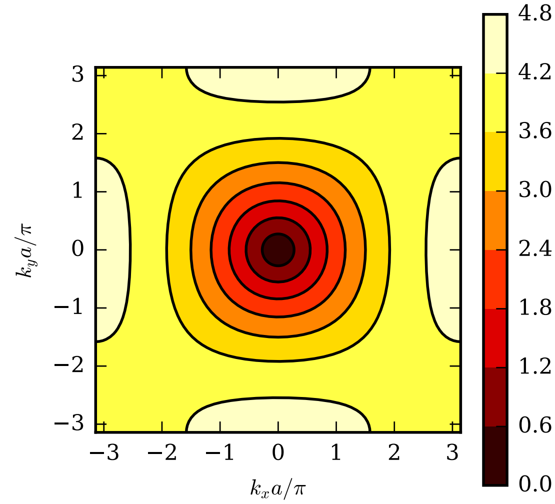
$$
\omega_1^2 = \frac{8c_1}{m}\sin^2\left(\frac{1}{2}k_x a\right) + \frac{4c_d}{m}\left[\sin^2\frac{1}{2}\left(k_x a + k_y b\right) + \sin^2\frac{1}{2}\left(k_x a - k_y b\right)\right] \tag{32}
$$

$$
\omega_2^2 = \frac{8c_2}{m}\sin^2\left(\frac{1}{2}k_y b\right) + \frac{4c_d}{m}\left[\sin^2\frac{1}{2}\left(k_x a + k_y b\right) + \sin^2\frac{1}{2}\left(k_x a - k_y b\right)\right] \tag{33}
$$

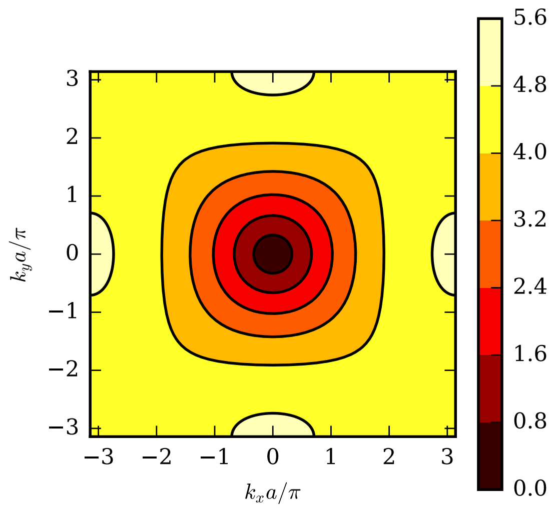
We recover the square lattice (without diagonals) making $c_d = 0$. The dispersion curves for this problem varying the ratio c_d/c are shown in Figure 16.



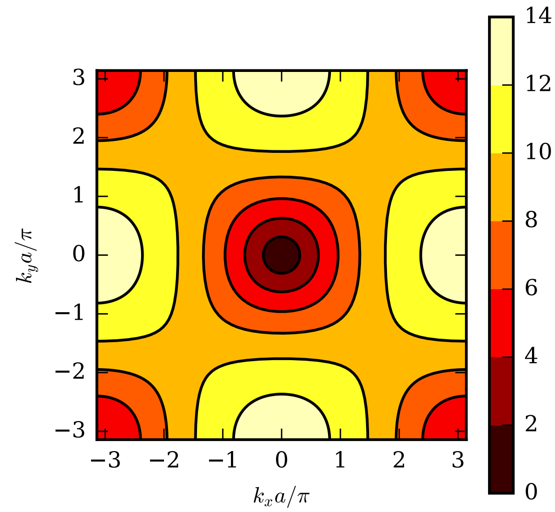
(a) $c_d/c = 0.1$ and $a = b$.



(b) $c_d/c = \sqrt{2}/2$ and $a = b$.

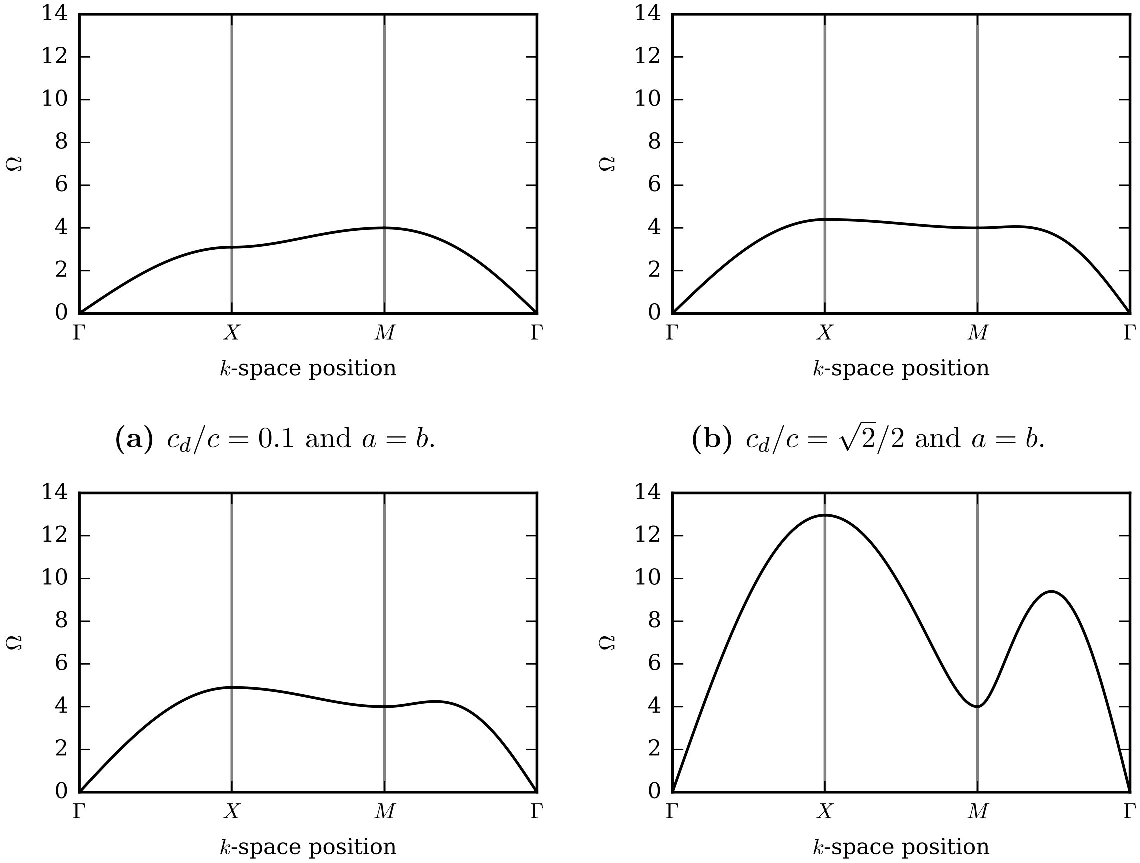


(c) $c_d/c = 1$ and $a = b$.



(d) $c_d/c = 10$ and $a = b$.

Figure 16. Dispersion curves for different values of spring ratios c_d/c for the 2D rectangular lattice with diagonal springs.



(a) $c_d/c = 0.1$ and $a = b$.

(b) $c_d/c = \sqrt{2}/2$ and $a = b$.

(c) $c_d/c = 1$ and $a = b$.

(d) $c_d/c = 10$ and $a = b$.

Figure 17. Dispersion curves for different values of spring ratios c_d/c for the 2D rectangular lattice with diagonal springs.

6 2D square lattice with body mass and diagonal springs

In this case we have a rectangular cell with springs with constant c in the sides. We added a second mass m_2 to the center of the cell, and diagonal springs with constant c_d (see Figure 18). It should be noted that the value c_d is the *effective* spring in the x and y directions –they are the same for a square lattice, in the case of $a \neq b$ the constants should vary.

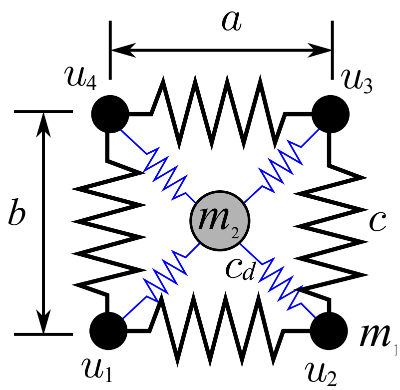


Figure 18. Unit cell for a two dimensional square lattice with a unique species in the corners and another one in the center that is linked by diagonal springs.

$$\mathbb{K}\begin{Bmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \\ u_3 \\ v_3 \\ u_4 \\ v_4 \\ u_5 \\ v_5 \end{Bmatrix} = -\omega^2 \mathbb{M}\begin{Bmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \\ u_3 \\ v_3 \\ u_4 \\ v_4 \\ u_5 \\ v_5 \end{Bmatrix} \tag{34}$$

with

$$\mathbb{K} = \begin{bmatrix} -c' & 0 & c_s & 0 & 0 & 0 & 0 & 0 & c_d & 0 \\ 0 & -c' & 0 & 0 & 0 & 0 & 0 & c_s & 0 & c_d \\ c_s & 0 & -c' & 0 & 0 & 0 & 0 & 0 & c_d & 0 \\ 0 & 0 & 0 & -c' & 0 & c_s & 0 & 0 & 0 & c_d \\ 0 & 0 & 0 & 0 & -c' & 0 & c_s & 0 & c_d & 0 \\ 0 & 0 & 0 & c_s & 0 & -c' & 0 & 0 & 0 & c_d \\ 0 & 0 & 0 & 0 & c_s & 0 & -c' & 0 & c_d & 0 \\ 0 & c_s & 0 & 0 & 0 & 0 & 0 & -c' & 0 & c_d \\ c_d & 0 & c_d & 0 & c_d & 0 & c_d & 0 & -4\,c_d & 0 \\ 0 & c_d & 0 & c_d & 0 & c_d & 0 & c_d & 0 & -4\,c_d \end{bmatrix},$$

$c' = c_s + c_d$, and

$$\mathbb{M} = \begin{bmatrix} \frac{m_1}{4}\mathbb{I}_6 & 0 \\ 0 & m_2\mathbb{I}_2 \end{bmatrix} .$$

After applying the Bloch theorem we obtain (showing just the lower diagonal due to the Hermiticity)

$$\mathbb{K}_R = \begin{bmatrix} -4\left[c_d - c_s(\cos(k_y a) - 1)\right] & \bullet & \bullet & \bullet \\ 0 & -4\left[c_d - c_s(\cos(k_y b) - 1)\right] & \bullet & \bullet \\ c_d\left(e^{i\,k_x a} + 1\right)\left(e^{i\,k_y b} + 1\right) & 0 & -4c_d & \bullet \\ 0 & c_d\left(e^{i\,k_x a} + 1\right)\left(e^{i\,k_y b} + 1\right) & 0 & -4c_d \end{bmatrix}$$

and

$$\mathbb{M}_R = \begin{bmatrix} m_1\mathbb{I}_2 & 0 \\ 0 & m_2\mathbb{I}_2 \end{bmatrix} \ .$$

The eigenvalues for this problem are lengthy, but a second order expansion around $(k_x, k_y) = (0, 0)$ (linear in the case o its square root) is shown

$$\begin{aligned}
\omega_1^2 =& \frac{2c_s(k_x a)^2 + c_d\left((k_x a)^2 + (k_y b)^2\right)}{m_1 + m_2} \\
\omega_2^2 =& \frac{2c_s(k_y b)^2 + c_d\left((k_x a)^2 + (k_y b)^2\right)}{m_1 + m_2} \\
\omega_3^2 =& \frac{2c_s(k_x a)^2 + 2c_d\left[2m_1^2 + 2m_2^2 + \left(4 - (k_x a)^2 + (k_y b)^2\right)m_1 m_2\right]}{m_1 m_2(m_2 + m_1)} \\
\omega_4^2 =& \frac{2c_s(k_y b)^2 + 2c_d\left[2m_1^2 + 2m_2^2 + \left(4 - (k_x a)^2 + (k_y b)^2\right)m_1 m_2\right]}{m_1 m_2(m_2 + m_1)} \ .
\end{aligned}$$

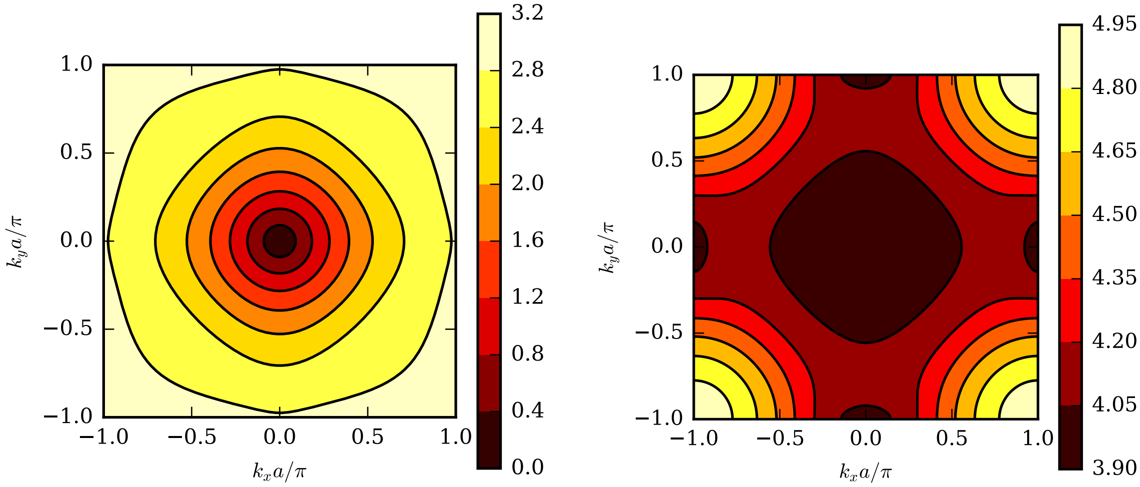
Assuming $a = b$, we can group the modes as degenerate ones and consider the most general propagation in the plane (due to the orthogonality)

$$\omega_{\text{low}}^2 = \frac{2(c_s + c_d)(k_x^2 + k_y^2)a^2}{m_1 + m_2} \equiv \frac{2(c_s + c_d)\mathbf{k}^2 a^2}{m_1 + m_2} \ ,$$

the same argument holds for the other two, giving

$$\omega_{\text{high}}^2 = \frac{2c_s\mathbf{k}^2 a^2 + 2c_d\left[4m_1^2 + 4m_2^2 + \left(8 - \mathbf{k}^2 a^2\right)m_1 m_2\right]}{m_1 m_2(m_2 + m_1)} \ .$$

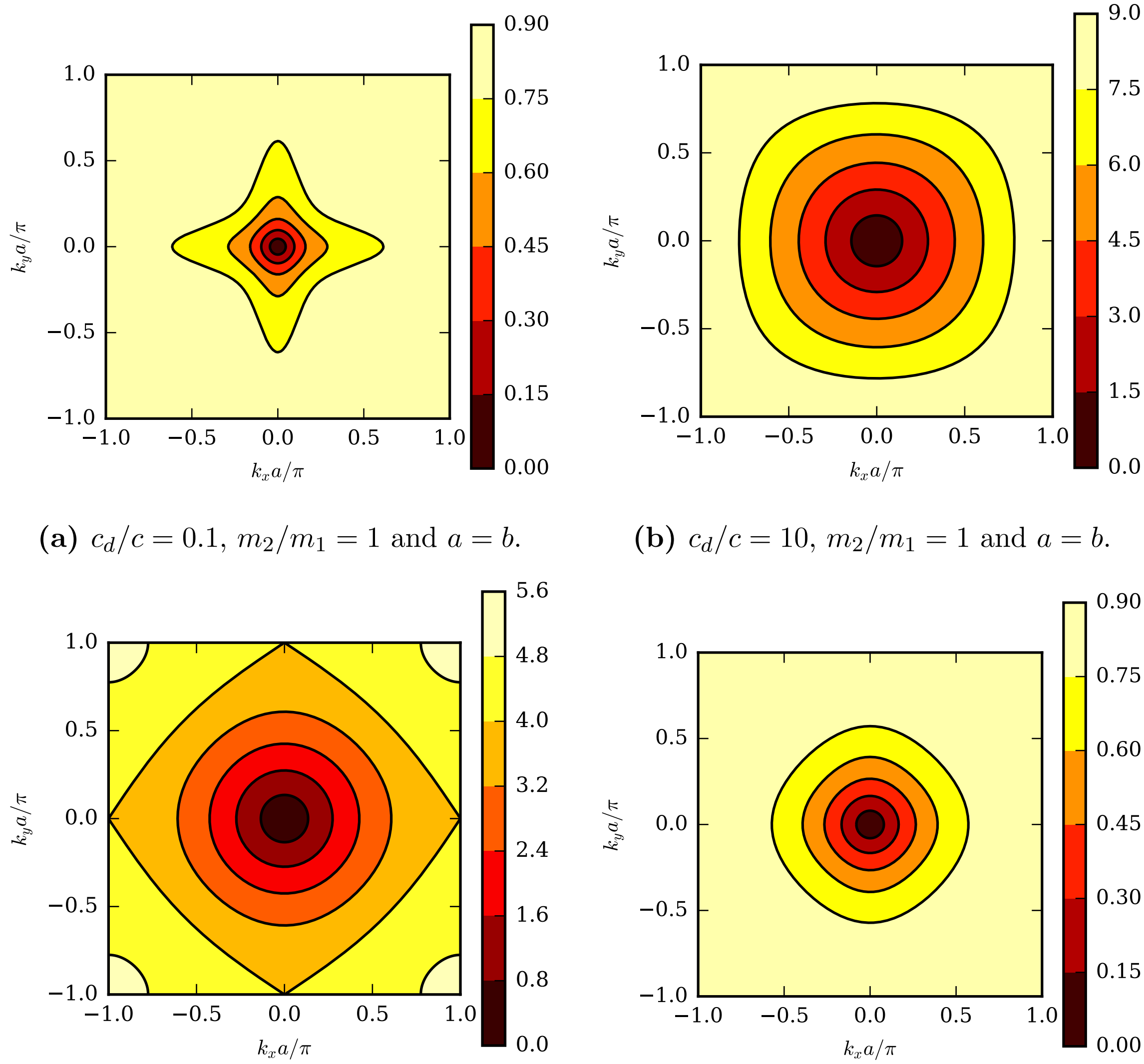
Figure 19 shows the dispersion modes for ratios $m_2/m_1 = 1$ and $c_d/c_s = 1$.



(a) First branch. **(b)** Second branch.

Figure 19. Dispersion relations for the square lattice with body mass and diagonal springs. The parameters are $c_d/c = 1$, $m_1/m_2 = 1$ and $a = b$.

Figure 20 shows the first branch of the dispersion curves for different ratios m_2/m_1 and c_d/c_s.



(a) $c_d/c = 0.1$, $m_2/m_1 = 1$ and $a = b$.

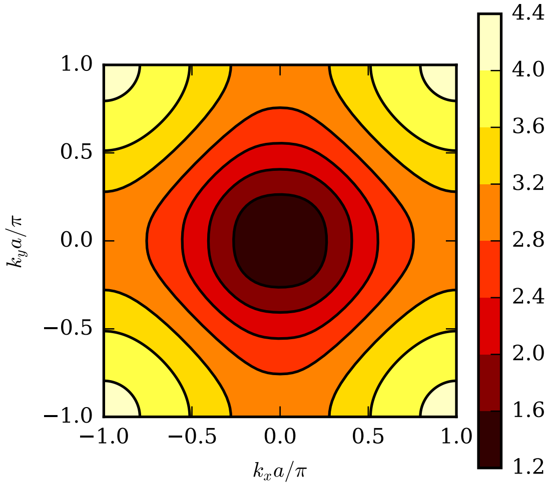
(b) $c_d/c = 10$, $m_2/m_1 = 1$ and $a = b$.

(c) $c_d/c = 1$, $m_2/m_1 = 0.1$ and $a = b$.

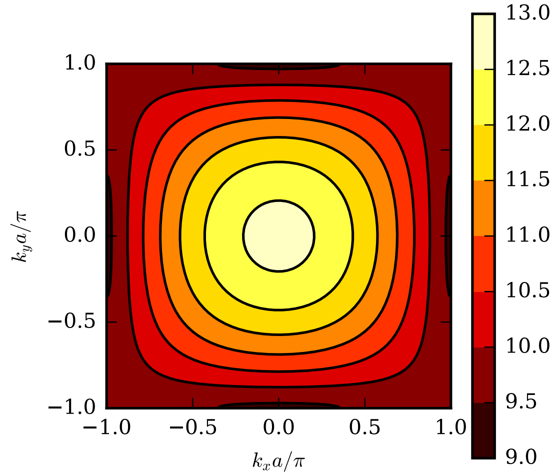
(d) $c_d/c = 1$, $m_2/m_1 = 10$ and $a = b$.

Figure 20. First branch of the dispersion curves for different ratios m_2/m_1 and c_d/c_s for the 2D square lattice with centered mass and digonal springs.

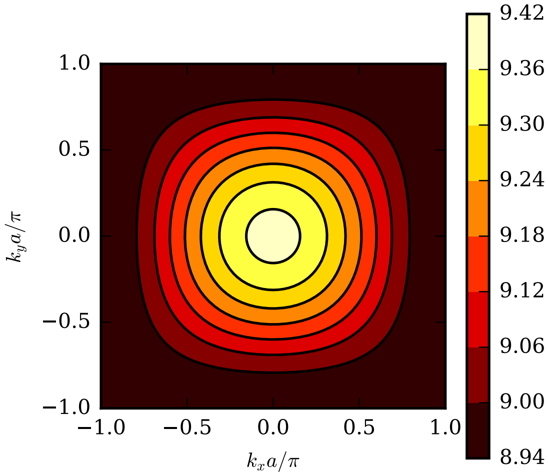
Figure 21 shows the second branch of the dispersion curves for different ratios m_2/m_1 and c_d/c_s.



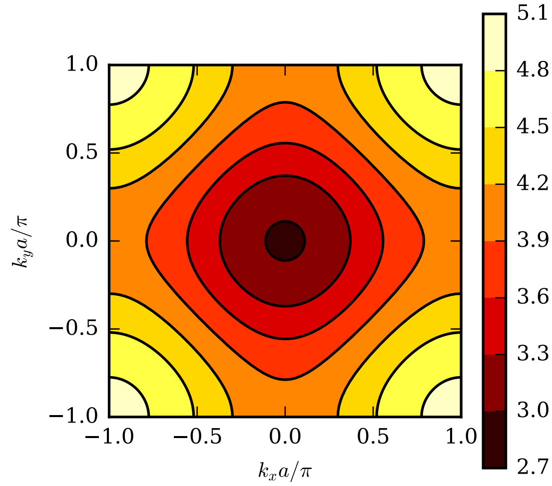
(a) $c_d/c = 0.1$, $m_2/m_1 = 1$ and $a = b$.



(b) $c_d/c = 10$, $m_2/m_1 = 1$ and $a = b$.

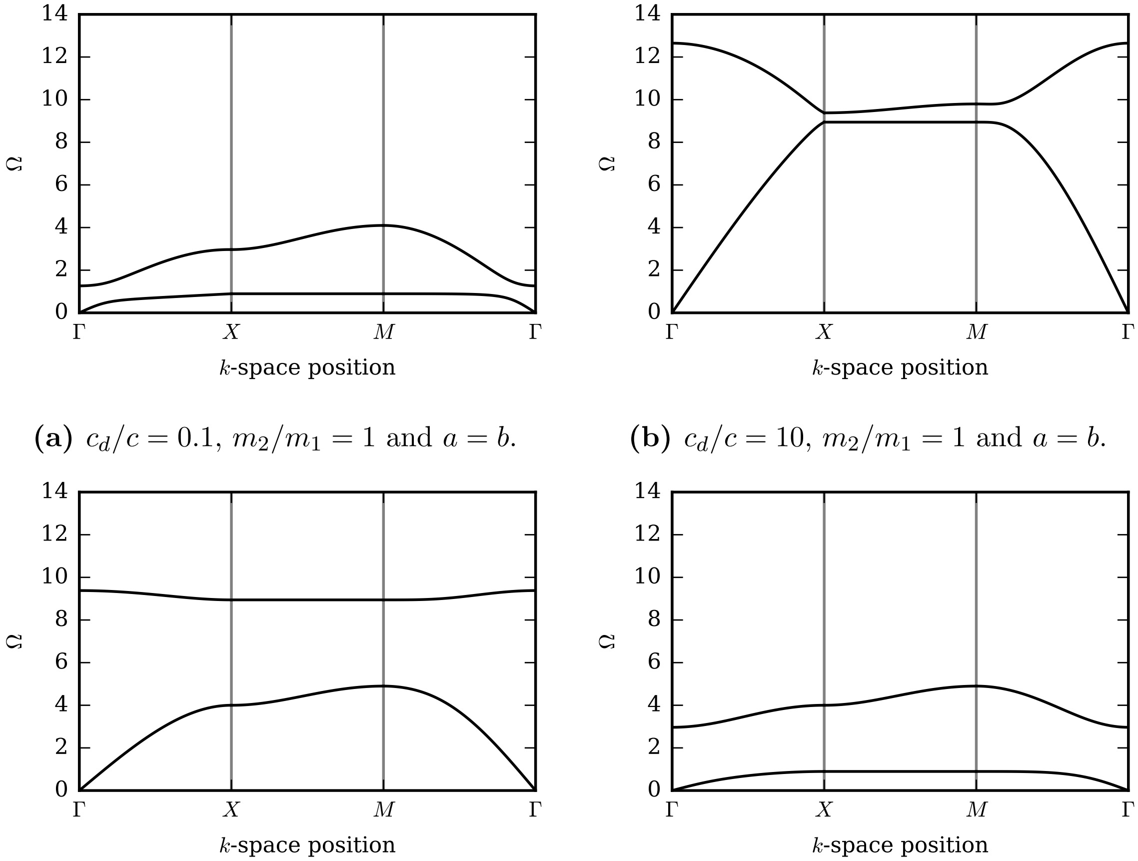


(c) $c_d/c = 1$, $m_2/m_1 = 0.1$ and $a = b$.



(d) $c_d/c = 1$, $m_2/m_1 = 10$ and $a = b$.

Figure 21. Second branch of the dispersion curves for different ratios m_2/m_1 and c_d/c_s for the 2D square lattice with centered mass and digonal springs.



(a) $c_d/c = 0.1$, $m_2/m_1 = 1$ and $a = b$.

(b) $c_d/c = 10$, $m_2/m_1 = 1$ and $a = b$.

(c) $c_d/c = 1$, $m_2/m_1 = 0.1$ and $a = b$.

(d) $c_d/c = 1$, $m_2/m_1 = 10$ and $a = b$.

Figure 22. Dispersion curves over the irreducible Brillouin zone for different ratios m_2/m_1 and c_d/c_s for the 2D square lattice with centered mass and digonal springs.

7 Hexagonal Lattice

In this case we have an hexagonal cell with springs with constant c in the sides (see Figure 23).

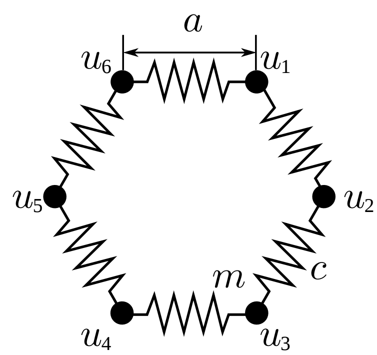


Figure 23. Unit cell for a two dimensional hexagonal lattice with a unique species in the corners.

The system of equations to solve is one more time

$$\mathbb{K}\begin{Bmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \\ u_3 \\ v_3 \\ u_4 \\ v_4 \\ u_5 \\ v_5 \\ u_6 \\ v_6 \end{Bmatrix} = -\omega^2\mathbb{M}\begin{Bmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \\ u_3 \\ v_3 \\ u_4 \\ v_4 \\ u_5 \\ v_5 \\ u_6 \\ v_6 \end{Bmatrix} \tag{35}$$

with

$$\mathbb{K} = \frac{c}{2}\begin{bmatrix} -3 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & -\sqrt{3} & 0 & \sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -2 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{3} & 0 & -2\sqrt{3} & 0 & \sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & -3 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{3} & 0 & -\sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & -3 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\sqrt{3} & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -2 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{3} & 0 & -2\sqrt{3} & 0 & \sqrt{3} \\ 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{3} & 0 & -\sqrt{3} \end{bmatrix}$$

and

$$\mathbb{M} = \frac{m}{3}\mathbb{I}_{12} \ .$$

After applying the Bloch theorem we obtain (showing just the lower diagonal due to the Hermiticity)

$$\mathbb{K}_R = c\begin{bmatrix} -4 & \bullet & \bullet & \bullet\\ 0 & -2\sqrt{3} & \bullet & \bullet\\ e^{\frac{\sqrt{3}\,ik_y a}{2}-\frac{ik_x a}{2}} + e^{-\frac{\sqrt{3}\,ik_y a}{2}-\frac{ik_x a}{2}} + 2\,e^{ik_x a} & 0 & -4 & \bullet\\ 0 & e^{\frac{\sqrt{3}ik_y a}{2}-\frac{ik_x a}{2}} + e^{-\frac{\sqrt{3}ik_y a}{2}-\frac{ik_x a}{2}} & 0 & -2\sqrt{3}\end{bmatrix}$$

and

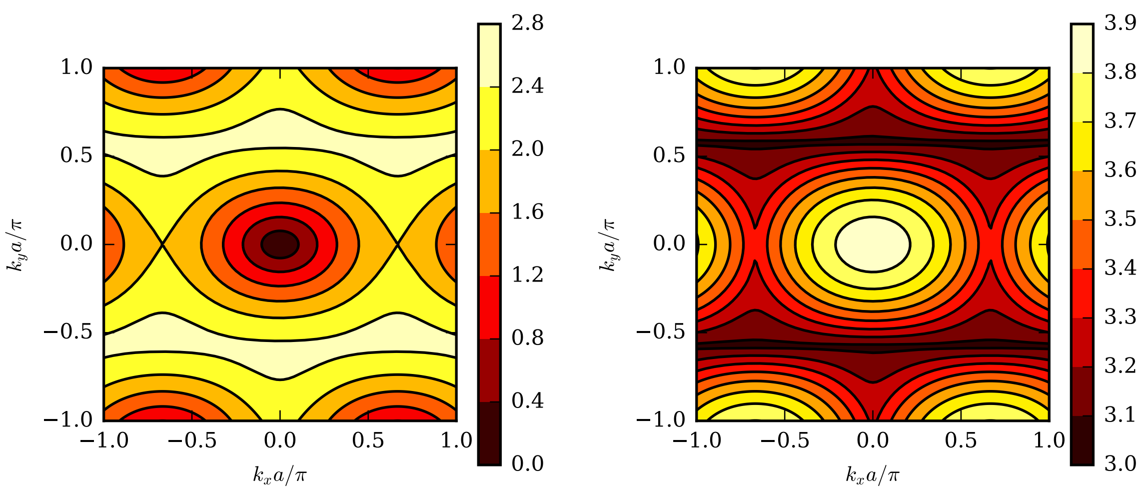
$$\mathbb{M}_R = m\mathbb{I}_4.$$

The eigenvalues for this problem are lengthy, but a second order expansion around $(k_x, k_y) = (0, 0)$ (linear in the case of its square root) is shown

$$\begin{aligned}\frac{\omega_1^2}{\omega_0^2} &= \frac{3^{\frac{3}{2}}\,k_y a^2}{4}\\ \frac{\omega_2^2}{\omega_0^2} &= \frac{6\,k_y a^2 + 9\,k_x a^2}{8}\\ \frac{\omega_3^2}{\omega_0^2} &= -\frac{3^{\frac{3}{2}}\,k_y a^2 - 16\,\sqrt{3}}{4}\\ \frac{\omega_4^2}{\omega_0^2} &= -\frac{6\,k_y a^2 + 9\,k_x a^2 - 64}{8}\ ,\end{aligned}$$

with $\omega_0^2 = c/m$.

Figure 24 shows the dispersion modes for ratios $m_2/m_1 = 1$ and $c_d/c_s = 1$.



(a) First branch. **(b)** Second branch.

Figure 24. Dispersion relations for the hexagonal unit cell.

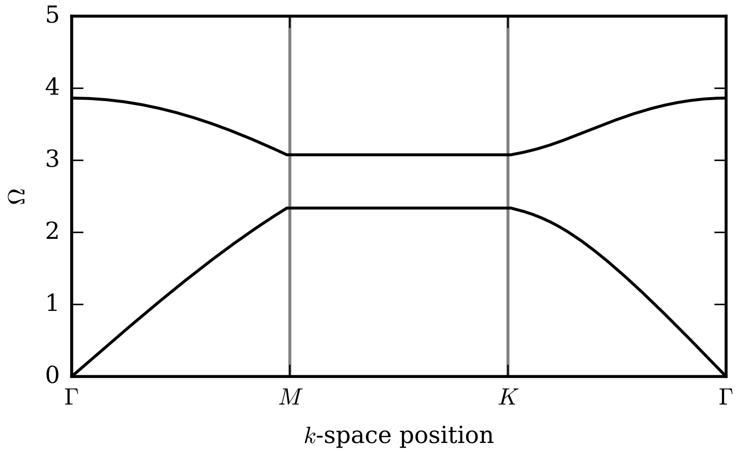


Figure 25. Dispersion curves over the irreducible Brillouin zone.

8 Hexagonal Lattice: 2 species

In this case we have an hexagonal cell with springs with constant c in the sides (see Figure 26).

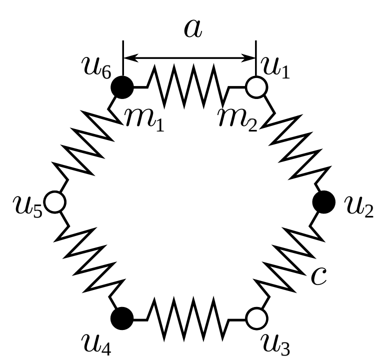
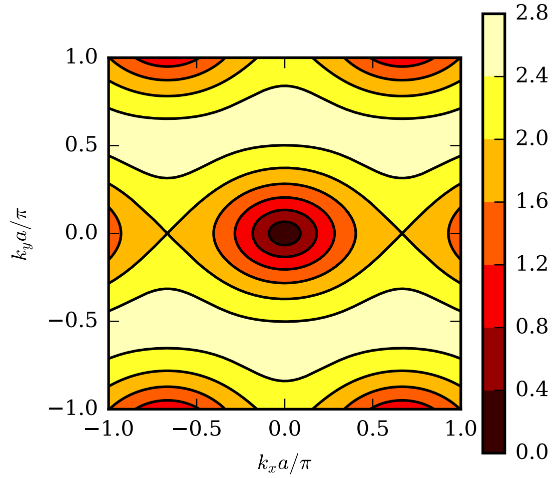


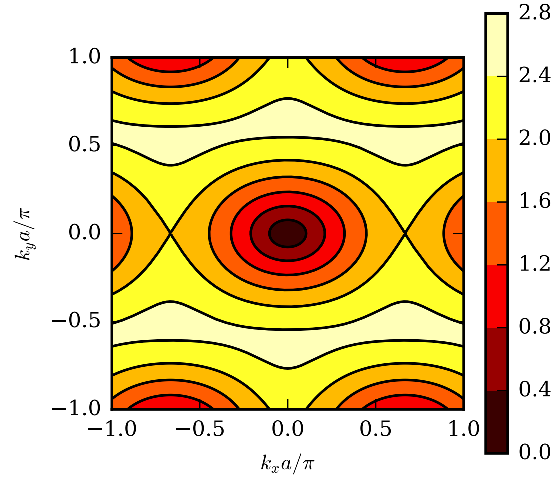
Figure 26. Unit cell for a two dimensional hexagonal lattice with two species in the corners.

The system of equations to solve is the same that the one for the hexagonal lattice with a single species. The mass matrix is different

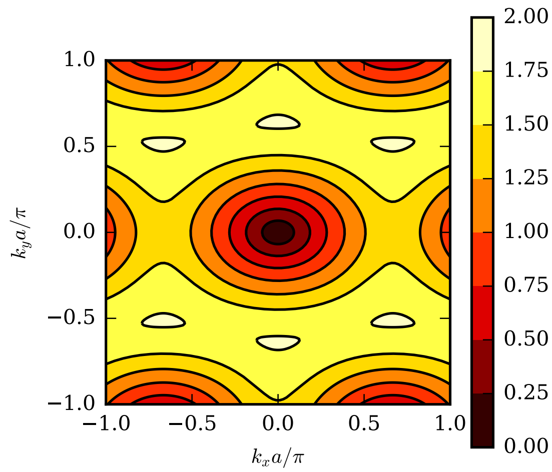
$$\mathbb{M} = \frac{m}{3}\begin{bmatrix} m_1\mathbb{I}_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & m_2\mathbb{I}_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & m_1\mathbb{I}_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & m_2\mathbb{I}_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & m_1\mathbb{I}_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & m_2\mathbb{I}_2 \end{bmatrix} .$$



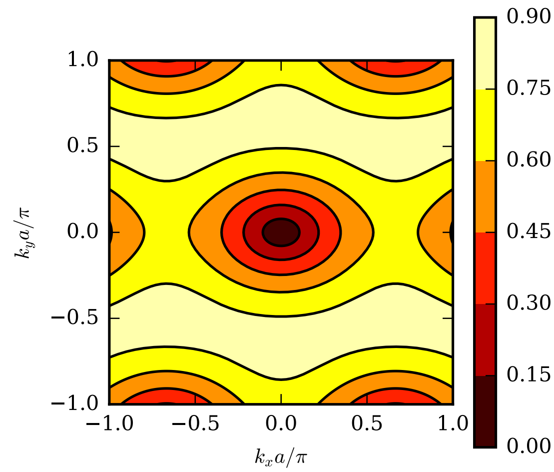
(a) $m_2/m_1 = 0.1$.



(b) $m_2/m_1 = 0.5$.

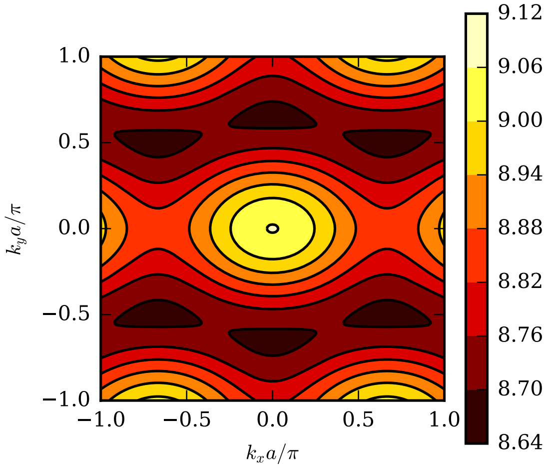


(c) $m_2/m_1 = 2$.

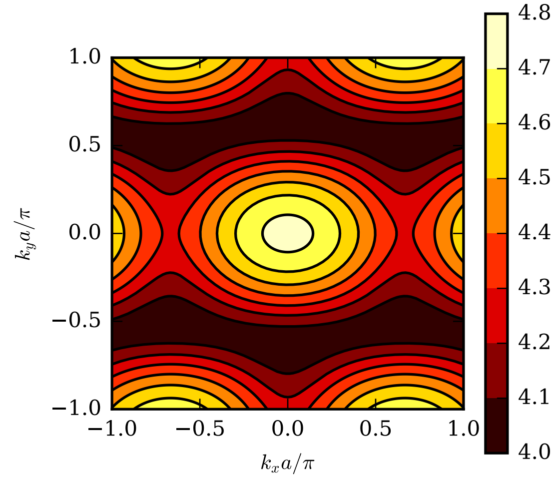


(d) $m_2/m_1 = 10$.

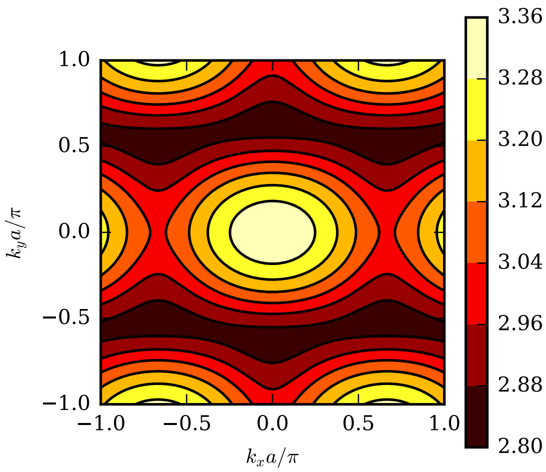
Figure 27. First branch of the dispersion curves for the hexagon with two species.



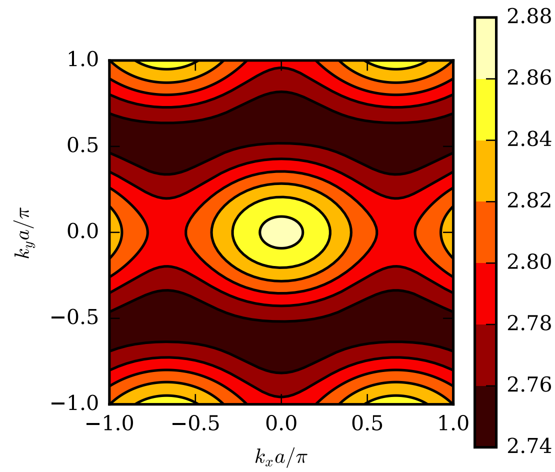
(a) $m_2/m_1 = 0.1$.



(b) $m_2/m_1 = 0.5$.



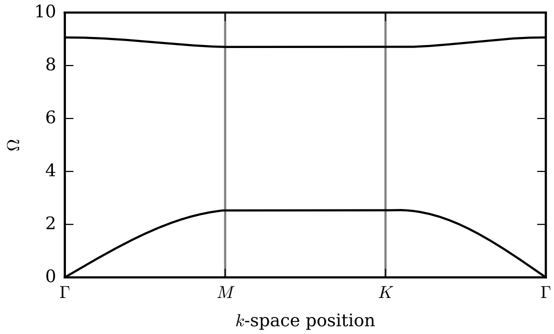
(c) $m_2/m_1 = 2$.



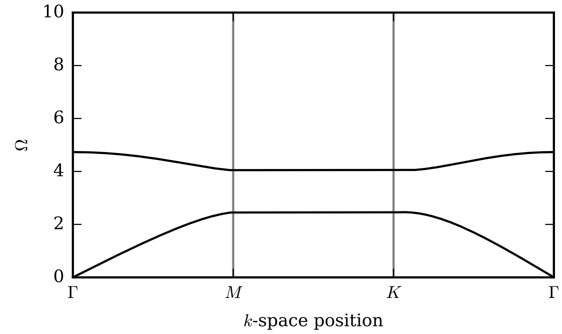
(d) $m_2/m_1 = 10$.

Figure 28. Second branch of the dispersion curves for the hexagon with two species.

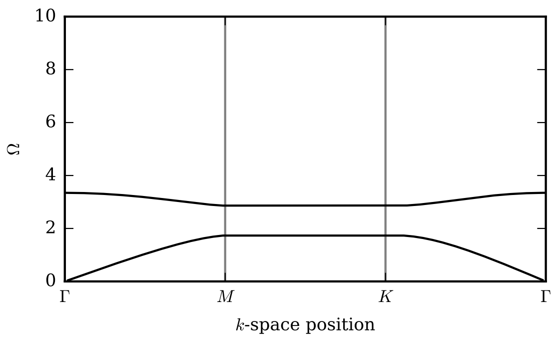
Figure 29 show the dispersion curves over the irreducible Brillouin zone of the two species hexagon.



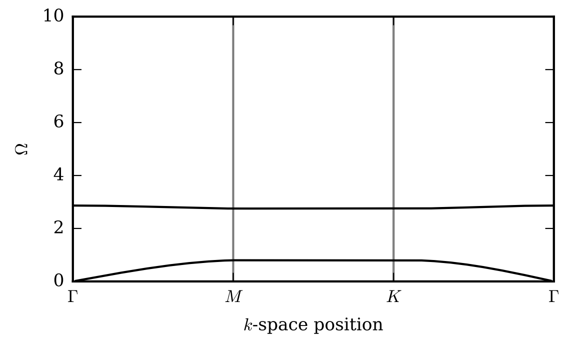
(a) $m_2/m_1 = 0.1$.



(b) $m_2/m_1 = 0.5$.



(c) $m_2/m_1 = 2$.



(d) $m_2/m_1 = 10$.

Figure 29. Dispersion curves over the irreducible Brillouin zone for the hexagonal lattice with two species.

9 Uncertainty quantification

In this section we would like to analyze the uncertainty in the dispersion relations taken the parameters, geometric at first, of the lattices.

We can approximate the moments of a function f of a random variable X using a Taylor series expansion. If we consider quadratic expansions in the standard deviation, σ_X^2, we obtain that [1]

$$\mathrm{E}[f(X)] \approx f(\mu_X) + f''(\mu_X)\frac{\sigma_X^2}{2} \tag{36}$$

$$\mathrm{Var}[f(X)] \approx f'(\mu_X)^2 \sigma_X^2 \,, \tag{37}$$

where E[] is the expected value, Var[] the variance, μ_X is the expected value of X and σ_X the standard deviation of X.

In the case of function of several variables we would need to performa a multivariate Taylor expansion.

9.1 Single-species lattice

In this case the dispersion relation reads

$$\Omega = 2\left|\sin\frac{1}{2}ka\right| ,$$

and let's take a as a random variable, and $\bar{a}$ as the expected value of a and σ_a as it's standard deviation.

Then, we have

$$\mathrm{E}[\Omega] \approx 2\left|\sin\frac{1}{2}k\bar{a}\right| - \frac{k^2\sigma_a^2}{4}\left|\sin\frac{1}{2}k\bar{a}\right| \tag{38}$$

$$\mathrm{Var}[\Omega] \approx k^2\sigma_a^2\cos^2\frac{1}{2}k\bar{a} \tag{39}$$

We can see a plot of the expected values and variances for different levels of standard deviation in Figure 30.

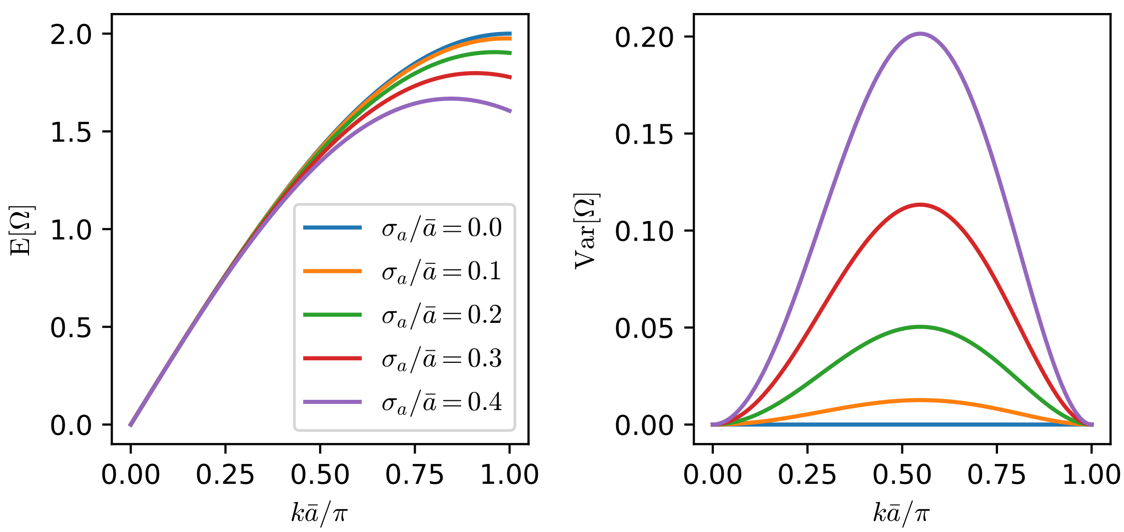


Figure 30. Dispersion curves over the first Brillouin zone for a single-species considering that the spacing in the lattice is a random variable.

In Figure 31

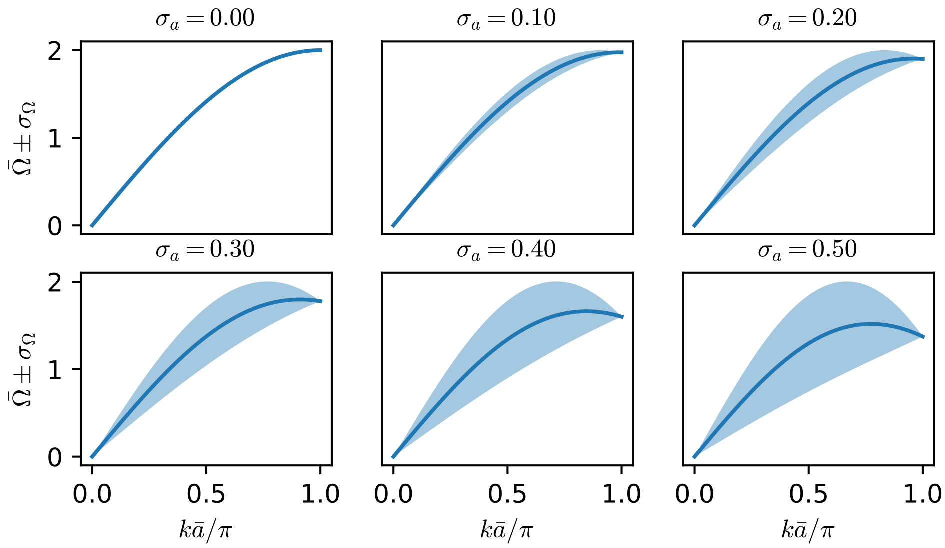


Figure 31. Dispersion curves over the first Brillouin zone for a single-species considering that the spacing in the lattice is a random variable.

9.2 Two-species lattice

For a two-species lattices the dispersion relation is

$$\Omega_{\mp} = \left[1 + \mu \pm \sqrt{(1+\mu)^2 - 2\mu(1 - \cos ka)}\right]^{1/2} ,$$

with

$$\mu = \frac{m_1}{m_2}, \quad \Omega^2 = \frac{\omega^2}{\omega_0^2}, \quad \omega_0^2 = \frac{c}{m_1} .$$

If we compute the expected value and variance up to second order (σ_a^2) terms, we obtain

$$\mathrm{E}[\Omega_\pm] \approx \Omega_\pm \pm \frac{k^2\sigma_a^2\mu^2}{4g^{1/2}\Omega_\pm}\left[\frac{\sin^2 k\bar{a}}{g} - \frac{\cos k\bar{a}}{\mu} - \frac{\sin^2 k\bar{a}}{2g^{1/2}\Omega_\pm}\right] \tag{40}$$

$$\mathrm{Var}[\Omega_\pm] \approx \frac{k^2\mu^2\sigma_a^2}{4g\Omega_\pm}\sin^2 k\bar{a}\,, \tag{41}$$

with

$$g = (1+\mu)^2 - 2\mu(-\cos k\bar{a})\,.$$

We can see a plot of the expected values and variances for different levels of standard deviation in Figure 32.

In Figure 33

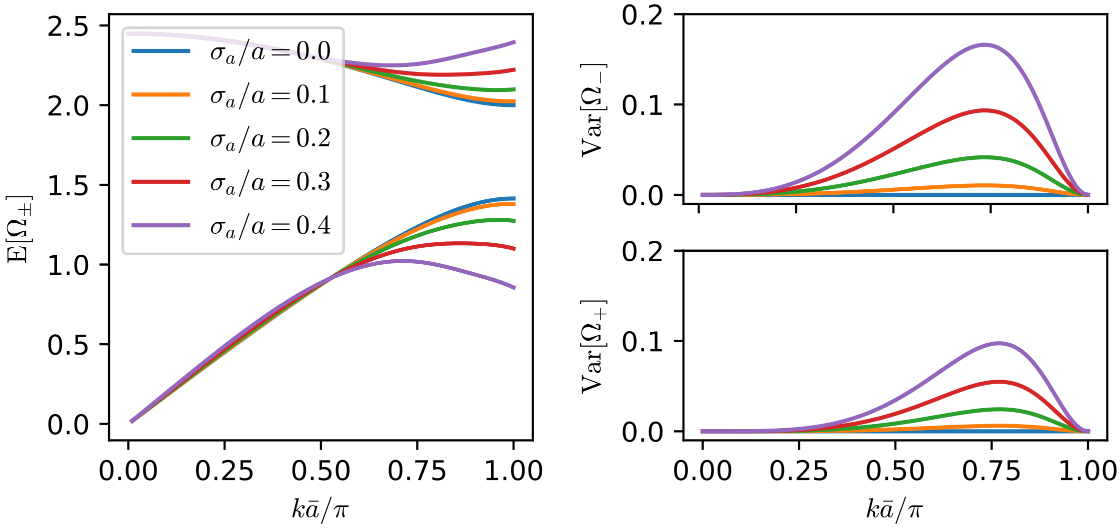


Figure 32. Dispersion curves over the first Brillouin zone for a two-species considering that the spacing in the lattice is a random variable and the ratio of masses $\mu = 2$.

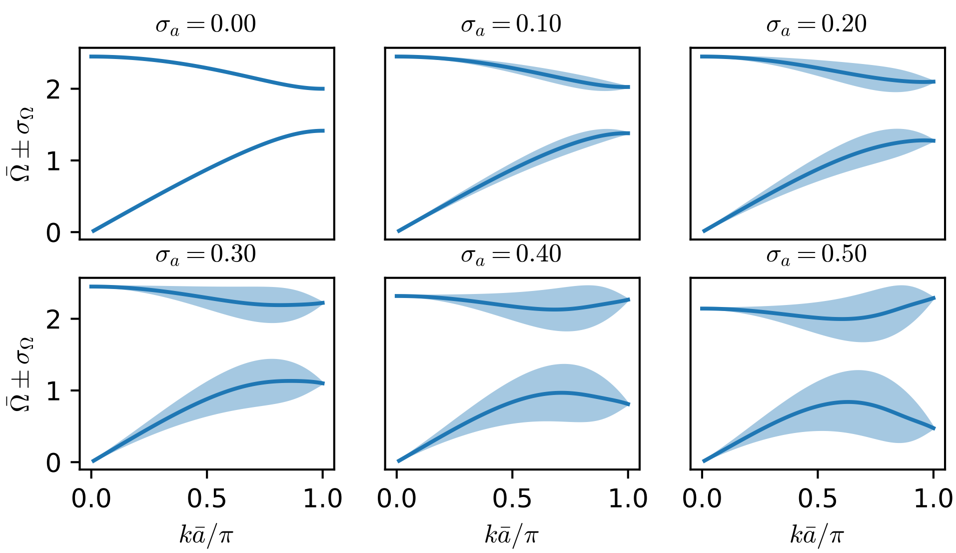


Figure 33. Dispersion curves over the first Brillouin zone for a single-species considering that the spacing in the lattice is a random variable.

We want to see how much the bandgap is affected by the increase in the standard deviation of the parameter a. The Figure 34 shows the bandgap size as a function of the normalized standard deviation $\sigma_a/\bar{a}$. The size is defined as the separation between the maximum and minimum of the two branches considering the first standard deviation in the frequency, i.e, the separation between the branches in Figure 33.

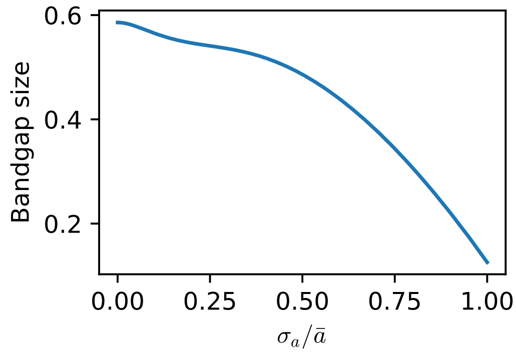


Figure 34. Bandgap size as a function of normalized standard deviation $\sigma_a/\bar{a}$.

References

[1] Haym Benaroya and Seon Mi Han, *Probability Models in Engineering and Science*, Taylor & Francis, 1st edition, 2005.