

Lattice-summation methods for band-gap evanescent waves

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1 Background

Band gap materials have a fundamental role in the engineering of wave-control devices, due to their ability to act as insulators for waves of certain frequencies. Here, a *band gap* is a range of frequencies at which waves cannot propagate, as illustrated in Figure 2. In other words, waves at band gap frequencies are evanescent (exponentially decaying), and band gap materials are cornerstone of the recent developments of wave localisation, guiding, and topological robustness [1, 2]. A fundamental quantity is the *decay rate* of evanescent waves, which can be represented through a complex wave momentum. Although its importance has long been recognised in engineering communities, there are few mathematical results or numerical methods to compute this decay rate.

Please note: The next section will give you some flavour of the project. Everything is very briefly described, and there will most likely be things you cannot follow. This is okay! If you are interested in the project, the best thing to do is to reach out directly to me to discuss.

2 Problem formulation

Band gap materials are typically *periodic crystals*. Here, we consider a d -dimensional crystal, for $d \in \{2, 3\}$, of resonators repeated periodically in a lattice Λ . In Figure 1, we sketch an example of a crystal with a square lattice. We let $l_1, \dots, l_d \in \mathbb{R}^d$ denote lattice vectors generating the lattice:

$$\Lambda := \{m_1 l_1 + \dots + m_d l_d \mid m_i \in \mathbb{Z}\}.$$

Bloch's theorem states, roughly speaking, that solutions u to differential equations with periodic coefficients are *quasiperiodic* in the sense that

$$u(x + \ell) = e^{ik \cdot \ell} u(x), \text{ for all } \ell \in \Lambda, \quad (1)$$

for some k , known as the *quasimomentum* of the wave. Here, “quasi-” refers to the fact that k is not uniquely defined, instead, it is defined modulo elements of the dual lattice Λ^* . The dual lattice is generated by lattice vectors $\alpha_1, \dots, \alpha_d$ satisfying $\alpha_i \cdot l_j = 2\pi \delta_{ij}$. The (real) Brillouin zone Y^* is defined as $Y^* := \mathbb{R}^d / \Lambda^*$. Observe that Y^* has the topology of a d -dimensional torus. For band gap modes, the complex Brillouin zone is given by $Y^* + i\mathbb{R}^d$. The *band structure*, or dispersion relationship, is a relationship between the frequency ω and the momentum k of waves.

A cornerstone quantity for band structure calculation is the *quasiperiodic Green's function*. For a real quasimomentum $k = \alpha \in Y^*$, the α -quasiperiodic Green's function $G^{\alpha, \omega}$ satisfies

$$\Delta G^{\alpha, \omega}(x) + \omega^2 G^{\alpha, \omega}(x) = \sum_{m \in \Lambda} \delta(x - m) e^{i\alpha \cdot m}, \quad (2)$$

and is given by

$$G^{\alpha, \omega}(x) = \frac{1}{|Y|} \sum_{q \in \Lambda^*} \frac{e^{i(\alpha + q) \cdot x}}{\omega^2 - |\alpha + q|^2}. \quad (3)$$

The series in (3) converges conditionally. Numerical evaluation of the series is challenging, since the naive idea of just truncating the series require an infeasible number of terms. Nevertheless, this is well-studied problem, and nowadays there exist accelerated, exponentially convergent, series representations [3].

Consider now the Helmholtz equation with complex quasimomentum:

$$\begin{cases} \Delta u + \omega^2 u = 0 \\ u(x + \ell) = e^{ik \cdot \ell} u(x), \quad \text{for all } \ell \in \Lambda. \end{cases} \quad (4)$$

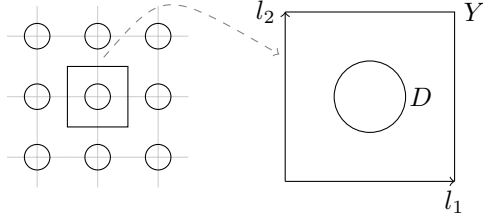


Figure 1: Illustration of the crystal in the case of a square lattice with a single resonator inside the unit cell.

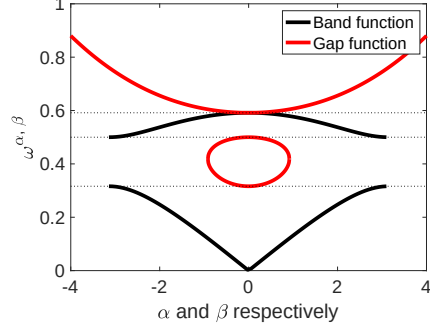


Figure 2: Sketch of the band functions (black) and the gap functions (red) of a band gap material. The regions where the gap functions are nonzero are band gaps, and the magnitude of β describes the decay rate of waves of those frequencies.

for $k = \alpha + i\beta$ for $\alpha \in Y^*$ and $\beta \in \mathbb{R}^d$. The solution $u(x)$ satisfies the complex Floquet condition $u(x + \ell) = e^{i\alpha \cdot \ell} e^{-\beta \cdot \ell} u(x)$. By a change of function, we can pull out the decaying envelope:

$$v(x) := e^{\beta \cdot x} u(x), \quad (5)$$

so that v is not decaying. Substituting into (4), we find that v satisfies

$$\begin{cases} \Delta v - 2\beta \cdot \nabla v + (k^2 + |\beta|^2)v = 0, \\ v(x + \ell) = e^{i\alpha \cdot \ell} v(x), \end{cases} \quad \text{for all } \ell \in \Lambda. \quad (6)$$

In other words, the PDE equation for v is no longer the Helmholtz equation, but v now satisfies the real Floquet-Bloch condition given by the last line of (6). The band gap Green's function $\tilde{G}$ can be defined in a similar fashion:

$$\tilde{G}^{\alpha, \beta, k}(x) = e^{\beta \cdot x} G^{\alpha, k}(x). \quad (7)$$

As a consequence, the band gap Green's function satisfies the following equation

$$\Delta \tilde{G}^{\alpha, \beta, k}(x) - 2\beta \cdot \nabla \tilde{G}^{\alpha, \beta, k}(x) + (k^2 + |\beta|^2) \tilde{G}^{\alpha, \beta, k}(x) = \sum_{m \in \Lambda} e^{i\alpha \cdot m} \delta(x - m), \quad (8)$$

and is given by

$$\tilde{G}^{\alpha, \beta, k}(x) = \frac{1}{|Y|} \sum_{q \in \Lambda^*} \frac{e^{i(\alpha+q) \cdot x}}{k^2 + |\beta|^2 - 2i\beta \cdot (\alpha + q) - |\alpha + q|^2}. \quad (9)$$

The central task lies in the evaluation of (9) or related series.

A simple way to accelerate the convergence is to instead compute the difference $\tilde{G}_R^{\alpha, \beta, k}$:

$$\tilde{G}_R^{\alpha, \beta, k}(x) := \tilde{G}^{\alpha, \beta, k}(x) - \tilde{G}^{\alpha, 0, k}(x) \quad (10)$$

$$= \frac{1}{|Y|} \sum_{q \in \Lambda^*} e^{i(\alpha+q) \cdot x} \frac{2i\beta \cdot (\alpha + q) - |\beta|^2}{((\omega^2 + |\beta|^2) - 2i\beta \cdot (\alpha + q) - |\alpha + q|^2)(\omega^2 - |\alpha + q|^2)}. \quad (11)$$

In two dimensions, the series defining $\tilde{G}_R^{\alpha, \beta, k}(x)$ is absolutely convergent. Although slow, it is now feasible to compute the lattice sums by truncating the series. Since the series is algebraically convergent, it is likely to be a bottleneck of any numerical algorithm. Moreover, this method fails in three dimensions, as the series (11) no longer converges absolutely. Instead, we should follow similar techniques as for the accelerated summation of (3) for computing (9) [3].

3 Goal of the project

The goal of this project is to generalise the lattice-summation methods from real quasimomentum to the case of complex quasimomentum, and use this formulation to compute gap functions associated to band

gap materials. Additionally, an important aspect is to consider exponentially localized defect modes, or topologically protected interface modes, and prove that the decay length can be predicted by the gap functions of the bulk material. Finally, the goal is to study modes in a neighbourhood of the *Rayleigh singularities*, which are points such that

$$|\alpha + q|^2 = \omega^2 + |\beta|^2, \quad \text{and} \quad (\alpha + q) \perp \beta. \quad (12)$$

for some $q \in \Lambda^*$. At these points, the series (9) is ill-defined.

4 Required background

The project is suitable for any student with a solid foundation of PDE-theory and numerical computations, who wants to work in the intersection of theoretical mathematics, numerical analysis, and wave physics. The project can be tailored to the specific background of the student, e.g., a physics-oriented student might focus more on the physical implications, and a numerics-oriented student might focus more on the numerical analysis and implementation.

References

- [1] Habib Ammari, Bryn Davies, and Erik Orvehed Hiltunen. Functional analytic methods for discrete approximations of subwavelength resonator systems. *arXiv preprint arXiv:2106.12301*, 2021.
- [2] Peter Kuchment. An overview of periodic elliptic operators. *Bulletin of the American Mathematical Society*, 53(3):343–414, 2016.
- [3] Chris M Linton. Lattice sums for the helmholtz equation. *SIAM review*, 52(4):630–674, 2010.