ÉCOLE DOCTORALE GALILÉE
Université Sorbonne Paris Nord

Sujet de thèse, École doctorale Galilée, Université Sorbonne Paris Nord

Modèles périodiques discrets pour la propagation des ondes : principe d'absorption limite et conditions limites transparentes.

Titre du sujet : Modèles périodiques discrets pour la propagation des ondes : principe d'absorption limite et conditions limites transparentes.

Unité de recherche : LAGA

Directrices de thèse : Bérangère Delourme (LAGA, Université Sorbonne Paris Nord), Sonia Fliss (POEMS, CNRS-Ensta, Inria)

Co-encadrement : Maxence Cassier (Institut Fresnel, CNRS, Aix-Marseille Université)

Domaine de recherche : mathématiques appliquées

Mots clés : propagation des ondes, EDP, théorie spectrale, analyse numérique

---

1 Resumé

Les cristaux photoniques sont des structures périodiques composées de matériaux di-électriques dans lesquels la propagation des ondes électromagnétiques est très similaire à celle des déplacements des électrons dans des cristaux : il existe des plages de fréquences appelées band gap dans lesquelles les ondes ne se propagent pas et d'autres plages de fréquences, appelées bandes spectrales, dans lesquelles la propagation est possible. Par ailleurs, des perturbations locales ou linéiques de ces structures permettent de créer des modes guidés ou piégés localisés près de la perturbation.

L'étude mathématique et numérique de l'équation des ondes électromagnétiques dans de tels milieux est délicate, notamment parce que le domaine de propagation est en général très grand devant la longueur d'onde, et est donc supposé infini. De plus, quand la fréquence est dans une bande spectrale, il n'y a pas de solution d'énergie finie mais une infinité de solutions bornées. Le principe d'absorption limite permet de restaurer le caractère bien posé du problème, mais son application est souvent complexe, en particulier au voisinage de certaines fréquences correspondant aux singularités dites de Van Hove. Numériquement, il faut pouvoir restreindre les calculs dans une région bornée autour d'une zone d'interet (autour des perturbations par exemple). Les méthodes classiques développées dans le cas où le milieu est homogène sont difficilement applicables dans le cas des milieux périodiques.

Dans cette thèse, nous nous intéresserons à ces 2 difficultés, théorique et numérique, tout d'abord pour des modèles périodiques discrets où des calculs analytiques sont possibles. Nous étudierons en particulier le principe d'absorption limite au niveau des singularités de type Dirac qui apparaissent pour la structure périodique présente une symétrie hexagonale. Pour les aspects numériques, nous adapterons la méthode des demi-espaces raccordés pour le problème avec dissipation (modélisé en rajoutant une petite partie imaginaire à la fréquence), nous ferons l'analyse numérique puis nous étendrons la méthode au cas sans dissipation tout d'abord pour les modèles discrets présentant des perturbations locales puis linéiques et enfin pour des modèles continus.

Summary

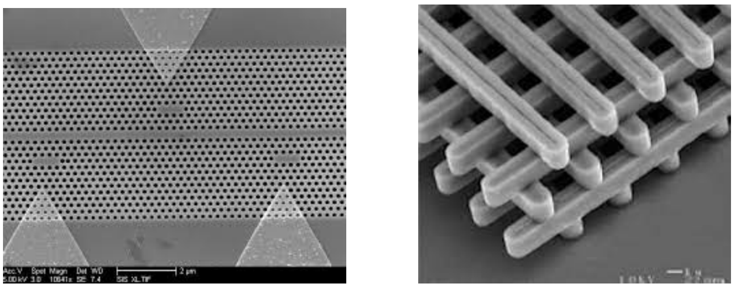
Photonic crystals are periodic structures composed of dielectric materials in which the propagation of electromagnetic waves is very similar to the motion of electrons in crystals: there exist frequency ranges called band gaps in which waves do not propagate, and other frequency ranges, called spectral bands, in which propagation is possible. Furthermore, local or linear perturbations of these structures allow the existence of guided or trapped modes localised near the perturbation.

The mathematical and numerical study of the electromagnetic wave equation in such media is challenging, in particular because the propagation domain is generally very large compared to the wavelength, and is therefore assumed to be infinite. Moreover, when the frequency lies within a spectral band, there is no finite-energy solution but rather infinitely many bounded solutions. The limiting absorption principle makes it possible to restore the well-posedness of the problem, but its application is often complex, particularly in the vicinity of certain frequencies corresponding to so-called Van Hove singularities. Numerically, one must be able to restrict computations to a bounded region around an area of interest (around the perturbations, for instance). Classical methods used when the medium is homogeneous are difficult to apply in the case of periodic media.

In this thesis, we will address these two difficulties — theoretical and numerical — first in the setting of discrete periodic models where analytical computations are possible. In particular, we will study the limiting absorption principle at Dirac-type singularities, which arise when the periodic structure exhibits hexagonal symmetry. Regarding the numerical aspects, we will adapt the half-space matching method to the dissipative problem (modelled by adding a small imaginary part to the frequency), carry out the numerical analysis, and then extend the method to the dissipation-free case, first for discrete models with a local perturbation, then with a line perturbation and finally for continuous models.

2 Scientific context

Photonic crystals, also known as electromagnetic band gap metamaterials, are 2D or 3D periodic media designed to control the light propagation. Indeed, the multiple scattering resulting from the periodicity of the material can give rise to destructive interferences at some range of frequencies. It follows that there might exist intervals of frequencies (called gaps) wherein the monochromatic waves cannot propagate. At the same time, a local perturbation of the crystal can produce defect mid-gap modes, that is to say solutions to the homogeneous time-harmonic wave equation, at a fixed frequency located inside one gap, that remains strongly localised in the vicinity of the perturbation. Those phenomena are of particular interest for a variety of promising applications in optics, for instance the design of highly efficient waveguides [10].



(a) Crystal perturbed on a line

(b) 3D crystal

Figure 1: Examples of photonic crystals that are perturbed (left) or not (right).

A recent advance in this field concerns topological insulators, in which the geometry (via symmetries) of the crystal plays a key role. Like graphene in solid-state physics, topological insulators in photonics are periodic structures that, for certain frequency ranges, behave as insulators in their volume but allow guided modes to propagate along a line defect in the crystal. Among these crystals, those with hexagonal symmetry have remarkable properties (see Fig. 2). On the one hand, some of their dispersion surfaces touch each other conically at points called Dirac points. On the other hand, by breaking the symmetry of the crystal, a gap can be opened at the Dirac points [13, 3] and, after a local perturbation, guided modes can be created: surface waves localised transversely to the defect. Unlike other structures, their existence is resistant to local variations in the defect. These are referred to as topologically protected modes [13]. For certain models, an equality has been demonstrated between a topological index, the Chern number (associated with the crystal), and a spectral flux, which counts the number of guided modes in a gap [5].

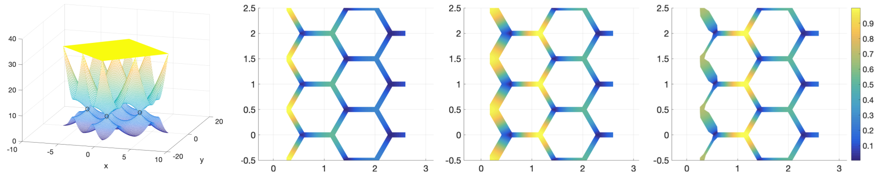


Figure 2: Conical point in the dispersion surfaces of a periodic medium with hexagonal symetry (left), localized guided modes (right)

Mathematically, the analysis (and simulations) of such media is particularly complicated by the fact that the medium is infinite. Indeed, it is easy to show that when the frequency lies in one of the band of the spectrum of the underlying operator, the problem is not well-posed in usual functional framework. In the one hand, in this case, the physical solution, when it exists, does not belong to L^2 due to wave propagation phenomena and a lack of decay at infinity. On the other hand, uniqueness of a bounded solution does not hold in general since within this framework, one cannot make the difference between the so-called outgoing wave (propagating towards infinity), the ingoing wave (propagating from infinity), or any linear combination of them. To select the physical and outgoing wave and restore the uniqueness, one has to add a so-called radiation or outgoing condition. To obtain such condition in practice, one uses the limiting absorption principle, which consists in

1. adding some dissipation, i.e. a small imaginary part to the frequency,
2. solving the well-posed problem with dissipation,
3. studying the limit of the corresponding solution when the dissipation tends to 0.

The limiting absorption principle is a classical approach to study time harmonic wave propagation problems in unbounded domain, see for instance [20, 1, 6]. More recently this approach has been successfully applied to periodic media [8, 16, 9, 11, 12, 19] for so called regular frequencies, frequencies for which the associated dispersion surfaces are regular enough. When the limiting absorption principle holds, the physical solution is defined as the limit solution. The next question concerns the asymptotic at infinity of the physical solution, which enables to derive a radiation condition. In homogeneous media, such radiation condition is the famous Sommerfeld radiation condition. For periodic media, such derivation has been obtained recently in [18, 14]. The final question concerns the well-posedness of the Helmholtz equation without dissipation completed with the radiation condition. This is difficult question that is based on the Rellich theorem for homogeneous media but it is still an open question for periodic media. It is worth mentioning that taking into account this radiation condition from a numerical point of view is also a real challenge.

From a numerical point of view, one has to derive a formulation that is suitable for discretization and simulations. There exist several methods that work well in homogeneous media but they are not adaptable for periodic media (among other the method based on perfectly matched layers). Few years ago, the Halfspace Matching Method has been designed and implemented for periodic media [7] (and also in other context [2]). The method is based on a fairly simple idea: whether the medium is homogeneous or periodic, the solution in a half-plane can be expressed, semi-explicitly, from its trace on the boundary by using an appropriate transformation (the so-called Floquet–Bloch transform). The approach then consists in coupling the representations of the solution in several half-planes with a representation of the solution around the defect. By ensuring compatibility of the representations in the overlapping regions, one arrives at a formulation that couples, through integral operators, the solution in a bounded domain containing the defect with its traces on the boundaries of the half-planes. At present, this is the only numerical method that makes it possible to compute the solution of these wave equations in periodic media. The formulation has been analysed from a theoretical point of view in the dissipative case. However the numerical analysis of the method is still an open question. Moreover, the extension of the method in the case without dissipation is a real challenge. The difficulties are linked to the theoretical ones. The idea will be to use the limiting absorption principle on each step of the method. This approach offers two key advantages: it characterises the physical solution and has a direct numerical counterpart.

3 Objective of the PhD thesis and work plan

The overall objective of this PhD thesis is to study the wave propagation in the frequency regime in perturbed periodic media, starting from the simple discrete graphs models (square and hexagonal lattices), where explicit computations can be done. Even if these problems are interesting by them selves, we aim also to extend the analysis and the method to continuous models. We shall follow two research directions, the first one related to the limiting absorption principle near Dirac points (only for hexagonal lattices), while the second one focuses on the characterization and the computation of the outgoing solution in perturbed periodic media.

Limiting absorption principle for discrete hexagonal graphs

In that part, we consider discrete graph models with honeycomb symmetry. As mentioned above, the dispersion surfaces associated with such a medium touch each other conically at points called Dirac points. The degeneracy (due to the local conical behaviour) of the dispersion surfaces raises intriguing questions about the validity of the limiting absorption principle. We point out that the limiting absorption principle is also strongly related to the limiting amplitude principle: under suitable hypotheses, the solution to the wave equation with harmonic source of the form $e^{\imath\omega t}f(x)$ is, in long time, the product of $e^{\imath\omega t}$ and a solution to the Hemlholtz equation. Understanding the time domain signature of Dirac point (existence of resonances, duration of the transition regime), is of particular interest. Moreover, this result would complete all the existing results on the limiting aborption principle established for so called "regular frequencies" that does not include such singularities.
Methodology and work plan: We shall start by investigating the limiting amplitude principle for hexagonal graphs for frequencies located just above or below the Diract point. Because the dispersion relation is explicit, the analysis results from explicit computations and applications of complex analysis tools [17, 18]. Then, we shall try to pass to the limit, as the frequency approaches the frequency of the Dirac point. We will study then the limiting amplitude principle to deduce how the presence of dirac

points change the behaviour of the solution of the time dependent equation. Possible extensions to quantum graph models and, by asymptotic analysis to two dimensional thin graph like structures [4] may be considered. The result will be illustrated by numerical time domain simulations, where we have to pay particular attention to the honeycomb symmetry in the discretisation step in order to keep the Dirac point.

Dirichlet to Neumann methods for discrete graphs

In this second topic extend the halfspace matching method in the context of periodic media, first for discrete models and then for continuous models. We shall consider theoretical and numerical analysis issues and carry out numerical simulations.

Methodology and work plan

- We shall start again by the analysis of the method with dissipation for square and hexagonal graph. This part appears as an application of [7] to discrete models, where all the unknowns are sequences instead of functions, the Floquet Bloch transform reduced a Fourier series, and the integral equations are replaced by discrete equations.
- We shall make the associated numerical analysis where, for discrete models, the infinite sums have to be truncated, leading to an approximation error that has to be controlled.
- We shall pass to the limit as the dissipation goes to zero. We shall consider (1)frequencies belonging to a gap of the spectrum of the associated operator, where the analysis should be easier since the solution being decaying at infinity, (2)frequencies in the bands of the spectrum of the operator.
- whereas the previous steps concern local perturbations, we shall consider also the presence of line perturbations. The last case is of practical interest for applications, in particular to study the robustness of guided modes that are so called topologically protected, to the presence of local perturbation [13].

All these steps would be achieved first for square and hexagonal discrete models, then to quantum graphs (extension should be almost straightforward), then to two dimensional thin structures that are asymptotically close to quantum graphs and, finally to 2D periodic continuous models. If time allows, we want to consider the presence of line perturbations or more generally the case of a junction of two, three or four waveguides, with possible application to the simulation of topologically stable guided modes. Finally, we have to compare the efficiency of the method with another numerical method that can be derived from [14, 18, 15].

References

[1] Agmon S. Spectral properties of Schrödinger operators and scattering theory. Annali della Scuola Normale Superiore di Pisa-Classe di Scienze. 1975;2(2):151-218.

[2] Anne-Sophie Bonnet-Ben Dhia, Fliss, Sonia, et Tonnoir, Antoine. The halfspace matching method: A new method to solve scattering problems in infinite media. Journal of Computational and Applied Mathematics, 2018, vol. 338, p. 44-68.

[3] M. Cassier and M. Weinstein, High contrast elliptic operators in honeycomb structures, SIAM Journal MMS 19 (4) (2021), pp. 1784-1856.

[4] B. Delourme and S. Fliss, Guided modes in a hexagonal periodic graph like domain, SIAM Journal MMS 22 (3) (2024), pp. 1196-1245

[5] Drouot, Alexis. The bulk-edge correspondence for continuous honeycomb lattices. Communications in Partial Differential Equations 44.12 (2019): 1406-1430.

[6] Eidus D. The limiting absorption and amplitude principles for the diffraction problem with two unbounded media. Communications in mathematical physics. 1986 Mar;107(1):29-38.

[7] Fliss, Sonia, and Patrick Joly. Exact boundary conditions for time-harmonic wave propagation in locally perturbed periodic media. Applied Numerical Mathematics 59.9 (2009): 2155-2178.

[8] Fliss S, Joly P. Solutions of the time-harmonic wave equation in periodic waveguides: asymptotic behaviour and radiation condition. Archive for rational mechanics and analysis. 2016 Jan;219(1):349-86.

[9] Hoang V. The limiting absorption principle for a periodic semi-infinite waveguide. SIAM Journal on Applied Mathematics. 2011;71(3):791-810.

[10] Johnson, Steven G., and John D. Joannopoulos. Photonic crystals: the road from theory to practice. Springer Science & Business Media, 2001.

[11] Kirsch A, Lechleiter A. A radiation condition arising from the limiting absorption principle for a closed full-or half-waveguide problem. Mathematical Methods in the Applied Sciences. 2018 Jul 15;41(10):3955-75.

[12] Kirsch A, Lechleiter A. The limiting absorption principle and a radiation condition for the scattering by a periodic layer. SIAM Journal on Mathematical Analysis. 2018;50(3):2536-65.

[13] Lee-Thorp, James P., Michael I. Weinstein, and Yi Zhu. "Elliptic operators with honeycomb symmetry: Dirac points, edge states and applications to photonic graphene." Archive for Rational Mechanics and Analysis 232.1 (2019): 1-63.

[14] Lescarret, Vincent. "Asymptotic expansion of wave scattering in a periodic plane." Journal of Mathematical Physics 65.12 (2024).

[15] E. Letournel, Analyse théorique et numérique de modèles statiques et dynamiques en calcul de structure électronique, PhD dissertation, (2024)

[16] Radosz, Maria. New limiting absorption and limit amplitude principles for periodic operators. Zeitschrift für angewandte Mathematik und Physik 66.2 (2015): 253-275.

[17] Shaban, W. et Vainberg, Boris. Radiation conditions for the difference Schrödinger operators. Applicable Analysis, 2001, vol. 80, no 3-4, p. 525-556.

[18] Shanin, Andrey V., et al. Double Floquet-Bloch transforms and the far-field asymptotics of Green's functions tailored to periodic structures. Physical Review B 110.2 (2024): 024310.

[19] Vainberg, B. Asymptotic methods in equations of mathematical physics. CRC Press, 2024

[20] Wilcox, Calvin H. Wave operators and asymptotic solutions of wave propagation problems of classical physics, Archive for Rational Mechanics and Analysis 22.1 (1966): 37-76.