Chapter 3

Discrete one dimensional systems

Learning goals

- You know the concept of a Brillouin zone.
- You know what an evanescent wave is.
- You know the relation between the number of elements in a unit cell and the the number of bands.
- You know the effect of a local resonance for wave propagation.

3.1 Discrete systems

So far, we have been considering the wave equation

$$\partial_x^2 u = \frac{\rho}{E}\partial_t^2 u \tag{3.1}$$

in a homogeneous and isotropic medium. As a first step towards understanding (periodically) structured metamaterials we study discrete systems. To prepare ourselves for this step, we first look at the translation "operator" $T_\Delta x$ that we encountered in the last section. So far, our system was "living" on the real axis

$$u(x,t) \qquad \text{with} \qquad x \in \mathbb{R}. \tag{3.2}$$

We found that an eigenmode labelled by the wave-number k has the property that

$$u(x,t) = e^{ik-i\omega t} \quad \Rightarrow \quad u(x+\Delta x,t) = e^{ik\Delta x}u(x,t). \tag{3.3}$$

Let us now consider the discrete system depicted in Fig. 3.1. Each local discrete element is

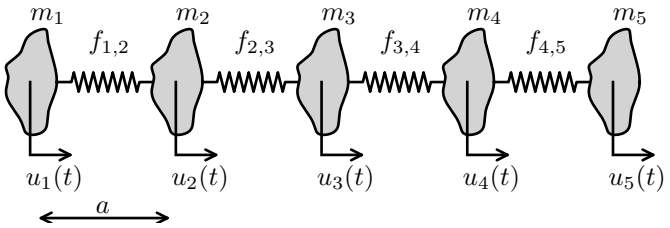


Figure 3.1: A discrete one dimensional chain.

considered rigid, having a mass m_i and it is connected to its neighbors via springs with spring constants $f_{n,n+1}$ and $f_{n,n-1}$. Each element, or mass, can be displaced by $u_n(t)$. But now, the displacement field $u_n(t)$ is actually living on the set of integer numbers $n \in \mathbb{Z}$ and not $\mathbb{R}$ as we have only a discrete number of displacements, one for each element located at $x_n = na$, where a is the lattice constant. (Of course, u, itself can still take values in $\mathbb{R}$, or $\mathbb{C}$, respectively).
This has immediate consequences for the possible wave-numbers that can appear. Assume again that plane waves are good solutions:

$$u_n(t) = e^{ikan - i\omega t}. \tag{3.4}$$

Therefore, we again have that the solution at n and at $n+1$ differ by

$$e^{ika}. \tag{3.5}$$

But now, $kna = 2\pi$ is really the same as $kna = 0$. Actually, all $k = k + 2\pi m$ with $m \in \mathbb{Z}$ are equivalent. Hence, we can confine the possible values of the wave-number to

$$k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right], \tag{3.6}$$

which is known as the first Brillouin zone. Equivalently, $k > \frac{2\pi}{a}$ would correspond to a wave with wavelength $\lambda < \frac{2\pi}{k} = a$. But as we have a mass only every a, there is nothing to be described with a wavelength smaller than the lattice spacing a.

3.2 The monoatomic chain

Let us now solve the problem sketched in Fig. 3.1. In a first step, we assume all masses to be the same $m_i = m$ and all springs to be identical with $f_{i,j} = f$. The equations of motion are then given by

$$m\ddot{u}_n(t) = f\left\{[u_{n-1}(t) - u_n(t)] - [u_n(t) - u_{n+1}(t)]\right\} \tag{3.7}$$

When assuming solutions of the form

$$u_n(t) = e^{ikna - i\omega t} \tag{3.8}$$

we find that the equation of motion reduces to

$$-m\omega^2 e^{inak - i\omega t} = f e^{inak - i\omega t}\left[e^{ika} - 1 - 1 + e^{ika}\right] \tag{3.9}$$

$$= -4f \sin^2\left(\frac{ka}{2}\right) e^{inak - i\omega t}. \tag{3.10}$$

With this we find the dispersion relation shown in Fig. 3.2

$$\boxed{\omega(k) = \sqrt{\frac{4f}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|.} \tag{3.11}$$

Again plane waves are good solutions! However, our dispersion relation changed. A few important observations

1. The dispersion $\omega(k)$ is periodic in k with period $2\pi/a$.
2. Around $k = 0$, the waves seem to still linear disperse with

$$c = a\sqrt{\frac{f}{m}}. \tag{3.12}$$

Where the spring constant f [N/m] replaced the Young's modulus E [N/m^2] and the mass m [kg] the mass density ρ [kg/m]. The fact that around $k = 0$ we recover the result for a continuous system is easily explained. At wavelengths much larger than the lattice spacing, the waves don't feel the granularity of the individual masses.

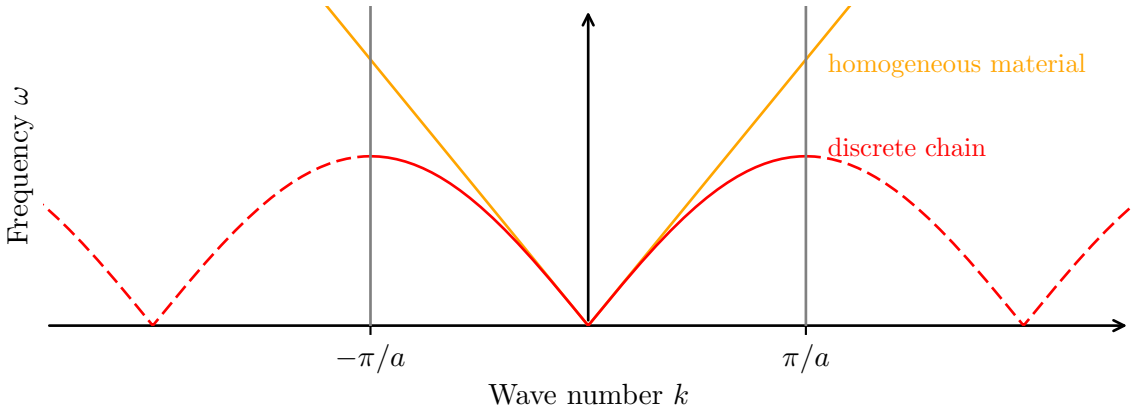


Figure 3.2: Dispersion relation of a mono-atomic chain.

3. Owing to the non-linearity of $\omega(k)$, group and phase velocity are not identical anymore.

There is another interesting property: The spectrum $\omega(k)$ of possible traveling waves is now bounded form above. That means, for frequencies

$$\omega > \omega_{\text{edge}} = \omega(\pi/a) = \sqrt{\frac{4f}{m}}, \tag{3.13}$$

there are no propagating solutions.

3.2.1 Evanescent waves

The fact that there are no propagating solutions does not mean that the mono-atomic chain is totally inert if we try to excite it with frequencies $\omega > \omega_{\text{edge}}$. Let us assume solutions

$$u_n^\xi(t) = e^{i\left(\pi + i\frac{1}{\xi}\right)na - \omega t}. \tag{3.14}$$

Inserted into (3.7), we find

$$-m\omega^2 u_n^\xi(t) = f u_n^\xi(t) e^{i\omega t}\left[e^{i\left(\pi+i\frac{1}{\xi}\right)} + e^{-i\left(\pi+i\frac{1}{\xi}\right)} - 2\right] \tag{3.15}$$

$$-m\omega^2 = f\left[-e^{-\frac{1}{\xi}} - e^{-\frac{1}{\xi}} - 2\right] = -f\left[2\cosh\left(\frac{1}{\xi}\right) + 2\right]. \tag{3.16}$$

And therefore

$$\omega(\xi) = \sqrt{\frac{4f}{m}} \underbrace{\sqrt{\frac{\cosh\left(\frac{1}{\xi}\right)+1}{2}}}_{\geq 1}. \tag{3.17}$$

This is a solution only for $\omega > \omega_{\text{edge}}$. We found that in this case, vibrations penetrate into the mono-atomic chain with a decay length ξ given by

$$\xi = \frac{1}{\sqrt{\operatorname{arccosh}\left(\frac{m\omega^2}{2f} - 1\right)}}. \tag{3.18}$$

We can summarize these findings in Fig. 3.3

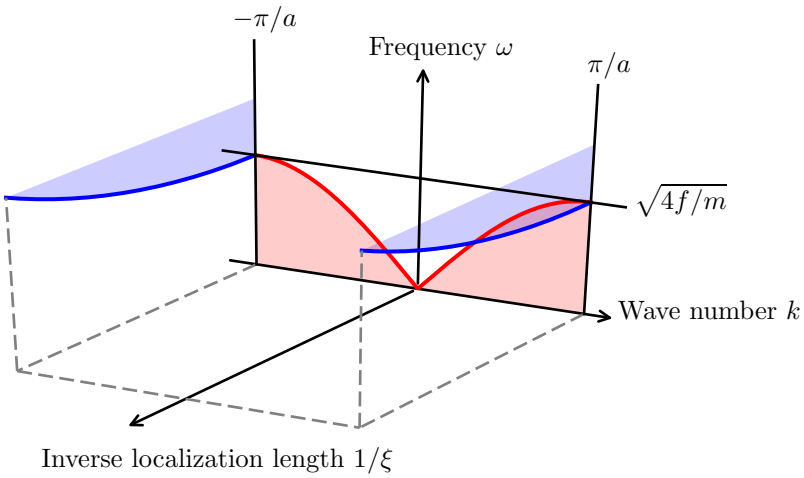
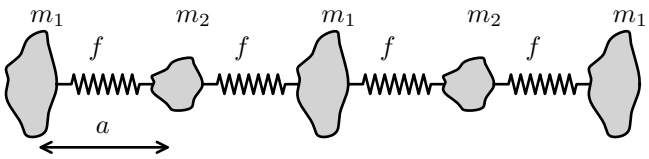


Figure 3.3: Summary of the mono-atomic chain: Up to a frequency $\omega = \sqrt{\frac{4f}{m}}$ waves propagate with a real wavenumber k. Above this cut-off frequency, evanescent waves with a decay length ξ can survive at the endpoints of the chain.

3.2.2 The diatomic chain

We are now in the position to embark on the first interesting example. Let us consider a system similar to the one above, but with alternating masses:



What of the analysis of the last section can we carry over to this problem? Remember that we knew $u_n^k(t)$ if we had $u_m^k(t)$ just by multiplying

$$u_n^k(t) = e^{ik(m-n)a} u_m^k(t). \tag{3.19}$$

This simple phase relation was due to the fact that our problem was symmetric under a shift by one lattice site. Now, that $m_1 \neq m_2$, we have no reason to assume that a simple relation as in (3.19) should hold. However, every second mass is identical! Therefore, let us assume the following structure for the eigenmodes

$$u_n^k(t) = e^{ikna - i\omega t} \times \begin{cases} a_k & n = 2s, \quad s \in \mathbb{Z}, \\ b_k & n = 2s+1, \quad s \in \mathbb{Z}. \end{cases} \tag{3.20}$$

In other words, we assume that from even to even and from odd to odd site we again have a simple phase factor

$$e^{ik2a}, \tag{3.21}$$

but that the structure within one unit cell is given by the relation between a_k and b_k. Note, that by virtue of this ansatz we have that

$$e^{2ika} = e^{2i(k+r\pi)a} \qquad \text{with} \qquad r \in \mathbb{Z}. \tag{3.22}$$

By doubling ($a \to 2a$) our unit cell size, we halved the sized of the first Brillouin zone.[1]
The equations of motion read

$$m_1 \ddot{u}_{2n} = f(u_{2n+1} + u_{2n-1} - 2u_{2n}), \tag{3.23}$$
$$m_2 \ddot{u}_{2n} = f(u_{2n} + u_{2n+2} - 2u_{2n+1}). \tag{3.24}$$

Inserting ansatz (3.20) into the above equation we find

$$-m_1\omega^2 a_k = f(b_k + e^{2iak} b_k - 2a_k), \tag{3.25}$$
$$-m_2\omega^2 b_k = f(a_k + e^{2iak} a_k - 2b_k). \tag{3.26}$$

We deal with a problem of the form

$$-\omega^2 \begin{pmatrix} m_1 & \\ & m_2 \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} = \begin{pmatrix} 2f & -f\left(1 + e^{-2iak}\right) \\ \left(1 + e^{2iak}\right) & 2f \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} \tag{3.27}$$

This is a generalized eigenvalue problem of the type $\alpha B x = A x$ with B positive definite and both $A = A^\dagger$ and $B = B^\dagger$. We could do

$$\alpha x = B^{-1} A x, \tag{3.28}$$

but we would not deal with a hermitian problem anymore. Let us write $B = LL^\dagger$ with

$$L = \begin{pmatrix} \sqrt{m_1} & \\ & \sqrt{m_2} \end{pmatrix}. \tag{3.29}$$

With this we obtain

$$\alpha L L^\dagger x = A (L^\dagger)^{-1} L^\dagger x \tag{3.30}$$
$$\alpha \underbrace{L^\dagger x}_{y} = \underbrace{L^{-1} A (L^\dagger)^{-1}}_{\tilde{A}} \underbrace{L^\dagger x}_{y}. \tag{3.31}$$

Therefore we deal with a regular eigenvalue problem

$$\alpha y = \tilde{A} y, \tag{3.32}$$

with the property

$$\tilde{A}^\dagger = [(L^\dagger)^{-1}]^\dagger A^\dagger (L^{-1})^\dagger = L^{-1} A (L^\dagger)^{-1} = \tilde{A}, \tag{3.33}$$

i.e., a hermitian eigenvalue problem. For us this means

$$\tilde{A} = \begin{pmatrix} \frac{1}{\sqrt{m_1}} & \\ & \frac{1}{\sqrt{m_2}} \end{pmatrix} \begin{pmatrix} 2f & -f\left(1 + e^{-2iak}\right) \\ \left(1 + e^{2iak}\right) & 2f \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{m_1}} & \\ & \frac{1}{\sqrt{m_2}} \end{pmatrix} = \tag{3.34}$$
$$= \begin{pmatrix} \frac{2f}{m_1} & -\frac{f}{\sqrt{m_1 m_2}}\left(1 + e^{-2iak}\right) \\ -\frac{f}{\sqrt{m_1 m_2}}\left(1 + e^{2iak}\right) & \frac{2f}{m_2} \end{pmatrix} \tag{3.35}$$
$$= f\left(\frac{1}{m_1} + \frac{1}{m_2}\right) \mathbb{1} - \underbrace{\frac{f}{m}(1 + cos(\varphi_k))}_{d_1(k)} \sigma_1 - \underbrace{\frac{f}{m} \sin(\varphi_k)}_{d_2(k)} \sigma_2 + \underbrace{f\left(\frac{1}{m_1} + \frac{1}{m_2}\right)}_{d_3(k)} \sigma_3 \tag{3.36}$$
$$= f\left(\frac{1}{m_1} + \frac{1}{m_2}\right) \mathbb{1} + \sum_{i=1}^{3} d_i(k) \sigma_i. \tag{3.37}$$

[1] You could argue that now there is a life below the wavelength $\lambda = 2a$ as there is "something" at a distance a rather than $2a$. But this degree of freedom is taken care of by the relation between a_k and b_k!

We introduced $m = \sqrt{m_1 m_2}$ and $\varphi_k = 2ak$. We can now capitalize on our knowledge of $2x2$ matrices written with Pauli matrices to immediately read off the eigenvalues

$$\alpha_\pm = f\left(\frac{1}{m_1} + \frac{1}{m_2}\right) \pm \frac{f}{m}\sqrt{\left(\frac{m}{m_1} - \frac{m}{m_2}\right)^2 + (1+\cos(\varphi_k))^2 + \sin(\varphi_k)^2} \tag{3.38}$$

$$= \frac{f}{m}\left(\sqrt{\frac{m_2}{m_1}} + \sqrt{\frac{m_1}{m_2}}\right) \pm \frac{f}{m}\sqrt{\left(\sqrt{\frac{m_2}{m_1}} - \sqrt{\frac{m_1}{m_2}}\right)^2 + 2 + 2\cos(2ka)}. \tag{3.39}$$

With this, we arrive at the dispersion

$$\boxed{\omega_\pm(k) = \sqrt{\frac{f}{m}}\sqrt{\left(r + \frac{1}{r}\right) \pm \sqrt{\left(r - \frac{1}{r}\right)^2 + 4\cos^2(ka)}},} \tag{3.40}$$

with $m = \sqrt{m_1 m_2}$ and $r = \sqrt{m_2/m_1}$. Let us inspect how this dispersion behaves for various values of the reduced mass m and ratio r. We see that we opened a band gap for $k = \frac{\pi}{2a}$ with magnitude $\sqrt{\frac{4f}{m}}\sqrt{r - \frac{1}{r}}$, which goes to zero for $r = 1$. In fact, for $r = 1$, we chose a unit cell which is too large, or equivalently, a too small Brillouin zone. We see that in the Fig. 3.4. that this leads to a "folding" of the spectrum.

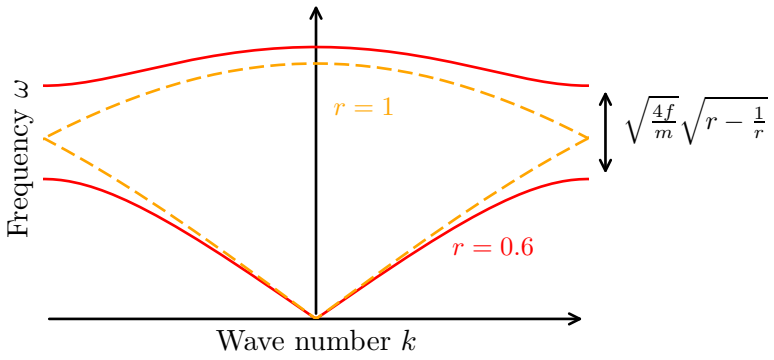


Figure 3.4: Dispersion of a diatomic chain.

We have now seen that by structuring our chain at the scale $2a$, we opened a band gap at $k = \pi/2a.$, and the frequency was hence dictated by $\omega_{k=\pi/a}$ of the undisturbed (mono-atomic) chain. We would like to see, if another design-principle exists that can beat this limit.

3.2.3 Locally resonant structures

We want to study the system shown in Fig. 3.5. The block system of masses m and spring constants f alone defines a regular mono-atomic chain with no band gap. We want to understand the effect of a added local resonators:

$$m\ddot{u}_i = f(u_{i-1} + u_{i+1} - 2u_i) + F(u_i - w_i), \tag{3.41}$$

$$M\ddot{w}_i = -F(w_i - u_i). \tag{3.42}$$

As usual, we assume plane waves and write the above equation in matrix form

$$-\begin{pmatrix} m & \\ & M \end{pmatrix}\omega^2\begin{pmatrix} u_k \\ w_k \end{pmatrix} = \begin{pmatrix} -(2f+F) + 2f\cos(ka) & F \\ F & -F \end{pmatrix}\begin{pmatrix} u_k \\ v_k \end{pmatrix}, \tag{3.43}$$

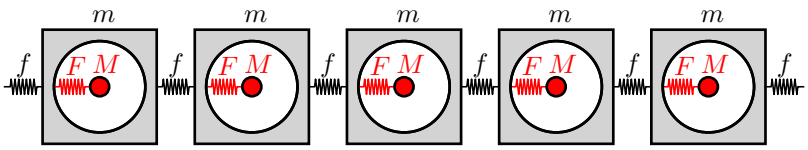


Figure 3.5: Resonantor-in-resonator setup.

where we assumed

$$u_n = u_k e^{ikna - i\omega t}, \tag{3.44}$$

$$w_n = w_k e^{ikna - i\omega t}. \tag{3.45}$$

We again transform $A \to \tilde{A}$ wiht $LL^\dagger = B$ to obtain

$$\tilde{A} = L^{-1}A(L^\dagger)^{-1} = \begin{pmatrix} \frac{(2f+F)-2f\cos(ka)}{m} & -\frac{1}{\sqrt{mM}}F \\ -\frac{1}{\sqrt{mM}}F & \frac{F}{M} \end{pmatrix} = \omega_0^2 \begin{pmatrix} \frac{1}{2}(1-\cos(k)) + \gamma^2\tilde{\omega}_L^2 & -\gamma\tilde{\omega}_L^2 \\ -\gamma\tilde{\omega}_L^2 & \tilde{\omega}_L^2 \end{pmatrix},$$

where we introduced

$$\tilde{\omega}_L = \frac{1}{2}\sqrt{\frac{m}{f}\frac{F}{M}}: \qquad \text{local resonance frequency in units of } \omega_0, \tag{3.46}$$

$$\gamma = \sqrt{\frac{M}{m}}: \qquad \text{“coupling strength”}, \tag{3.47}$$

$$\omega_0 = \sqrt{\frac{4f}{m}}: \qquad \text{overall frequency scale.} \tag{3.48}$$

With these abbreviations we can write

$$\frac{1}{\omega_0^2}\tilde{A} = \frac{1}{2}\left\{\frac{1}{2}[1-\cos(ka)] + \tilde{\omega}_L^2(\gamma^2+1)\right\}\mathbb{1} + \sum_{i=1}^{3} d_i(k)\sigma_i, \tag{3.49}$$

with

$$\mathbf{d}(k) = \left(-\gamma^2\tilde{\omega}_0^2, 0, \left\{\tfrac{1}{2}[1-\cos(ka)] + \tilde{\omega}_L^2(\gamma^2-1)\right\}\right). \tag{3.50}$$

And again, we just read off the dispersion relation

$$\boxed{\omega_\pm(k) = \omega_0\sqrt{\frac{1}{2}\left\{\frac{1}{2}[1-\cos(ka)] + \tilde{\omega}_L^2(1+\gamma^2) \pm \sqrt{4(\gamma\tilde{\omega}_L^2)^2 + \left[\frac{1}{2}[1-\cos(ka)] + \tilde{\omega}_L^2(\gamma^2-1)\right]^2}\right\}}}$$

The dispersion is displayed in Fig. 3.6. We see that for the case of a local resonance a band gap is opening not at a specific k but at a specific $\tilde{\omega}_L$. Moreover, the stronger the resonance is coupled, the bigger the band gap.

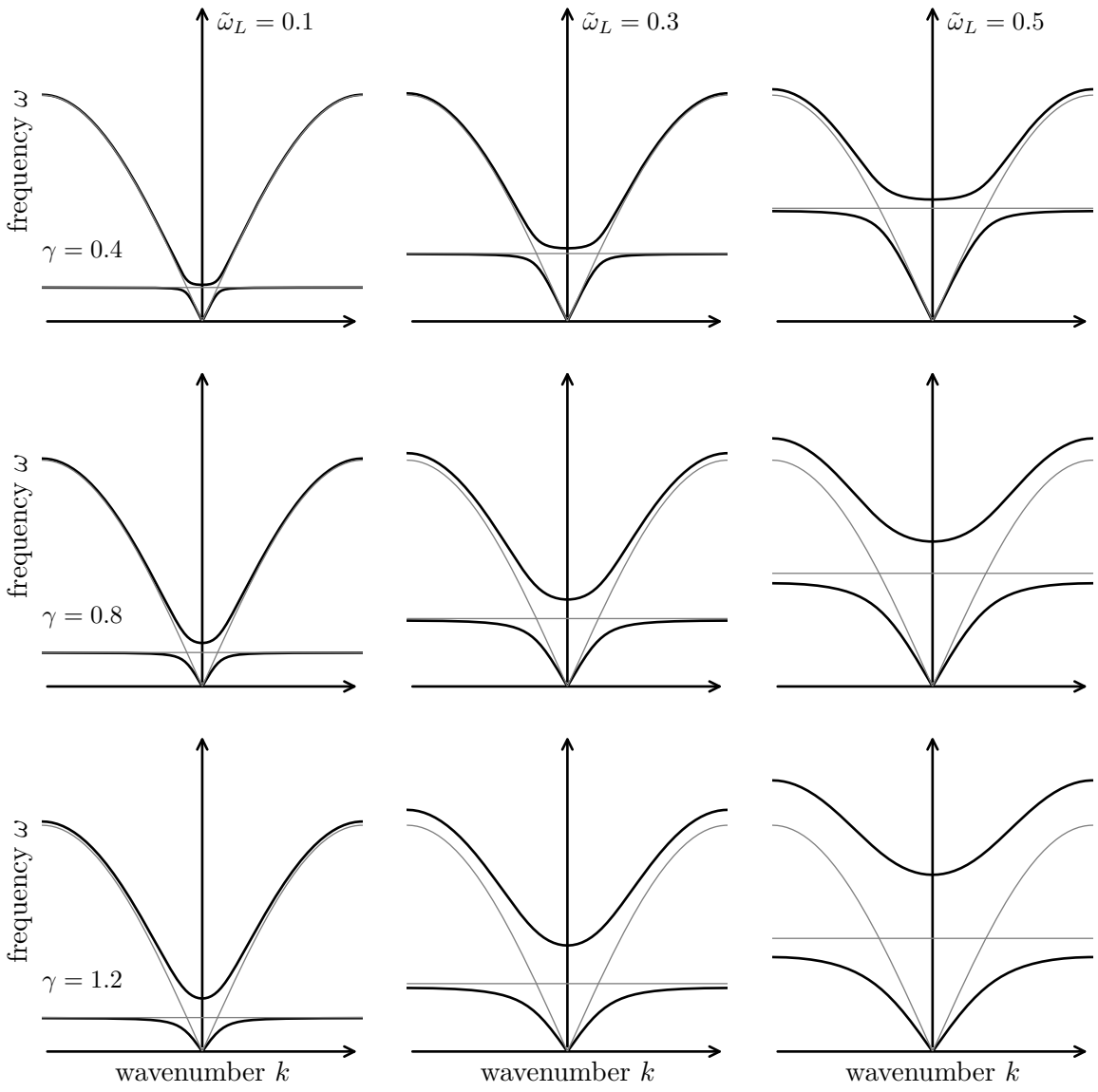


Figure 3.6: Dispersion for a chain made of local resonators.