

Fine tuning topological waveguides using asymptotic analysis

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ABSTRACT

We use asymptotic methods to quantify the properties of topological waveguides and show how these concise results can be used very efficiently to design materials with specific, custom specifications. This work presents a general method for studying localised eigenmodes in periodic media with defects. The results of this analysis characterise the existence of localised eigenmodes, determine their eigenfrequencies and quantify the rate at which they decay away from the defect. These results are obtained using both high-frequency homogenisation and transfer matrix analysis, with good agreement between the two methods. This approach is ideally suited to studying problems arising in topological wave physics and we demonstrate its efficacy by studying materials based on the famous Su-Schrieffer-Heeger model.

1. INTRODUCTION

A powerful phenomenon in the design of waveguides is the principle that if a perturbation is made to a periodic structure, then there is a tendency for specific frequencies to be strongly localised in a region of that defect. These localised eigenmodes (often known as defect modes) have eigenfrequencies that are within a stop band of the spectrum of the unperturbed periodic structure and typically decay exponentially away from the defect. This phenomenon can be used to build powerful waveguides, capable of guiding waves of specific frequencies both along straight lines and around corners [1,2]. As is true for metamaterials in general, the increasing complexity and sophistication of these waveguides poses an ever greater challenge for computational simulation. In order to be able to fine tune and optimise designs, it is important that we find novel ways to describe the fundamental properties of these materials with minimal computational cost.

In this work, we will consider metamaterial versions of the famous Su–Schrieffer–Heeger (SSH) model [3]. This model arose in the study of electron localisation in polyacetylene, which features alternating 'weak' and 'strong' coupling between adjacent atoms. Since its discovery, the SSH model has been canonised as the simplest periodic structure with non-trivial topology. There have been many subsequent studies in settings including acoustics [4], photonics [5], elastic plates [6] and mechanical systems [7]. The motivation for studying these topological waveguides is that they enjoy enhanced robustness properties compared to other defect modes.

We will consider two versions of the SSH model. In both models, we arrange metaatoms in an SSH-type pattern, with short and long separation distances playing the role of the 'weak' and 'strong'

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Figure 1: The two SSH-type metamaterials that we will consider in this work. Left: a sequence of lamina, arranged in an SSH-type pattern, which we study using high-frequency homogenisation. Right: an array of three-dimensional bounded material inclusions arranged according to an SSH-type pattern in one dimension, which we study under a high-contrast assumption. In both cases, the lengths l and l' are the crucial parameters which describe the materials' topological wave transmission properties. The materials are periodic with periodicity length L = l + l'.

coupling. The first model is a sequence of lamina, arranged in an SSH-type pattern, which can be described by a one-dimensional equation (on the left in Figure 1). We will perform asymptotic analysis in terms of the scale of periodicity, to compute homogenised fields. The second model is an array of three-dimensional bounded material inclusions arranged according to an SSH-type pattern in one dimension (on the right in Figure 1). We will study the three-dimensional differential problem under a high-contrast assumption: we will assume that the density of the material inside the inclusions is much less than that of the background material and perform asymptotic analysis in terms of the material contrast parameter. This approach will yield a concise characterisation of the subwavelength resonant modes of the system, in terms of the eigenstates of the generalized capacitance matrix. In both models, we will create a localised defect mode by introducing a dislocation to the periodic structure. We will see that by varying the size of the dislocation we are able to create localised eigenmodes with any localised frequency within the band gap. In the case of the one-dimensional model, homogenisation will also allow us to estimate the rate at which the localised eigenmode decays away from the defect, in addition to quantifying its resonant frequency.

2. HOMOGENISATION OF A ONE-DIMENSIONAL MODEL

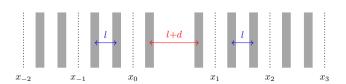
We begin by studying the mathematically simpler one-dimensional model. We model the transmission of time-harmonic waves by studying the Helmholtz problem $u''(x) + \omega^2 c^{-2}(x)u(x) = 0$. Here, c is the material shown in Figure 1 which has c = 1 in the background and $c \ne 1$ on strips that are arranged according to an SSH-type pattern. We can introduce a defect by dislocating, as shown in Figure 2.

Introducing the mesh $\{x_n = 2n : n \in \mathbb{Z}\}$, as shown in Figure 2, we can define transfer matrices $T = T(\omega)$ and $D = D(\omega)$ to be such that

$$\begin{pmatrix} u(x_{n+1}) \\ u'(x_{n+1}) \end{pmatrix} = T \begin{pmatrix} u(x_n) \\ u'(x_n) \end{pmatrix} + \delta_{n,0}(D - T) \begin{pmatrix} u(x_n) \\ u'(x_n) \end{pmatrix}, \quad \text{for } n \in \mathbb{Z}.$$
 (1)

An important goal of this work is to estimate the rate at which a localised eigenmode decays away from the interface. We can estimate this from (1) based on the eigenvalues of the transfer matrices. We immediately have that $u(x_n) = O(|\lambda_1|^n)$ as $n \to \infty$, where λ_1 is the eigenvalue of T with $|\lambda_1| < 1$. Similarly, using the symmetry of the material, we can see that $u(x_n) = O(|\lambda_1|^{-n})$ as $n \to -\infty$. These estimates provide upper bounds on the exponentially decaying envelope of the localised eigenmode, which are observed to be tight. This is indicated by the circles in Figure 3, for the localised eigenmode that exists when $\epsilon = 0.05$.

As well as studying the decay of localised modes, we can use this framework to find their eigenfrequencies. In particular, using ideas from [8], we can show that in order for an eigenmode to



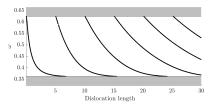


Figure 2: Introducing a dislocation to the one-dimensional SSH structure causes topologically protected mid-gap modes to be introduced. Their eigenfrequencies appear one side of the band gap and successively cross the band gap as the dislocation length increases.

decay its eigenfrequency ω must satisfy

$$\left(-V_{21}(\omega) \quad V_{11}(\omega)\right)D(\omega)\begin{pmatrix} V_{11}(\omega) \\ -V_{21}(\omega) \end{pmatrix} = 0, \tag{2}$$

where $(V_{11}(\omega), V_{21}(\omega))^{\top}$ is the eigenvector of $T(\omega)$ associated to the eigenvalue $|\lambda_1| < 1$. This formula, which was proved in [9, Theorem 2.4], provides an efficient way to find the eigenfrequencies of the localised eigenmodes. This is shown on the right in Figure 2. We see that the dislocation cause successive localised modes to be introduced to the band gap and that their eigenfrequencies cross the band gap as the dislocation length increases.

In the case that the dislocation is small, $d = \epsilon \ll 1$, we can use high-frequency homogenisation, as introduced in [9,10], to approximate the profiles of the localised modes. We assume that the localised eigenmode is a perturbation of the Bloch modes that exist at the edges of the band gap and which are anti-periodic in the sense that $u(x_{n+1}) = -u(x_n)$ for all $n \in \mathbb{Z}$. Introducing the continuous long-scale variable $\eta = \epsilon n$, we express the short-scale discrete variable relative to a single reference mass and set

$$u(x_n) = u(\eta, 0)$$
 and $u(x_{n\pm 1}) = u(\eta \pm \epsilon, \pm 1) = -u(\eta \pm \epsilon, 0).$ (3)

Further to this, we suppose that the localised eigenmode can be approximated as $u = u_0 + \epsilon u_1 + \ldots$ with its eigenfrequency given by $\omega = \omega_0 + \epsilon \omega_1 + \ldots$. This ansatz means the transfer matrices $T^L = T^L(\omega)$ and $T^R = T^R(\omega)$, which depend on ω , support similar expansions in terms of ϵ : $T^L = T_0^L + \epsilon T_2^L + \ldots$ and $T^R = T_0^R + \epsilon T_1^R + \ldots$. Under these approximations, (1) reduces to a hierarchy of equations. Solving these reveals that $u_0(\eta, 0) = f(\eta)$ for some function $f : \mathbb{R} \to \mathbb{R}$ which satisfies the equation

$$0 = f''(\eta) - \mathcal{T}^2 f(\eta) + \delta(\eta) \left[P_{11} f(0) + P_{12} g(0) \right] + \delta(\eta - \epsilon) \left[P_{11} f(0) - P_{12} g(0) \right], \tag{4}$$

where P is the matrix such that $\epsilon P = D - T$, \mathcal{T} is a real-valued constant and g is the envelope of the derivative of the localised mode, which satisfies a similar second-order ordinary differential equation [9]. Solving these equations gives that a localised eigenmode must satisfy

$$|u(x_n)| = \exp\left(-\left((D_0^L)_{11} - (T_0)_{11}\right)|n - 1/2|\right) + O(\epsilon) \quad \text{for } n \in \mathbb{Z},\tag{5}$$

when normalised such that $\max_n |u(x_n)| = 1$. An example of a mode is shown in Figure 3. We see that the homogenised envelope agrees closely with the decay of the eigenmode, as well as with the aforementioned decay estimate in terms of the transfer matrix eigenvalues.

3. ASYMPTOTIC ANALYSIS OF A THREE-DIMENSIONAL MODEL

We now consider the array of three-dimensional material inclusions, which we will study under an assumption of high material contrast. We will use boundary integral operators to characterise the

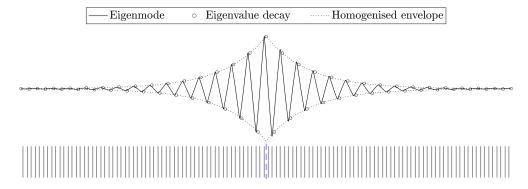


Figure 3: The localised eigenmode for an array of SSH lamina with dislocation size $d = \epsilon = 0.05$. The envelope of the decaying mode is accurately estimated by both the eigenvalues of the transfer matrices (shown by circles) and by the homogenised field (dotted line).

scattering of waves by the inclusions, which can have general (smooth) shapes. Once again, to model the propagation of time-harmonic waves, we study a Helmholtz transmission problem $\Delta u + \omega^2 u = 0$ in $\mathbb{R}^3 \setminus \partial D$ where $D = \bigcup_{n \in \mathbb{Z}} ((D_1 + nL) \cup (D_2 + nL))$ is the union of all the material inclusions. We assume transmission conditions on the boundary ∂D , given by

$$u|_{+} = u|_{-} \quad \text{and} \quad \delta \frac{\partial u}{\partial \nu}|_{+} = \frac{\partial u}{\partial \nu}|_{-},$$
 (6)

where ν is the outward facing unit normal vector and the subscript + and – denote the limits from outside and inside the boundary, respectively. We use Floquet-Bloch to seach for solutions that satisfy $u(x_1, x_2, x_3) = e^{i\alpha L}u(x_1 + L, x_2, x_3)$. We also impose the Sommerfeld radiation condition in the far field on $u - u^{\text{in}}$ where u^{in} is the incoming wave. δ is the material contrast parameter and we will assume that we are in a high-contrast regime such that $0 < \delta \ll 1$. In the case of an acoustic metamaterial, δ is the ratio of the density inside the material inclusions to that in the background material. The small δ regime corresponds to the material inclusions being much less dense than the background and is motivated by the Minnaert resonance of an air bubble in water. Metamaterials based on these principles have been realised by injecting bubbles into polymers [11,12].

We define a resonant mode to be a non-zero solution that exists when $u^{\rm in}=0$. We are interested in characterising the *subwavelength* resonant modes of the system so, in the asymptotic regime when $\delta \to 0$, we search for resonant modes for which $\omega \to 0$ continuously as $\delta \to 0$. This asymptotic approach was developed in [13] and has since been generalised to many different settings, including non-Hermitian and time-varying metamaterials [14]. The main result of the approach is the following theorem, proved in [14], which characterises the subwavelength resonant frequencies of the system in terms of the eigenvalues of the generalized capacitance matrix.

Lemma 1 Given a system of N bounded material inclusions $D_1, \ldots, D_N \in \mathbb{R}^3$ which is repeated periodically in one direction to give $D = \bigcup_{n \in \mathbb{Z}} ((D_1 + nL) \cup \cdots \cup (D_N + nL))$, we can define the associated single layer potential $S_D^{\alpha}: L^2(\partial D) \to H^1(\partial D)$ as

$$\mathcal{S}_D^{\alpha}[\phi](x) = \int_{\partial D} - \sum_{m \in \mathbb{Z}} \frac{\exp(\mathrm{i}\alpha m L)}{4\pi |x-y-mL|} \phi(y) \, \mathrm{d}\sigma(y), \quad \phi \in L^2(\partial D), \ x \in \mathbb{R}^3.$$

Then, S_D^{α} is invertible as a map from $L^2(\partial D)$ to $H^1(\partial D)$, provided $\alpha/L \notin \mathbb{Z}$. Further, we can define the associated generalized capacitance matrix $C^{\alpha} \in \mathbb{C}^{N \times N}$ as

$$C_{ij}^{\alpha} = -\int_{\partial D_i} (\mathcal{S}_D^{\alpha})^{-1} [\chi_{\partial D_J}] \, \mathrm{d}\sigma.$$

Then, C is a Hermitian matrix with real, positive entries on the diagonal.



Figure 4: Introducing a dislocation to the three-dimensional SSH structure causes two topologically protected mid-gap modes to be introduced at either end of the dislocation. Their eigenfrequencies appear at either side of the band gap and converge on a single position within the band gap as the dislocation becomes arbitrarily large.

Theorem 1 A system of N bounded material inclusions $D_1, \ldots, D_N \in \mathbb{R}^3$ which is repeated periodically in one direction to give $D = \bigcup_{n \in \mathbb{Z}} ((D_1 + nL) \cup \cdots \cup (D_N + nL))$ has N subwavelength resonant frequencies, with positive real parts, which are given by

$$\omega_n = \sqrt{\delta \lambda_n} + O(\delta),$$

as $\delta \to 0$, for n = 1, ..., N, where $\lambda_n, n = 1, ..., N$, are the eigenvalues of the associated generalized capacitance matrix.

A consequence of this asymptotic characterisation is that we can use it to show when the SSH structure has a spectral band gap. In particular, in [15] it was proved that (provided the material inclusions are small relative to the distances between them) if $l \neq l'$ then

$$\max_{\alpha} \operatorname{Re}\left(\omega_{1}^{\alpha}\right) = \omega_{1}^{\pi/L} < \omega_{2}^{\pi/L} = \min_{\alpha} \operatorname{Re}\left(\omega_{2}^{\alpha}\right) \tag{7}$$

On top of this, we can use the generalized capacitance matrix to understand the extent to which this band gap is topologically non-trivial. That is, we can use it to calculate topological indices associated to the structure. In particular, we have that the Zak phase [16] is defined as

$$\varphi_j^z := i \int_{V^*} \langle u_j^{\alpha}, \frac{\partial}{\partial \alpha} u_j^{\alpha} \rangle d\alpha, \tag{8}$$

where $\langle \cdot, \cdot \rangle$ denotes the $L^2(D)$ -inner product. Then, we have that

$$\varphi_j^z = -\frac{1}{2} \left[\theta_\alpha \right]_{Y^*} + O(\delta) \tag{9}$$

as $\delta \to 0$, from which we can show that, provided that δ is small and the material inclusions are small relative to the distances between them [17],

$$\varphi_j^z = \begin{cases} 0, & \text{if } l < l', \\ \pi, & \text{if } l > l'. \end{cases}$$
 (10)

This demonstrates that the band gap is topologically non-trivial when l > l'. This is the key property that tells us that, provided we insert the dislocation in one of the shorter gaps (as shown in Figure 4) topologically protected localised modes will be created.

We can introduce localised edge modes by introducing a defect to the SSH structure. (10) tells us that we should introduce the dislocation in one of the short gaps in order to get topologically protected modes. This is sketched in Figure 4. Some of the localised modes are shown in Figure 5. The two localised modes that exist for a finite dislocation are shown. For comparison, we also show the edge mode that exists for the half-infinite structure. The system with finite dislocation can be viewed as a coupled system of two of these half-infinite structures.

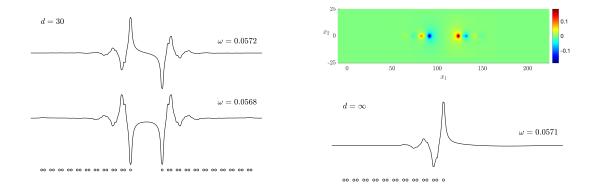


Figure 5: Left: The two localised mid-gap modes that exist for the three-dimensional SSH structure with dislocation length d=30. Top right: A cross section of the higher-order mode with frequency $\omega=0.0572$ and dislocation d=30, to show the decay in all directions (the system is radially symmetric). Bottom right: The localised edge mode that exists in the limiting case, when $d\to\infty$. This is the mode that both of the two mid-gap localised modes converge to.

4. CONCLUSIONS

In conclusion, we have developed a range of asymptotic methods for studying localised modes in periodic and quasiperiodic media. The concise, explicit formulae that are the results of this analysis allow us to fine tune and optimise designs of the waveguides, without the need for expensive simulations. We demonstrated this on waveguides based on the SSH model here, but it could easily be extended to other metamaterial waveguides, offering a convenient approach to study the rich variety of topological waveguides that have been developed.

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