Topological States Due to Third-Neighbor Coupling in Diatomic Linear Elastic Chains

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The vibrations of a diatomic linear chain exhibit two bands, the acoustic and the optical one. In the case of equal masses and nearest-neighbor spring constants, no gap exists. The effects of nearest, next-nearest, and third-nearest neighbor coupling with different spring constants are analyzed. Nearest neighbor coupling leads to two topologically different bulk states with winding numbers $\nu = 0$ and $-1$. Next-nearest neighbor coupling does not change the topological properties and introduces only a trivial “Semenov” gap. Third-nearest neighbor coupling leads to four distinct topological bulk phases with winding numbers $\nu = 0$, $\pm 1$, and $-2$.

1. Introduction

The concept of topological phases is nowadays considered for surprisingly many systems. The ideas were initially developed for solitons in polymers. The concepts for the explanation of quantum Hall states are closely related to the physics in quasi-1D conductors as pointed out in the study by Schrieffer and coworkers. The lattice vibrations in a solid are typically introduced in textbooks with a linear chain model. To allow for acoustic and optical branches, a diatomic unit cell is used. Herein, we like to point out some topological aspects of this rather simple classical system.

The diatomic linear chain with nearest-neighbor and third-neighbor coupling is schematically shown in Figure 1. We will show that the diatomic chain with nearest-neighbor coupling has two different topological bulk states. It is generally known that going beyond nearest-neighbor coupling can change the topological properties. The introduction of next-neighbor coupling (Figure 1a) only opens a trivial gap and is thus considered only briefly. The main aspect of this article is to analyze the effect of third-neighbor coupling (Figure 1b) on the dispersion and the bulk winding number; it will lead to four distinct topological bulk phases.

2. Dispersion Relations

2.1. Nearest Neighbor Coupling

It is well known that a gap forms at the X point for $C_1 \neq C_2$. The lower branch is termed “acoustic” branch, the upper one the “optical.” At the X points ($k = \pm \pi$), the lower and the upper branches have the frequencies (in units of $\sqrt{C/M}$)

$$\omega_{\pm}(X) = \sqrt{C_1 + C_2 \pm |C_1 - C_2|}$$

the width of the gap $\omega_b(X) = \omega_+(X) - \omega_-(X)$ being

$$\omega_b(X) = \sqrt{2} \sqrt{C_1 + C_2 \left[ 1 - \sqrt{1 - \frac{(C_1 - C_2)^2}{(C_1 + C_2)^2}} \right]}$$

At the $\Gamma$ point

$$\omega_-(\Gamma) = 0$$

$$\omega_+(\Gamma) = \sqrt{2} \sqrt{C_1 + C_2}$$

2.2. Next-Nearest Neighbor Coupling

At the X points, the lower and the upper branches have the frequencies...
2.3. Third-Neighbor Coupling Dispersion Relation

Herein, we consider $C_1 = C_2 = C = 1$ and $C_A = C_B = 0$ for simplicity. The general dispersion is given by (in units of $\sqrt{C/M}$)

$$\omega_{\pm}(X) = \sqrt{\frac{C_1 + C_2 + 2(C_A + C_B)}{\pm \sqrt{(C_1 - C_2)^2 + 4(C_A - C_B)^2}}}
$$

(5)

with a gap forming for $C_1 \neq C_2$ and/or $C_A \neq C_B$. At the $\Gamma$ point, (3) and (4) remain valid.

The dispersion is shown in Figure 2a for $C' = 1/2$ and in addition to the zero gap at the X point ($k = \pm \pi$), another degeneracy exists at $k = \pm 2\pi/3$ which we denote as $\pm \psi'$. Generally, for $C_1' = C_2'$, the chain is monoatomic and has actually a periodicity of $a/2$ and the doubled Brillouin zone, as shown in Figure 2b, is actually folded. In Figure 2b, also the dispersions for $C' = 0, 1/8, 1/3, 1/2$ and $C' = 1$ are shown.

A variation of $C_1$ and $C_2$ will open these two gaps and generate topologically different states. Around the $\Gamma$ point in the lower branch is a region of imaginary frequencies which indicates frustration.

A representation of the $(C_1', C_2')$ parameter space is shown in Figure 3b. Along the two diagonals, the band structure has no gap, as detailed in the following.

Generally, $\omega_{\pm}' = \omega_{\pm}(X) - \omega_{\pm}(X)$, the gap at the X point, is given as

$$\omega_{\pm}' = 2\sqrt{1 - \sqrt{\frac{1 + C_1 - C_2}{2} \left( \frac{1 - C_1' - C_2'}{2} \right)}}.
$$

(8)

Thus, only for $C_2' = C_1'$ the gap at X is closed (it is open along the other diagonal $C_3 = C_1' = C_2' \neq 1/2$).

For $C_1' = C_2' = C'$, the k-position of the second gap is given by $k = \text{arccos}[(C' - 1)/(2C')]$ and the second gap exists for $C' > 1/3$ (cmp. the red curve in Figure 2b for $C' = 1/3$). As noted before, for $C' = 1/2$, the gap is at the X point, $k = \pm 2\pi/3$. For $C_2' = 1 - C_1'$, the second gap is always closed and located at the X' points.

**Figure 1.** Schematic of the diatomic linear chain with atomic sites A and B that have nearest-neighbor coupling $C_1$ and $C_2$ and a) next-nearest neighbor coupling $C_A$ and $C_B$ or b) third-nearest neighbor coupling $C_1'$ and $C_2'$.

**Figure 2.** a) Dispersion of the diatomic linear chain ($C_1 = C_2 = 1$) with third-nearest neighbor coupling $C_1' = C_2' = C' = 1/2$. Real and imaginary frequencies are depicted with “solid” and “dashed” lines, respectively. b) Dispersion of the real frequencies in the doubled (unfolded) Brillouin zone for various values of $C' = 0$ (dispersion of the conventional monoatomic chain with nearest-neighbor coupling) and $C' = 1/8, 1/3, 1/2$, and 1. For $C' = 1/3$ (red curve), the dispersion has zero slope (and zero curvature) at $k = \pm \pi$. 

**Figure 3.** Schematic of the diatomic linear chain with atomic sites A and B that have nearest-neighbor coupling $C_1$ and $C_2$ and a) next-nearest neighbor coupling $C_A$ and $C_B$ or b) third-nearest neighbor coupling $C_1'$ and $C_2'$. 

![Schematic diagram of the diatomic linear chain](image-url)
Therefore, in summary, a band structure with zero gap exists for $C_2 = C_1$ and $C_2 = 1 - C_1$. These two cases are represented by the diagonal black lines in Figure 3b. For all other combinations of $C_1$ and $C_2$, the band structure has a gap. For these cases, we will calculate the winding number as topological invariant in the next section.

3. Winding Numbers

From the eigenproblem, the eigenvectors of type

\[ u_\pm(k) = \left( u_{A,\pm}(k), u_{B,\pm}(k) \right) = (1, \exp[\mp i \delta \phi(k)]) \]  

(9)

with the relative phase $\delta \phi$ of A and B sites are obtained for both bands ($\pm$ indicating the upper and lower bands); the phases of the lower and upper bands are related by a factor of $-1$. The important quantity is the change of phase within a band when traversing the Brillouin zone from $-\pi$ to $+\pi$. As the physical properties are periodic with the Brillouin zone, this total phase change must be an integer multiple of $2\pi$. To properly account for the change in phase, the property $A_\pm$

\[ A_\pm(k) = i u_\pm^* (k) \frac{\partial u_\pm(k)}{\partial k} \]  

(10)

a 1D Berry connection, is calculated and integrated over the Brillouin zone, resulting in the associated Berry phase. The resulting winding number is (for a gapped system) an integer as topological invariant of a 1D BDI-type system\cite{12}

\[ \nu = \frac{1}{2\pi} \int_{-\pi}^{+\pi} A_\pm(k) dk, \quad \nu \in \mathbb{Z} \]  

(11)

3.1. Nearest Neighbor Coupling

The winding number for the diatomic chain with nearest neighbor coupling is (for the nonzero gap case) $\nu = 0$ for $C_1 > C_2$ and $\nu = -1$ for $C_1 < C_2$. This is similar to the Su–Schrieffer–Heeger tight-binding model\cite{3} for linear molecules with alternating bonds and nearest neighbor hopping parameters and related works.\cite{16,17} Thus, these two cases of intra- and interdimer spring constants are topologically different. This seems to be largely ignored in literature so far and presents a simple example of topologically different states. In the zero-gap case ($C_1 = C_2$), each band has a formal winding number of $-1/2$.

We note that different masses $M_1 \neq M_2$ introduce a gap ("Semenov" insulator\cite{18}) but do not lead to a change of winding number; in particular, for the gapless case $C_1 = C_2$, different masses leave the winding number for the two bands at $-1/2$ and topologically the bulk band structure is trivial. This can also be seen (without further discussion here) from the properties of a finite chain (due to the general bulk-boundary correspondence).

For a topologically nontrivial gap as for $C_1 \neq C_2$, end/edge states can develop for a finite chain with fixed ends. For $M_1 \neq M_2$ and $C_1 = C_2$, a frequency gap develops but no end states exist for any finite chain.

3.2. Next-Nearest Neighbor Coupling

The winding numbers for the cases $C_1 \neq C_2$ do not change upon the introduction of next-nearest neighbor coupling. Thus, the topological properties are not changed, as shown in Figure 3a. In the case of $C_1 = C_2$, values $C_\delta \neq C_0$ introduce a frequency gap at the X points but the winding numbers of the two branches remain $-1/2$ as in the zero-gap case. Thus, the cases $C_1 = C_2$ and $C_\delta \neq C_0$ are topologically trivial (again a "Semenov" insulator\cite{18}).

3.3. Third-Nearest Neighbor Coupling

For the cases with nonzero gap, the winding number can take four values, $\nu = 0, \pm 1, -2$ as shown in Figure 3b. For selected parameters, these four cases are shown with their dispersion and the phase visualized as color in Figure 4. The phase of the lower band and for the four cases is shown also as line graph in Figure 5. At the $\Gamma$ and X points, the modes have defined even ($\delta \phi = 2n\pi, n \in \mathbb{Z}$) or odd ($\delta \phi = (2n + 1)\pi, n \in \mathbb{Z}$) parity. Also, around the second gap, the parity is defined for a certain $k$. Across the Brillouin zone, the parity changes 2\nu times. The case $\nu = 0$ is topologically the simplest as parity does not change within a band. This means that the typical "expectation," that the lower (acoustic) band has even parity (A and B sites are in phase) and the upper (optical) band has odd parity (A and B sites are out-of-phase), is fulfilled.

We note that, however, the choice of unit cell is free and could also be a B–A dimer. Then the winding numbers will be different as the role of $C_1$ and $C_2$ are exchanged but the general scheme of Figure 3b remains the same.

3.4. Higher-Order Neighbor Coupling

As generalization of Equation (6), coupling of higher-order $n$-th neighbors will introduce terms of type $\cos nk$. Thus, in general, further degeneracy points are possible for certain elastic parameters. These can split into gaps and generate topological states with higher winding numbers; for odd $n = 2m + 1$ ($m \geq 0$), we expect $\nu = -m - 1, \ldots, m$. 

4. Conclusions and Outlook

The rather elementary model of the diatomic linear chain can serve as simple example to understand the concept of topologically different bulk states. For the trivial chain with equal nearest-neighbor coupling, the third-neighbor coupling has gapless states for two conditions, namely $C_0^2 = C_0^1$ and $C_0^2 = 1/C_0 C_0^1$. For the other cases, the dispersion has a gap (and is an insulator in the terminology of topological states) and takes one of four distinct topological states. However, while our model can be executed with arbitrary model parameters, realistic parameters are $C' \ll C$ and the cases $\nu = 0$ and $\nu = -1$ known from nearest-neighbor coupling dominate, whereas the cases $\nu = +1$ and $\nu = -2$ will hardly occur naturally.

Our model has direct application to the maybe unexpected mechanical properties of linear molecules with alternating “short” and “long,” i.e., stiffer and softer, bonds such as, for example, in trans-polyacetylene. However, the topological states arise only when the ends of the chain are fixed, and the first spring is the stiffer one. We note that if only one end is fixed like that, accordingly one topological state can exist at this end. Such could be the case for molecules in a confined space or if they are sufficiently strongly attached or bonded to another entity. As is known \cite{12,13} 2D and 3D mechanical systems also can exhibit topological states, and it remains to be seen whether, e.g., topological vibrational motions in 2D molecules become an interesting field.

Conflict of Interest

The author declares no conflict of interest.

Keywords

lattice vibrations, linear chains, topological states, winding numbers

Received: March 25, 2020
Revised: June 9, 2020
Published online: June 16, 2020

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