Wave propagation in mechanical metamaterials

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Chapter 5

Defects in twisted kagome lattices: gap modes

In the previous chapter, we have studied the perfect twisted kagome lattices. In this chapter, we study the effect of defects on lattice vibrations in the framework of lattice dynamics [79, 82, 83]. As in chapter 3, we model a defect by changing the stiffness constant of one spring (Fig. 5.1).

As we shall see, such defects can induce localized and spectrally isolated modes inside the bulk band gap. We investigate such gap modes in detail for varying twisting angles. Remarkably, when several defects are present, the resulting vibrational modes can be understood in terms of the hybridization of single-defect modes. We investigate this situation through an effective tight-binding theory.

5.1 A single defect: localized gap modes

In this section we study a lattice where the stiffness of a single spring is changed from the uniform value k_0 to k. Due to the lattice symmetry, all springs in a perfect kagome lattice are equivalent, so we can modify any of them and get the same system. When a spring is removed, i.e. when $k/k_0 = 0$, the phonon spectrum is modified, going from Fig. 4.7 to Fig. 5.2.

When the twisting angle θ is low and the phonon spectrum is not gapped,

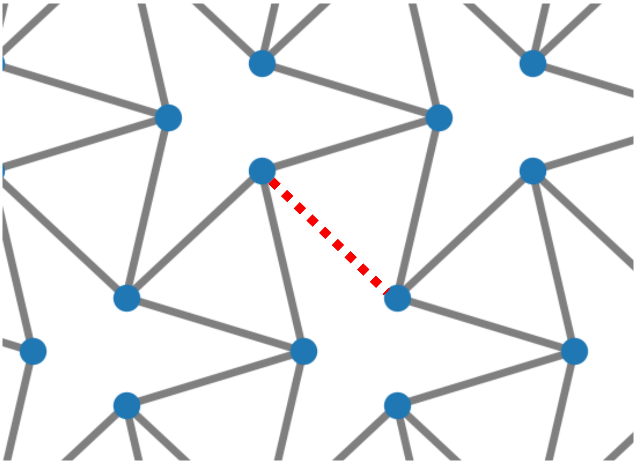


Figure 5.1. The twisted kagome lattice that has a defect of a single spring (dashed red line) whose stiffness constant k_0 is changed from the uniform value k of all other springs (solid gray lines).

there is no visible change. However, when the gap opens, for a twisting angle $\theta > 22°$, then we see that a vibrational mode appears inside the bulk band gap. Notably, this gap mode, due to the existence of the defect, is exponentially localized around the defect (see Fig. 5.3), i.e. $\phi(r) \sim e^{-r/\xi}$ where ϕ is the vibrational amplitude, r is the distance from the defect and ξ is a decay length.

The frequency of the defect mode slightly depends on the twisting angle and reaches its maximum at the critical twisting angle[1] $\theta = 45°$ (see Fig. 5.4). Interestingly, the maximum frequency $\omega/\omega_0 = 1$ is the frequency for a simple harmonic oscillator with the same spring and mass as those of the perfect kagome lattice. The underlying reason for this has yet to be understood.

The same effect can be observed when the defect spring stiffness $k/k_0 < 1$ is finite, see Fig. 5.5. When $k/k_0 > 1$, the defect mode leaves the optical band from its top. See the treatise by Maradudin [79] for the explanation of this behavior.

[1] See 4.5 for a discussion on the critical twisting angle.

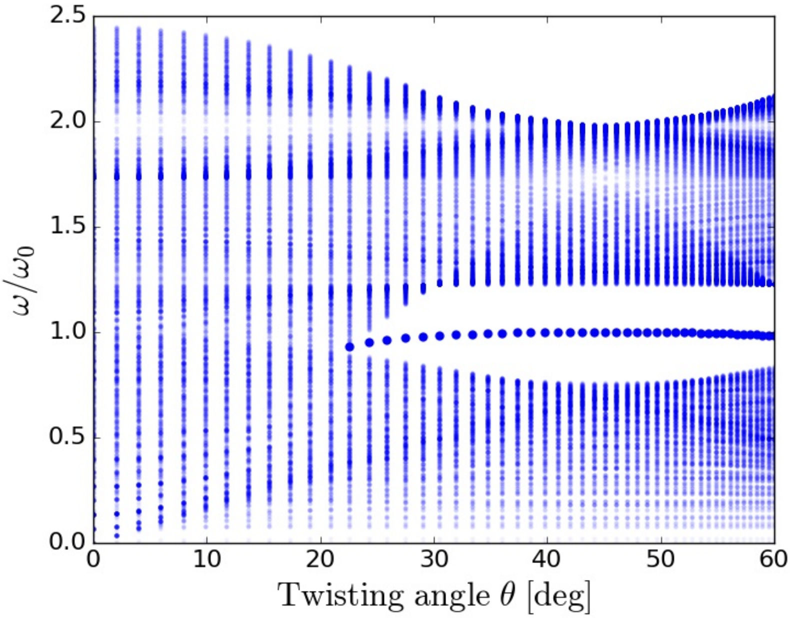
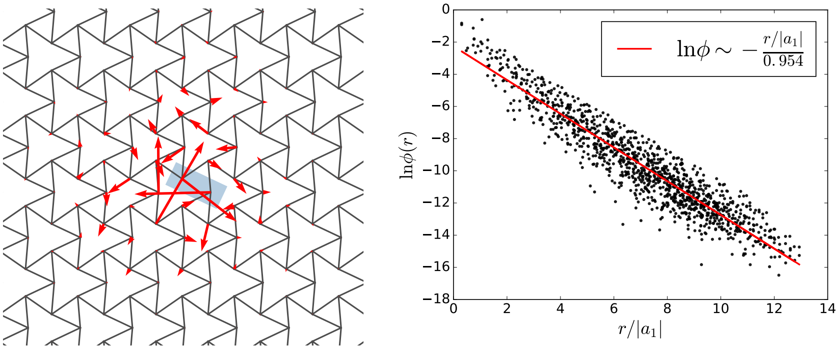


Figure 5.2. The phonon spectrum of the kagome lattice with varied twisting angle. The opacity of the data points indicates the density of states at each frequency bin. A band gap opens up at around $\theta = 22°$. The defect mode in the gap is emphasized via big solid dots. The system has 20×20 unit cells with periodic boundary conditions.

5.2 A pair of defects: the tight-binding theory

We have studied the system with a single defect. We can also consider multiple defects, and the most simple case is a pair of defects. When the two defects are far away from each other, the corresponding defect modes can be considered as single isolated defect modes, with the same frequency and mode pattern. This is because the defect modes are exponentially localized. When the defects are brought closer and closer, they hybridize, and the frequencies and mode patterns of the defect modes change. Crucially, we can understand this change through an effective tight-binding theory[2].

[2]While several combinations of pairs of defects are possible, corresponding to different removed springs in the unit cell, all of them have the same qualitative properties, and we focus



(a) **(b)**

Figure 5.3. The defect mode is localized. (**a**) The kagome lattice with one removed spring indicated in the shaded blue region. The defect mode is depicted by arrows representing the mode displacement of the masses. (**b**) The amplitude of the mode displacement decays exponentially with the normalized distance $r/|a_1|$ from the defect, where a_1 is a lattice vector in Eq. 4.2. Here we find the decay length $\xi/|a_1| = 0.954$. The twisting angle is $\theta = 34.7°$, and the system has 20×20 unit cells with periodic boundary conditions.

When only one defect is present, there is a single-defect mode ϕ with frequency ω_s. Let us now consider a lattice with two defects located respectively at the x_1th and the x_2th unit cell along the same horizontal line and separated by a distance $d = |x_1 - x_2|$ (see Fig. 5.6).

The dynamical matrix of the lattice $\boldsymbol{D}$ has two gap modes, which we denote as ψ_+ and ψ_-. By definition, we have

$$\boldsymbol{D}\psi_\pm = \omega_\pm^2 \psi_\pm, \tag{5.1}$$

where $\omega_\pm^2$ is the square of the gap-mode frequencies. ϕ's and ψ's are assumed to be normalized.

Following the principle of tight-binding models[3], we try to express ψ as a linear combination of the two single-defect modes ϕ_1 and ϕ_2, where $\phi_{1(2)}$

on only one of them.

[3]It is also known as the Hückel model or Linear Combination of Atomic Orbitals (LCAO) approximation in the context of quantum chemistry.

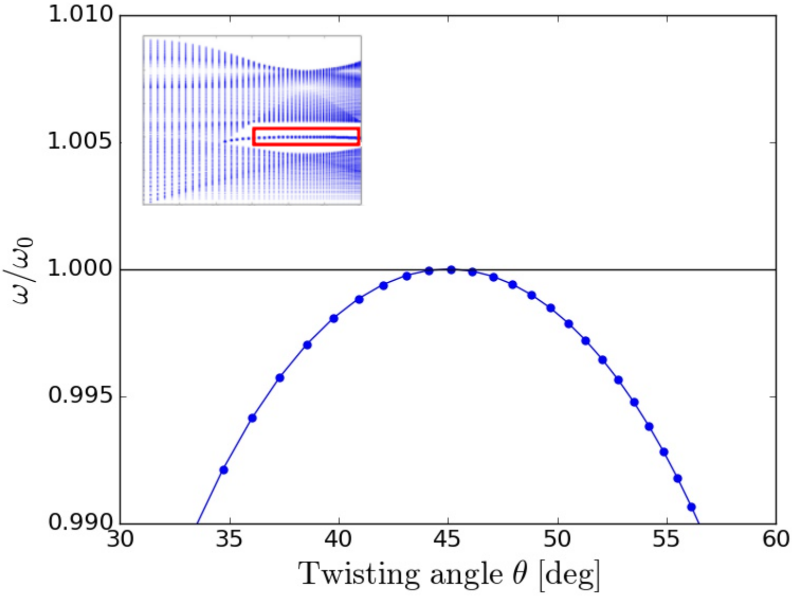


Figure 5.4. Zoom of Fig. 5.2. The gap mode that has its maximum frequency of $\omega/\omega_0 = 1$ at $\theta = 45°$.

corresponds to the single defect located at $x_{1(2)}$ (See Fig. 5.7). To do so, let us write

$$\psi_{\text{TB}} = c_1\phi_1 + c_2\phi_2, \tag{5.2}$$

where c_1 and c_2 are scalar constants. Multiplying both sides of Eq. 5.1 by ϕ_1 and ϕ_2 respectively, we get

$$c_1\langle\phi_1, \boldsymbol{D}\phi_1\rangle + c_2\langle\phi_1, \boldsymbol{D}\phi_2\rangle = \omega_{\text{TB}}^2(c_1\langle\phi_1,\phi_1\rangle + c_2\langle\phi_1,\phi_2\rangle) \tag{5.3}$$
$$c_1\langle\phi_2, \boldsymbol{D}\phi_1\rangle + c_2\langle\phi_2, \boldsymbol{D}\phi_2\rangle = \omega_{\text{TB}}^2(c_1\langle\phi_2,\phi_1\rangle + c_2\langle\phi_2,\phi_2\rangle) \tag{5.4}$$

or in the matrix form:

$$\begin{pmatrix}\alpha & \beta\\ \beta & \alpha\end{pmatrix}\begin{pmatrix}c_1\\ c_2\end{pmatrix} = \omega_{\text{TB}}^2\begin{pmatrix}1 & S\\ S & 1\end{pmatrix}\begin{pmatrix}c_1\\ c_2\end{pmatrix} \tag{5.5}$$

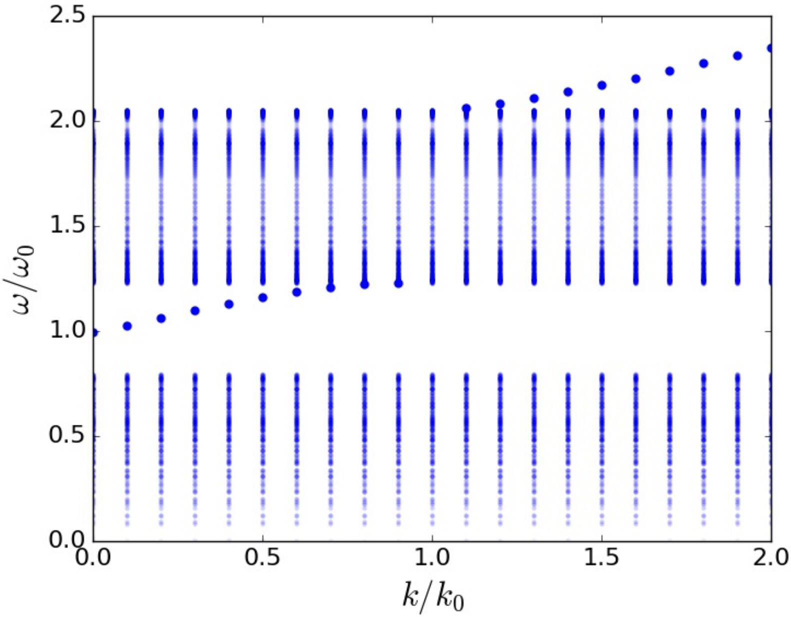


Figure 5.5. The spectrum with varying spring stiffness k. k_0 is the stiffness of the spring stiffness in perfect lattices. The system parameters are the same as Fig. 5.3.

where we defined $\alpha = \langle \phi_1, \boldsymbol{D}\phi_1 \rangle = \langle \phi_2, \boldsymbol{D}\phi_2 \rangle$, $\beta = \langle \phi_1, \boldsymbol{D}\phi_2 \rangle = \langle \phi_2, \boldsymbol{D}\phi_1 \rangle$ as $\boldsymbol{D}$ is hermitian, and the overlap integral $S = \langle \phi_2, \phi_1 \rangle$. The solution to the above eigenvalue problem is:

$$\omega_{+\mathrm{TB}}^2 = \frac{\alpha + \beta}{1 + S}, \quad \omega_{-\mathrm{TB}}^2 = \frac{\alpha - \beta}{1 - S}. \tag{5.6}$$

When the defects are far away from each other, i.e. $d \gg \xi$, both the overlap integral S and the matrix element β vanish as ϕ_1 and ϕ_2 are localized. In this case,

$$\omega_{+\mathrm{TB}}^2 = \omega_{-\mathrm{TB}}^2 = \alpha = \omega_s^2, \tag{5.7}$$

that is to say, the frequencies of both gap modes equal the single-defect gap mode frequency.

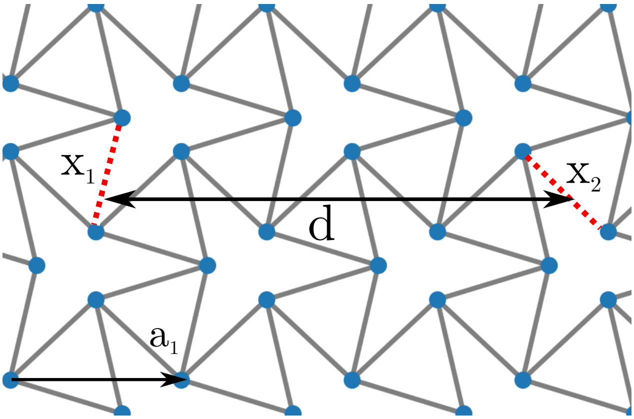


Figure 5.6. The twisted kagome lattice that has two defects located respectively at the x_1 and x_2 along the same horizontal line and separated by a distance $d = |x_1 - x_2|$. a_1 is a lattice vector.

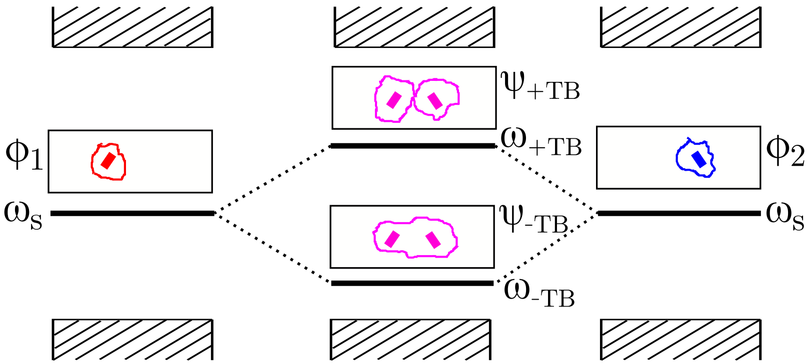


Figure 5.7. The scheme of tight-binding models for gap modes.

In Fig. 5.8, we compare this result with the values directly obtained from the diagonalization of $\boldsymbol{D}$. We see that the tight-binding theory predicts the hybridization frequency level quite well, even though it only keeps track of only two degrees of freedom ϕ_1 and ϕ_2. The reason why the theory works so well is because the defect modes lie in the band gap and therefore are spectrally isolated from the other vibrational modes. Notice there is a small discrepancy between the tight-binding prediction and the direct diagonalization values.

We also compute the eigenvectors ψ_- and plot them in Fig. 5.9.

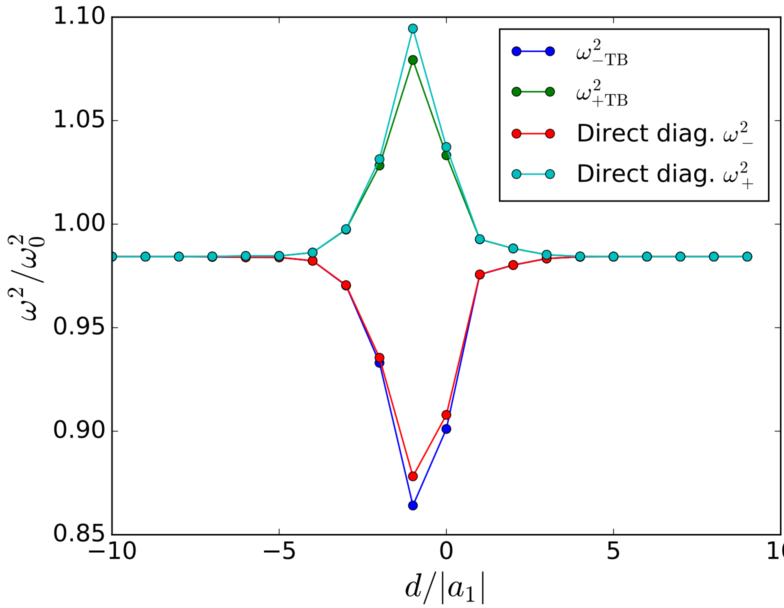


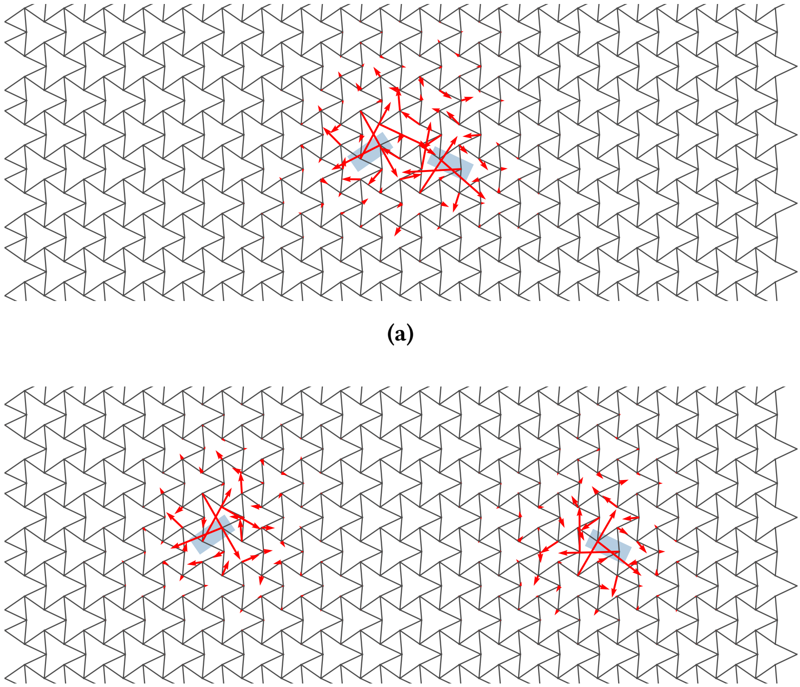
Figure 5.8. A comparison of the squared frequencies between the tight-binding theory and the direct diagonalization of the dynamical matrix. The defects are separated by a distance d. The system parameters are the same as Fig. 5.3.

5.3 Towards multiple defects

For a system with multiple defects, we raise two specific questions about the gap modes. While we do not include the results of these investigations in this thesis, it is worth pointing out the directions.

First, since the tight binding theory works for a pair of defects, we can wonder whether there is a hybridization of gap modes of multiple defects, just like the formation of a molecule out of multiple atoms via chemical bonds.

Second, for a perfect system, the band gap in the spectrum forbids signals to propagate. But the gap mode associated with each defect can help



(a)

(b)

Figure 5.9. Lowest frequency gap modes ψ_- for (**a**) $d/|a_1| = 2$ and (**b**) $d/|a_1| = 10$. The shaded blue regions indicate the defects of removed springs. The system parameters are the same as Fig. 5.3.

mediate the forbidden signal. As we keep introducing defects into the system, there is presumably a percolation phenomenon in terms of the mechanical signal at the band-gap frequencies. The same concepts have been realized and investigated in the systems of continuum media like photonic [84] and phononic crystals [85], but never in the discrete mechanical lattice systems to the knowledge of the author.