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PAPER

Topological states of the diatomic linear chain: effect of impedance matching to the fixed ends

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Abstract

The diatomic linear chain with nearest-neighbor spring constants C_1 and C_2 has topologically different bulk states for $C_1 \gtrless C_2$. A finite chain of N unit cells and fixed ends (the first and last spring is C_1) exhibits two topological end states within the gap for $C_1 > C_2$. We investigate the effect of an impedance mismatch by varying the first and last 'boundary' spring constant termed C_F from its ideal value C_1. $C_F = 0$ represents an open end and does never lead to topological states. $C_F \to \infty$ means that also the next site to the boundary is fixed, leading to topological states only for $C_1 < C_2$ since now the first movable spring is C_2. Within a range of C_F around C_1 topological end states are preserved for $C_1 > C_2$. For $C_2 > C_1$, topological end states occur when C_F exceeds a certain value.

1. Introduction

In this paper we like to analyze the simplest mechanical model for a non-trivial linear molecule with alternating short/strong and long/weak bonds, such as e.g. trans-polyacetylene, being attached to a surface. While the electronic topological properties of such molecules have been treated with Su–Schrieffer–Heeger [1] type models in detail [2, 3], the impact of the topological nature on mechanical properties, in particular the robustness of the topological gap states with respect to the mechanical coupling to the environment has not been considered.

Since the topological gap state has maximum amplitude at the end(s) of the chain, it could be responsible for the detachment (i.e. ripping off) of a molecule bonded to another (heavy) entity such as a surface or a nanoparticle. We investigate in this paper, for what range of bonding strengths the well-localized gap state of the topological chain exists.

Topological mechanical systems can be generally mapped to quantum mechanical Hamiltonians and can this way be classified [4, 5]. Specific linear (1D) mechanical systems have been treated with regard to their topological properties, however, they were more complicated, containing pivots [5, 6] or a double chain with cross-connects [7].

Here, we assume the simplest mechanical model with topological properties, namely the diatomic linear chain model (DLCM) [8–10] of dimers with sites A and B having the same mass M. The inter-dimer (A–B) spring constant shall be C_1 and the intra-dimer (B–A) spring constant C_2 (figure 1(a)). We denote $\xi = C_2/C_1$. For $\xi = 1$ there is no gap. For $\xi \neq 1$, the diatomic linear chain has two topologically different bulk states for $\xi < 1$ and $\xi > 1$ [11]. For a finite chain with N dimers, topological end states can form within the gap. We fix the leftmost A-site and the rightmost B-site, leaving $2N - 2$ oscillators. In this case topological end states develop for $\xi < 1$ [11]. We note that the first (leftmost) and last (rightmost) spring are of type C_1. Obviously, if now the second site (B-type) and the second-to-last site (A-type) are additionally fixed, reducing the number of oscillators to $2N - 4$, the chain has topological end states for $\xi > 1$ since C_2-springs are now the first oscillating spring type.

Here, we are interested in the impedance matching of the chain to the fixed ends and its impact on the topological end states. The spring constant of the first and last spring shall now be varied (between 0 and

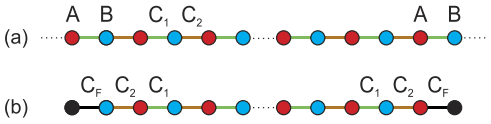

Figure 1. (a) DLCM with A–B dimers in an infinite chain; A-sites (B-sites) are shown in *red* (*blue*); the connecting springs have force constants C_1 (*green*) and C_2 (*orange*), respectively. (b) DLCM with finite number of dimers with both end sites fixed (shown in *black*). The first and last spring (coupling to the fixed ends) have the spring constant C_F.

∞) and is denoted by C_F (figure 1(b)). $C_F = C_1$ is the 'natural' or 'ideal' matching spring constant. $C_F = 0$ represents an open end and $C_F \to \infty$ leads to the fixation of the second *and* second-to-last site as discussed above. Our question here is what deviations of C_F from C_1 (for $\xi < 1$) still support topological end states.

2. Bulk states

The bulk dispersion within the 1D Brillouin zone X–Γ–X with $k \in [-\pi, \ldots, 0, \ldots, +\pi]$ is given by [10] (upper sign for the upper branch)

$$\omega_\pm(k) = \frac{\omega_{\max}}{\sqrt{2}} \sqrt{1 \pm \sqrt{1 - [\gamma \, \sin(k/2)]^2}}, \tag{1}$$

with $\gamma = \sqrt{C_1 \, C_2}/\bar{C}$, $\bar{C} = (C_1 + C_2)/2$ and the maximum phonon frequency given by $\omega_{\max} = \omega_+(\Gamma)$,

$$\omega_{\max} = \sqrt{2 \, \frac{C_1 + C_2}{M}} = 2 \sqrt{\frac{\bar{C}}{M}}. \tag{2}$$

In the following, the frequencies for a given system will be depicted as scaled by $\omega_{\max}$ such that the maximum frequency of the upper band is 1.

3. Finite 'long' chain with fixed ends

Now we consider a finite chain with $N \ggg 1$ dimers ($2N$ oscillators). The two ends are fixed as shown in figure 1(b), thus $2N - 2$ oscillators can move. On the left end the A-site, on the right end the B-site shall be fixed. The vector $\boldsymbol{u}$ contains displacements for the A- and B-sites of the dimer n, u_n^{A} and u_n^{B},

$$\boldsymbol{u} = (u_1^{\mathrm{A}}, u_1^{\mathrm{B}}, u_2^{\mathrm{A}}, u_2^{\mathrm{B}}, \ldots, u_N^{\mathrm{A}}, u_N^{\mathrm{B}})^{\mathrm{T}} \tag{3}$$

$$= (\tilde{u}_1, \tilde{u}_2, \tilde{u}_3, \tilde{u}_4, \ldots, \tilde{u}_{2N-1}, \tilde{u}_{2N})^{\mathrm{T}} \tag{4}$$

The displacements $\tilde{u}_i$ represent another way of counting the oscillators with an index $i = 1, \ldots, 2N$.

With the ends fixed, $u_1^{\mathrm{A}} = \tilde{u}_1 = 0$ and $u_N^{\mathrm{B}} = \tilde{u}_{2N} = 0$, the equations of motion can be written as $\boldsymbol{C}\,\boldsymbol{u} = M\,\omega^2\,\boldsymbol{u}$ with the upper left corner of the matrix $\boldsymbol{C}$ being,

$$\frac{\boldsymbol{C}}{C_1} = \begin{pmatrix} 0 & 0 & 0 & 0 & \ldots \\ 0 & 1+\xi & -\xi & 0 & \ldots \\ 0 & -\xi & 1+\xi & -1 & \ldots \\ 0 & 0 & -1 & 1+\xi & \ldots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{5}$$

For the left end gap mode, $u_n^{\mathrm{A}} = 0$ for all n in the ideal case of an infinitely long chain for which the right end gap mode does not overlap. The frequency of the double degenerate gap mode is then given from the second row of (5) as

$$\omega_{\mathrm{g}} = \sqrt{\frac{C_1 + C_2}{M}} = \frac{\omega_{\max}}{\sqrt{2}}. \tag{6}$$

This value is also equal to $\omega_-(X) = \omega_+(X)$ for the gapless case $C_1 = C_2$. For the right end gap mode, $u_n^{\mathrm{B}} = 0$ for many $n = N, N-1, \ldots$ and (6) holds. The orthonormal mode patterns of the two eigenstates shall be $\boldsymbol{u}_{\mathbf{g},1}$ and $\boldsymbol{u}_{\mathbf{g},2}$.

We note that due to the frequency degeneracy, other combinations such as $(\boldsymbol{u}_{\mathbf{g},1} + \boldsymbol{u}_{\mathbf{g},2})/\sqrt{2}$ and $(\boldsymbol{u}_{\mathbf{g},1} - \boldsymbol{u}_{\mathbf{g},2})/\sqrt{2}$ are also eigenstates. In order to avoid such ambiguity in our calculations and for obtaining

solutions that are localized at the ends (and not symmetric and antisymmetric 'hybridized' modes), a minute mass difference $(M_A - M_B)/(M_A + M_B) = 5 \times 10^{-4}$ has been used in the calculations. In this case of different masses of A- and B-sites [12], the two gaps states are no longer degenerate and the eigenfrequency at the left (right) end is given by ω_g^B (ω_g^A),

$$\omega_g^A = \sqrt{\frac{C_1 + C_2}{M_A}}, \tag{7}$$

$$\omega_g^B = \sqrt{\frac{C_1 + C_2}{M_B}}. \tag{8}$$

The gap modes decay exponentially from the ends; from the third row of (5) we obtain $C_2\, u_1^B + C_1\, u_2^B = 0$, and generally,

$$u_{n+1}^B = -\xi\, u_n^B. \tag{9}$$

for many $n = 1, 2, \ldots$ The solution is

$$u_n^B = (-\xi)^{n-1}\, u_1^B. \tag{10}$$

In the case of a gap state, $\xi < 1$, and the amplitude decays in a geometrical series with alternating sign.

4. Finite chain with different fixtures

The first and last spring shall now be different and have the spring constant C_F. The matrix $\boldsymbol{C}$ then is given by (11).

$$\frac{\boldsymbol{C}}{C_1} = \begin{pmatrix} 0 & 0 & 0 & 0 & \ldots \\ 0 & \zeta + \xi & -\xi & 0 & \ldots \\ 0 & -\xi & 1 + \xi & -1 & \ldots \\ 0 & 0 & -1 & 1 + \xi & \ldots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{11}$$

The variation of C_F changes the impedance matching to the fixed ends. For the 'impedance matched' condition $C_F = C_1$ ($\zeta = C_F/C_1 = 1$), the two gap states are given by (6).

In figure 2 we show the eigenspectra for a $N = 2^5$ chain as a function of ζ for $\xi = 1/2$. Most of the states are essentially independent of C_F while two degenerate states (red solid line in figure 2) move from the top of the lower band to the bottom of the upper band. We note that eventually for C_F/C_1 larger than about 2, two degenerate states develop with frequency larger than ω_{max} (dashed red line in figure 2) where eventually only the outer sites oscillate, going asymptotically to

$$\omega_{top} = \sqrt{\frac{C_F + C_2}{M}} \tag{12}$$

(black thick line in figure 2). This formula can be obtained from the solution of the 2×2 problem in (11) for the two left- or rightmost oscillators. The amplitude ratio of the end oscillator and the next one is $|u_2^B/u_1^B| \approx C_2/C_F = \xi/\zeta \ll 1$. Formula (12) also gives the correct value (6) for $\zeta = 1$ as visualized in figure 2.

A special case is $\zeta = 2$. It entertains a solution with $\tilde{u}_{n+1} = -\tilde{u}_n$ ($n = 2, 3, \ldots, 2N - 1$) and the frequency $\omega_{max} = \sqrt{(2 + \xi)\, C_1/M}$ as can be seen from the first rows of (11). Thus the chain acts as if no fixed borders are present, ergo also no end state is present. The value $\zeta = 2$ therefore separates the regime of end states in the gap $\zeta < 2$ from the regime of the top state $\zeta > 2$ with $\omega > \omega_{max}$.

For the case $\xi > 1$, no gap states exist for fixed ends and $\zeta = 1$. However, $C_F \to \infty$ means that the second inner site becomes fixed which is a B-site on the left and an A-site on the right end. Then the roles of inter- and intra-dimer springs are exchanged and a gap state exists for $\xi > 1$. As depicted in figure 3, a gap state starts to develop for $\zeta > 2$.

Now we investigate the impact of the coupling to the ends C_F on the gap state (for $\xi < 1$) in more detail. The nature of the 'ideal' gap state (for $\zeta = 1$) is that only one type of sites oscillates (B-sites on the left end if the A-site is fixed). Parameters to quantify this are the average position of the mode, counting the oscillators $\nu = 1, \ldots, 2N$ (cmp. (4))

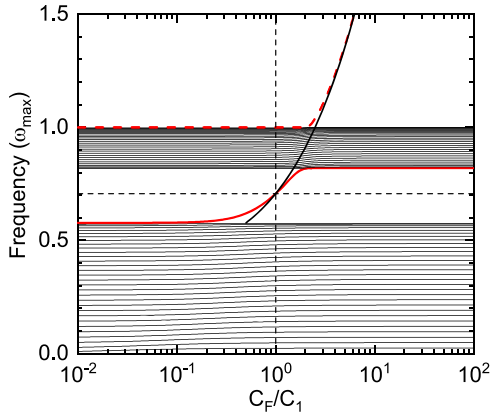

Figure 2. Eigenfrequency spectra of a DLCM with 2^5 dimers and fixed ends as a function of $\zeta = C_F/C_1$ for $\xi = C_2/C_1 = 1/2$. The frequency is scaled to the maximum value from equation (2) for all parameters. The gap states are highlighted in *solid red*, the highest states in *dashed red*. The *black thick line* follows ω_{top} of equation (12).

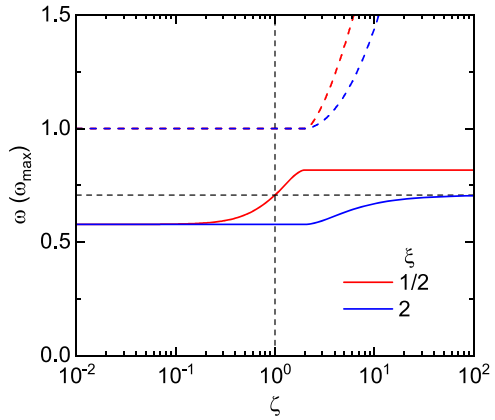

Figure 3. Eigenfrequency spectra of a DLCM with 2^7 dimers and fixed ends as a function of $\zeta = C_F/C_1$ for $\xi = 1/2$ (*red*, same as in figure 2) and $\xi = 2$ (*blue*). The frequency is scaled to the maximum value from equation (2) for all parameters. Only the gap states *solid lines* and the highest states *dashed lines* are shown. The *horizontal dashed line* represents the gap mode energy according to equation (6).

$$\langle \nu \rangle = \sum_{i=1}^{2N} \tilde{u}_i^2 \, i, \tag{13}$$

the standard deviation as width of the mode,

$$\sigma^2 = \sum_{i=1}^{2N} \tilde{u}_i^2 \, (i - \langle \nu \rangle)^2, \tag{14}$$

and the difference of amplitudes of the A- and B-sites, also termed momentum,

$$P = \left| \sum_{i=1}^{N} (u_i^{A\,2} - u_i^{B\,2}) \right| \tag{15}$$

which is 1 for the gap state at $\zeta = 1$ and 0 (or very small for finite chains) for bulk states. For these calculations of course the displacements are normalized with

$$\sum_{i=1}^{2N} \tilde{u}_i^2 = 1. \tag{16}$$

The average position of the gap modes is shown as a function of $\zeta = C_F/C_1$ in figure 4 for the two cases $\xi = 1/2$ and $\xi = 2$. When the gap mode is actually a topological state at the ends, the position is close to oscillators 2 or $2N - 1$, otherwise, when the gap mode is close the top of the bottom band or the bottom of

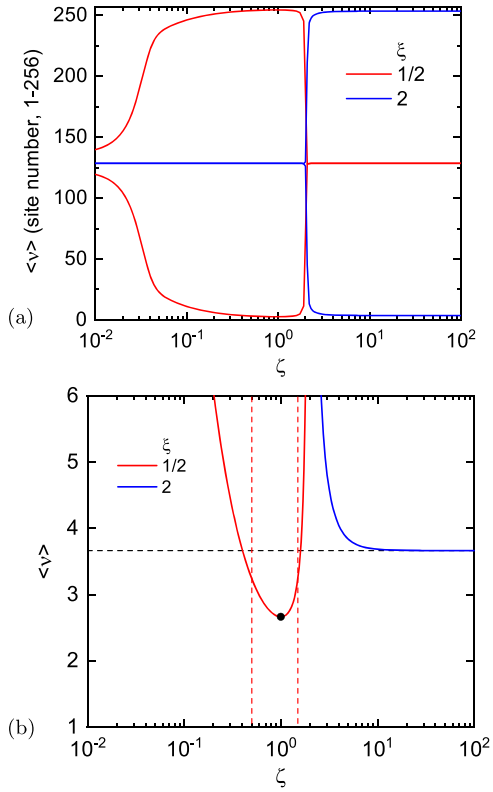

Figure 4. (a) Average position $\langle\nu\rangle$ according to (13) of the two (degenerate) gap modes of a DLCM with 2^7 dimers and fixed ends as a function of C_F/C_1 for $\xi = 1/2$ (*red*) and $\xi = 2$ (*blue*). (b) Zoom into the left end of the chain. The *dot* indicates the analytical result according to (17), the *dashed line* the result from (17) for fixed ends at oscillator positions 2 and $2N-1$. The *dashed red lines* indicate an estimate of the C_F-range for gap states according to (19).

the top band (cmp. figure 3), the average position is in the middle of the chain. There is a rather steep transition between the two regimes. For $\zeta = 1$, the average position can be calculated analytically (for $N \gg 1$) as ($0 < \xi = C_2/C_1 < 1$),

$$\langle\nu\rangle = \frac{2}{1-\xi^2}. \tag{17}$$

Let us look at the vicinity of $\zeta = 1$ (for three different values of ξ, $\xi < 1$) in more detail as depicted in figure 5. For $\zeta = 1$, the momentum is exactly 1, for values around 1 it remains close to but smaller than 1. Then there is a rather sharp transition to values close to zero indicating completely delocalized bulk modes involving both sites. Also the width of the mode follows such scheme. From the solution (10), the width can be calculated in the case $C_F/C_1 = 1$ and large N as

$$\sigma = \frac{2\,\xi}{1-\xi^2} = \xi\,\langle\nu\rangle. \tag{18}$$

These values are indicated in figure 5 as dots and agree with the numerical calculation. Certainly, for (18) to be correct, it is required that the chain is sufficiently long, $2N \gg \sigma$.

End states are generally possible for $0 < \zeta < 2$ (for $\xi < 1$). An estimation of the range of C_F for which a strongly localized gap state exists can be obtained from the condition that the approximation ω_{top} lies within the bandgap, $\omega_{top}(C_F) = \omega_{\pm}(X)$ (cf figure 2). This condition leads to $C_1 - |C_1 - C_2| \leqslant C_F \leqslant C_1 + |C_1 - C_2|$, i.e. $C_2 \leqslant C_F \leqslant 2C_1 - C_2$ for $C_1 > C_2$, or

$$\xi < \zeta < 2 - \xi, \tag{19}$$

as shown as vertical dashed lines in figures 4 (b) and 5.

For 'short' chains, the end modes from the two ends can overlap and results start to deviate from the calculations with $N \ggg 1$. As example the mode width is shown in figure 6 for chains of lengths 2^4, 2^5 and 2^6. In the given plot, no change occurs for $N > 2^6$.

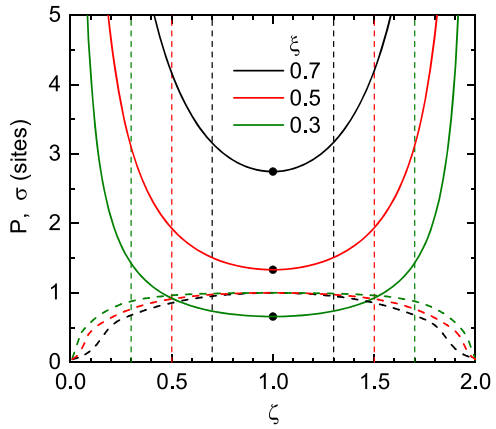

Figure 5. Mode width σ (*solid lines*) according to (14) and momentum P (*dashed lines*) according to (15) for a DLCM with 2^7 dimers and fixed ends as a function of ζ for three different values of $\xi = 0.3, 1/2$ and 0.7 as labeled. The *dots* indicate analytical results according to (18).

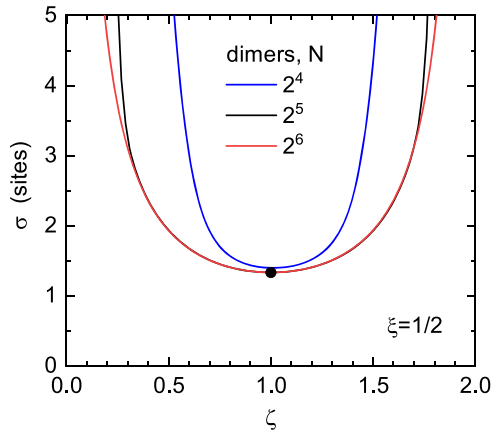

Figure 6. Mode width σ (*solid lines*) according to (14) for a DLCM with N dimers as labeled and fixed ends as a function of ζ for $\xi = 1/2$. The *dot* indicates the analytical result according to (18).

5. Summary

A diatomic linear chain with different inter- and intra-dimer spring constants and fixed ends exhibits topological edge states when the outmost spring has the larger spring constant. The end state tolerates a deviation of the last spring from its ideal stiffness as long as it is smaller than twice that value. The resulting topological state deviates from its ideal frequency value (higher or lower), moves inward the chain and broadens. Analytical results have been given for the ideal chain and selected cases.

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[12] The maximum frequency is then given by $\omega^2_{\max} = (4/\gamma)C_1C_2/(M_AM_B)$. We note that a trivial gap occurs for $M_A \neq M_B$, i.e. for $C_1 = C_2$, the two cases $M_A \gtrless M_B$ are topologically equivalent. A fixed chain with $C_1 = C_2$ and different masses does not exhibit end states