# Chapter 3

# Discrete one dimensionsal systems

Learning goals

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

# 3. Discrete systems

So far, we have been considering the wave equation

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

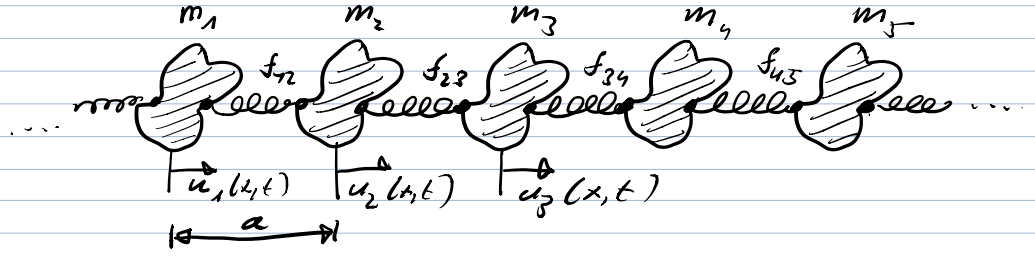
in a homogeneous and isotropic medium. As a first step towards understanding (periodically) structured metamaterials we study discrete systems. To prepare for this step, we first look at the translation "operator" the we encountered last time. So far our system was "living" on the real axis

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

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

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

Let us now consider a discrete system:



Each local discrete element is considered rigid, having a mass $m_i$ and it is connected to its neighbors via springs $f_{i,i+1}$ and $f_{i,i-1}$. Each element, or mass, can be displaced by $u_i(x,t)$. But now the displacement field $u_i(x,t)$ is actually living on the integer numbers and not $\mathbb{R}$:

$$u_i(x,t) = u_i(i\cdot a, t)$$

as we only have a discrete number of displacements, one for each element.

This has immediate consequences for the possible wave-numbers that can appear. Assume that again plane waves are good solutions:

$$u_n(x,t) = e^{ikan - i\omega t}$$

$\Rightarrow$ We again have that the solution at $n$ and $n+1$ differ by

$$e^{ikna}.$$

But now $kna = 2\pi$ is the same as $kna = 0$. Actually any $k \hat{=} k + 2\pi m$ $\forall m$. Hence, we can confine the possible values of the wave numbers to

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

which is known as the *first Brillouine zone*. Equivalently, $k > \frac{2\pi}{a}$ corresponds to a wave with wavelength $\lambda < \frac{2\pi}{k} = a$. But as we have a mass only every $a$, there is nothing to describe with a wavelength smaller than the lattice-spacing $a$.

## 3.1 The monoatomic chain

Let us now solve the problem sketched above. In a first step, we assume all masses to be the same $m_i \equiv m$ and all springs to be identical with $f_i \equiv f$. The equations of motion are the given by

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

When assuming solutions of the form

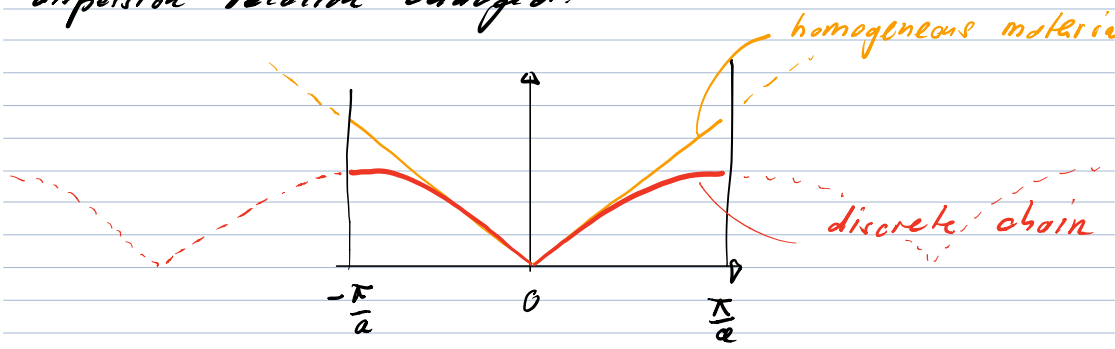
$$u_n(t) = e^{ina k - i\omega t}$$

we find

$$\begin{aligned} -m\omega^2 e^{ina k - i\omega t} &= f e^{ina k - i\omega t} \times \\ &\quad \left[e^{-ika} - 1 - 1 + e^{ika}\right] \\ &= -4f \sin^2\left(\frac{ka}{2}\right) e^{ina k - i\omega t} \end{aligned}$$

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

Again plane waves are good solutions! However, our dispersion relation changed.




A few important observations:

a.) The dispersion $\omega(k)$ is periodic in $k$ with period $2\pi$

b.) Around $k = 0$, the waves seem to still linearly disperse with

$$c = a\sqrt{\frac{f}{m}},$$

where the spring constant $f$ [N/m] replaced the Young's modulus $E$ [N/m$^2$] and the mass $m$ [kg] the mass density $\rho$ [kg/V]

c.) Owing to the non-linearity of $\omega(k)$, $v_g \neq v_\varphi$!

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

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

there are no propagating solutions!

### 3.1.1 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 $\omega > \sqrt{\frac{4f}{m}}$. Let us assume solutions

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

$\Rightarrow$ inserted into (1) we find

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

$$-m\omega^2 = f \left[ -e^{-\frac{1}{\xi}} - e^{\frac{1}{\xi}} - 2 \right]$$

$$= -f \left[ 2\cosh\frac{1}{\xi} + 2 \right]$$

$$\Rightarrow \quad \omega(\xi) = \sqrt{\frac{4f}{m}} \underbrace{\sqrt{\frac{\cosh\frac{1}{\xi} + 1}{2}}}_{\geq 1}$$

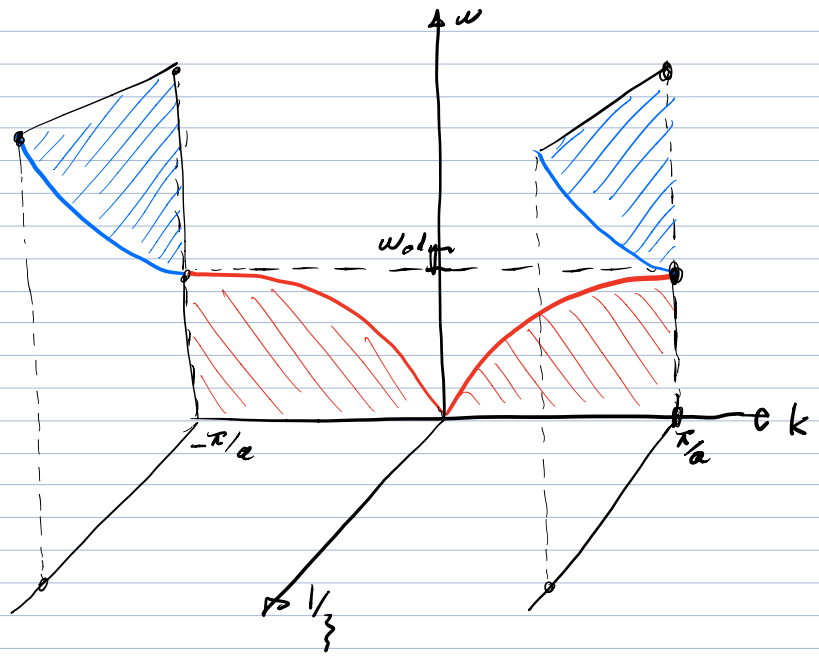
$\Rightarrow$ This is a solution only for

$$\omega > \omega_{edge} = \sqrt{\frac{4f}{m}}$$

We found that for $\omega > \omega_{edge}$, vibrations penetrate into the mono-atomic chain with a decay length $\xi$ given by

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

We can summarize these findings in the following plot



## 3.2 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 in 3.1 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

$$u_n^k(t) = e^{ik(n-m)} u_m^k(t). \tag{2}$$

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 such a simple relation as (2) should hold.

However, every second mass is identical! Therefore, let us assume the following structure for the eigenmodes

$$u_n^k(t) = \begin{cases} e^{ikn-i\omega t} a_k & n = 2s, \; s \in \mathbb{Z}, \\ e^{ikn-i\omega t} b_k & n = 2s+1, \; s \in \mathbb{Z}. \end{cases} \tag{3}$$

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

$$e^{ik\,2a},$$

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

$$e^{ik\,2a} = e^{i(k+\pi r)2a} \qquad \text{with } r \in \mathbb{Z}$$

$\Rightarrow$ By doubling ($a \to 2a$) our unit-cell size we halve to size of the Brillouine zone.

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

The equations of motion read

$$m_1 \ddot{u}_{2n} = f(u_{2n+1} + u_{2n-1} - 2u_{2n})$$
$$m_2 \ddot{u}_{2n+1} = f(u_{2n} + u_{2n+2} - 2u_{2n+1})$$

Inserting ansatz (3) into the above equation we find

$$-m_1\omega^2 a_k = f(b_k + e^{-2iak} b_k - 2a_k),$$

$$-m_2\omega^2 b_k = f\left(a_k + e^{2iak}a_k - 2b_k\right).$$

We deal with a problem of the form

$$\omega^2 \underbrace{\begin{pmatrix} m_1 & \\ & m_2 \end{pmatrix}}_{B} \underbrace{\begin{pmatrix} a_k \\ b_k \end{pmatrix}}_{x} = \underbrace{\begin{pmatrix} 2f & -f(1+e^{-2iak}) \\ -f(1+e^{-2iak}) & 2f \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} a_k \\ b_k \end{pmatrix}}_{x}, \qquad \varphi = 2ka$$

$$\alpha \quad B \quad x = \quad A \quad x$$

This is a generalized eigenvalue problem $\alpha B x = Ax$ with $B$ positive definit and both $A = A^+$ and $B = B^+$. We could do

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

but we would not deal with a hermitian problem anymore. Let us write $B = LL^+$ with $L = \begin{pmatrix} \sqrt{m_1} & \\ & \sqrt{m_2} \end{pmatrix}$

Then we write

$$\alpha LL^+ x = A(L^+)^{-1}L^+ x$$

$$\alpha \underbrace{L^+ x}_{y} = L^{-1}A(L^+)^{-1}\underbrace{L^+ x}_{y}$$

$$\alpha y = \tilde{A} y$$

with $\tilde{A}^+ = (L^+)^{-1+}A^+(L^{-1})^+ = L^{-1}A(L^+)^{-1} = \tilde{A}$.

For our problem we find

$$\tilde{A} = \begin{pmatrix} \frac{1}{\sqrt{m_1}} & \\ & \frac{1}{\sqrt{m_2}} \end{pmatrix} \begin{pmatrix} 2f & -f(1+e^{-i\varphi}) \\ -f(1+e^{i\varphi}) & 2f \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{m_1}} & \\ & \frac{1}{\sqrt{m_2}} \end{pmatrix} =$$

$$= \begin{pmatrix} \frac{2f}{m_1} & -\frac{f}{\sqrt{m_1 m_2}}(1+e^{-i\varphi}) \\ -\frac{f}{\sqrt{m_1 m_2}}(1+e^{i\varphi}) & \frac{2f}{m_2} \end{pmatrix} \qquad m = \sqrt{m_1 m_2}$$

$$= f\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\mathbb{1} - \underbrace{\frac{f}{m}(1+\cos\varphi)}_{d_1}\sigma_x \underbrace{- \frac{f}{m}\sin\varphi}_{d_2}\sigma_y$$

$$\underbrace{+ f\left(\frac{1}{m_1} - \frac{1}{m_2}\right)}_{d_3}\sigma_z$$

$$= f\left(\frac{1}{m_1} + \frac{1}{m_2}\right)\mathbb{1} + \sum_{i=1}^{3} d_i(k)\sigma_i$$

$$\Rightarrow \quad \omega^2(k) = f\left(\frac{1}{m_1} + \frac{1}{m_2}\right) \pm \frac{f}{m}\sqrt{\left(\frac{m}{m_1} - \frac{m}{m_2}\right)^2 + (1+\cos\varphi)^2 + \sin^2\varphi}$$

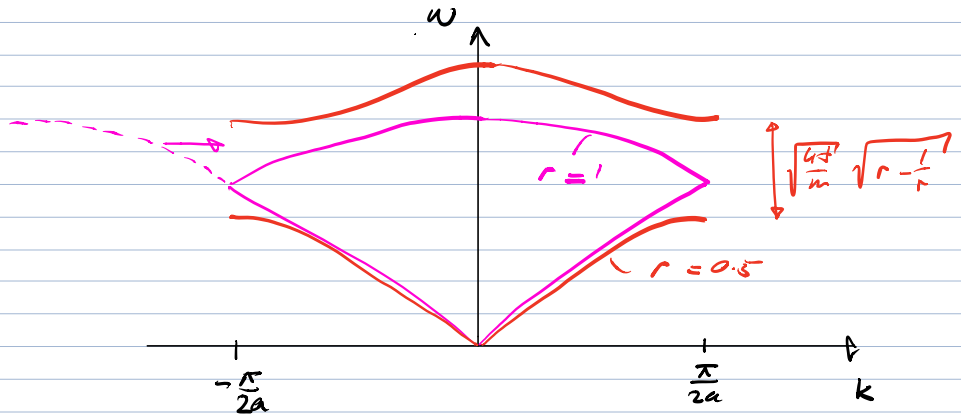
$$= \frac{f}{m}\left(\sqrt{\frac{m_2}{m_1}} + \sqrt{\frac{m_1}{m_2}}\right) \pm \frac{f}{m}\sqrt{\left(\sqrt{\frac{m_2}{m_1}} - \sqrt{\frac{m_1}{m_2}}\right)^2 + 2 + 2\cos(2ka)}$$

With this we arrive at the dispersion

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

$m = \sqrt{m_1 m_2} \qquad r = \sqrt{\frac{m_2}{m_1}}$

Let us inspect how this dispersion behavare for various values of the mass ratio $r$.

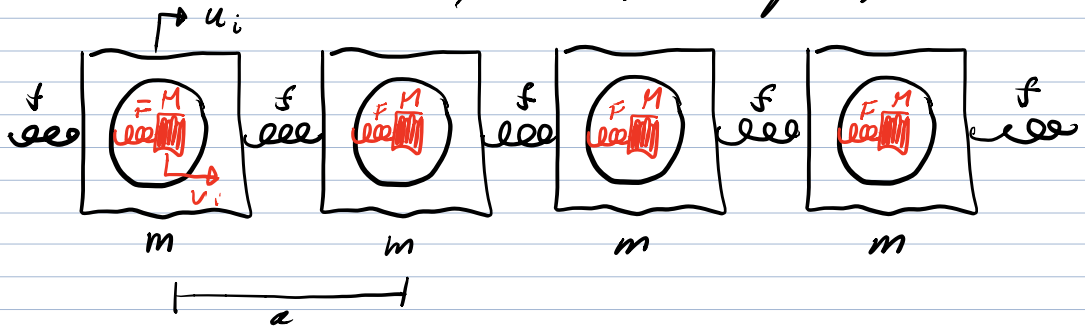



We see that we opened a band gap for $k = \frac{\pi}{2a}$ with magnitude $\sqrt{\frac{4\beta}{m}}\sqrt{r-\frac{1}{r}}$ which goes to zero for $r = 1$. In fact, for $r = 1$, we chose an unit cell which is too large, or equivalently, a too small Brillouine zone. We see in the figure above, that this leads to a "folding" of the spectrum.

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

## 3.3 Locally resonant structures

We want to study the following system




The block system $(m, f)$ alone defines a regular monoatomic chain with no band gap. We want to understand the effect of the added local resonators

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

$$\Rightarrow -\underbrace{\begin{pmatrix} m & \\ & M \end{pmatrix}}_{B} \omega^2 \begin{pmatrix} u_k \\ w_k \end{pmatrix} = \underbrace{\begin{pmatrix} -(2f+F)+2f\cos ak & F \\ F & -F \end{pmatrix}}_{A} \begin{pmatrix} u_k \\ v_k \end{pmatrix}$$

Where we assumed $u_i = u_k e^{iak - i\omega t}$

$$v_i = v_k e^{iak - i\omega t}$$

we again transform $A \to \tilde{A}$ with $L L^t = B$

$$\tilde{A} = L^{-1} A L^{t\,-1} =$$

$$= \begin{pmatrix} \frac{(2f+F) - 2f\cos k}{m} & -\frac{1}{\sqrt{mM}} F \\ -\frac{1}{\sqrt{mM}} & +\frac{F}{M} \end{pmatrix}$$

$$= \frac{4f}{m} \begin{pmatrix} \frac{1}{2}(1-\cos k) + \frac{F}{4f} & -\sqrt{\frac{m}{M}}\frac{F}{4f} \\ -\sqrt{\frac{m}{M}}\frac{F}{4f} & +\frac{1}{4}\frac{m}{M}\frac{F}{f} \end{pmatrix}$$

$$= \omega_0^2 \begin{pmatrix} \frac{1}{2}(1-\cos k) + \mu^2 \tilde{\omega}_L^2 & -\mu\tilde{\omega}_L^2 \\ -\mu\tilde{\omega}_L^2 & \tilde{\omega}_L^2 \end{pmatrix}$$

$$\tilde{\omega}_L = \frac{1}{2}\sqrt{\frac{m}{f}\frac{F}{M}} \; ; \quad \mu = \sqrt{\frac{M}{m}} \; ; \quad \omega_0 = \sqrt{\frac{4f}{m}}$$

$\tilde{\omega}_L$: local resonance frequency in units of $\omega_0$

$\mu$: "coupling strength"

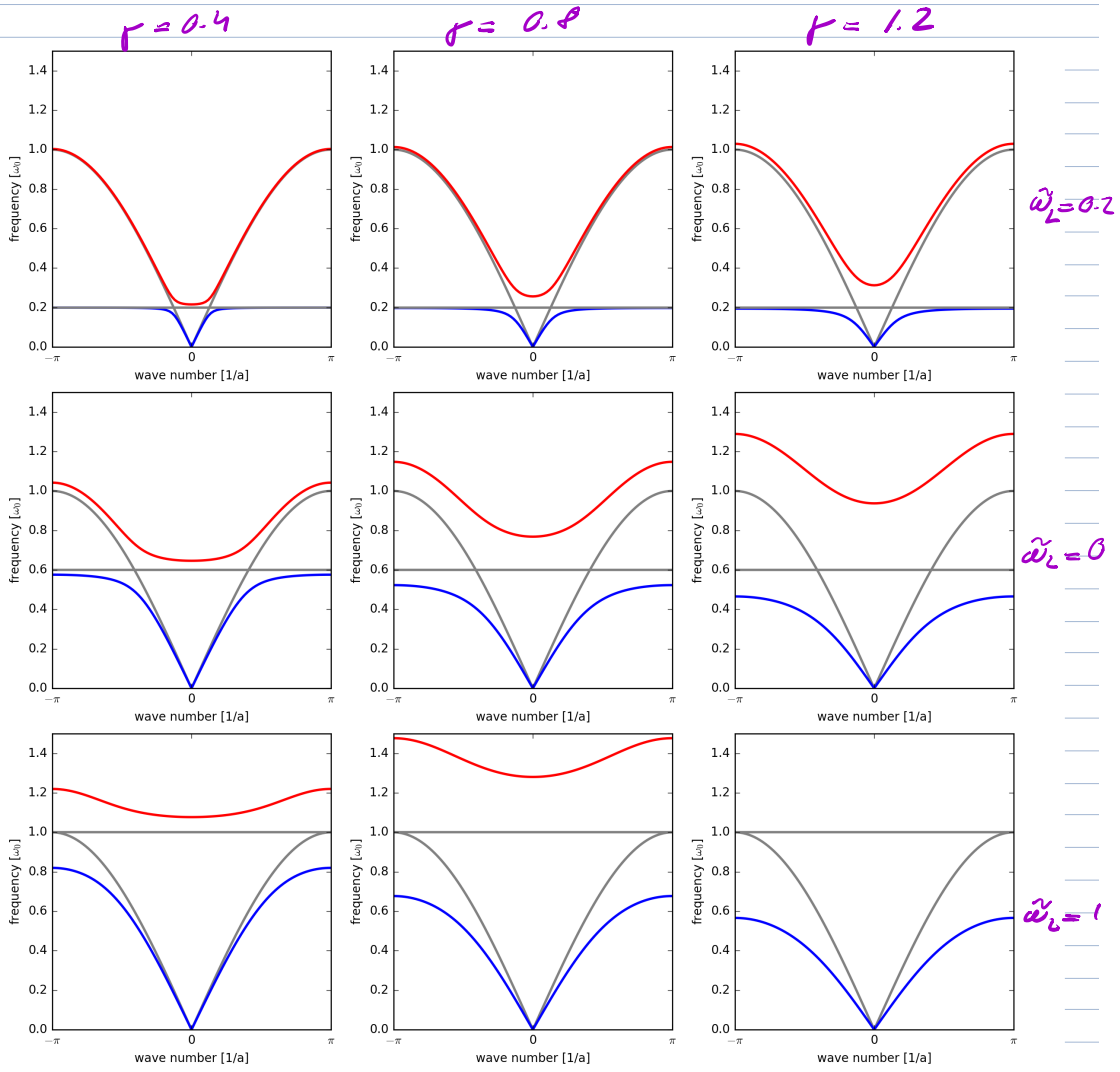
$\omega_0$: overall frequency scale

$$\Rightarrow \frac{1}{\omega_0^2}\tilde{A} = \frac{1}{2}\left\{\frac{1}{2}\left[1-\cos(k)\right] + \tilde{\omega}_L^2(\mu^2+1)\right\} \mathbb{1} + \sum_i d_i(k)\sigma_i$$

with $\vec{d} = \left(-\gamma\tilde{\omega}_L^2,\ 0,\ \frac{1}{2}\left\{\frac{1}{2}\left[1-\cos(k)\right] + \tilde{\omega}_L^2(\gamma^2-1)\right\}\right)$

from wich we immediately read off the dispersion relation:

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



From the above figure we see that for the case of local resonances a band gap is opening to at a specific $\underline{k}$ but at a given $\underline{\omega}$, namely $\omega \approx \omega_L$. Moreover, the stronger the resonance is coupled

$$\gamma = \sqrt{\frac{M}{m}},$$

the bigger the band gap.