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PHONONIC LATTICES AND TIME-VARYING PARAMETERS

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ABSTRACT

The propagation of linear and nonlinear waves (phonons) in finite 1-D lattices with different interaction potentials is numerically studied. These potentials are elastic linear potentials (the classical mass-spring system), and Coulomb-type potentials (nonlinear magnetic coupling). To excite the waves in the lattice, harmonic driving at the boundary is considered. We show the presence of different modes as higher harmonics and sub-harmonics, induced by the non-linearity of the system. The study is also focused on the influence of the time dependence of lattice parameters (mass and coupling strength) in the mode excitation. This analysis of time varying lattices is performed for a simple mass-spring system, and reveals novel features of wave phenomena characteristic of discrete systems.

Key words **—** Metamaterials, dispersion relation, 1-D lattice, phononic crystal, waves propagation

1. INTRODUCTION

In order to understand the behavior of periodic materials & structures, we can at first approximate the system to a 1-D lattice, and then expand to 2-D & 3-D. This paper will only deal with 1-D lattice. We are using two different models to model the lattice: the first one is the classical mass-spring system, in which the interaction potentials are linear; and the second one is a magnets chain, where the interaction potentials are non-linear (Coulomb-type). All the simulations with these models are made using a FDTD method. Mono- and diatomic cases are considered for each model. Finally, time-varying parameters on a simple mass-spring system are studied. These results can then be expanded to a more complex in the future.

2. MASS-SPRING CHAIN

The first model we will study is the classical mass-spring chain. Two cases are considered for this: monoatomic, and diatomic chain. A monoatomic chain is a chain where each element has the same parameters. In our case, all the masses are the same and all the springs have the same stiffness. The diatomic chain is a chain with two different values for the masses, stiffness of the springs, and length of the springs. The studied chain is shown in Figure 1.

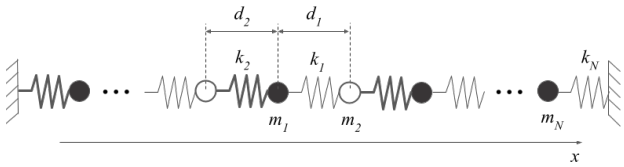

Figure 1. Layout of the studied mass-spring system.

In this figure, d_1 and d_2 are the inter-atomic distances between the atoms being at their equilibrium position x_{0n} (thus the length of the springs at rest). N is the number of atoms in the chain, m_1 *and* m_2 are the masses of the atoms, k_1 and k_2 are the stiffnesses of the springs. We define the relative position of the n-th atom with respect to its equilibrium position as $u_n = x_n - x_{0n}$.

2.1. Dispersion relation

To obtain the dispersion relation of the diatomic chain, we need at first to get the motion equation of both possible situations for an atom in this chain: either with mass m_1 and the spring with k_1 and d_1 parameters on its right, and the other spring on its left, or with mass m_2 and the inverted

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order for the springs. Assuming the first situation happens for the n-th atom, the motion equations are expressed as such:

$$-m_1\ddot{u}_n = k_2 u_{n-1} + (-k_1 - k_2)u_n + k_1 u_{n+1} \quad (2)$$

$$-m_2\ddot{u}_{n+1} = k_1 u_n + (-k_1 - k_2)u_{n+1} + k_2 u_{n+2} \quad (3)$$

We can then assume the general solution for u_n:

$$u_n = A_1 \cdot \exp\left(i\left(\frac{n+1}{2}d_1 + \frac{n-1}{2}d_2\right)k_w - \omega t\right) \quad (4)$$

$$u_{n+1} = A_2 \cdot \exp\left(i\frac{n+1}{2}(d_1 + d_2)k_w - \omega t\right) \quad (5)$$

With A_1 and A_2 two amplitudes, i the imaginary unit and ω the frequency of the wave inside the chain. Then, by respectively implementing eqs. (4) and (5) in eqs. (2) and (3) we obtain the following system:

$$\begin{cases} A_1\left(-m_1\omega^2 + k_1 + k_2\right) + A_2\left(-k_2 e^{-id_1 k_w} - k_1 e^{id_2 k_w}\right) = 0 \\ A_1\left(-k_1 e^{-id_2 k_w} - k_2 e^{id_1 k_w}\right) + A_2\left(-m_2\omega^2 + k_1 + k_2\right) = 0 \end{cases} \quad (6)$$

Then we express this system in a matrix form as such:

$$\begin{bmatrix} -m_1\omega^2 + k_1 + k_2 & -k_2 e^{-id_1 k_w} - k_1 e^{id_2 k_w} \\ -k_1 e^{-id_2 k_w} - k_2 e^{id_1 k_w} & -m_2\omega^2 + k_1 + k_2 \end{bmatrix} \cdot \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = 0 \quad (7)$$

This implies that the determinant of the first matrix is null. We can obtain ω by solving the equation for the determinant, and we finally get:

$$\omega^2 = \frac{k_1 + k_2}{2M} \pm \sqrt{\left(\frac{k_1 + k_2}{2M}\right)^2 - 2k_1 k_2 (1 - \cos((d_1 + d_2))k_w)}, \quad M = \left(\frac{1}{m_1} + \frac{1}{m_2}\right)^{-1} \quad (8)$$

This implies the existence of two solutions for ω, and hence the existence of two different branches for the dispersion relation as we can see of Figure 2. These two branches correspond to two different vibration behaviors: in the acoustical branch (in red on the graph), consecutive atoms in the chain move more less in phase; in the optical branch (in blue on the graph), they move more or less out of phase.

We can also see that the two branches are separated by a band gap. The width of this band gap can easily be determined by subtracting the maximum of the acoustical branch to the minimum of the optical branch, which gives:

$$\Delta\omega = \sqrt{\left(\frac{k_1 + k_2}{M} - 4\sqrt{\frac{k_1 k_2}{m_1 m_2}}\right)} \quad (9)$$

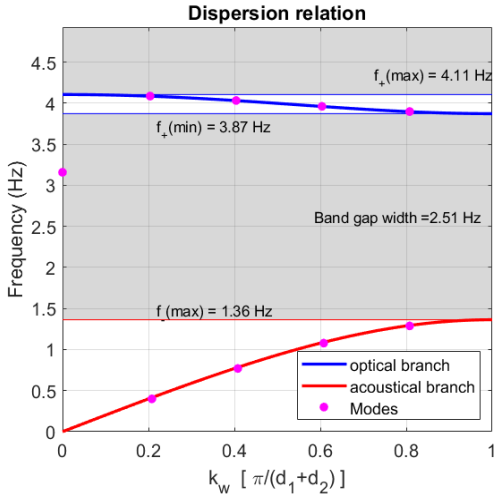

Figure 2. Dispersion relation for a chain with N=9, m_1 = 0.1, m_2 = 0.145, k_1 = 3,86, k_2 = 29,8, d_1 = 0.28, d_2 = 0.325.

On Figure 2, we can observe the presence of a mode in the band gap. During the solving of the eigenproblem, the eigenfrequency for this mode was determined. But since it's located in the band gap, it manifests itself as an evanescent resonance. Thus, it happens only when the chain is externally stimulated, around the excitation point.

2.2. Motion study

We are now exciting the chain with a sinusoidal force on the first atom. Results are obtained via an FDTD method. The FDTD scheme used is the following:

$$u_n(t) = 2u_n(t - \Delta t) - u_n(t - 2\Delta t) + \frac{\Delta t^2}{m_n}F_D(t - \Delta t) - \frac{\Delta t^2}{m_n}k_{n-1}(u_n(t - \Delta t) - u_{n-1}(t - \Delta t)) - \frac{\Delta t^2}{m_n}k_n(u_n(t - \Delta t) + u_{n+1}(t - \Delta t)) \quad (10)$$

With the driving force $F_D = A_D \sin(\omega t)$, A_D the amplitude of the force, m_n the mass of the n-th atom, k_n the stiffness of the n-th spring, and Δt the time step for the method. Figure 3 shows the power spectral density (PSD) for the motion of each atom in the chain, with the same parameters as for Figure 1. At first, the chain is stimulated at the eigenfrequency located in the band gap. For all the atoms,

we see all the propagative modes being stimulated, and the evanescent one previously discussed is only visible around the excitation point. This allows us to see the modal distribution of the chain. The two branches are easily noticeable, as well as the band gap. Then we excite the chain at half the frequency of mode 4 to see if there is any kind of harmonics generation due to some nonlinear behavior that can stimulate this mode. We then see that some other modes are stimulated, but only because the system is discrete, implying that waves can only propagate at modal frequencies. The aimed mode (*i.e.* mode 4) isn't stimulated, we can then assume that the system doesn't generate harmonics, hence behaves mainly linearly.

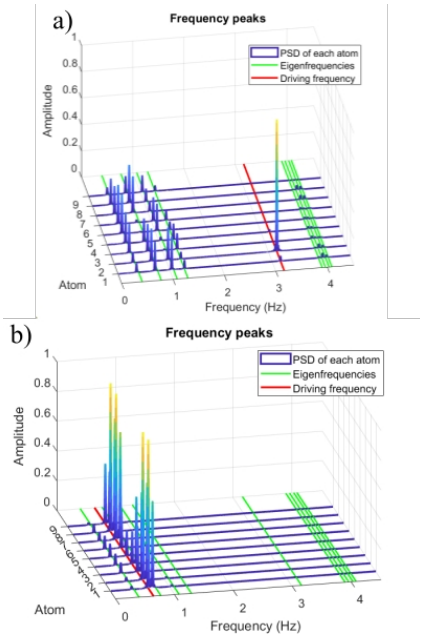

Figure 3. Normalized PSDs of the atoms with excitation on the first atom. a) with the driving frequency at the evanescent resonance. b) with the driving frequency at half of the mode 4.

3. MONOATOMIC MAGNETS CHAIN

The springs are now replaced by repulsive magnetic potentials. By doing as such, we make the interatomic potentials non-linear. This implies some changes in the behavior of the chain, as well as its layout, as shown in Figure 4. All magnets have the same mass m and are separated from a distance d at rest state. The α parameter can change depending on the particular system. For instance, α = 2 for electrically charged particles, or α = 4 for distant magnetic dipoles. β is the strength of the magnets.

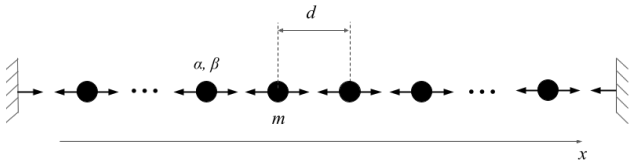

Figure 4. Monoatomic magnets lattice layout.

3.1. Dispersion relation

A good model to describe this system is provided and described in Ref. [1]. For such a system, the dispersion relation is expressed as such :

$$\omega = \omega_m \cdot \sqrt{\sin^2\left(\frac{k_w}{2}\right)}, \qquad \omega_m = \sqrt{\frac{4\alpha\beta}{m d^{\alpha+1}}} \tag{11}$$

Where ω_m is the maximum frequency for propagative waves in the lattice, and k_w is again the wavenumber for the wave propagating in the chain. The chain being monoatomic, the dispersion relation only has one branch, and is pretty similar to the monoatomic mass-spring one [2]. Figure 5. shows the dispersion relation for this chain, restricted to the half period for the same reasons as for the mass-spring chain.

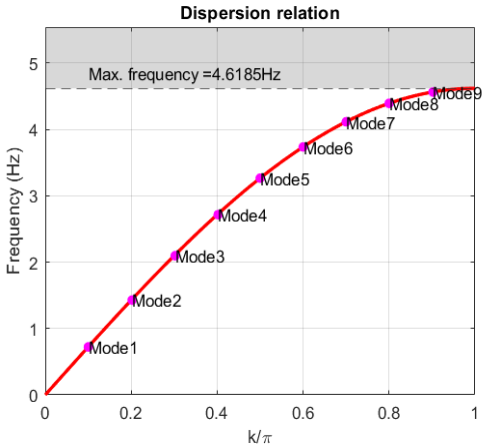

Figure 5. Dispersion relation for a magnets chain with $N = 9$, $\alpha = 4$, $\beta = 5$, $d = 1$.

3.2. Motion study

We now excite the chain in the same way as before. The FDTD scheme used for the calculations is expressed as such:

$$u_n(t)=2u_n(t-\Delta t)-u_n(t-2\Delta t)+\frac{\Delta t^2}{m}\cdot(\gamma+F_D(t-\Delta t)),$$
$$\gamma=\beta\cdot\left(\frac{1}{d-u_{n+1}(t-\Delta t)+u_n(t-\Delta t)^\alpha}-\frac{1}{d-u_n(t-\Delta t)+u_{n-1}(t-\Delta t)^\alpha}\right) \quad (12)$$

The γ term induces the non-linearities of the system, that we will observe with Figure 6., which shows the normalized PSDs of the motion of the atoms in different situations: lower or higher amplitude of excitation, and two different driving frequencies. The main phenomenon to observe here is that with a higher amplitude of excitation, the system generates more harmonics, as visible comparing Figures 6.a and 6.c. There is also a strong generation of harmonics when the driving frequency is half of an eigenfrequency, even visible at lower amplitudes of excitation.

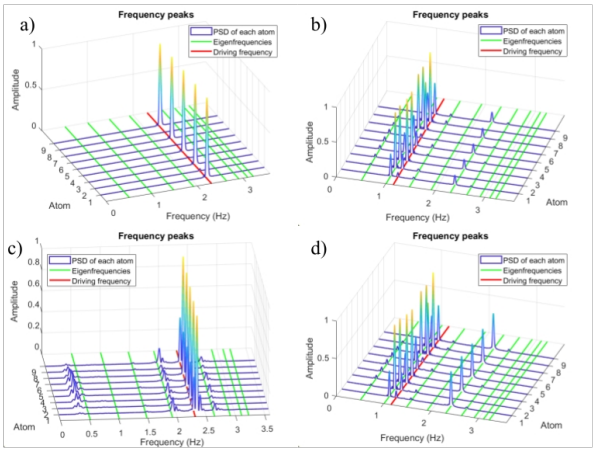

Figure 6. Normalized PSDs of the atoms with excitation at the first atom. a) low amplitude, driving frequency equal to the 5th eigenfrequency. b) low amplitude, driving frequency equal to half of the 5th eigenfrequency. c) high amplitude, driving frequency equal to the 5th eigenfrequency. d) high amplitude, driving frequency equal to half of the 5th eigenfrequency.

4. TIME-VARYING PARAMETERS

We finally study the behavior of a simple mass-spring system with time-varying mass and stiffness. The goal of this chapter is to get a first understanding of the behavior of a lattice with time-varying parameters, that could be then expanded to a full lattice (linear or non-linear). The studied system is described in Figure 7.

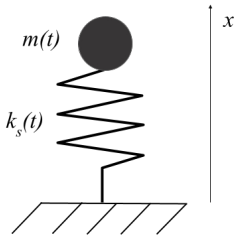

Figure 7. Mass-spring system with time-varying mass and stiffness.

The mass and stiffness are expressed as such :

$$m(t)=m_0+A_m\sin(2\pi f_m t) \quad (13)$$
$$k(t)=k_0+A_k\sin(2\pi f_k t) \quad (14)$$

With m_0 and k_0 the static parts, A_m and A_k the modulation amplitudes, and f_m and f_k the modulation frequencies, all respectively of the mass and the stiffness. The following equation shows the FDTD scheme used for the simulations of this system:

$$u(t)=2u(t-\Delta t)-u(t-2\Delta t) - \frac{\Delta t^2}{m(t-\Delta t)}[k(t-\Delta t)u(t-2\Delta t)-F_D(t-2\Delta t)] \quad (15)$$

With $u(t)$ the relative displacement of the mass along the x-axis with respect to its equilibrium position, and F_D the driving frequency. Figure 8 shows the PSDs of the system with and without modulations of the mass and stiffness.

The most visible phenomenon is that the higher the amplitude, the higher the number of harmonics there will be. The harmonics are centered both around the driving frequency, and the resonance frequency, and are regularly scattered, separated by the difference between these frequencies and the modulation frequency. There is also a shift of the resonant frequency for both modulations when the amplitude is higher, and the scattering of the harmonics follows this shift too. The harmonics generation for the stiffness modulation tends to be focused around the resonant frequency and less near the driving frequency, whereas the mass modulation generates harmonics around both frequencies. Another interesting phenomenon is that since the mass and stiffness are varying, the eigenfrequency is also varying in time, creating a resonance "range", as show the gray regions on Figure 8. In this range, the harmonics don't decrease as much as outside of it.

This system does possess some non-linear properties that we can find as well in the magnets chain, in a more predictable way (evenly scattered harmonics, centered about the driving and resonant frequencies,...).

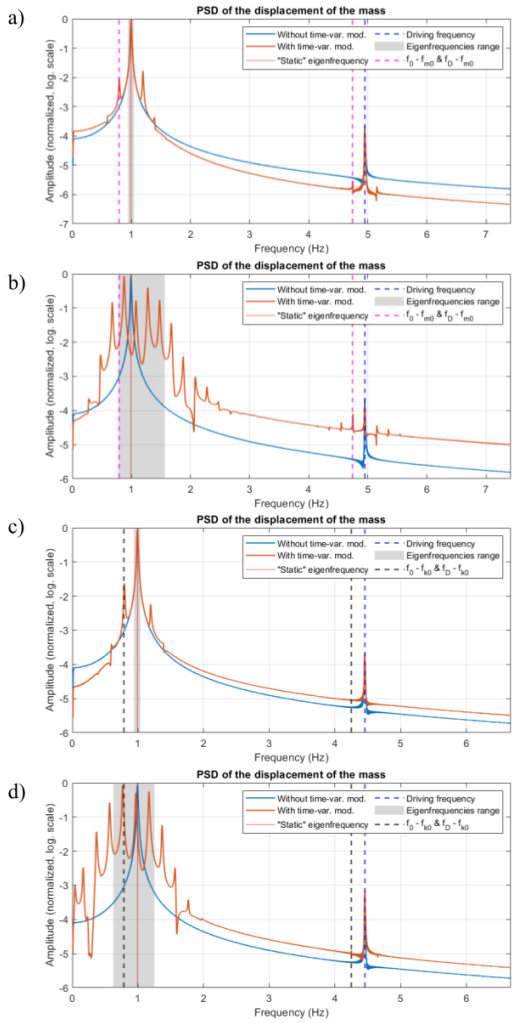

Figure 8. PSD of the motion of the atom with $m_0 = 0.1$ and $k_0 = 3.86$. a) low amplitude of modulation, mass modulation. b) high amplitude, mass modulation. c) low amplitude, stiffness modulation. d) high amplitude, stiffness modulation.

5. CONCLUSION

Two different types of 1-D discrete lattices have been studied, with different interaction potentials that imply different types of behavior. Some non-linear phenomena have been enlightened, mostly due to the excitation amplitude on the chain. Then a first glance at time-varying parameters structures has been made, by studying the motion of a simple mass-spring system with varying mass and stiffness with respect to time. Time-varying structures are complex and still to be studied. Although the results obtained in this paper are only numerical, they can already give the idea of some features and behaviors of potential real systems. Results from chapter 4 could be then extrapolated to more complex lattices, such as the two lattices studied in this paper. Making a real system with time-varying masses seems to be quite complex, but modulating other parameters, such as the interactions between the elements of the chain, has already been made and shows interesting results [3].

12. REFERENCES

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