Wave propagation in mechanical metamaterials

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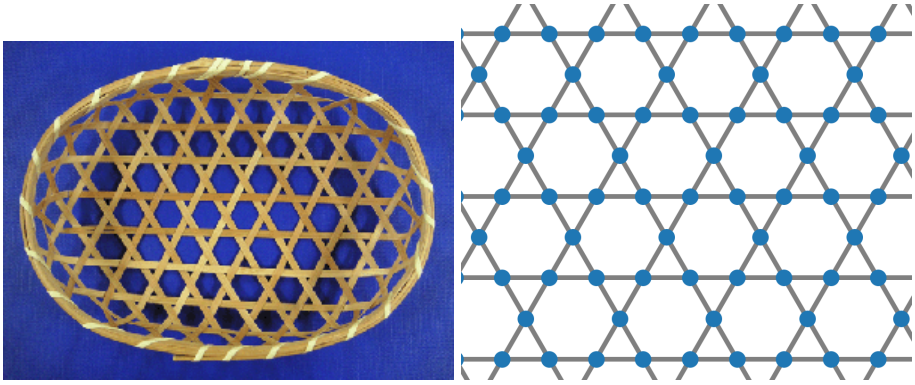
Chapter 4

Twisted kagome lattices: band structure analysis

4.1 What is a kagome lattice

In this chapter we study the so-called kagome lattice. The name kagome comes from Japanese, where "kago" means "basket", and "me" means "eye". As shown in Fig. 4.1a, it is a pattern that has been used in Japanese basketry for a long time [68, 69]. If we extend this pattern into an infinite lattice, and put a mass at each crossing point of the bamboo ribbons and a spring between each pair of neighboring masses, then we obtain a mechanical model of kagome lattice (see Fig. 4.1b). It can be seen as a network of corner-sharing equilateral triangles. There are other ways of building a mechanical kagome lattice, such as pin-jointing rigid triangular plaquettes (Fig. 4.2) or rigid bars (Fig. 4.3).

The kagome lattice as a mechanical model has been studied quite extensively in terms of phonon spectrum, elasticity, and rigidity [13, 14, 26, 28, 42, 69, 71–73]. It features an internal zero-energy motion, in which neighboring triangles are twisted towards alternating directions [25, 43, 53, 74–77] (see Fig. 4.2 or Fig. 4.3). This is a finite "collapsing" mechanism that changes the geometry of the unit cell. We call it the *twisting mechanism*. Its infinitesimal counterpart is termed the *twisting mode*, which is known as a Guest-Hutchinson mode [74].



(a) (b)

Figure 4.1. (**a**) A basket with kagome pattern. The figure is from Ref. [70]. (**b**) A mechanical kagome lattice of masses and springs.

The infinitesimal vibrations of the lattice are described, in the harmonic approximation, by a phonon band structure. This band structure is determined by the content and geometry of the lattice unit cell. As the twisting mechanism changes the geometry without costing any energy, it turns out to be an easy way to tune the vibrational properties of the lattice. Although this idea has been considered before [53], we investigate it in a more detailed way and present the results in the following sections.

The twisting mechanism is the integrated version of the twist mode. As it has only one degree of freedom, it can be described by the twisting angle θ of each triangle around its center. We define ϑ to be the angle between two lines connecting two centers of adjacent triangles (see Fig. 4.4). Then θ is defined as

$$\theta = (180^\circ - \vartheta)/2 \tag{4.1}$$

In this work, θ ranges from 0° to 60°. When the lattice is untwisted, $\theta = 0^\circ$ (Fig. 4.2a). When the twisted triangles touch each other, $\theta = 60^\circ$ (Fig. 4.2d).

We choose a unit cell which has the shape of a rhombus with angle 60° and consists of two triangles (see Fig. 4.4). The Bravais lattice primitive vectors

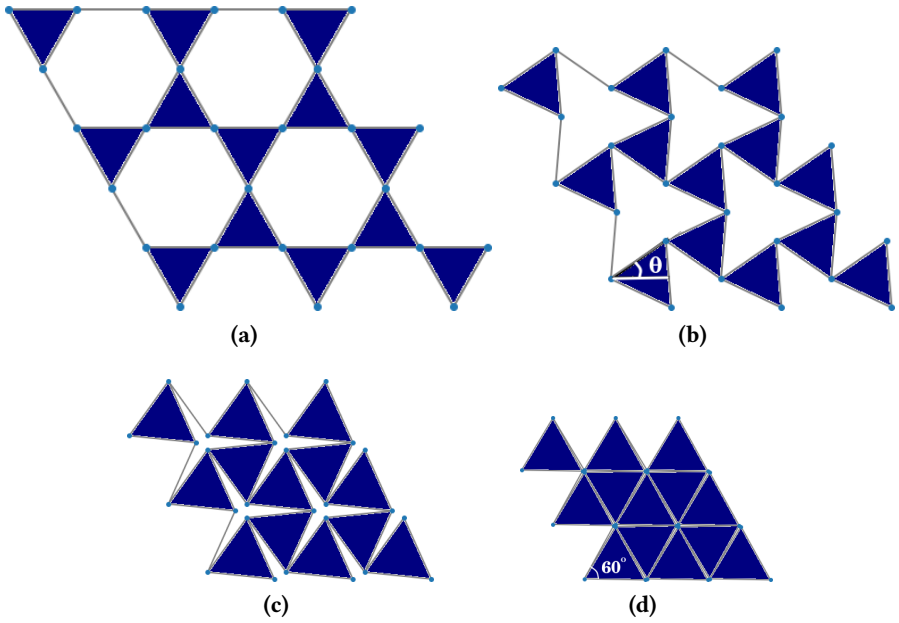


Figure 4.2. A mechanical kagome model made of triangular plaquettes. The framework collapses through a zero-energy mechanism without deformation of its rigid components.

are

$$a_1 = (2\ell\cos\theta, 0), \tag{4.2}$$

$$a_2 = (\ell\cos\theta, \sqrt{3}\ell\sin\theta), \tag{4.3}$$

where ℓ is the spring length.

The coordinates of the masses are

$$(x_1, y_1) = \left\{\frac{1}{3}\ell\left(\sin\left(30^\circ - \theta\right) + \cos\theta\right), \frac{1}{2}\ell\left(\sqrt{3}\cos\theta - \sin\theta\right)\right\}, \tag{4.4}$$

$$(x_2, y_2) = \left\{\ell\left(\frac{\sin\theta}{\sqrt{3}} + \cos\theta\right), 0\right\}, \tag{4.5}$$

$$(x_3, y_3) = \left\{-\frac{1}{6}\ell\left(\sqrt{3}\sin\theta - 9\cos\theta\right), \frac{1}{2}\ell\left(\sin\theta + \sqrt{3}\cos\theta\right)\right\}. \tag{4.6}$$

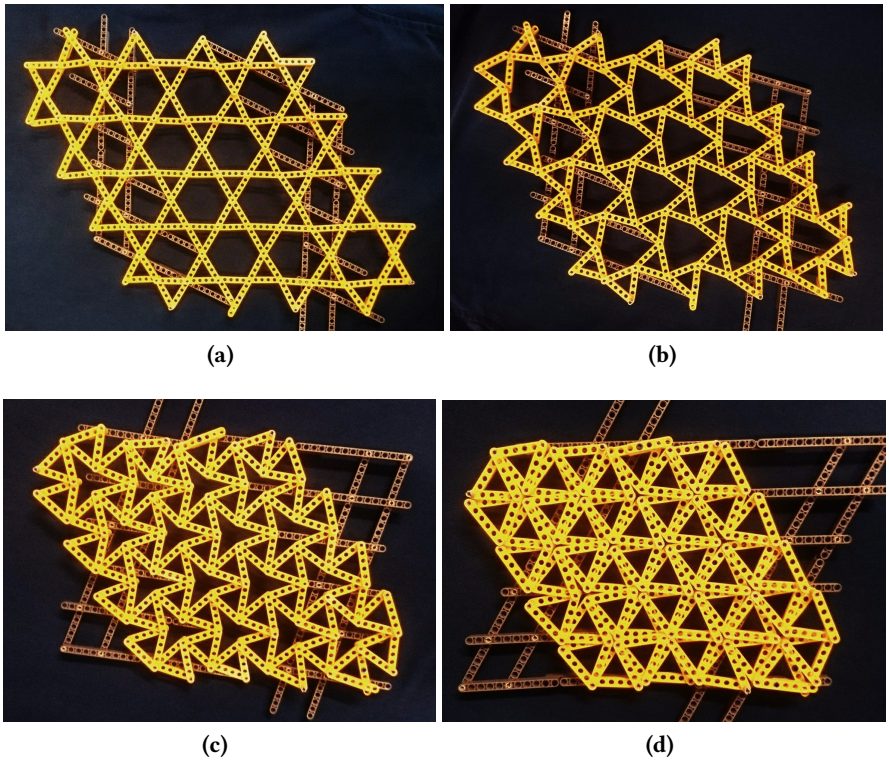


Figure 4.3. A mechanical kagome model made of LEGO. The yellow bars consist of the kagome framework, while the gray bars provide the handle for the twisting mechanism.

4.2 Lattice dynamics of kagome lattices

Since we study the vibrational properties of kagome lattices, we first briefly explain the theory of lattice dynamics, and concept of the phonon band structure. For rigorous details, we refer to the textbooks [78–80].

We study the harmonic oscillation of a lattice system of masses. Its equa-

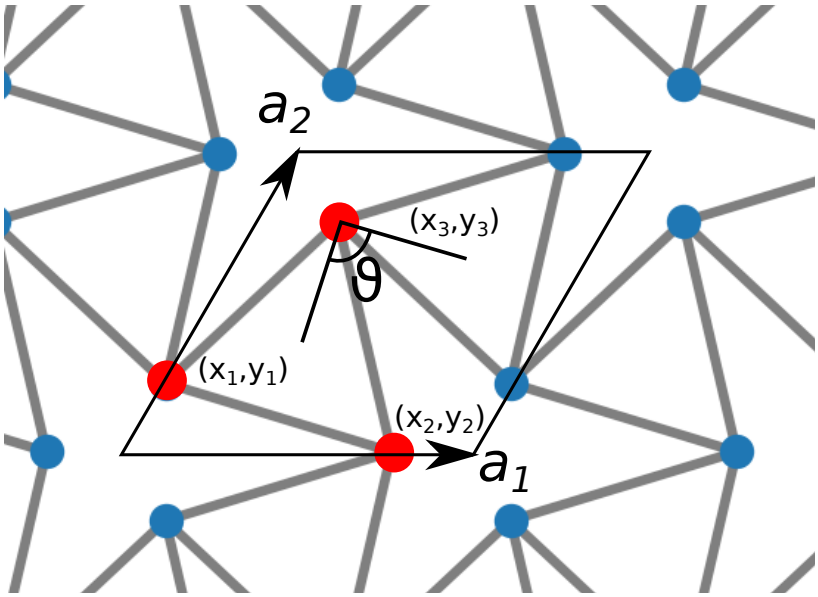


Figure 4.4. Our choice of the unit cell for the twisted kagome lattice. The masses inside the unit cell are shown in red. ϑ is the angle between two lines connecting two centres of adjacent triangles. The twisting angle $\theta = (180^\circ - \vartheta)/2$.

tion of motion in real space can be written as:

$$\boldsymbol{M}\ddot{\boldsymbol{u}} = -\partial_{\boldsymbol{u}}\Phi \approx -\left(\partial_{\boldsymbol{u}}^2\Phi\right)\Big|_{\boldsymbol{u}=0}\boldsymbol{u}, \tag{4.7}$$

where $\boldsymbol{M}$ is the mass matrix, Φ is the total potential energy, and $\boldsymbol{u}$ is the displacement vector of masses. We take the time Fourier transform of the Eqn. (4.7) to obtain the secular equation

$$\omega^2\hat{\boldsymbol{u}} = \boldsymbol{D}\hat{\boldsymbol{u}} \tag{4.8}$$

where $\boldsymbol{D} = -\boldsymbol{M}^{-1}\left(\partial_{\boldsymbol{u}}^2\Phi\right)\Big|_{\boldsymbol{u}=0}$ is the dynamical matrix in real space, and ω is the oscillation frequency.

Since the lattice is spatially periodic, we can decompose all solutions in terms of plane waves of the form

$$\boldsymbol{u}(\boldsymbol{x}, t) = \boldsymbol{\epsilon} \exp\left[i(\boldsymbol{k} \cdot \boldsymbol{x} - \omega t)\right], \tag{4.9}$$

where $\boldsymbol{\epsilon}$ is a polarization vector giving the displacement of the masses in a unit cell, $\boldsymbol{k}$ is the wave vector, $\boldsymbol{x}$ is a Bravais vector giving the position of unit cells, and t is time. This allows us to define the Fourier transformed dynamical matrix $\boldsymbol{D}(\boldsymbol{k})$ such as

$$\omega^2 \boldsymbol{\epsilon} = \boldsymbol{D}(\boldsymbol{k}) \boldsymbol{\epsilon}. \tag{4.10}$$

The eigenvalues $\omega(\boldsymbol{k})$ and eigenvectors $\boldsymbol{\epsilon}(\boldsymbol{k})$ of $\boldsymbol{D}(\boldsymbol{k})$ are called the dispersion relation and the polarization vectors. They form a complete set of solutions of the equation of motion of the lattice called normal modes, which describe the small oscillations of the lattice around its equilibrium configuration.

The wave vector $\boldsymbol{k}$ also lives in a periodic space called the reciprocal space. Its has a primitive cell in which the points are closer to the origin than any to any other reciprocal lattice points. It is uniquely defined as the first Brillouin zone. The first Brillouin zone of the kagome lattice is shown in Fig. 4.5. The points of high symmetry are denoted.

Now we study the eigenvalue equation (4.10) carefully. Since it is Fourier transformed, the dimension of $\boldsymbol{\epsilon}(\boldsymbol{k})$ equals the number of degrees of freedom in a unit cell. For the kagome lattice, each unit cell has six degrees of freedom. This means that $\boldsymbol{D}(\boldsymbol{k})$ is a 6×6 matrix. As it can be shown that $\boldsymbol{D}(\boldsymbol{k})$ is Hermitian [1], it has six real eigenvalues for each $\boldsymbol{k}$. Since the wave vector $\boldsymbol{k}$ can vary continuously, each eigenvalue $\omega(\boldsymbol{k})$ as a continuous function forms a "band" in the reciprocal space. We plot $\omega(\boldsymbol{k})$ to show the six phonon bands (see Fig. 4.6). Two bands whose frequencies equal zero at the Γ point in the reciprocal space are conventionally called acoustic bands, while the other four bands are optical bands.

We see that each of the six modes at the Γ point are identical in all unit cells. Among them are the two global translation modes, the twisting mode,

[1] With our convention, $\boldsymbol{D}(\boldsymbol{k})$ is only pseudo-Hermitian, but it is possible to define a Hermitian one. See Ref. [79].

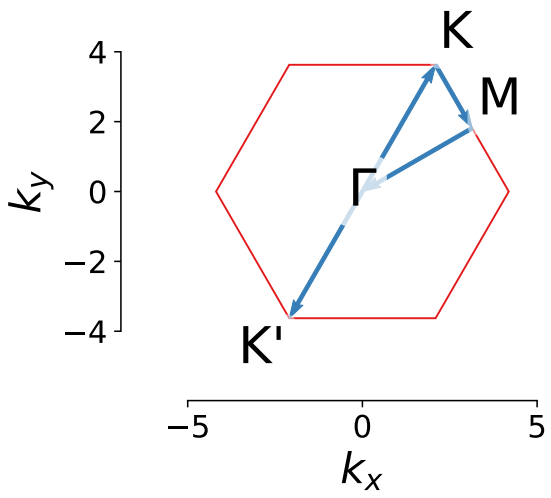


Figure 4.5. The first Brillouin zone of the kagome lattice, with its high symmetry points of $\Gamma = (0, 0)$, $K = (2\pi/3, 2\sqrt{3}\pi/3)$, $K' = (-2\pi/3, -2\sqrt{3}\pi/3)$ and $M = (\pi, \sqrt{3}\pi/3)$, in unit of $|a_1|^{-1}$, and a path used for the band structure in the following.

and three others. Notice that the frequency of the twisting mode is not zero for general twisting angle, which seems to be contradictory with what is said in the previous section that the twisting mechanism is a zero-energy finite motion. The subtlety is that we have to allow the unit cell to deform to be compatible with the changing framework along the finite mechanism. In this way the twisting mode is made to be a zero mode. This detail is well explained in Ref. [74–76]. Here in the theory of lattice dynamics, we do not make this assumption of deformable unit cell, so the twisting mode does not have zero frequency.

The phonon spectrum is obtained by projecting all the phonon bands to the ω axis. The density of states of phonons describes the number of states per interval of frequency and shows directly important lattice vibrational properties such as the band gaps, a frequency interval where no normal mode lies in. To estimate it, we compute the histogram of the phonon modes with respect to the frequency. We will show this in the next section in detail.

4.3 Influence of the twist: the band gap opens up

In the previous section, we show the linear theory of lattice motion, and ultimately, the phonon band structure. Usually, a mechanical lattice with give geometrical parameters of its component has fixed structure. If we forbid any process that costs energy such as deforming springs, then the lattice cannot change form. So the band structure associated with the lattice does not change either. However, as we mentioned before, the kagome lattice has a global zero-energy twisting mode. This enables us to deform the kagome lattice in a certain way, keep it at equilibrium state all along, and study how the band structure changes accordingly (see Fig. 4.6). [2].

First we notice that a gap opens when the twisting angle goes above $22°$. This is clearly shown in the phonon spectrum in Fig. 4.7. Looking at the band structure, we see that the band associated with the twisting mode lifts up. It is this process that opens up the gap, when the minimum of this band exceeds the maximum of the acoustic bands. In the next chapter, we will see how the band gap is used in studying the vibrational modes of the kagome lattice with defects.

Second we see there are linear crossings at K point for small θ and at Γ point for $\theta = 45°$. Such linear crossings are also related to the vanishing density of states in the spectrum at $\omega/\omega_0 = 2.0$ for small θ and at $\omega/\omega_0 = 1.7$ for $\theta = 45°$.

Third we find that at both $\theta = 30°$ and $\theta = 60°$, one of the bands becomes flat. The effect of flat bands on mechanical lattices has been studied in Ref. [81].

When the lattice is untwisted, the twisting mode has zero frequency. This has to do with the fact that the straight lines of connected springs across the unit cell form states of self stress. The twisting mode is just a linear combination of all the zero modes corresponding to these states of self stress.

4.4 Symmetry of twisted kagome lattices

To better understand the influence of the twisting angle on the band structure, it is useful to study the symmetry of the lattice. The plane symmetry group of

[2] Similar work has been done in phononic material as continuous media, but so far as we know, there is no such study on the discrete lattice network.

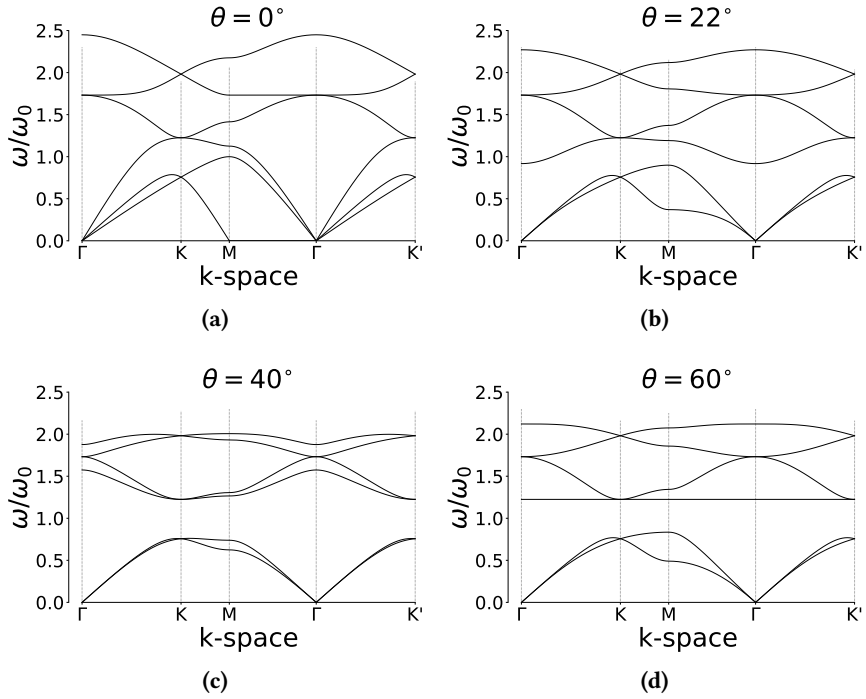


Figure 4.6. The band structure of the kagome lattice with varying twisting angle θ. The unit frequency ω_0 equals $\sqrt{k_0/m}$, where k_0 is the spring stiffness constant and m is the mass.

the twisted kagome lattice is p31m. The point group symmetry is 31m, which contains the identity, two three-fold rotation operation, and three mirror opertions (see Fig. 4.8).

Now we consider the effect of point group symmetry on the lattice vibration modes $\boldsymbol{u}(\boldsymbol{k})$. When acting upon a two-dimensional vector (x, y) in real space, the point group symmetry has the matrix representation:

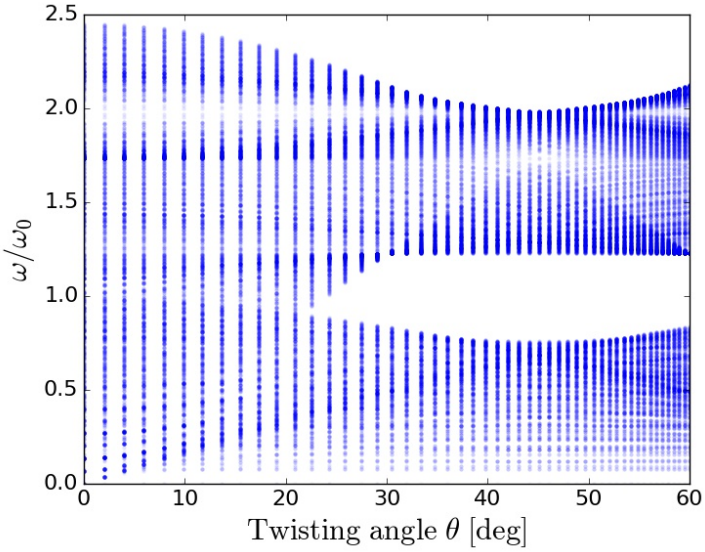


Figure 4.7. The phonon spectrum of the kagome lattice with varying twisting angle. The opacity of the data points indicates the density of states at each frequency bin. A band gap opens up at around $\theta = 22°$. The system has 20×20 unit cells with periodic boundary conditions.

$$
\begin{aligned}
R(1) &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, R(3^+) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \\
R(3^-) &= \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, R(m_{-12}) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \\
R(m_{2-1}) &= \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}, R(m_{11}) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}.
\end{aligned}
\tag{4.11}
$$

For the three masses in the unit cell, the point group symmetry has the representation

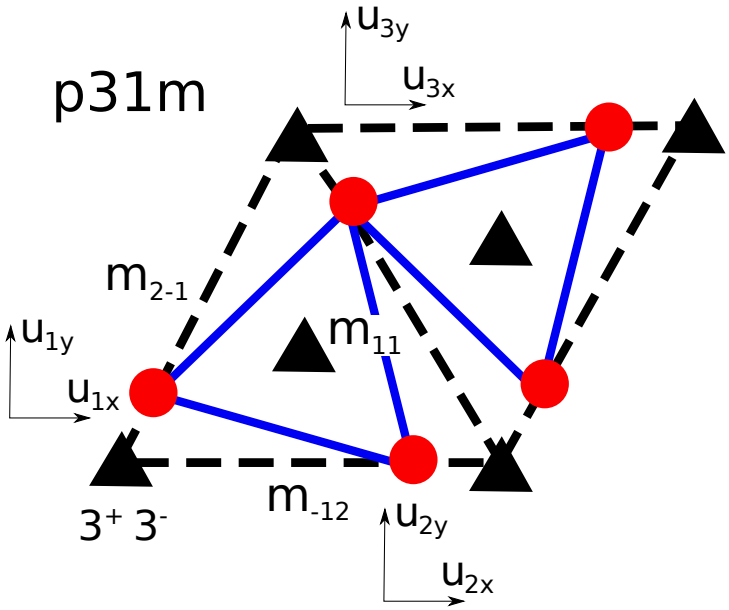


Figure 4.8. The unit cell of the twisted kagome lattice. The masses are the red dots. The bonds are the blue lines. The point group symmetries – the three-fold rotational axes and the mirrors – are labeled in black triangles and dashed lines respectively. The six components of vibrational modes – (u_{ix}, u_{iy}) for $i = 1, 2, 3$ – are also labeled near each mass.

$$
\begin{aligned}
P(1) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, P(3^+) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \\
P(3^-) &= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, P(m_{-12}) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \\
P(m_{2-1}) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, P(m_{11}) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.
\end{aligned} \tag{4.12}
$$

Now the representation S of the point group symmetry on the six-dimensional vector $\boldsymbol{u}(\boldsymbol{k})$ is just the direct product of R and P

$$S(g) = R(g) \otimes P(g), \tag{4.13}$$

where g is a symmetry operation.

In general the effect of the symmetries on the dynamical matrix is

$$S(g)\boldsymbol{D}(\boldsymbol{k})S(g^{-1}) = \boldsymbol{D}(R(g)\cdot\boldsymbol{k}). \tag{4.14}$$

At high symmetry point $\boldsymbol{k}^*$ such as Γ and K, where $R(g)\cdot\boldsymbol{k}^* - \boldsymbol{k}^*$ is a reciprocal lattice vector, we find that $S(g)$ commutes with the dynamical matrix $\boldsymbol{D}(\boldsymbol{k})$

$$S(g)\boldsymbol{D}(\boldsymbol{k})S(g^{-1}) = \boldsymbol{D}(\boldsymbol{k}). \tag{4.15}$$

This explains the degeneracies at the high symmetry points observed in Fig. 4.6.

4.5 Critical twisting angle: double degeneracy

When the twist angle $\theta = 45°$, the lattice dynamics shows very special phenomena, which we will study in this section.

The first and the most obvious phenomenon is in the band structure. The six phonon bands collapse into three pairs everywhere in the Brillouin zone (see Fig. 4.9). In other words, the dynamical matrix $\boldsymbol{D}(\boldsymbol{k})$ has doubly degenerate eigenvalues everywhere in the reciprocal space. Notice that a four-band linear crossing occurs at the Γ point.

Besides the degenerate eigenvalues ω, we also investigate the eigenvectors $\boldsymbol{\epsilon}$. The second special phenomenon is that all the eigenvectors $\boldsymbol{\epsilon}(\boldsymbol{k})$ of $\boldsymbol{D}(\boldsymbol{k})$ have equal mode amplitude on each of the three masses, i.e. the norm of the vector $(\epsilon_{ix}, \epsilon_{iy})$ is identical for $i = 1, 2, 3$.

When approaching the critical twisting angle, for $\theta \to 45°$, we also find that for each pair of the almost degenerate eigenvectors $\boldsymbol{\epsilon}^a$ and $\boldsymbol{\epsilon}^b$ which are orthogonal as they are have different eigenvalues, the sub-vectors $(\epsilon^a_{ix}, \epsilon^a_{iy})$ and $(\epsilon^b_{ix}, \epsilon^b_{iy})$ are also orthogonal for $i = 1, 2, 3$, namely $\langle(\epsilon^a_{ix}, \epsilon^a_{iy}), (\epsilon^b_{ix}, \epsilon^b_{iy})\rangle = 0$.

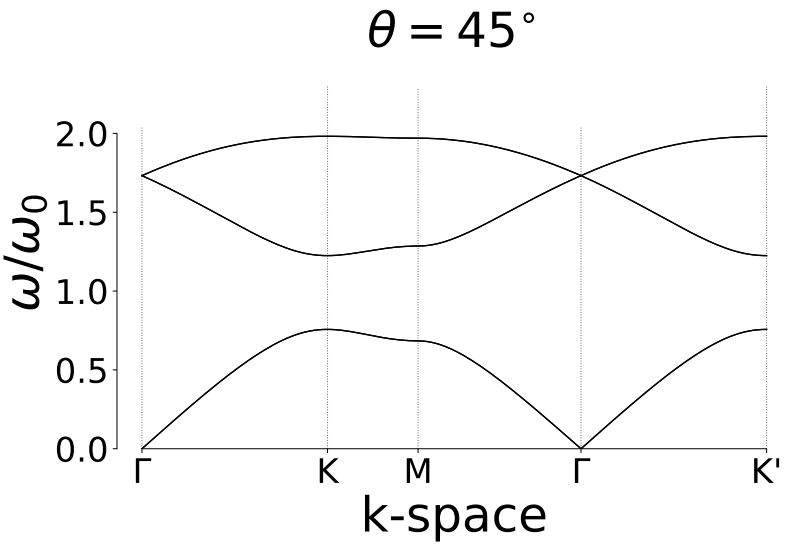


Figure 4.9. The band structure of the kagome lattice with the twisting angle $\theta = 45°$. The six bands are doubly degenerate everywhere in the reciprocal space, so only three bands can be seen in the figure. One of the finite-frequency vibrational modes at the four-band crossing at the Γ point is shown on the cover of this thesis.

All these phenomena together strongly imply that there is probably a symmetry of the dynamical matrix relating the eigenvectors in a special way. Currently we are still seeking the analytical form of this symmetry.

Mathematically, the expected symmetry operation with a matrix representation $\boldsymbol{S}$ in terms of the lattice vibration should commute with the dynamical matrix $\boldsymbol{D}(\boldsymbol{k})$ for all $\boldsymbol{k}$. This can be seen in the following. For each pair of bands, its eigenvectors $\boldsymbol{\epsilon}^a$ and $\boldsymbol{\epsilon}^b$ are related by this symmetry $\boldsymbol{S}$. Then we have

$$\boldsymbol{D}(\boldsymbol{k})\boldsymbol{S}\boldsymbol{\epsilon}^a = \boldsymbol{D}(\boldsymbol{k})\boldsymbol{\epsilon}^b = \lambda^b\boldsymbol{\epsilon}^b \tag{4.16}$$

and

$$\boldsymbol{S}\boldsymbol{D}(\boldsymbol{k})\boldsymbol{\epsilon}^a = \boldsymbol{S}\lambda^a\boldsymbol{\epsilon}^a = \lambda^a\boldsymbol{\epsilon}^b. \tag{4.17}$$

Since $\boldsymbol{D}(\boldsymbol{k})\boldsymbol{S} = \boldsymbol{S}\boldsymbol{D}(\boldsymbol{k})$, it means $\lambda^a = \lambda^b$, hence the degeneracy.

We know that $\boldsymbol{S}$ cannot simply be any point group symmetry, because the latter only commutes with $\boldsymbol{D}$ at certain high symmetry points, as we have seen in Eqn. (4.15).