Mathematical Modeling in Optics

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Thèse présentée pour obtenir le grade de

DOCTEUR DE L'ÉCOLE POLYTECHNIQUE

spécialité : Mathématiques Appliquées

par

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Quelques Modélisations Mathématiques en Optique

Soutenue le 24 septembre 2004 devant le jury composé de

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	Jean-Claude Nédélec	Président

à mon grand-père,
pour son immense générosité,
et les merveilleux souvenirs qu'il m'a laissés.

à ma mère et à mon père.

Nous ne vivons que pour découvrir la beauté.
Tout le reste n'est qu'une forme d'attente.
Khalil Gibran 1883–1931

Je ne me demande même pas si, aux yeux de l'Eglise, je passe pour un croyant, à mes yeux un croyant est simplement celui qui croit en certaines valeurs – que je résumerais en une seule : la dignité de l'être humain. Le reste n'est que mythologies, ou espérances.

Amin Maalouf (Les Identités meurtrières)

Moi, Hassan fils de Mohamed le peseur, moi, Jean-Léon de Médicis, circoncis de la main d'un barbier et baptisé de la main d'un pape, on me nomme aujourd'hui l'Africain, mais d'Afrique ne suis, ni d'Europe, ni d'Arabie. On m'appelle aussi le Grenadin, le Fassi, le Zayyati, mais je ne viens d'aucun pays, d'aucune cité, d'aucune tribu. Je suis fils de la route, ma patrie est caravane, et ma vie la plus inattendue des traversées.

Mes poignets ont connu tour à tour les caresses de la soie et les injures de la laine, l'or des princes et les chaînes des esclaves. Mes doigts ont écarté mille voiles, mes lèvres ont fait rougir mille vierges, mes yeux ont vu agoniser des villes et mourir des empires.

De ma bouche, tu entendras l'arabe, le turc, le castillan, le berbère, l'hébreu, le latin et l'italien vulgaire, car toutes les langues, toutes les prières m'appartiennent. Mais je n'appartiens à aucune. Je ne suis qu'à Dieu et à la terre, et c'est à eux qu'un jour prochain je reviendrai.

Et tu resteras après moi, mon fils. Et tu porteras mon souvenir. Et tu liras mes livres. Et tu reverras alors cette scène : ton père, habillé en Napolitain sur cette galée qui le ramène vers la côte africaine, en train de griffonner, comme un marchand qui dresse son bilan au bout d'un long périple.

Mais n'est-ce pas un peu ce que je fais : qu'ai-je gagné, qu'ai-je perdu, que dire au Créancier suprême ? Il m'a prêté quarante années, que j'ai dispersées au gré des voyages : ma sagesse a vécu à Rome, ma passion au Caire, mon angoisse à Fès, et à Grenade vit encore mon innocence.

Amin Maalouf (Léon l'Africain)

– Dove ce li ha, gli occhi, il mare?
– ...
– Perché ce l'ha, vero?
– Sì.
– E dove cavolo sono?
– Le navi.
– Le navi cosa?
– Le navi sono gli occhi del mare.
Rimane di stucco, Bartleboom. Questa non gli era proprio venuta in mente.
– Ma ce n'è a centinaia di navi...
– Ha centinaia di occhi, lui. Non vorrete mica che se la sbrighi con due.
Effettivamente. Con tutto il lavoro che ha. E grande com'è. C'è del buon senso, in tutto quello.
– Sì, ma allora, scusa...
– Mmmmh.
– E i naufraghi? Le tempeste, i tifoni, tutte quelle cose lì... Perché mai dovrebbe ingoiarsi quelle navi, se sono i suoi occhi?
Ha l'aria perfino un po' spazientita, Dood, quando si gira verso Bartleboom e dice
– Ma voi... voi non li chiudete mai gli occhi?

Alessandro Baricco (Oceano Mare)

Remerciements

Je tiens d'abord à remercier Habib Ammari pour m'avoir accueilli au CMAP et proposé un sujet de thèse. Je lui suis très reconnaissant pour la confiance qu'il m'a accordée et l'encadrement dont j'ai bénéficié. Son activité débordante ne l'a pas empêché d'être toujours à l'écoute, partageant sa manière d'aborder les mathématiques qui les rend merveilleuses.

Ses talents scientifiques exceptionnels ne sauraient masquer ses qualités humaines tout aussi exceptionnelles. Sa modestie, sa sincérité, sa générosité et bien d'autres qualités encore ont largement contribué à faire de cette thèse une aventure agréable.

Cher Habib, je t'exprime ma plus profonde gratitude. GRAZIE MILLE ! !

Eric Bonnetier, malgré un emploi du temps chargé a accepté avec enthousiasme de rapporter sur cette thèse. Je lui suis infiniment reconnaissant pour le travail qu'il a effectué.

Je suis tout aussi reconnaissant à David Dobson pour l'intérêt qu'il a porté à mon travail en acceptant d'être rapporteur pour cette thèse.

C'est un honneur pour moi de compter Guy Bouchitté et Patrick Joly parmi les membres de mon jury. Je suis sensible à leur présence et je les en remercie.

Enfin, il m'est bien difficile d'exprimer en quelques mots l'honneur et le plaisir que me fait Jean-Claude Nédélec en acceptant de présider mon jury.

A mon arrivée au CMAP, j'ai trouvé une ambiance merveilleuse. J'ai fait la connaissance de tant de personnes qui contribuent à la bonne ambiance dans le labo. Parmi ces personnes, je citerais Jeanne. Bien plus que secrétaire du laboratoire, c'est une mère, une amie et une fée capable de faire disparaître par un coup de baguette magique toutes les tracasseries administratives qui puissent exister. Je n'oublierais pas non plus Liliane et Véronique toujours souriantes et extrêmement serviables. J'ai aussi eu la chance d'assister à la dernière année de Geo au sein du labo et je n'oublierai jamais sa gentillesse.

Mes problèmes informatiques, de quelque nature qu'ils aient pu être, n'ont jamais pu me tracasser assez longtemps. Il suffisait que je m'adresse à l'un des informaticiens du labo : Sylvain, Aldjia, Natacha ou Erwan, pour que le problème soit aussitôt résolu. Tous sont aussi compétents que serviables.

Aldjia a été une véritable amie. Discuter avec elle a toujours été un moment très agréable. J'apprécie beaucoup sa franchise et sa générosité sans limites.

Sylvain a été un ami très précieux. Il a toujours été là quand surgissait une tracasserie informatique, surtout quand je l'invitais autour d'une tasse de "thé". Bien que, assez rapidement, nos voies aient divergé, lui vers l'Est, moi vers la Méditerranée, qu'il vante les mérites de la Vodka artisanale et que je continue à lui préférer, et de loin, le Limoncello et l'Amaro, qu'il adore le goulasch et que je me régale avec la pizza napolitaine et le panino à la rate de Palerme, notre amitié reste intacte.

Robert Brizzi (à prononcer à l'italienne) aussi a été un très grand ami. Toujours souriant et aimable, sauf quand on osait défendre le libéralisme en salle café. Là, il suffit à l'égaré de se rappeler la couleur très sombre de la ceinture de karaté de Bob pour qu'il rentre aussitôt dans le rang et entonne l'Internationale. Avec moi, il ne risque pas de se fâcher : je connais par cœur *Bella ciao* et *Fischia il vento*.

Et puis comment allais-je oublier Vincent, notre très cher directeur, toujours disponible et de bonne humeur. J'apprécie la confiance qu'il accorde aux membres du labo autant que les chocolats qu'il dispose sur son bureau et qu'il m'arrive quelquefois d'en piquer à son insu.

Je citerais aussi Hervé Maillot, François Jouve, Kamel Hamdache, François James, Christian Léonard, Patrick Cattiaux, Sylvie Mas-Gallic, Rémi Munos, Toufic Abboud, Kamal Abboud dont l'amitié m'est très chère.

Il y a aussi les thésards et ex-thésards : Charles, Karima, Benjamin, Patrice, Katia, Kaouthar, Erwan, Ignacio, Gabriel, Sébastian, Karim, Habib...

Je voudrais saluer par ailleurs les Italiens qui sont passés par le labo et grâce auxquels j'ai énormément progressé en italien. Je citerais : Paola, Luca, Annalisa Buffa et la récemment arrivée Claudia. *Vi ringrazio tanto per questo, l'Italia è bella con voi!!*

Mes remerciements vont aussi à Gang Bao qui m'avait accueilli au Michigan State University pour mon stage de DEA et qui continue à porter un intérêt à mon travail.

Enfin, tout récemment j'ai pu faire la connaissance d'Elisa Francini, Elena Beretta, Rolando Magnanini et son étudiant Giulio Ciraolo à Florence. J'ai été très touché par leur hospitalité et par l'enthousiasme qu'ils ont manifesté à ma thèse. *Spero di ritrovarvi un giorno a Firenze!*

Enfin, je tiens à remercier mes parents pour leur soutien et leurs encouragements omniprésents.

La liste des personnes que je dois remercier est bien longue encore et si je devais m'étendre sur les qualités de chacun, je risquerais de faire subir à ma thèse ce que *Ibn Khaldûn*, à une autre échelle, a fait subir à son livre d'histoire universelle *Kitab al-'Ibar*. Cet historien et sociologue tunisien du XIV^e^ siècle, qui, voulant écrire une introduction à son livre, a réalisé un traité de sociologie. Aujourd'hui, tous ceux qui le connaissent le présentent comme l'auteur de *Al Muqaddima* (L'Introduction), bien peu connaissent *Kitab al-'Ibar*.

En conséquence, j'implore l'indulgence de ceux qui ne se verront pas cités, qu'ils sachent que je ne les oublierai jamais.

GRAZIE MILLE A TUTTI!!!

Contents

Présentation générale

Cette thèse étudie trois problèmes émanant de deux grands sujets de l'optique : les matériaux non linéaires et les matériaux à bandes interdites de photons (BIP) connus aussi sous le nom de cristaux photoniques. Un intérêt particulier est accordé à la formulation des problèmes mathématiques et à leur analyse rigoureuse. L'importance fondamentale de ces deux sujets de l'optique est incontestable. Ils présentent des sources potentielles de solutions technologiques applicables à des domaines industriels tels que les télécommunications, le calcul ou le stockage de données.

Tous les milieux optiques sont non linéaires. Cependant, les effets non linéaires sont en général tellement faibles qu'il est quasiment impossible de les observer sans le recours à des impulsions laser de haute intensité. La modélisation mathématique de l'optique non linéaire dans les couches minces est plus complexe que celle de l'optique linéaire étudiée dans la littérature par plusieurs auteurs [14, 15, 16, 3, 4]. Dans le cas non linéaire, la propagation des ondes électromagnétiques obéit au système d'équations de Maxwell non linéaires, d'où la nécessité de l'étude des EDP non linéaires. Il faut noter aussi que l'amplitude de l'onde incidente, qui ne joue aucun rôle dans le cas linéaire, acquiert de l'importance dans le cas non linéaire. Par ailleurs, comme les propriétés des matériaux non linéaires sont généralement caractérisées par des tenseurs, les modèles vectoriels deviennent inévitables dans les situations générales.

L'objectif du Chapitre 2 est l'étude de la théorie électromagnétique de la diffraction par des couches minces non linéaires dans le cadre de l'approximation de la pompe non déplétée. Depuis son apparition au début des années 1960, un progrès rapide et continu a été réalisé dans le domaine de l'optique non linéaire. Une des innombrables applications importantes des phénomènes de l'optique non linéaire est une méthode permettant d'obtenir des émissions cohérentes à des longueurs d'onde plus courtes que celles des lasers disponibles, à travers le procédé de la génération de la seconde harmonique.

Notre motivation principale dans le Chapitre 2 est de donner une formulation rigoureuse de l'effet des couches minces de matériaux non linéaires dans l'approximation de la pompe non déplétée. Dans cette approximation, les équations de Maxwell sont réduites à un système d'équations de Helmholtz couplées qui sont vérifiées par le champ fondamental et par la seconde harmonique. Nous déduisons de façon rigoureuse des formules asymptotiques pour les champs bidimensionnels de l'onde fondamentale et de la seconde harmonique associées à la couche mince de matériau non linéaire. Notre approche est basée sur les techniques de potentiel de couche à travers les formules de représentation intégrale des champs permettant de se passer de l'utilisation (et de son adaptation à notre contexte) du résultat de régularité hautement non trivial de Li et Vogelius [50].

Notre intérêt pour de telles formules asymptotiques est dû au fait qu'elles fournissent des outils très puissants pour la résolution de problèmes d'optimisation [12, 51, 55]. Dans [67, 7, 5, 3], des développements asymptotiques de ce type pour des inclusions électromagnétiques (de matériau linéaire) de petit diamètre ont déjà été explicités. Cependant, ces développements sont par nature totalement différents de ceux trouvés dans ce chapitre. La dégénérescence des courbes associées à la couche mince rend compliquée une dérivation rigoureuse, basée sur les potentiels de couche, des perturbations de premier ordre des champs fondamental et de seconde harmonique.

Les Chapitres 3 et 4 sont consacrés à la modélisation mathématique des cristaux photoniques.

Les cristaux photoniques sont des structures périodiques composées de matériaux diélectriques conçues afin de présenter des propriétés intéressantes, telles que des gaps dans leurs spectres, pour la propagation des ondes électromagnétiques classiques. En d'autres termes, les ondes électromagnétiques monochromatiques de certaines fréquences ne peuvent pas exister dans de telles structures. Les milieux avec des bandes interdites ont plusieurs applications potentielles, par exemple, dans les communications optiques, les filtres, les lasers et les micro-ondes. Voir [37, 38, 60, 47] pour une introduction aux cristaux photoniques. Le phénomène de bandes interdites de photons peut être réalisé dans des matériaux structurés périodiquement ayant une périodicité de l'ordre de la longeur d'onde optique. Avec un choix adéquat de la structure du cristal photonique, de la dimension de la cellule fondamentale et des matériaux diélectriques composant le cristal, les ondes électromagnétiques dans certaines bandes de fréquence peuvent être bannies du cristal [69]. Alors que les conditions nécessaires pour l'existence de bandes interdites dans le cas général ne sont pas connues, Figotin et Kuchment ont donné un exemple de milieux périodiques à haut contraste d'indice où les bandes interdites existent et peuvent être caractérisées [34, 35]. D'autres structures à bandes interdites ont été trouvées à travers des approches numériques ou par la physique expérimentale. Voir [24, 22, 25, 9, 28].

Dans le but de réaliser des lasers, des filtres, des fibres ou des guides d'ondes, il est nécessaire d'avoir des modes autorisés dans le gap. Ces modes sont obtenus en introduisant des défauts localisés à la périodicité et correspondent à des valeurs propres isolées de multiplicité finie à l'intérieur du gap. La fréquence du mode de défaut dépend fortement de la nature du défaut. Figotin et Klein ont prouvé rigoureusement que l'introduction de défaut à la structure périodique, c'est-à-dire une perturbation à support compact, peut créer des modes de défaut, qui sont des ondes stationnaires à décroissance exponentielle loin de la perturbation dont la fréquence se situe dans le gap [30, 31, 29]. Voir aussi Ammari et Santosa [6] et Kuchment et Ong [48] pour les preuves d'existence de modes, exponentiellement localisés, guidés par un défaut linéaire dans les cristaux photoniques.

Les modes de défaut aussi bien que les modes guidés associés respectivement à des défauts compacts et linéaires sont calculés par une technique dite de la *supercell*. Cette technique consiste en la restriction des calculs à un domaine borné englobant le défaut et contenant assez de cellules du cristal photonique de référence avec des conditions aux limites périodiques sur le bord du domaine.

Les conditions aux limites sur la *supercell* sont, en principe, sans importance si le mode est suffisamment confiné. Comme on veut déterminer uniquement les modes de défaut ou les modes guidés situés dans le gap, sans encombrement de calcul et de mémoire dû à la détermination de toutes les valeurs propres associées à la *supercell* situées dans le spectre continu, on formule le problème comme étant celui de la détermination des valeurs propres les plus proches de la fréquence centrale du gap.

La méthode de la *supercell* montre un très bon accord avec les résultats expérimentaux et semble d'une très grande précision. Cependant, les études analytiques et les preuves rigoureuses de la convergence de cette technique font largement défaut.

Dans le Chapitre 3, nous démontrons la convergence de cette méthode numérique et quantifions sa précision. Bien qu'on puisse obtenir des résultats analogues pour le cas des équations de Maxwell, nous n'étudions que les cas des ondes électromagnétiques polarisées TM et TE dans les cristaux photoniques bidimensionnels. Des résultats d'expériences numériques sont présentés afin d'illustrer les principaux résultats de convergence.

Les fibres optiques photoniques constituent le thème central du dernier chapitre.

Les fibres optiques trouvent aujourd'hui de grands domaines d'application tels que les télécommunications, les capteurs, la spectroscopie et la médecine [17]. Les fibres optiques ordinaires guident la lumière par réflexion interne totale ce qui nécessite un indice de réfraction dans le cœur plus grand que celui de l'enveloppe. Ce mécanisme physique a été découvert et exploité technologiquement depuis plusieurs années. Cependant, dans la dernière décennie, la recherche dans la conception de nouveaux matériaux a donné la possibilité de localiser et de contrôler la lumière dans les cavités et les guides d'onde par l'effet des bandes interdites de photons.

Dans [46], Knight et ses collègues décrivent un type de fibres optiques totalement différent, dont le cœur possède un indice de réfraction inférieur à celui du milieu environnant ce qui anéanti la possibilité de réflexion interne totale. Ce mécanisme permet d'acheminer la lumière dans de l'air retardant ainsi l'apparition des effets non linéaires.

Le cœur de la nouvelle fibre est principalement un défaut entouré par une structure périodique de trous d'air allant le long de la fibre. La lumière, expulsée de la structure périodique entourant le cœur, ne peut que se propager le long du défaut. La nouvelle fibre opère effectivement par l'effet de bande interdite. Nous appellerons de telles structures des fibres optiques photoniques (FOP).

Dans le Chapitre 4, nous modélisons la propagation des ondes électromagnétiques dans les fibres optiques photoniques. Nous donnons un cadre mathématique permettant de comprendre leurs propriétés inhabituelles comparées aux fibres optiques classiques opérant par le mécanisme de réflexion totale et nous développons des outils théoriques pour la modélisation de ces fibres optiques photoniques. Nous étudions leurs propriétés de dispersion et vérifions le confinement exponentiel des modes guidés. Enfin, nous illustrons les principaux résultats par des exemples numériques.

Les trois chapitres de ce document sont autonomes et peuvent être lus indépendamment.

Chapter 1

Introduction

This thesis addresses three problems in two areas of optical science: nonlinear materials and photonic band gap structures, also known as photonic crystals. Particular emphasis is put on the formulation of the mathematical problems and their rigorous analysis. The fundamental importance of these two areas of optics is clear. They provide enabling technology potentially applicable to numerous industries, including communication, computing, and data storage.

All optical media are nonlinear. However, the nonlinearity is generally so weak that is impossible to observe without the use of high intensity laser beams. Mathematical modeling of nonlinear optics in thin layers is more difficult than that of linear optics studied in the literature by many authors [14, 15, 16, 3, 4]. In the nonlinear case, the electromagnetic wave propagation is now governed by the system of nonlinear Maxwell's equations, *i.e.*, nonlinear PDEs need to be studied. Also, the amplitude of the incident wave, which has no role in the linear case, plays an important role in the nonlinear case. Furthermore, since nonlinear material properties are usually characterized by tensors, vectorial models become inevitable in the general situation.

The purpose of Chapter 2 is to study the electromagnetic theory of diffraction from nonlinear thin layers in the undepleted-pump approximation. Since its birth in the early 1960s, rapid and continuous progress has been made in the field of nonlinear optics. One of the many important applications of nonlinear optical phenomena is a method for obtaining coherent radiation at a wavelength shorter than that of available lasers, through the process of second-harmonic generation (SHG).

Our main aim in Chapter 2 is to rigorously derive the effect of thin layers of nonlinear material in the undepleted-pump approximation. In this approximation, the nonlinear Maxwell equations reduce to two coupled Helmholtz equations for the fundamental and the second-harmonic fields. We rigorously derive asymptotic formulas for two-dimensional fundamental and second-harmonic fields associated with thin layers of nonlinear materials. Our approach is based on layer potential techniques through integral representation formulas of the fields, avoiding the use (and the adaptation to our context) of the highly-nontrivial regularity results of Li and Vogelius [50].

Our interest in such asymptotic formulas owes to the fact that they provide extremely powerful tools to solve optimization problems [12, 51, 55]. In [67, 7, 5, 3], asymptotic expansions of this kind for electromagnetic inclusions (of linear material) of small diameter have been already derived. However, they are by nature completely different from those derived in this chapter. The degeneracy of the curves associated with the thin layer complicates a mathematically rigorous derivation, based on layer potentials, of the leading-order perturbations in the fundamental and second-harmonic fields.

Chapters 3 and 4 are devoted to mathematical modeling of photonic crystals.

Photonic crystals are periodic structures composed of dielectric materials and designed to exhibit interesting properties, such as spectral band gaps, in the propagation of classical electromagnetic waves. In other words, monochromatic electromagnetic waves of certain frequencies do not exist in these structures. Medium with band gaps have many potential applications, for example, in optical communications, filters, lasers, and microwaves. See [37, 38, 60, 47] for an introduction to photonic crystals. The photonic band gap (PBG) effect may be achieved in periodically structured materials having a periodicity on the scale of the optical wavelength. By appropriate choice of the crystal structure, the dimensions of the periodic lattice, and the properties of the component materials, propagation of electromagnetic waves in certain frequency bands (the photonic band gaps) may be forbidden within the crystal [69]. While necessary conditions under which band gaps exist in general are not known, Figotin and Kuchment have produced an example of high-contrast periodic medium where band gaps exist and can be characterized [34, 35]. Other band gap structures have been found through computational and physical experiments. See [24, 22, 25, 9, 28].

In order to fabricate lasers, filters, fibers, or waveguides, allowed modes are required in the band gaps. These modes are obtained by creating localized defects in the periodicity and correspond to isolated eigenvalues with finite multiplicity inside the gaps. The defect mode frequency strongly depends on the defect nature. Figotin and Klein rigorously proved that when a defect is introduced into the periodic structure, *i.e.*, a perturbation with compact support, it is possible to create a defect mode, which is an exponentially confined standing wave whose frequency lies in the band gap [30, 31, 29]. See also Ammari and Santosa [6] and Kuchment and Ong [48] for the issue of existence of exponentially confined modes guided by line defects in photonic crystals.

The defect modes as well as the guided modes associated with compact and line defects, respectively, are computed via the supercell technique. This technique consists in restricting the computations on a domain surrounding the defect with sufficient bulk crystal with periodic conditions on its boundary. The boundary conditions on the supercell are, in principle, irrelevant if the mode is sufficiently confined. Since one would like to compute only the defect or the guided modes in the band gap, without the waste of computation and memory of finding all the eigenvalues associated with the supercell belonging to the continuous spectrum, one states the problem as one of finding the eigenvalues and eigenvectors closest to the mid-gap frequency.

The supercell method shows very good concordance with experimental results and seems to be very accurate. However, analytic studies and rigorous proofs of convergence of this technique are essentially absent.

In Chapter 3 we address some of the basic issues of the supercell method, prove the convergence of this numerical technique, and quantify its accuracy. Although one can obtain analogous results for the case of full Maxwell equations, we only address the cases of transverse electric (TE) and transverse magnetic

(TM) polarized electromagnetic waves in two-dimensional photonic structures. Results of numerical experiments are given to illustrate our main findings.

The central topic of Chapter 4 is photonic crystal fibers.

Optical fibers know today a wide use in areas covering telecommunications, sensor technologies, spectroscopy, and medicine [17].

Ordinary optical fibers guide light by total internal reflection, which relies on the refractive index of the central core being greater than that of the surrounding cladding. This physical mechanism has been known and exploited technologically for many years. However, within the past decade the research in new purpose-built materials has opened up the possibilities of localizing and controlling light in cavities and waveguides by the photonic band gap effect (PBG).

In [46], Knight and colleagues describe a fundamentally different type of optical fiber, one that has a core with a lower refractive index than the cladding and so rules out the possibility of internal reflection. Instead, light is guided by a mechanism which allows it to be piped through air.

The core of the new fiber is essentially a defect surrounded by a periodic array of air holes running along the entire length of the fiber. The defect acts like the core of an optical fiber. Light, which is expelled from the periodic structure surrounding the core, can only propagate along it. The new fiber operates truly by the photonic band gap effect. We refer to such a structure as a photonic crystal fiber (PCF).

In Chapter 4 we model the propagation of electromagnetic waves in photonic crystal fibers. We give a mathematical framework for understanding their very unusual properties compared with the conventional fibers, attributed to an operation of the well-known mechanism of total reflection, and develop theoretical tools for the modeling of these photonic crystal fibers. We study their dispersion properties and verify the exponential confinement of guided modes. We illustrate the main findings of the investigation in numerical examples.

The three chapters of this manuscript are self-contained and can be read independently.

Chapter 2

Second-harmonic generation in the undepleted-pump approximation

2.1 Introduction

In this chapter, we study the electromagnetic theory of diffraction from nonlinear thin layers in the undepleted-pump approximation. Since its birth in the early 1960s, rapid and continuous andvances have been made in the field of nonlinear optics. One of the many important applications of nonlinear optical phenomena is a method for obtaining coherent radiation at a wavelength shorter than that of available lasers, through the process of second-harmonic generation (SHG).

All optical media are nonlinear. However, the nonlinearity is generally so weak that it is impossible to be observed without the use of high intensity laser beams. Mathematical modeling of nonlinear optics in thin layers is more difficult than that of linear optics studied in the literature by many authors [14, 15, 16, 3, 4]. In the nonlinear case, the electromagnetic wave propagation is now governed by the system of nonlinear Maxwell's equations, *i.e.*, nonlinear PDEs need to be studied. Also, the amplitude of the incident wave, which has no role in the linear case, plays an important role in the nonlinear case. Further, since nonlinear material properties are usually characterized by tensors, vectorial models become inevitable in the general situation.

The main aim of this chapter is to rigorously derive the effect of thin layers of nonlinear material in the undepleted-pump approximation. In this approximation, the nonlinear Maxwell equations reduce to two coupled Helmholtz equations for the fundamental and the second-harmonic fields. We derive asymptotic formulas for two-dimensional fundamental and second-harmonic fields associated with thin layers of nonlinear materials. Our approach is based on layer potential techniques through integral representation formulas of the fields, avoiding the use (and the adaptation to our context) of the highly-nontrivial regularity results of Li and Vogelius [50]. See for a similar approach Beretta and Francini [14].

Our interest in such asymptotic formulas owes to the fact that they provide extremely powerful tools to solve optimization problems [12, 51, 55]. In [67, 7, 5, 3], asymptotic expansions of this kind for electromagnetic inclusions (of linear material) of small diameter have been already derived. However, they are by nature completely different from those derived in this chapter. The degeneracy of the curves associated with the thin layer complicates a mathematically rigorous derivation, based on layer potentials, of the leading-order perturbations in the fundamental and second-harmonic fields.

This chapter is organized in the following way. In Section 2.2 we formulate the problem and state our main results. Section 2.3 is devoted to the proof of existence and uniqueness of the fundamental and second-harmonic fields that are solution of two coupled Helmholtz equations. In Section 2.4 we review some well-known properties of the layer potentials and prove some useful identities. In Sections 2.5 and 2.6 we give an integral representation of the fundamental field and prove a regularity result necessary to show existence of the second-harmonic field. In Section 2.7 we provide a rigorous derivation of the leading-order perturbation term in its asymptotic expansion due to the nonlinear thin layer. Our aim in Sections 2.8 and 2.9 is to provide a rigorous derivation of leading-order term in the asymptotic expansion of the second-harmonic field.

2.2 Problem formulation

We start from the following Maxwell's equations, which are the general laws governing electromagnetic fields interacting with (nonmagnetic) matter

$$\nabla \times \mathbf{E} = -\frac{i\omega}{c}\mathbf{H}, \tag{2.2.1}$$

$$\nabla \times \mathbf{H} = \frac{i\omega}{c}(\mathbf{E} + 4\pi \mathbf{P}), \tag{2.2.2}$$

where c is the speed of light, ω is the angular frequency, $\mathbf{E}$ and $\mathbf{H}$ are the electric and magnetic fields, respectively, and $\mathbf{P}$ is the polarization.

These two Maxwell equations combine into

$$\nabla \times \nabla \times \mathbf{E} - \frac{\omega^2}{c^2}(\mathbf{E} + 4\pi \mathbf{P}) = 0.$$

It is obvious that we need the information on the relationship between $\mathbf{P}$ and $\mathbf{E}$ to proceed further. This is where the optical nonlinearities are introduced. In general, the nonlinear responses are orders of magnitude smaller than the linear response and the displacement vector of a medium can be expanded according to the power of the applied electric field $\mathbf{E}$. The case of most general interest, which is the subject of the investigations described later in the chapter, is the second-harmonic generation (SHG). In this case we have

$$4\pi \mathbf{P} = (\epsilon - 1)\mathbf{E} + \chi^{(2)}(x, \omega) : \mathbf{E}\mathbf{E},$$

where ϵ is the dielectric coefficient, and $\chi^{(2)}$ is the second-order nonlinear susceptibility tensor of third rank, *i.e.*, $\chi^{(2)} : \mathbf{E}\mathbf{E}$ is a vector whose jth component is $\sum_{k,l=1}^{3} \chi^{(2)}_{jkl} : \mathbf{E}_k \mathbf{E}_l$.

For simplicity, we assume that the nonlinear polarization term $\mathbf{P}$ contains only the sum-frequency generation of the second-harmonic from the fundamental frequency and ignore all other $\chi^{(2)}$ phenomena such as difference-frequency generation, optical rectification, or cascaded nonlinear effects, as is consistent with the undepleted-pump approximation. Thus the polarization $\mathbf{P}$ at the fundamental frequency $\omega_1 = \omega$ and the second-harmonic frequency $\omega_2 = 2\omega$ may be written as

$$4\pi\mathbf{P}(x,\omega_1) = (\epsilon(x,\omega_1) - 1)\mathbf{E}(x,\omega_1),$$

and

$$4\pi\mathbf{P}(x,\omega_2) = (\epsilon(x,\omega_2) - 1)\mathbf{E}(x,\omega_2) + \chi^{(2)}(x,\omega_2) : \mathbf{E}(x,\omega_1)\mathbf{E}(x,\omega_1).$$

Assume that the depletion of energy from the pump waves (at the fundamental frequency ω_1) may be neglected. Then, using the above expression of the undepleted-pump nonlinear polarization, we can decompose the Maxwell equations (2.2.1)-(2.2.2) into two sets of coupled partial differential equations at the fundamental and second-harmonic frequencies.

Suppose that all fields are invariant in the x_3 direction. In the linear case, in transverse electric (TE) polarization the electric field is transversal to the (x_1, x_2)-plane, and in transverse magnetic (TM) polarization the magnetic field is transversal to the (x_1, x_2)-plane. In the nonlinear case, however, the polarization is determined by group symmetry properties of $\chi^{(2)} = (\chi^{(2)}_{njl})^3_{n,j,l=1}$. In this work, we assume that the electromagnetic fields are TE polarized at the fundamental frequency ω_1 and TM polarized at the second-harmonic frequency ω_2. This polarization assumption is known to support a large class of nonlinear optical materials, for example, crystals with cubic symmetry structures. See [61].

Therefore,

$$\mathbf{H}(x,\omega_1) = u(x_1,x_2,\omega_1)\vec{x}_3,$$

$$\mathbf{E}(x,\omega_2) = v(x_1,x_2,\omega_2)\vec{x}_3.$$

Define for the sake of simplicity

$$\epsilon_j = \epsilon(x_1,x_2,\omega_j), \quad j = 1,2,$$

$$\kappa_j = \frac{\omega_j}{c}\sqrt{\epsilon_j}, \quad \Im\kappa_j \geq 0, \quad j = 1,2.$$

At the fundamental frequency ω_1, the system (2.2.1)-(2.2.2) can be simplified to

$$\nabla \cdot \left(\frac{1}{\kappa_1^2}\nabla u\right) + u = 0.$$

We deduce the expression of the electric field at the fundamental frequency ω_1

$$\begin{aligned}\mathbf{E}(x,\omega_1) &= \frac{c}{i\omega_1\epsilon_1}\nabla \times \mathbf{H}(x,\omega_1) \\ &= \frac{c}{i\omega_1\epsilon_1}(\partial_{x_2}u, -\partial_{x_1}u, 0).\end{aligned}$$

Hence the second-harmonic field satisfies

$$\begin{aligned}(\Delta + \kappa_2^2)\, v &= -\frac{4\pi\omega_2^2}{c^2} \sum_{j,l=1,2,3} \chi^{(2)}_{3jl}(x,\omega_2)(\mathbf{E}(x,\omega_1))_j(\mathbf{E}(x,\omega_1))_l \\ &= \sum_{j,l=1,2} \chi_{jl}\partial_{x_j}u\partial_{x_l}u,\end{aligned}$$

where $\chi_{jl} = (-1)^{j+l}(16\pi/\epsilon_1^2)\chi^{(2)}_{3jl}(x,\omega_2)$.

Then (u,v) satisfies in the nonlinear material the following two coupled Helmholtz equations

$$\nabla \cdot \left(\frac{1}{\kappa_1^2}\nabla u\right) + u = 0, \tag{2.2.3}$$

$$\Delta v + \kappa_2^2 v = \sum_{j,l=1,2} \chi_{jl}\partial_{x_j}u\partial_{x_l}u. \tag{2.2.4}$$

Let us now specify the geometry of the problem. Let Ω be a bounded $\mathcal{C}^3$-domain in $\mathbb{R}^2$. Let $\tau(x)$ and $\nu(x)$ denote a unit tangential and a unit (exterior to Ω) normal field to $\partial\Omega$. For a function f defined on $\mathbb{R}^2 \setminus \partial\Omega$, we denote $[f(x)]_{\partial\Omega} = f|_+ - f|_-$ where $f|_+ = \lim_{\delta\to 0^+} f(x+\delta\nu(x))$ and $f|_- = \lim_{\delta\to 0^+} f(x-\delta\nu(x))$, if the limits exist.

We consider a layer of nonlinear material of the form

$$\mathcal{O}_\delta = \left\{ x + \eta\nu(x) : x \in \partial\Omega, \eta \in (0,\delta) \right\},$$

where the thickness, $\delta > 0$, is a small parameter. Let $\Omega_\delta^i = \overline{\Omega} \cup \mathcal{O}_\delta$, $\Omega_\delta^e = \mathbb{R}^2 \setminus \overline{\Omega_\delta^i}$.

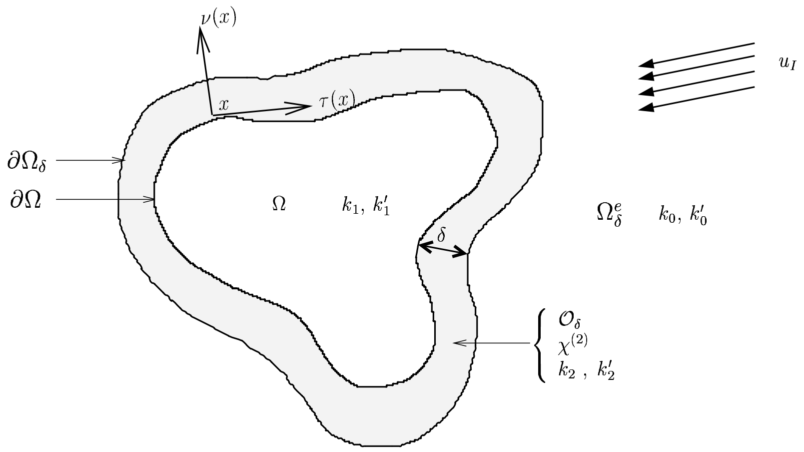


Figure 2.1: The dielectric medium.

Throughout this chapter we suppose that the susceptibility tensor is of the form

$$\chi_{jl}(x+\eta\nu) = \tilde{\chi}_{jl}\left(x, \frac{\eta}{\delta}\right), \qquad x \in \partial\Omega\ ,\ 0 < \eta < \delta\ ,$$

where $\tilde{\chi}_{jl} \in L^\infty(\overline{\mathcal{O}}_\delta)$ are independent of δ, and define

$$k(x) = \begin{cases} k_1 & \text{for } x \in \Omega, \\ k_2 & \text{for } x \in \mathcal{O}_\delta, \\ k_0 & \text{for } x \in \Omega_\delta^e, \end{cases}$$

where k_1, k_2, k_0 are positive constants. We also introduce a function $k'(x)$ defined analogously with positive constants k'_1, k'_2, k'_0. We assume in all what follows that $k_2 \neq k_1$, $k_2 \neq k_0$, $k'_2 \neq k'_1$, and $k'_2 \neq k'_0$.

By $\partial\Omega_\eta$, for $\eta \in (0, \delta)$, we denote

$$\partial\Omega_\eta = \left\{ x + \eta\nu(x) : x \in \partial\Omega \right\},$$

with the convention $\partial\Omega_0 = \partial\Omega$. We denote by $\rho(x)$ the curvature at the point $x \in \partial\Omega$. If ds denotes the surface measure on $\partial\Omega$ then the corresponding surface measure on $\partial\Omega_\eta$ is related to ds at the point $x \in \partial\Omega$ through the relation $ds_\eta(x + \eta\nu(x)) = (1 + \eta\rho(x))\ ds(x)$.

Consider an incident plane wave given by $u_I(x) = U_I e^{ik_I \cdot x}$ where $k_I \in \mathbb{R}^2$ is the wave-vector with $|k_I| = k_0$ and $U_I \in \mathbb{R}$ is a positive constant. Then (u, v) is solution of the following problem

$$\begin{cases} \nabla \cdot \dfrac{1}{k^2} \nabla u + u & = & 0, \\ \Delta v + k'^2 v & = & \displaystyle\sum_{j,l=1,2} \chi_{jl} \partial_{x_j} u \partial_{x_l} u \, \mathrm{I}_{\mathcal{O}_\delta}, \\ \displaystyle\lim_{|x| \to +\infty} \sqrt{|x|} \left(\frac{\partial(u - u_I)}{\partial|x|} - ik_0(u - u_I) \right) & = & 0, \\ \displaystyle\lim_{|x| \to +\infty} \sqrt{|x|} \left(\frac{\partial v}{\partial|x|} - ik'_0 v \right) & = & 0, \end{cases} \tag{2.2.5}$$

where $\mathrm{I}_{\mathcal{O}_\delta}$ is the characteristic function of $\mathcal{O}_\delta$.

The equations (2.2.5) may alternatively be formulated as follows

$$\begin{cases} \Delta u + k_1^2 u = 0 & \text{in } \Omega, \\ \Delta u + k_2^2 u = 0 & \text{in } \mathcal{O}_\delta, \\ \Delta u + k_0^2 u = 0 & \text{in } \Omega_\delta^e, \\ [u]_{\partial\Omega} = [u]_{\partial\Omega_\delta} = 0, \\ \left[\dfrac{1}{k^2}\dfrac{\partial u}{\partial\nu}\right]_{\partial\Omega} = \left[\dfrac{1}{k^2}\dfrac{\partial u}{\partial\nu}\right]_{\partial\Omega_\delta} = 0, \\ \displaystyle\lim_{|x| \to \infty} \sqrt{|x|} \left| \frac{\partial(u - u_I)}{\partial|x|} - ik_0(u - u_I) \right| = 0, & \text{uniformly in } \dfrac{x}{|x|}, \end{cases} \tag{2.2.6}$$

and

$$\begin{cases} \Delta v + k_1'^2 v = 0 & \text{in } \Omega, \\ \Delta v + k_2'^2 v = \displaystyle\sum_{j,l=1,2} \chi_{jl} \partial_{x_j} u \partial_{x_l} u & \text{in } \mathcal{O}_\delta, \\ \Delta v + k_0'^2 v = 0 & \text{in } \Omega_\delta^e, \\ [v]_{\partial\Omega} = [v]_{\partial\Omega_\delta} = 0, \\ \left[\dfrac{\partial v}{\partial \nu}\right]_{\partial\Omega} = \left[\dfrac{\partial v}{\partial \nu}\right]_{\partial\Omega_\delta} = 0, \\ \displaystyle\lim_{|x|\to\infty} \sqrt{|x|} \left| \frac{\partial v}{\partial |x|} - i k_0' v \right| = 0, & \text{uniformly in } \dfrac{x}{|x|}. \end{cases} \tag{2.2.7}$$

In the remainder of this chapter U shall always refer to the solution of

$$\begin{cases} \Delta U + k_1^2 U = 0 & \text{in } \Omega, \\ \Delta U + k_0^2 U = 0 & \text{in } \mathbb{R}^2 \setminus \overline{\Omega}, \\ [U]_{\partial\Omega} = 0, \\ \left[\dfrac{1}{\tilde{k}^2} \dfrac{\partial U}{\partial \nu}\right]_{\partial\Omega} = 0, \\ \displaystyle\lim_{|x|\to\infty} \sqrt{|x|} \left| \frac{\partial (U - u_I)}{\partial |x|} - i k_0 (U - u_I) \right| = 0, & \text{uniformly in } \dfrac{x}{|x|}, \end{cases} \tag{2.2.8}$$

where the function $\tilde{k}(y)$ is given by

$$\tilde{k}(y) = \begin{cases} k_1 & \text{for } y \in \Omega\ , \\ k_0 & \text{for } y \in \mathbb{R}^2 \setminus \overline{\Omega}\ . \end{cases}$$

Before giving a precise formulation of the main results of this chapter we need to introduce some additional notation. By G, we denote the fundamental solution of the following transmission problem

$$\begin{cases} \Delta_y G(x,y) + k_0^2 G(x,y) = \delta_x(y) & \text{for } y \in \mathbb{R}^2 \setminus \overline{\Omega}\ , \\ \Delta_y G(x,y) + k_1^2 G(x,y) = \delta_x(y) & \text{for } y \in \Omega\ , \\ \left[\tilde{k}^2 G(x,\cdot)\right] = 0 \quad \text{on } \partial\Omega\ , \\ \left[\dfrac{\partial G(x,\cdot)}{\partial \nu(y)}\right] = 0 \quad \text{on } \partial\Omega\ , \\ \displaystyle\lim_{|y|\to\infty} \sqrt{|y|} \left| \frac{\partial G(x,y)}{\partial |y|} - i k_0 G(x,y) \right| = 0, & \text{uniformly in } \dfrac{y}{|y|}. \end{cases}$$

We will also need the function G' that is the solution to

$$\begin{cases} \Delta_y G'(x,y) + (k_0')^2 G'(x,y) = \delta_x(y) \quad \text{for } y \in \mathbb{R}^2 \setminus \overline{\Omega} \,, \\ \Delta_y G'(x,y) + (k_1')^2 G'(x,y) = \delta_x(y) \quad \text{for } y \in \Omega \,, \\ [G'(x,\cdot)] = 0 \quad \text{on } \partial\Omega \,, \\ \left[\dfrac{\partial G'(x,\cdot)}{\partial \nu(y)}\right] = 0 \quad \text{on } \partial\Omega \,, \\ \lim\limits_{|y|\to\infty} \sqrt{|y|} \left| \dfrac{\partial G'(x,y)}{\partial |y|} - i k_0' G'(x,y) \right| = 0, \qquad \text{uniformly in } \dfrac{y}{|y|}, \end{cases}$$

where the function $\tilde{k}'(y)$ is defined analogously to $\tilde{k}(y)$.

Define the symmetric matrix $\mathcal{A}(x), x \in \partial\Omega$, by

$$\begin{aligned} &\mathcal{A} \text{ has eigenvectors } \tau(x) \text{ and } \nu(x), \\ &\text{the eigenvalue corresponding to } \tau(x) \text{ is } (\frac{k_0}{k_2})^2 - 1, \\ &\text{the eigenvalue corresponding to } \nu(x) \text{ is } 1 - (\frac{k_2}{k_0})^2. \end{aligned} \tag{2.2.9}$$

It is clear that $\mathcal{A}$ is positive definite if $k_0 > k_2$, and negative definite if $k_0 < k_2$. We also need the matrix $\mathcal{A}'(x), x \in \partial\Omega$, defined by

$$\begin{aligned} &\mathcal{A}' \text{ has eigenvectors } \tau(x) \text{ and } \nu(x), \\ &\text{the eigenvalue corresponding to } \tau(x) \text{ is } 1, \\ &\text{the eigenvalue corresponding to } \nu(x) \text{ is } (\frac{k_2}{k_0})^2. \end{aligned} \tag{2.2.10}$$

The main achievement of this chapter consists in the following asymptotic formulas concerning the perturbation, $u - U$, and the second-harmonic field v, enhanced by the thin layer of nonlinear material $\mathcal{O}_\delta$ in the undepleted-pump approximation.

Theorem 2.2.1 *Let u and v be the solutions to (2.2.6) and (2.2.7), respectively, and let $\mathcal{A}$ and $\mathcal{A}'$ be the matrices defined by (2.2.9) and (2.2.10), respectively. Then, for $x \in \mathbb{R}^2 \setminus \overline{\Omega}$ bounded away from $\partial\Omega$, the following pointwise expansions hold:*

$$u(x) = U(x) + \delta \int_{\partial\Omega} \nabla_y G(x,y) \Big|_+ \cdot \mathcal{A} \nabla U(y) \Big|_+ \, ds(y) + o(\delta) \,, \tag{2.2.11}$$

and

$$\begin{aligned} v(x) = \delta \sum_{j,l=1,2} \int_{\partial\Omega} & G'(x,y) \Big|_+ \\ & \left(\int_0^1 \tilde{\chi}_{jl}(y,\theta)\, d\theta\right) \left(\mathcal{A}' \nabla U(y) \Big|_+\right)_j \left(\mathcal{A}' \nabla U(y) \Big|_+\right)_l ds(y) \\ & + o(\delta) \,, \end{aligned} \tag{2.2.12}$$

where the remainder terms $o(\delta)$ are independent of x.

This result generalizes those of E. Beretta, E. Francini, and M. Vogelius in [15] and of E. Beretta and E. Francini in [14] to the case of a thin layer of nonlinear material. Its main particularity is the fact that it is based on integral equations and layer potentials rather than variational techniques avoiding the use (and the adaptation to our context) of the highly-nontrivial regularity results of Li and Vogelius [50].

It is worth noticing that from the nature of our derivations it follows that we cannot expect the remainder terms in (2.2.11) and (2.2.12) to be uniform in $\mathbb{R}^2 \setminus \partial\Omega$. Rather, these terms are uniform at fixed distance away from $\partial\Omega$, but the estimates (2.2.11) and (2.2.12) degenerate as x approaches $\partial\Omega$. Indeed, the transmission problem for U and the first order correction

$$u_1 = \int_{\partial\Omega} \nabla_y G(x,y)\Big|_+ \cdot \mathcal{A}\nabla U(y)\Big|_+ \, ds(y)$$

are not posed on the same domain – the transmission problem for U is posed on the whole $\mathbb{R}^2$, but the one for u_1 is naturally posed on $\mathbb{R}^2 \setminus \partial\Omega$. This significantly complicates our derivation of the expansions (2.2.11) and (2.2.12) and makes our analysis nontrivial.

2.3 Well-posedness

In this section, we will prove existence and uniqueness of the fundamental field u. Even though these results are classical we give their proof for the reader's convenience. The proof of existence and uniqueness of the second-harmonic field v is exactly the same as for the fundamental field u since, as will be shown later in Corollary 2.6.1, $\sum_{j,l=1,2} \chi_{jl} \partial_{x_j} u \partial_{x_l} u$ belongs to $L^2(\mathcal{O}_\delta)$.

We start by formulating the problem (2.2.6) in a bounded domain. Consider the disc B_R centered at the origin with radius R large enough to have $\overline{\Omega} \subset B_R$ and denote by S_R its boundary. The scattered field $u - u_I$ satisfy in $\mathbb{R}^2 \setminus \overline{B_R}$ the Helmholtz equation

$$\Delta(u-u_I) + k_0^2(u-u_I) = 0 \,,$$

together with the (outgoing) radiation condition

$$\lim_{r\to+\infty} \sqrt{r}\left(\frac{\partial(u-u_I)}{\partial r} - ik_0(u-u_I)\right) = 0 \,.$$

Taking the Fourier series $(u^n - u_I^n)(r)$ with respect to the angular variable θ, where (r,θ) are the polar coordinates, we get

$$(u^n - u_I^n)''(r) + \frac{1}{r}(u^n - u_I^n)'(r) + (k_0^2 - \frac{n^2}{r^2})(u^n - u_I^n)(r) = 0 \quad \text{for } r > R.$$

Therefore

$$(u^n - u_I^n)(r) = A_n H_n^{(1)}(k_0 r) + B_n H_n^{(2)}(k_0 r) \,,$$

where A_n and B_n are constants, and $H_n^{(1)}$ and $H_n^{(2)}$ denote the Hankel functions of the first and the second kind, respectively. However, only $H_n^{(1)}(k_0 r)$ satisfies the above radiation condition. Thus,

$$(u-u_I)(r,\theta) = \sum_{n\in\mathbb{Z}} A_n H_n^{(1)}(k_0 r) e^{in\theta} \quad \text{for } r > R \text{ and } \theta \in [0, 2\pi) \,.$$

Using this Fourier expansion we can express the trace of $(u-u_I)$ and $\dfrac{\partial(u-u_I)}{\partial\nu}$ on S_R as follows

$$(u-u_I)(R,\theta) = \sum_{n\in\mathbb{Z}} A_n H_n^{(1)}(k_0R)e^{in\theta} ,$$

$$\frac{\partial(u-u_I)}{\partial\nu}(R,\theta) = \sum_{n\in\mathbb{Z}} A_n k_0 H_n^{(1)\prime}(k_0R)e^{in\theta} ,$$

from which we readily get that

$$\left(\frac{\partial(u-u_I)}{\partial\nu}\right)^n(R) = k_0\frac{H_n^{(1)\prime}(k_0R)}{H_n^{(1)}(k_0R)}(u-u_I)^n(R) .$$

Let C_R be the mapping defined by

$$\begin{array}{llll} C_R : & H^{1/2}(S_R) & \to & H^{-1/2}(S_R) \\ & f = \sum_{n\in\mathbb{Z}} f^n e^{in\theta} & \mapsto & C_R(f) = \displaystyle\sum_{n\in\mathbb{Z}} k_0\frac{H_n^{(1)\prime}(k_0R)}{H_n^{(1)}(k_0R)} f^n e^{in\theta} . \end{array}$$

The proof of uniqueness of a solution to (2.2.6) relies on the following important properties of the so-called Dirichlet-to-Neumann map C_R. We refer to Appendix A.2 for a proof.

Lemma 2.3.1 *The mapping C_R defines a bounded operator from $H^{1/2}(S_R)$ into $H^{-1/2}(S_R)$. Furthermore, we have*

$$\Im\int_{S_R} C_R(u)\overline{u} > 0 \quad \forall u \in H^{1/2}(S_R) \ , u \neq 0 , \tag{2.3.13}$$

$$\Re\int_{S_R} C_R(u)\overline{u} \leq 0 \quad \forall u \in H^{1/2}(S_R) . \tag{2.3.14}$$

Now we can formulate (2.2.6) in the bounded domain B_R using the Dirichlet-to-Neumann map C_R. Introduce the following transmission problem

$$\begin{cases} \Delta u + k_1^2 u = 0 & \text{in } \Omega, \\ \Delta u + k_2^2 u = 0 & \text{in } \mathcal{O}_\delta, \\ \Delta u + k_0^2 u = 0 & \text{in } \Omega_\delta^e \cap B_R, \\ [u]_{\partial\Omega} = [u]_{\partial\Omega_\delta} = 0, \\ \left[\dfrac{1}{k^2}\dfrac{\partial u}{\partial\nu}\right]_{\partial\Omega} = \left[\dfrac{1}{k^2}\dfrac{\partial u}{\partial\nu}\right]_{\partial\Omega_\delta} = 0 , \\ \dfrac{\partial u}{\partial\nu} = C_R(u) + g & \text{on } S_R, \end{cases} \tag{2.3.15}$$

where $g := \dfrac{\partial u_I}{\partial\nu} - C_R(u_I)$ on S_R.

Lemma 2.3.2 *To each solution u to the problem (2.2.6) corresponds one and only one solution u^i to the problem (2.3.15) that is its restriction to B_R.*

Proof. Let u be a solution to (2.2.6). Since $(u - u_I)$ satisfies the Helmholtz equation $\Delta(u - u_I) + k_0^2(u - u_I) = 0$ in $\mathbb{R}^2 \setminus \overline{B}_R$ and the radiation condition, it immediately follows that

$$\frac{\partial(u - u_I)}{\partial \nu} = C_R(u - u_I) \quad \text{on } S_R,$$

which is equivalent to

$$\frac{\partial u}{\partial \nu} = C_R(u) + g \quad \text{on } S_R.$$

The restriction of u to B_R is then a solution to (2.2.6).

Conversely, let u^i be a solution to (2.3.15). Let $f = u^i|_{S_R}$. It is well known from the potential theory that the following exterior problem

$$\begin{cases} \Delta u^e + k_0^2 u^e = 0 & \text{in } \mathbb{R}^2 \setminus \overline{B}_R, \\ u^e = f - u_I & \text{on } S_R \ , \\ \lim\limits_{|x|\to\infty} \sqrt{|x|} \left| \dfrac{\partial u^e}{\partial |x|} - ik_0 u^e \right| = 0 & \text{uniformly in } \dfrac{x}{|x|}, \end{cases} \tag{2.3.16}$$

has a unique solution u^e. Define u by

$$u = \begin{cases} u^i & \text{in } B_R \ , \\ u^e + u_I & \text{in } \mathbb{R}^2 \setminus \overline{B}_R \ , \end{cases}$$

It is easy to check that u satisfies (2.2.6). □

We are now ready to prove the well-posedness of the problem (2.3.15). We introduce the bilinear form $a(u, w)$ on $H^1(B_R) \times H^1(B_R)$ by

$$a(u, w) = \int_{B_R} \frac{1}{k^2} \nabla u \cdot \nabla \overline{w} - \int_{B_R} u\overline{w} - \frac{1}{k_0^2} \int_{S_R} C_R(u)\overline{w} \ . \tag{2.3.17}$$

We can immediately see that a function $u \in H^1(B_R)$ is a weak solution to (2.3.15) if and only if it is a solution to the variational problem

$$a(u, w) = \frac{1}{k_0^2} \int_{S_R} g\overline{w} \quad \forall w \in H^1(B_R). \tag{2.3.18}$$

The following lemma gives a classical existence and uniqueness result that can be found in [57]. We give its proof for reader's convenience.

Proposition 2.3.1 *There exists a unique weak solution to the problem (2.3.15) in $H^1(B_R)$.*

Proof. Since $k^2(x)$ is bounded away from 0 and ∞, there exists a constant $C > 0$ such that

$$\Re a(u, u) \geq C \int_{B_R} |\nabla u|^2 - \int_{B_R} |u|^2 \ . \tag{2.3.19}$$

It is also obvious that the bilinear form a is bounded. Since the embedding of $H^1(B_R)$ into $L^2(B_R)$ is compact, the Fredholm alternative holds and existence will follow from uniqueness.

In order to prove the uniqueness, suppose that there exists $u \in H^1(B_R)$ satisfying

$$a(u, w) = 0 \quad \forall w \in H^1(B_R) .$$

Therefore

$$\Im a(u, u) = 0 = \Im \int_{S_R} C_R(u)\overline{u} ,$$

and thus, using (2.3.13), we deduce that u belongs to $H_0^1(B_R)$ and satisfies

$$\int_{B_R} \frac{1}{k^2} \nabla u \cdot \nabla \overline{w} - \int_{B_R} u\overline{w} = 0 \ , \forall w \in H^1(B_R) . \qquad (2.3.20)$$

This means that u is a weak solution to

$$\begin{cases} \nabla \cdot \dfrac{1}{k^2} \nabla u + u = 0 \quad \text{in } B_R , \\ u = 0 \quad \text{on } S_R , \\ \dfrac{\partial u}{\partial \nu} = 0 \quad \text{on } S_R . \end{cases}$$

Finally, since k^2 is piecewise constant in B_R, the unique continuation theorem for the Helmholtz equation applies to ensure the uniqueness of a solution. The proof of the proposition is complete. $\square$

2.4 Preliminary results

Let us first review some well-known properties of the layer potentials for the Helmholtz equation and prove some useful identities.

Let $k > 0$ be a given constant and let Γ_k and Γ_0 be the fundamental (outgoing) solutions of $\Delta + k^2$ and Δ, respectively, which are defined by

$$\Gamma_k(x) = -\frac{i}{4} H_0^1(k|x|), \quad x \in \mathbb{R}^2,$$

$$\Gamma_0(x) = \frac{1}{2\pi} \log(|x|), \quad x \in \mathbb{R}^2,$$

for $x \neq 0$.

Let $\eta \geq 0$ be small enough. We define the slightly modified single layer potential S_η^k and double layer potential D_η^k for a density $\varphi \in L^2(\partial\Omega)$ by the following

$$S_\eta^k \varphi(x) = \int_{\partial\Omega} \Gamma_k(x - y - \eta\nu(y))(1 + \eta\rho(y))\varphi(y)\, ds(y) , \quad x \in \mathbb{R}^2,$$

$$D_\eta^k \varphi(x) = \int_{\partial\Omega} \frac{\partial \Gamma_k(x - y - \eta\nu(y))}{\partial \nu(y)} (1 + \eta\rho(y))\varphi(y)\, ds(y) , \quad x \in \mathbb{R}^2 \setminus \partial\Omega_\eta,$$

We also define the operators K_η^k, its L^2-adjoint $(K_\eta^k)^*$, and M_η^k by

$$K_\eta^k \varphi(x) = \int_{\partial\Omega} \frac{\partial \Gamma_k(x - y + \eta(\nu(x) - \nu(y)))}{\partial \nu(y)} (1 + \eta\rho(y))\varphi(y)\, ds(y) , \quad x \in \partial\Omega ,$$

$$(K_\eta^k)^*\varphi(x) = \int_{\partial\Omega} \frac{\partial \Gamma_k(x-y+\eta(\nu(x)-\nu(y)))}{\partial\nu(x)}(1+\eta\rho(y))\varphi(y)\,ds(y) , \quad x \in \partial\Omega ,$$

$$M_\eta^k\varphi(x) = \int_{\partial\Omega}\left(\frac{\partial^2}{\partial\nu(x)^2}+\frac{\partial^2}{\partial\nu(x)\partial\nu(y)}\right)\Gamma_k(x-y+\eta(\nu(x)-\nu(y))) \\ (1+\eta\rho(y))\varphi(y)\,ds(y) ,$$

for $x \in \partial\Omega$.

Finally, we introduce the following notations for $\eta, \delta \geq 0$ small enough and $x \in \partial\Omega$:

$$S_{\eta,\delta}^k\varphi(x) = S_\eta^k\varphi(x+\delta\nu(x)) , \quad x \in \mathbb{R}^2 ,$$

and

$$D_{\eta,\delta}^k\varphi(x) = D_\eta^k\varphi(x+\delta\nu(x)) , \quad x \in \mathbb{R}^2 \setminus \partial\Omega_{\eta-\delta} .$$

The functions $S_\eta^k\varphi$ and $D_\eta^k\varphi$ are in fact the single and double layer potentials of the density $\tilde{\varphi}(y+\eta\nu(y)) = \varphi(y)$ on the curve $\partial\Omega_\eta$.

We recall the following classical result.

Lemma 2.4.1 *For any $k > 0$, the function $\Gamma_k - \Gamma_0$ is continuous.*

Proof. From

$$\Delta(\Gamma_k - \Gamma_0) + k^2(\Gamma_k - \Gamma_0) = -k^2\Gamma_0 ,$$

and since Γ_0 is in $L^2_{\text{loc}}(\mathbb{R}^2)$, we deduce by applying classical results on elliptic regularity [27] and the Sobolev embedding theorem [2] that $\Gamma_k - \Gamma_0$ is a continuous function. □

From the properties of S_η^0 and D_η^0, see [19], we can obtain that

$$\frac{\partial(S_\eta^k\varphi)_\pm}{\partial\nu}(x) = \left(\pm\frac{1}{2}I + (K_\eta^k)^*\right)\varphi(x) , \quad \text{a.e. } x \in \partial\Omega_\eta, \tag{2.4.21}$$

$$(D_\eta^k\varphi)_\pm(x) = \left(\mp\frac{1}{2}I + K_\eta^k\right)\varphi(x) , \quad \text{a.e. } x \in \partial\Omega_\eta, \tag{2.4.22}$$

for $\varphi \in L^2(\partial\Omega)$, where

$$\frac{\partial(u)_\pm}{\partial\nu}(x) := \lim_{h\to+0} \nu(x)\cdot\nabla u(x \pm h\nu(x)) ,$$

and

$$u_\pm(x) := \lim_{h\to+0} u(x\pm h\nu(x)) .$$

From standard potential theory, we also have the following results.

Lemma 2.4.2 *Suppose $\partial\Omega$ is $\mathcal{C}^2$. For $\eta \geq 0$ small enough, the following operators*

$$S_{\eta,\eta}^k : L^2(\partial\Omega) \to H^1(\partial\Omega) ,$$

$$K_\eta^k, (K_\eta^k)^* : L^2(\partial\Omega) \to H^1(\partial\Omega) ,$$

$$M_\eta^k, (\partial_\nu S_{\eta,\eta}^k)_\pm, (D_{\eta,\eta}^k)_\pm : L^2(\partial\Omega) \to L^2(\partial\Omega) ,$$

are bounded.

We can prove that the following expansions hold. See Appendix A.3 for the proof.

Lemma 2.4.3 *For any $\eta > 0$ small enough and for any $\varphi \in L^2(\partial\Omega)$, we have*

$$S^k_{\delta,\delta}\varphi(x) = S^k_{0,0}\varphi(x) + \delta\left(K^k_0\varphi(x) + (K^k_0)^*\varphi(x) + S^k_{0,0}(\rho\varphi)(x)\right) + O(\delta^2)\ ,$$

$$(K^k_\delta)^*\varphi(x) = (K^k_0)^*\varphi(x) + \delta\left(M^k_0\varphi(x) + (K^k_0)^*(\rho\varphi)(x)\right) + O(\delta^2)\ ,$$

where $O(\delta^2)$ is in $H^1(\partial\Omega)$ in the first equation and in $L^2(\partial\Omega)$ in the second one.

The following lemma is of importance to us. We refer the reader to Appendix A.4 for its proof.

Lemma 2.4.4 *There exists $\varepsilon_\delta > 0$ satisfying $\lim\limits_{\delta\to 0}\varepsilon_\delta = 0$ such that for any $\varphi \in L^2(\partial\Omega)$ and $s = 0, 1$, the following estimates hold:*

$$\|S^k_{0,\delta}\varphi - S^k_{0,0}\varphi\|_{H^{s+1}(\partial\Omega)} \le \varepsilon_\delta\|\varphi\|_{H^s(\partial\Omega)}\ ,$$

$$\|S^k_{\delta,\delta}\varphi - S^k_{\delta,0}\varphi\|_{H^{s+1}(\partial\Omega)} \le \varepsilon_\delta\|\varphi\|_{H^s(\partial\Omega)}\ ,$$

$$\left\|\frac{\partial(S^k_{0,\delta}\varphi)}{\partial\nu} - \frac{\partial(S^k_{0,0}\varphi)_+}{\partial\nu}\right\|_{H^s(\partial\Omega)} \le \varepsilon_\delta\|\varphi\|_{H^s(\partial\Omega)}\ ,$$

$$\left\|\frac{\partial(S^k_{\delta,\delta}\varphi)_-}{\partial\nu} - \frac{\partial(S^k_{\delta,0}\varphi)}{\partial\nu}\right\|_{H^s(\partial\Omega)} \le \varepsilon_\delta\|\varphi\|_{H^s(\partial\Omega)}\ .$$

The estimates for $s = 1$ hold under the assumption that $\partial\Omega$ is of class $\mathcal{C}^3$.

The following result on the spectral radius of K^k_0 is also of use to us.

Lemma 2.4.5 *For any λ satisfying $|\lambda| > \frac{1}{2}$ and any $k > 0$, the operator $\lambda I + (K^k_\eta)^*$ defined from $L^2(\partial\Omega)$ into $L^2(\partial\Omega)$ is invertible.*

Proof. It has been proved by Kellog in [44] that when $|\lambda| > \frac{1}{2}$, the operator $\lambda I + (K^0_\eta)^*$ is invertible on $L^2(\partial\Omega)$. Lemma 2.4.1 shows that $(K^k_\eta)^* - (K^0_\eta)^*$ is compact on $L^2(\partial\Omega)$. Therefore the Fredholm alternative holds. It remains then to prove the injectivity of $\lambda I + (K^k_\eta)^*$. Let us suppose that we have $\varphi \in L^2(\partial\Omega)$ satisfying

$$\left(\lambda I + (K^k_\eta)^*\right)\varphi = 0\ .$$

Define u on $\mathbb{R}^2$ by $u(x) = S^k_\eta\varphi(x)$. It is clear that u satisfies the Helmholtz equation in $\mathbb{R}^2 \setminus \partial\Omega_\eta$ together with the radiation condition as $|x| \to +\infty$. Moreover, it can be easily seen that

$$u_+ = u_- \quad \text{on } \partial\Omega_\eta\ , \tag{2.4.23}$$

$$\frac{1}{-\frac{1}{2}-\lambda}\partial_\nu(u)_- = \frac{1}{\frac{1}{2}-\lambda}\partial_\nu(u)_+ = \varphi \quad \text{on } \partial\Omega_\eta\ . \tag{2.4.24}$$

Consequently

$$\begin{aligned}
\Im\int_{\partial\Omega_\eta}\partial_\nu(u)_+\overline{u} &= \frac{\frac{1}{2}-\lambda}{-\frac{1}{2}-\lambda}\Im\int_{\partial\Omega_\eta}\partial_\nu(u)_-\overline{u} \\
&= \frac{\frac{1}{2}-\lambda}{-\frac{1}{2}-\lambda}\Im\int_{\Omega^i_\eta}(\Delta u\overline{u} + |\nabla u|^2) = 0\ .
\end{aligned}$$

Applying Lemma A.A.1.2, we obtain that $u \equiv 0$ in Ω_η^e. From the expression of $\partial_\nu (u)_+$ we finally conclude that $\varphi \equiv 0$ which ends the proof. $\square$

2.5 Representation formula for the fundamental field

In this section, we state and prove a representation formula of the solution of (2.2.6) which will be the main tool for deriving the asymptotic expansions of the fundamental and second-harmonic fields. A similar representation formula for the transmission problem for the harmonic equation was found in [39, 40]. See also [3].

By X and Y let us denote

$$X := L^2(\partial\Omega)^2 \, , \quad Y := H^1(\partial\Omega) \times L^2(\partial\Omega).$$

The following theorem is of particular importance to us for establishing our representation formula.

Theorem 2.5.1 *Suppose k_0^2, k_2^2 are not Dirichlet eigenvalues for $-\Delta$ on Ω. There exists $\delta_0 > 0$ such that, for $0 < \delta < \delta_0$, for each $(f_1, f_2, g_1, g_2) \in Y^2$, there exists a unique solution $\Phi = (\varphi_1, \varphi_2, \psi_2, \varphi_0) \in X^2$ to the system of integral equations*

$$\left\{ \begin{array}{l} S_{0,0}^{k_1}\varphi_1 - S_{0,0}^{k_2}\varphi_2 - S_{\delta,0}^{k_2}\psi_2 = f_1, \\ \displaystyle \frac{1}{k_1^2}\frac{\partial(S_{0,0}^{k_1}\varphi_1)_-}{\partial\nu} - \frac{1}{k_2^2}\frac{\partial(S_{0,0}^{k_2}\varphi_2)_+}{\partial\nu} - \frac{1}{k_2^2}\frac{\partial(S_{\delta,0}^{k_2}\psi_2)}{\partial\nu} = f_2, \\ S_{0,\delta}^{k_2}\varphi_2 + S_{\delta,\delta}^{k_2}\psi_2 - S_{\delta,\delta}^{k_0}\varphi_0 = g_1, \\ \displaystyle \frac{1}{k_2^2}\frac{\partial(S_{0,\delta}^{k_2}\varphi_2)}{\partial\nu} + \frac{1}{k_2^2}\frac{\partial(S_{\delta,\delta}^{k_2}\psi_2)_-}{\partial\nu} - \frac{1}{k_0^2}\frac{\partial(S_{\delta,\delta}^{k_0}\varphi_0)_+}{\partial\nu} = g_2 \end{array} \right. \tag{2.5.25}$$

on $\partial\Omega$.

To prove this theorem, we need some preliminary results. First, define the operator T from X^2 into Y^2 by $T(\Phi) = (f_1, f_2, g_1, g_2)$ where (f_1, f_2, g_1, g_2) is given as in (2.5.25), and let the operator T_0 from X^2 into Y^2 be given by $T_0(\Phi) = (f_1, f_2, g_1, g_2)$ where

$$\left\{ \begin{array}{l} S_{0,0}^{k_2}\varphi_1 - S_{0,0}^{k_2}\varphi_2 = f_1, \\ \displaystyle \frac{1}{k_1^2}\frac{\partial(S_{0,0}^{k_2}\varphi_1)_-}{\partial\nu} - \frac{1}{k_2^2}\frac{\partial(S_{0,0}^{k_2}\varphi_2)_+}{\partial\nu} = f_2, \\ S_{\delta,\delta}^{k_2}\psi_2 - S_{\delta,\delta}^{k_2}\varphi_0 = g_1, \\ \displaystyle \frac{1}{k_2^2}\frac{\partial(S_{\delta,\delta}^{k_2}\psi_2)_-}{\partial\nu} - \frac{1}{k_0^2}\frac{\partial(S_{\delta,\delta}^{k_2}\varphi_0)_+}{\partial\nu} = g_2 \end{array} \right.$$

on $\partial\Omega$.

Then the following lemma holds.

Lemma 2.5.1 *The operator $T_0 : X^2 \to Y^2$ is invertible.*

Proof. Let us solve the equation $T_0(\Phi) = (f_1, f_2, g_1, g_2)$. Since the two first equations are decoupled from the two last ones, we start by solving the system

$$\begin{cases} S_{0,0}^{k_2}\varphi_1 - S_{0,0}^{k_2}\varphi_2 = f_1 \\ \dfrac{1}{k_1^2}\dfrac{\partial(S_{0,0}^{k_2}\varphi_1)_-}{\partial\nu} - \dfrac{1}{k_2^2}\dfrac{\partial(S_{0,0}^{k_2}\varphi_2)_+}{\partial\nu} = f_2 \end{cases} \quad \text{on } \partial\Omega.$$

Since k_2^2 is not a Dirichlet eigenvalue of $-\Delta$ in Ω, the operator $S_{0,0}^{k_2} : L^2(\partial\Omega) \to H^1(\partial\Omega)$ is invertible and so we have

$$\varphi_1 = \varphi_2 + \left(S_{0,0}^{k_2}\right)^{-1} f_1\ .$$

Substituting this into the second equation, we get

$$\left(\frac{1}{k_1^2} - \frac{1}{k_2^2}\right)\left(\lambda + \left(K_0^{k_2}\right)^*\right)\varphi_2 = f_2 - \frac{1}{k_1^2}\left(-\frac{1}{2} + \left(K_0^{k_2}\right)^*\right)\left(S_{0,0}^{k_2}\right)^{-1} f_1\ ,$$

where λ is given by

$$\lambda = -\frac{1}{2}\frac{\frac{1}{k_1^2} + \frac{1}{k_2^2}}{\frac{1}{k_1^2} - \frac{1}{k_2^2}}.$$

Since $|\lambda| > \dfrac{1}{2}$ for any positive constants $k_1 \neq k_2$, applying Lemma 2.4.5 yields that $\lambda I + \left(K_0^{k_2}\right)^* : L^2(\partial\Omega) \to L^2(\partial\Omega)$ is invertible. We can then express φ_2 in terms of (f_1, f_2), and the expression of φ_1 follows immediately.

On the other hand, it is well-known that for δ small enough, k_2^2 is not a Dirichlet eigenvalue of $-\Delta$ in $\overline{\Omega} \cup \mathcal{O}_\delta$. See, for example, [43]. We can then express analogously (ψ_2, φ_0) in terms of (g_1, g_2). □

Lemma 2.5.2 *The operator $T - T_0 : X^2 \to Y^2$ is compact.*

Proof. Let $\Phi = (\varphi_1, \varphi_2, \psi_2, \varphi_0) \in X^2$, then $(T - T_0)\Phi$ is given by

$$(T - T_0)\Phi = \begin{pmatrix} \left(S_{0,0}^{k_1} - S_{0,0}^{k_2}\right)\varphi_1 - S_{\delta,0}^{k_2}\psi_2 \\ \dfrac{1}{k_1^2}\dfrac{\partial\left((S_{0,0}^{k_1} - S_{0,0}^{k_2})\varphi_1\right)_-}{\partial\nu} - \dfrac{1}{k_2^2}\dfrac{\partial S_{\delta,0}^{k_2}\psi_2}{\partial\nu} \\ S_{0,\delta}^{k_2}\varphi_2 - \left(S_{\delta,\delta}^{k_0} - S_{\delta,\delta}^{k_2}\right)\varphi_0 \\ \dfrac{1}{k_2^2}\dfrac{\partial S_{0,\delta}^{k_2}\varphi_2}{\partial\nu} - \dfrac{1}{k_0^2}\dfrac{\partial\left((S_{\delta,\delta}^{k_0} - S_{\delta,\delta}^{k_2})\varphi_0\right)_+}{\partial\nu} \end{pmatrix}.$$

Since $\Gamma_k - \Gamma_{k_1}$ is smooth, we can easily see that $S_{\eta,\eta}^{k} - S_{\eta,\eta}^{k_2} : L^2(\partial\Omega) \to H^1(\partial\Omega)$ is a compact operator, and so is $\dfrac{\partial(S_{\eta,\eta}^{k})_\pm}{\partial\nu} - \dfrac{\partial(S_{\eta,\eta}^{k_2})_\pm}{\partial\nu} : L^2(\partial\Omega) \to L^2(\partial\Omega)$. It is also clear, since the layer potential of a curve is smooth away from its curve, that $S^k_{0,\delta}, S^k_{\delta,0} : L^2(\partial\Omega) \to H^1(\partial\Omega)$ and $\dfrac{\partial S^k_{\delta,0}}{\partial\nu}, \dfrac{\partial S^k_{0,\delta}}{\partial\nu} : L^2(\partial\Omega) \to L^2(\partial\Omega)$ are compact operators which ends the proof. □

Now we are ready to prove Theorem 2.5.1.

Proof of Theorem 2.5.1. Since T_0 is invertible and $T - T_0$ is compact, the Fredholm alternative holds and existence follows from uniqueness.

Let $\Phi = (\varphi_1, \varphi_2, \psi_2, \varphi_0) \in X^2$ satisfy $T\Phi = 0$. Consider the function u defined as follows

$$u(x) = \begin{cases} S_0^{k_1}\varphi_1(x) & x \in \Omega\ , \\ S_0^{k_2}\varphi_2(x) + S_\delta^{k_2}\psi_2(x) & x \in \mathcal{O}_\delta\ , \\ S_\delta^{k_0}\varphi_0(x) & x \in \Omega_\delta^e. \end{cases}$$

This function satisfies the equations in (2.2.6) with the incident field $u_I \equiv 0$. Moreover,

$$\begin{aligned} \int_{\partial\Omega_\delta} \frac{\partial u}{\partial\nu}\Big|_+ \overline{u}\, ds &= \frac{k_0^2}{k_2^2}\int_{\partial\Omega_\delta} \frac{\partial u}{\partial\nu}\Big|_- \overline{u}\, ds \\ &= \frac{k_0^2}{k_2^2}\int_{\mathcal{O}_\delta} \left(|\nabla u|^2 - k_2^2|u|^2\right) dy + \frac{k_0^2}{k_2^2}\int_{\partial\Omega} \frac{\partial u}{\partial\nu}\Big|_+ \overline{u}\, ds \\ &= \frac{k_0^2}{k_2^2}\int_{\mathcal{O}_\delta} \left(|\nabla u|^2 - k_2^2|u|^2\right) dy + \frac{k_0^2}{k_1^2}\int_{\partial\Omega} \frac{\partial u}{\partial\nu}\Big|_- \overline{u}\, ds \\ &= \frac{k_0^2}{k_2^2}\int_{\mathcal{O}_\delta} \left(|\nabla u|^2 - k_2^2|u|^2\right) dy + \frac{k_0^2}{k_1^2}\int_{\Omega} \left(|\nabla u|^2 - k_1^2|u|^2\right) dy. \end{aligned}$$

Thus

$$\Im \int_{\partial\Omega_\delta} \frac{\partial u}{\partial\nu}\Big|_+ \overline{u}\, ds = 0.$$

Since u satisfies the radiation condition, using Lemma A.A.1.2 we deduce that $u \equiv 0$ in Ω_δ^e. Then, u satisfies the Helmholtz equation in $\mathcal{O}_\delta$ with $u = \frac{\partial u}{\partial\nu} = 0$ on $\partial\Omega_\delta$. By the unique continuation theorem, we conclude that $u \equiv 0$ in $\mathcal{O}_\delta$ and in the same way we get $u \equiv 0$ in Ω.

Now let us define $\tilde{u}$ by

$$\tilde{u}(x) = S_\delta^{k_0}\varphi_0(x) \quad \text{for } x \in \mathbb{R}^2.$$

Then $\tilde{u}$ is a solution to $\Delta\tilde{u} + k_0^2\tilde{u} = 0$ in Ω_δ^i with zero Dirichlet boundary condition. Since k_0^2 is not a Dirichlet eigenvalue for $-\Delta$ on Ω, there exists $\delta_0 > 0$ such that, for $0 \le \delta \le \delta_0$, k_0^2 is not a Dirichlet eigenvalue for $-\Delta$ on Ω_δ^i, and for such δ, we have necessarily $\tilde{u} = 0$ in Ω_δ^i. From the jump of the normal derivative, we obtain

$$\varphi_0 = \frac{\partial\tilde{u}}{\partial\nu}\Big|_+ - \frac{\partial\tilde{u}}{\partial\nu}\Big|_- = 0 \quad \text{on } \partial\Omega_\delta.$$

Consider now the function $\tilde{v}$ defined by

$$\tilde{v}(x) := S_0^{k_2}\varphi_2(x) + S_\delta^{k_2}\psi_2(x) \quad \text{for } x \in \mathbb{R}^2,$$

which satisfies the Helmholtz equation on $\Omega \cup \mathcal{O}_\delta \cup \Omega_\delta^e$ together with the radiation condition. Since $\tilde{v}(x) = 0$ on $\partial\Omega_\delta$, it follows by Lemma A.A.1.2 that $\tilde{v} = 0$ in Ω_δ^e. We also notice that $\tilde{v} = 0$ on $\partial\Omega$. Since k_2^2 is not a Dirichlet eigenvalue for $-\Delta$ on Ω, $\tilde{v} = 0$ in Ω, and so $\tilde{v} \equiv 0$ in $\mathbb{R}^2$. Then, we get

$$\varphi_2 = \frac{\partial(\tilde{v})_+}{\partial\nu} - \frac{\partial(\tilde{v})_-}{\partial\nu} = 0 \quad \text{on } \partial\Omega.$$

$$\psi_2 = \frac{\partial(\tilde{v})_+}{\partial\nu} - \frac{\partial(\tilde{v})_-}{\partial\nu} = 0 \quad \text{on } \partial\Omega_\delta.$$

Define $\hat{v}(x) = S_0^{k_1}\varphi_1(x)$ in $\mathbb{R}^2$. It is already proved that $\hat{v}(x) = 0$ and

$$\frac{\partial(S_0^{k_1}\varphi_1)_-}{\partial\nu}(x) = 0$$

on $\partial\Omega$. We deduce by Lemma A.A.1.2 that $\dfrac{\partial(S_0^{k_1}\varphi_1)_+}{\partial\nu}(x) = 0$ on $\partial\Omega$. It then follows that

$$\varphi_1 = \frac{\partial(S_0^{k_1}\varphi_1)_+}{\partial\nu} - \frac{\partial(S_0^{k_1}\varphi_1)_-}{\partial\nu} = 0 \quad \text{on } \partial\Omega.$$

This ends the proof of the theorem. □

At this point we have all the necessary ingredients to state and prove the following representation formula.

Theorem 2.5.2 *Suppose k_0^2, k_2^2 are not Dirichlet eigenvalues for $-\Delta$ on Ω. There exists $\delta_0 > 0$ such that for $0 < \delta < \delta_0$, if u is the solution of the problem (2.2.6) and $\Phi = (\varphi_1, \varphi_2, \psi_2, \varphi_0) \in X^2$ is the unique solution of*

$$\begin{cases} S_{0,0}^{k_1}\varphi_1 - S_{0,0}^{k_2}\varphi_2 - S_{\delta,0}^{k_2}\psi_2 = 0, \\ \dfrac{1}{k_1^2}\dfrac{\partial(S_{0,0}^{k_1}\varphi_1)_-}{\partial\nu} - \dfrac{1}{k_2^2}\dfrac{\partial(S_{0,0}^{k_2}\varphi_2)_+}{\partial\nu} - \dfrac{1}{k_2^2}\dfrac{\partial(S_{\delta,0}^{k_2}\psi_2)}{\partial\nu} = 0, \\ S_{0,\delta}^{k_2}\varphi_2 + S_{\delta,\delta}^{k_2}\psi_2 - S_{\delta,\delta}^{k_0}\varphi_0 = u_I(x+\delta\nu(x)), \\ \dfrac{1}{k_2^2}\dfrac{\partial(S_{0,\delta}^{k_2}\varphi_2)}{\partial\nu} + \dfrac{1}{k_2^2}\dfrac{\partial(S_{\delta,\delta}^{k_2}\psi_2)_-}{\partial\nu} - \dfrac{1}{k_0^2}\dfrac{\partial(S_{\delta,\delta}^{k_0}\varphi_0)_+}{\partial\nu} = \dfrac{1}{k_0^2}\dfrac{\partial u_I}{\partial\nu}(x+\delta\nu(x)), \end{cases} \tag{2.5.26}$$

where $x \in \partial\Omega$, then u can be represented as

$$u(x) = \begin{cases} S_0^{k_1}\varphi_1(x) & \text{for } x \in \Omega\,, \\ S_0^{k_2}\varphi_2(x) + S_\delta^{k_2}\psi_2(x) & \text{for } x \in \mathcal{O}_\delta \\ u_I + S_\delta^{k_0}\varphi_0(x)\,, & \text{for } x \in \Omega_\delta^e\,. \end{cases} \tag{2.5.27}$$

Proof. In fact, the function defined as in (2.5.27) clearly satisfies the Helmholtz equations, the transmission conditions and the radiation condition in (2.2.6). □

2.6 Regularity result

In order to rigorously derive the asymptotic expansions of the fundamental and the second-harmonic fields u and v, we will need to prove a more refined regularity result for the solution Φ in X^2 of the system of integral equations (2.5.26).

Lemma 2.6.1 *Let Φ be the solution in X^2 of the system of integral equations (2.5.26), then $\Phi \in \left(\mathcal{C}^1(\partial\Omega)\right)^4$.*

Proof. From (2.5.26), we have

$$T_0\Phi = \begin{pmatrix} S_{\delta,0}^{k_2}\psi_2 + (S_{0,0}^{k_2} - S_{0,0}^{k_1})\varphi_1 \\ \dfrac{1}{k_2^2}\dfrac{\partial S_{\delta,0}^{k_2}\psi_2}{\partial\nu} + \dfrac{1}{k_2^2}\left((K_0^{k_2})^* - (K_0^{k_1})^*\right)\varphi_1 \\ -S_{0,\delta}^{k_2}\varphi_2 + \left(S_{\delta,\delta}^{k_0} - S_{\delta,\delta}^{k_2}\right)\varphi_0 + u_I(x+\delta\nu(x)) \\ -\dfrac{1}{k_2^2}\dfrac{\partial S_{0,\delta}^{k_2}\varphi_2}{\partial\nu} + \dfrac{1}{k_0^2}\left((K_\delta^{k_0})^* - (K_\delta^{k_2})^*\right)\varphi_0 + \dfrac{1}{k_0^2}\dfrac{\partial u_I}{\partial\nu}(x+\delta\nu(x)) \end{pmatrix}.$$

Since $\partial\Omega$ is $\mathcal{C}^2$ we can deduce from the right-hand side of the previous identity that $T_0\Phi \in \left(\mathcal{C}^2(\partial\Omega)\times\mathcal{C}^1(\partial\Omega)\right)^2$. Another immediate consequence of the regularity of $\partial\Omega$ is that the following operators

$$\begin{aligned} S_{0,0}^{k} &: \mathcal{C}^1(\partial\Omega) \to \mathcal{C}^2(\partial\Omega)\,, \\ \lambda I + (K_{0,0}^{k})^* &: \mathcal{C}^1(\partial\Omega) \to \mathcal{C}^1(\partial\Omega)\,, \end{aligned}$$

with $|\lambda| > \frac{1}{2}$ and $k > 0$, are invertible with bounded inverse. The proof can be found, for example, in [44].

From the expression of $(T_0)^{-1}$ in the proof of Lemma 2.5.1 we can then deduce that $\Phi \in \left(\mathcal{C}^1(\partial\Omega)\right)^4$. □

As a direct consequence of the previous lemma and the following integral representation for u in $\mathcal{O}_\delta$:

$$u(x) = S_0^{k_2}\varphi_2(x) + S_\delta^{k_2}\psi_2(x)\,,$$

the following regularity result holds.

Corollary 2.6.1 *Let u be the solution to the problem (2.2.6). Then $\nabla u \in L^\infty(\overline{\mathcal{O}}_\delta)$.*

This result is important to us for establishing the well-posedness of problem (2.2.7). Estimates with uniform bounds will be proved later when looking for the main term of the second harmonic field.

Corollary 2.6.2 *Let Φ be the solution in X^2 of the system (2.5.26), then $\Phi \in \left(H^1(\partial\Omega)\right)^4$.*

With this higher regularity for Φ, we can define higher-order derivatives of the single layer potential. The following lemma holds.

Lemma 2.6.2 *Let $\varphi \in H^1(\partial\Omega)$. Then the first and second order normal derivatives of the single layer potential exist and are continuous from $H^1(\partial\Omega)$ into $H^1(\partial\Omega)$ and $L^2(\partial\Omega)$, respectively. In particular, we have*

$$\begin{aligned}
S^k_{0,\delta}\varphi &= S^k_{0,0}\varphi + \delta \frac{\partial (S^k_{0,0}\varphi)_+}{\partial \nu} + o(\delta) ,\\
\frac{\partial S^k_{0,\delta}\varphi}{\partial \nu} &= \frac{\partial (S^k_{0,0}\varphi)_+}{\partial \nu} + \delta \frac{\partial^2 (S^k_{0,0}\varphi)_+}{\partial \nu^2} + o(\delta) ,\\
S^k_{\delta,0}\varphi &= S^k_{\delta,\delta}\varphi + \delta \frac{\partial (S^k_{0,0}\varphi)_-}{\partial \nu} + o(\delta) ,\\
\frac{\partial S^k_{\delta,0}\varphi}{\partial \nu} &= \frac{\partial (S^k_{\delta,\delta}\varphi)_-}{\partial \nu} + \delta \frac{\partial^2 (S^k_{0,0}\varphi)_-}{\partial \nu^2} + o(\delta) ,
\end{aligned}$$

where $o(\delta)$ is in $H^1(\partial\Omega)$ in the first and third equations and in $L^2(\partial\Omega)$ in the remaining ones.

2.7 Asymptotic expansion of the fundamental field

Given sufficient regularity of $\partial\Omega$, we establish in this section the asymptotic formula (2.2.11) for the fundamental field u. We first introduce some notations. Define the operators Q_δ, R_δ and W_δ from X into Y by

$$\begin{aligned}
Q_\delta(\varphi,\psi) &:= \left(S^{k_1}_{0,0}\varphi - S^{k_0}_{\delta,\delta}\psi, \frac{1}{k_1^2}\frac{\partial (S^{k_1}_{0,0}\varphi)_-}{\partial\nu} - \frac{1}{k_0^2}\frac{\partial (S^{k_0}_{\delta,\delta}\psi)_+}{\partial\nu} \right) ,\\
R_\delta(\varphi,\psi) &:= \Bigg((S^{k_2}_{0,\delta} - S^{k_2}_{0,0})\varphi + (S^{k_2}_{\delta,\delta} - S^{k_2}_{\delta,0})\psi,\\
&\qquad \frac{1}{k_2^2}\frac{\partial}{\partial\nu}\Big((S^{k_2}_{0,\delta}\varphi) - (S^{k_2}_{0,0}\varphi)_+ + (S^{k_2}_{\delta,\delta}\psi)_- - (S^{k_2}_{\delta,0}\psi)\Big)\Bigg) ,\\
W_\delta(\varphi,\psi) &:= \left(S^{k_2}_{0,0}\varphi + S^{k_2}_{\delta,0}\psi, \frac{1}{k_2^2}\frac{\partial (S^{k_2}_{0,0}\varphi)_+}{\partial\nu} + \frac{1}{k_2^2}\frac{\partial (S^{k_2}_{\delta,0}\psi)}{\partial\nu} \right) ,\\
W_0(\varphi,\psi) &:= \left(S^{k_2}_{0,0}\varphi + S^{k_2}_{0,0}\psi, \frac{1}{k_2^2}\frac{\partial (S^{k_2}_{0,0}\varphi)_+}{\partial\nu} + \frac{1}{k_2^2}\frac{\partial (S^{k_2}_{0,0}\psi)_-}{\partial\nu} \right) ,
\end{aligned}$$

and the function U_I^δ on $\partial\Omega$ by

$$U_I^\delta(x) := \left(u_I(x+\delta\nu(x)), \frac{1}{k_0^2}\frac{\partial u_I}{\partial\nu}(x+\delta\nu(x)) \right) .$$

The following lemma holds.

Lemma 2.7.1 *Let $\Phi = (\varphi_1, \varphi_2, \psi_2, \varphi_0) \in X^2$ be the unique solution of (2.5.26), then (φ_1, φ_0) and (φ_2, ψ_2) are solutions of the following equations*

$$\begin{aligned} Q_\delta(\varphi_1, \varphi_0) &= U_I^\delta - R_\delta(\varphi_2, \psi_2) , \\ W_\delta(\varphi_2, \psi_2) &= \left((S_{0,0}^{k_1}\varphi_1), \frac{1}{k_1^2} \frac{\partial (S_{0,0}^{k_1}\varphi_1)_-}{\partial \nu} \right) . \end{aligned} \tag{2.7.28}$$

In order to expand Φ with respect to the thickness δ, we need to prove a stability result when δ goes to 0, provided $\partial\Omega$ is sufficiently regular.

Proposition 2.7.1 *The operators Q_δ and W_δ converge uniformly to Q_0 and W_0 respectively. Moreover, assuming $\partial\Omega$ of class $\mathcal{C}^3$, Q_0 and W_0 are invertible from X into Y and from $(H^1(\partial\Omega))^2$ into $H^2(\partial\Omega) \times H^1(\partial\Omega)$.*

Proof. The uniform convergence is a consequence of Lemmas 2.4.3 and 2.4.4. Let us prove the invertibility of Q_0. We write Q_0 as

$$\begin{aligned} Q_0(\varphi, \psi) &= \left(S_{0,0}^{k_1}\varphi - S_{0,0}^{k_1}\psi, \frac{1}{k_1^2}\frac{\partial (S_{0,0}^{k_1}\varphi)_-}{\partial \nu} - \frac{1}{k_0^2}\frac{\partial (S_{0,0}^{k_1}\psi)_+}{\partial \nu} \right) \\ &\quad + \Bigg(- (S_{0,0}^{k_0} - S_{0,0}^{k_1})\psi, \\ &\quad - \frac{1}{k_0^2} \frac{\partial ((S_{0,0}^{k_0} - S_{0,0}^{k_1})\psi)_+}{\partial \nu} \Bigg) , \end{aligned}$$

where the first operator is invertible and the second one is compact. The Fredholm alternative holds. It remains then to prove the injectivity of Q_0. Let $(\varphi, \psi) \in X$ be satisfying $Q_0(\varphi, \psi) = 0$. We define u in $\mathbb{R}^2$ by

$$u(x) = \begin{cases} S_0^{k_1}\varphi(x) & \text{for } x \in \Omega, \\ S_0^{k_0}\psi(x) & \text{for } x \in \mathbb{R}^2 \setminus \overline{\Omega}. \end{cases}$$

In a similar way as for Theorem 2.5.1, we prove that

$$\Im \int_{\partial\Omega} \frac{\partial (u)_+}{\partial \nu} \overline{u}\, ds = 0 ,$$

from which we get that, since u satisfies the outgoing radiation condition, $u \equiv 0$ in $\mathbb{R}^2 \setminus \overline{\Omega}$ and so, by the unique continuation theorem, we obtain that $u \equiv 0$ in $\mathbb{R}^2$. Since k_0^2 is not a Dirichlet eigenvalue for $-\Delta$ on Ω, it follows that $S_0^{k_0}\psi \equiv 0$ in $\mathbb{R}^2$ and from the jump of its normal derivative on $\partial\Omega$, we can deduce that $\psi \equiv 0$. We prove in a similar way that $S_0^{k_1}\varphi \equiv 0$ in $\mathbb{R}^2$ and then from the jump of its normal derivative, we get $\varphi \equiv 0$. The invertibility of Q_0 is then proved.

To prove that W_0 is invertible, let us suppose that we have $(\varphi, \psi) \in X$ and $(f, g) \in Y$ satisfying

$$\begin{cases} S_{0,0}^{k_2}\varphi + S_{0,0}^{k_2}\psi &= f , \\ \dfrac{1}{k_2^2}\dfrac{\partial (S_{0,0}^{k_2}\varphi)_+}{\partial \nu} + \dfrac{1}{k_2^2}\dfrac{\partial (S_{0,0}^{k_2}\psi)_-}{\partial \nu} &= g . \end{cases}$$

Then we deduce from the first equation, since k_2^2 is not a Dirichlet eigenvalue of $-\Delta$ on Ω, that

$$\varphi + \psi = (S_{0,0}^{k_2})^{-1} f \ .$$

Inserting this into the second equation together with the expression of the jump of the normal derivative of the single layer potential, we obtain

$$\varphi = k_2^2 g - (-\frac{1}{2} + (K_{0,0}^{k_2})^*)(S_{0,0}^{k_2})^{-1} f),$$

which gives us the expression of ψ and proves the invertibility of W_0.

The invertibility of Q_0 and W_0 from $(H^1(\partial\Omega))^2$ into $H^2(\partial\Omega) \times H^1(\partial\Omega)$ can be proved in the same way. □

Proposition 2.7.2 *Suppose that $\partial\Omega$ is of class $\mathcal{C}^3$. Let $\Phi = (\varphi_1, \varphi_2, \psi_2, \varphi_0) \in X^2$ be the unique solution of (2.5.26), then there exists a constant $C > 0$ such that*

$$\|\Phi\|_{H^1(\partial\Omega)^4} \leq C \ .$$

Proof. Since W_δ converges uniformly to W_0 and since W_0 is invertible from $(H^1(\partial\Omega))^2$ into $H^2(\partial\Omega) \times H^1(\partial\Omega)$, then in view of (2.7.28) it can be seen that there exist two constants $C, C_1 > 0$ such that

$$\begin{aligned} \|(\varphi_2, \psi_2)\|_{(H^1(\partial\Omega))^2} &\leq C_1 \left\| \left(S_{0,0}^{k_1}\varphi_1, \frac{\partial (S_{0,0}^{k_1}\varphi_1)_-}{\partial \nu} \right) \right\|_{H^2(\partial\Omega)\times H^1(\partial\Omega)} \\ &\leq C \|\varphi_1\|_{H^1(\partial\Omega)} \ . \end{aligned}$$

Combining the facts that Q_δ converges to Q_0 uniformly together with the fact that Q_0 is invertible, we show that there exist constants $C', C_1' > 0$ and ε_δ small such that for δ small enough, we have from Lemma 2.4.3 that

$$\begin{aligned} \|(\varphi_1, \varphi_0)\|_{(H^1(\partial\Omega))^2} &\leq C_1' \left\| U_I^\delta - R_\delta(\varphi_2, \psi_2) \right\|_{H^2(\partial\Omega)\times H^1(\partial\Omega)} \\ &\leq C_1 + \varepsilon_\delta \|\varphi_1\|_{H^1(\partial\Omega)} \ . \end{aligned}$$

Here $\varepsilon_\delta \to 0$ as $\delta \to 0$. It then follows that φ_1 and φ_0 are bounded in $H^1(\partial\Omega)$ which also implies that φ_2 and ψ_2 are bounded in $H^1(\partial\Omega)$. □

Proposition 2.7.3 *Let $\Phi^\delta = (\varphi_1^\delta, \varphi_2^\delta, \psi_2^\delta, \varphi_0^\delta) \in X^2$ be the unique solution of (2.5.26), then $(\varphi_1^\delta, \varphi_0^\delta)$ and $(\varphi_2^\delta, \psi_2^\delta)$ converge to $(\varphi_1^0, \varphi_0^0)$ and (φ_2^0, ψ_2^0) respectively in $(H^1(\partial\Omega))^2$ where $(\varphi_1^\delta, \varphi_0^\delta, \varphi_2^\delta, \psi_2^\delta)$ are the unique solutions to the decoupled systems of integral equations*

$$Q_0(\varphi_1^0, \varphi_0^0) = U_I^0 \ ,$$

and

$$W_0(\varphi_2^0, \psi_2^0) = \left((S_{0,0}^{k_1}\varphi_1^0), \frac{1}{k_1^2} \frac{\partial (S_{0,0}^{k_1}\varphi_1^0)_-}{\partial \nu} \right) \ . \tag{2.7.29}$$

Proof. Recalling that φ_2^δ and ψ_2^δ are bounded in $H^1(\partial\Omega)$, we have

$$U_I^\delta - R_\delta(\varphi_2^\delta, \psi_2^\delta) \to U_I^0$$

uniformly in $H^2(\partial\Omega) \times H^1(\partial\Omega)$. Since Q_δ converges uniformly to Q_0, $(\varphi_1^\delta, \varphi_0^\delta)$ converges to $(\varphi_1^0, \varphi_0^0)$ in $(H^1(\partial\Omega))^2$. It follows that, since W_δ converges uniformly to W_0, $(\varphi_2^\delta, \psi_2^\delta)$ converges to (φ_2^0, ψ_2^0) in $(H^1(\partial\Omega))^2$ which ends the proof of the proposition. □

It is worth noticing that the limit $(\varphi_1^0, \varphi_0^0)$ represents the solution of the problem without the thin coating. In fact, if we define U by

$$U(x) := \begin{cases} S_0^{k_1}\varphi_1^0(x) & \text{for } x \in \Omega\,, \\ S_0^{k_0}\varphi_0^0(x) + u_I(x) & \text{for } x \in \mathbb{R}^2 \setminus \overline{\Omega}\,, \end{cases} \tag{2.7.30}$$

then U is the unique solution to the problem (2.2.8).

The following proposition is a direct consequence of Lemmas 2.4.3 and 2.6.2.

Proposition 2.7.4 *The following expansions hold.*

$$Q_\delta(\varphi,\psi) = Q_0(\varphi,\psi) - \delta Q_1(\psi) + O(\delta^2)\,, \quad \forall\, \varphi,\psi \in H^1(\partial\Omega)\,, \tag{2.7.31}$$
$$R_\delta(\varphi,\psi) = \delta R_1(\varphi,\psi) + o(\delta)\,, \quad \forall\, \varphi,\psi \in H^1(\partial\Omega)\,, \tag{2.7.32}$$

where the remainder terms $O(\delta^2)$ and $o(\delta)$ are in $H^1(\partial\Omega) \times L^2(\partial\Omega)$, and

$$R_1(\varphi,\psi) := \Bigg(\frac{\partial(S_{0,0}^{k_2}\varphi)_+}{\partial\nu} + \frac{\partial(S_{0,0}^{k_2}\psi)_-}{\partial\nu}, \tag{2.7.33}$$
$$-\frac{1}{k_2^2}\left(\rho\frac{\partial(S_{0,0}^{k_2}\varphi)_+}{\partial\nu} + \rho\frac{\partial(S_{0,0}^{k_2}\psi)_-}{\partial\nu} + \frac{\partial^2 S_{0,0}^{k_2}(\varphi+\psi)}{\partial\tau^2} + k_2^2 S_{0,0}^{k_2}(\varphi+\psi)\right)\Bigg)\,,$$

$$Q_1(\varphi) := \Bigg(\frac{\partial(S_{0,0}^{k_0}\varphi)_+}{\partial\nu} + S_{0,0}^{k_0}(\rho\varphi) + (D_{0,0}^{k_0}\varphi)_+, \tag{2.7.34}$$
$$\frac{1}{k_0^2}\left(-\rho\frac{\partial(S_{0,0}^{k_0}\varphi)_+}{\partial\nu} - \frac{\partial^2(S_{0,0}^{k_0}\varphi)}{\partial\tau^2} - k_0^2(S_{0,0}^{k_0}\varphi) + \frac{\partial(S_{0,0}^{k_0}\rho\varphi)_+}{\partial\nu} + \frac{\partial(D_{0,0}^{k_0}\varphi)}{\partial\nu}\right)\Bigg)\,.$$

Proof. Since, for $\varphi \in H^1(\partial\Omega)$, $S_0^k\varphi$ satisfies the Helmholtz equation in $\mathbb{R}^2 \setminus \partial\Omega$ then

$$\frac{\partial^2(S_{0,0}^k\varphi)_\pm}{\partial\nu^2} = -\rho\frac{\partial(S_{0,0}^k\varphi)_\pm}{\partial\nu} - \frac{\partial^2(S_{0,0}^k\varphi)}{\partial\tau^2} - k^2 S_{0,0}^k\varphi \quad \text{on } \partial\Omega,$$

and equation (2.7.32) follows immediately from Lemma 2.6.2. Here we have expressed the Laplacian in the local coordinates

$$\Delta = \frac{\partial^2}{\partial\nu^2} + \rho\frac{\partial}{\partial\nu} + \frac{\partial^2}{\partial\tau^2} \quad \text{on } \partial\Omega. \tag{2.7.35}$$

Applying Lemma 2.4.3, we obtain (2.7.31) for $(\varphi,\psi) \in (L^2(\partial\Omega))^2$ with

$$Q_1(\psi) = \left(K_0^k\psi + (K_0^k)^*\psi + S_{0,0}^k(\rho\psi), \frac{1}{k_0^2}(M_0^k\psi + (K_0^k)^*(\rho\psi))\right)\,.$$

It remains then to prove that for $\psi \in H^1(\partial\Omega)$ this expression is identical to the one defined in (2.7.34).

In view of identities (2.4.21) and (2.4.22), it is easy to see that

$$K_0^k\psi + (K_0^k)^*\psi = \frac{\partial(S_{0,0}^k\psi)_+}{\partial\nu} + (D_{0,0}^k\psi)_+ \,.$$

On the other hand, by using the local coordinates (2.7.35) it follows that

$$\begin{aligned} M_0^k\psi + (K_0^k)^*(\rho\psi) &= -\rho\frac{\partial(S_{0,0}^{k_0}\varphi)_+}{\partial\nu} - \frac{\partial^2(S_{0,0}^{k_0}\varphi)}{\partial\tau^2} - k_0^2(S_{0,0}^{k_0}\varphi) \\ &\quad + \frac{\partial(S_{0,0}^{k_0}\rho\varphi)_+}{\partial\nu} + \frac{\partial(D_{0,0}^{k_0}\varphi)}{\partial\nu} \,, \end{aligned}$$

as desired. The proof is complete. □

Proposition 2.7.5 *Let* $(\varphi_1^{1,\delta}, \varphi_0^{1,\delta}) \in X$ *be defined as*

$$(\varphi_1^{1,\delta}, \varphi_0^{1,\delta}) := \left(\frac{\varphi_1^\delta - \varphi_1^0}{\delta}, \frac{\varphi_0^\delta - \varphi_0^0}{\delta}\right) \,.$$

Then, for $\delta \to 0$, $(\varphi_1^{1,\delta}, \varphi_0^{1,\delta})$ *converges in* X *to the pair* $(\varphi_1^{1,0}, \varphi_0^{1,0})$ *which satisfies*

$$Q_0(\varphi_1^{1,0}, \varphi_0^{1,0}) = U_I'(x) + Q_1(\varphi_0^0) - Z(\varphi_1^0) \,, \tag{2.7.36}$$

where

$$\begin{aligned} U_I'(x) &:= \left(\frac{\partial u_I}{\partial\nu}(x), -\frac{1}{k_0^2}\rho\frac{\partial u_I}{\partial\nu}(x) - \frac{1}{k_0^2}\frac{\partial^2 u_I}{\partial\tau^2}(x) - u_I(x)\right) \,, \quad x \in \partial\Omega \,, \\ Z(\varphi) &:= \left(\frac{k_2^2}{k_1^2}\frac{\partial(S_{0,0}^{k_1}\varphi)_-}{\partial\nu}, -\frac{1}{k_1^2}\rho\frac{\partial(S_{0,0}^{k_1}\varphi)_-}{\partial\nu} - \frac{1}{k_2^2}\frac{\partial^2 S_{0,0}^{k_1}(\varphi)}{\partial\tau^2} - S_{0,0}^{k_1}(\varphi)\right) \,. \end{aligned}$$

Proof. Since $(\varphi_2^\delta, \psi_2^\delta)$ converges to (φ_2^0, ψ_2^0) and $(\varphi_1^\delta, \varphi_0^\delta)$ converges to $(\varphi_1^0, \varphi_0^0)$ in $H^1(\partial\Omega)$, the following equation holds.

$$Q_0(\varphi_1^{1,\delta}, \varphi_0^{1,\delta}) = U_I'(x) + Q_1(\varphi_0^0) - R_1(\varphi_2^0, \psi_2^0) + o(1) \,,$$

where $o(1)$ is in Y. We can then state that $(\varphi_1^{1,\delta}, \varphi_0^{1,\delta})$ converges to $(\varphi_1^{1,0}, \varphi_0^{1,0})$ that is a solution of

$$Q_0(\varphi_1^{1,0}, \varphi_0^{1,0}) = U_I'(x) + Q_1(\varphi_0^0) - R_1(\varphi_2^0, \psi_2^0) \,.$$

From equation (2.7.29), we see that

$$\begin{aligned} S_{0,0}^{k_2}(\varphi_2^0 + \psi_2^0) &= S_{0,0}^{k_1}\varphi_1^0 \,, \\ \frac{\partial(S_{0,0}^{k_2}\varphi_2^0)_+}{\partial\nu} + \frac{\partial(S_{0,0}^{k_2}\psi_2^0)_-}{\partial\nu} &= \frac{k_2^2}{k_1^2}\frac{\partial(S_{0,0}^{k_1}\varphi_1^0)_-}{\partial\nu} \,, \end{aligned}$$

which gives

$$R_1(\varphi_2^0, \psi_2^0) = Z(\varphi_1^0) \,.$$

The proposition is then proved. $\square$

Finally, the following proposition provides the expansion of $(\varphi_1^\delta, \varphi_0^\delta)$ as δ goes to zero.

Proposition 2.7.6 *The following expansions hold.*

$$\begin{aligned} \varphi_1^\delta &= \varphi_1^0 + \delta \varphi_1^{1,0} + o(\delta) \ , \\ \varphi_0^\delta &= \varphi_0^0 + \delta \varphi_0^{1,0} + o(\delta) \ , \end{aligned}$$

where $o(\delta)$ is bounded in $L^2(\partial\Omega)$ by $C\delta$, C being a positive constant.

Proof of formula (2.2.11) in Theorem 2.2.1. From the representation formula and the expansion of (φ_1, φ_0) we can write

$$u(x) = U(x) + \delta u_1(x) + o(\delta) \ ,$$

where

$$u_1(x) = \begin{cases} S_0^{k_1} \varphi_1^{1,0}(x) & \text{for } x \in \Omega, \\ S_0^{k_0} \varphi_0^{1,0}(x) + D_0^{k_0} \varphi_0^0(x) + S_0^{k_0}(\rho \varphi_0^0)(x) & \text{for } x \in \mathbb{R}^2 \setminus \overline{\Omega}. \end{cases}$$

Consider now the unique solution to the following problem

$$\begin{cases} \Delta w_1 + k_1^2 w_1 = 0 & \text{for } x \in \Omega, \\ \Delta w_1 + k_0^2 w_1 = 0 & \text{for } x \in \mathbb{R}^2 \setminus \overline{\Omega}, \\ [w_1]_{\partial\Omega} = (D_{0,0}^{k_0} \varphi_0^0)_+ + S_{0,0}^{k_0}(\rho \varphi_0^0) & \text{on } \partial\Omega, \\ \left[\dfrac{1}{k^2} \dfrac{\partial w_1}{\partial \nu} \right]_{\partial\Omega} = \dfrac{1}{k_0^2} \dfrac{\partial (S_{0,0}^{k_0}(\rho \varphi_0^0))_+}{\partial \nu} + \dfrac{1}{k_0^2} \dfrac{\partial (D_{0,0}^{k_0} \varphi_0^0)}{\partial \nu} & \text{on } \partial\Omega, \\ w_1 \text{ satisfies the (outgoing) radiation condition.} \end{cases} \tag{2.7.37}$$

The function w_1 can be expressed using the Green's function G as follows

$$\begin{aligned} w_1(x) &= -\int_{\partial\Omega} \frac{\partial G}{\partial \nu}(x,y) \left((D_{0,0}^{k_0} \varphi_0^0)_+ + S_{0,0}^{k_0}(\rho \varphi_0^0) \right) ds(y) \\ &\quad + \int_{\partial\Omega} k_0^2 (G(x,y))_+ \left(\frac{1}{k_0^2} \frac{\partial (S_{0,0}^{k_0}(\rho \varphi_0^0))_+}{\partial \nu} + \frac{1}{k_0^2} \frac{\partial (D_{0,0}^{k_0} \varphi_0^0)}{\partial \nu} \right) ds(y). \end{aligned}$$

On the other hand, we can see that

$$w_1(x) = \begin{cases} 0 & \text{for } x \in \Omega \ , \\ D_0^{k_0} \varphi_0^0(x) + S_0^{k_0}(\rho \varphi_0^0)(x) & \text{for } x \in \mathbb{R}^2 \setminus \overline{\Omega} \ , \end{cases}$$

since this last function satisfies all the conditions in (2.7.37). We also introduce the function w_2 defined on $\mathbb{R}^2$ by

$$w_2(x) = \begin{cases} S_0^{k_1} \varphi_1^{1,0}(x) & \text{for } x \in \Omega \ , \\ S_0^{k_0} \varphi_0^{1,0}(x) & \text{for } x \in \mathbb{R}^2 \setminus \overline{\Omega} \ . \end{cases}$$

Since $(\varphi_1^{1,0}, \varphi_0^{1,0})$ satisfies the system (2.7.36), we can express w_2 using G as follows

$$
\begin{aligned}
w_2(x) &= \int_{\partial\Omega} \frac{\partial G}{\partial \nu}(x,y) \\
&\left(\frac{\partial u_I}{\partial \nu} + \frac{\partial (S_{0,0}^{k_0}\varphi_0^0)+}{\partial \nu} + S_{0,0}^{k_0}(\rho\varphi_0^0) + (D_{0,0}^{k_0}\varphi_0^0)_+ - \frac{k_2^2}{k_1^2}\frac{\partial (S_{0,0}^{k_1}\varphi_1^0)-}{\partial \nu} \right) ds(y) \\
&+ \int_{\partial\Omega} k_0^2 (G(x,y))_+ \left(\frac{1}{k_0^2}\rho \frac{\partial u_I}{\partial \nu}(x) + \frac{1}{k_0^2}\frac{\partial^2 u_I}{\partial \tau^2}(x) + u_I + \frac{1}{k_0^2}\rho \frac{\partial (S_{0,0}^{k_0}\varphi_0^0)+}{\partial \nu} \right. \\
&+ \frac{1}{k_0^2}\frac{\partial^2 (S_{0,0}^{k_0}\varphi_0^0)}{\partial \tau^2} + (S_{0,0}^{k_0}\varphi_0^0) - \frac{1}{k_0^2}\frac{\partial (S_{0,0}^{k_0}(\rho\varphi_0^0))+}{\partial \nu} - \frac{1}{k_0^2}\frac{\partial (D_{0,0}^{k_0}\varphi_0^0)}{\partial \nu} \\
&\left. - \frac{1}{k_1^2}\rho \frac{\partial (S_{0,0}^{k_1}\varphi_1^0)-}{\partial \nu} - \frac{1}{k_2^2}\frac{\partial^2 S_{0,0}^{k_1}(\varphi_1^0)}{\partial \tau^2} - S_{0,0}^{k_1}(\varphi_1^0) \right) ds(y).
\end{aligned}
$$

Since

$$
u_1(x) = w_1(x) + w_2(x) \ ,
$$

we conclude that

$$
\begin{aligned}
u_1(x) &= (k_0^2 - k_2^2) \int_{\partial\Omega} \left[\frac{\partial G}{\partial \nu}(x,y) \frac{1}{k_0^2} \left(\frac{\partial U}{\partial \nu}(y) \right)_+ \right. \\
&\left. - \left(\frac{1}{k_0^2} - \frac{1}{k_2^2} \right) \int_{\partial\Omega} k_0^2 (\frac{\partial G}{\partial \tau}(x,y))_+ \frac{\partial U}{\partial \tau}(y) \right] ds(y) \ ,
\end{aligned}
$$

which ends the proof of the first asymptotic expansion in Theorem 2.2.1. □

2.8 Representation formula for the second-harmonic field

In this section, we derive a representation formula for the solution of (2.2.7). The formula is essentially the same as for the fundamental field. However, we give its proof in order to make sure that the assumptions $k_2 \neq k_0$ and $k_2 \neq k_1$ do not play any role in the proof of Theorem 2.5.2.

The following holds.

Theorem 2.8.1 *Suppose $k_0'^2$, $k_2'^2$ are not Dirichlet eigenvalues for $-\Delta$ on Ω. Then, there exists $\delta_0 > 0$ such that, for $0 < \delta < \delta_0$, for each $(f_1, f_2, g_1, g_2) \in Y^2$, there exists a unique solution $\tilde{\Phi} = (\tilde{\varphi}_1, \tilde{\varphi}_2, \tilde{\psi}_2, \tilde{\varphi}_0) \in X^2$ to the system of integral* *equations*

$$\left\{\begin{array}{l} S^{k'_1}_{0,0}\tilde{\varphi}_1 - S^{k'_2}_{0,0}\tilde{\varphi}_2 - S^{k'_2}_{\delta,0}\tilde{\psi}_2 = f_1,\\ \dfrac{\partial(S^{k'_1}_{0,0}\tilde{\varphi}_1)_-}{\partial\nu} - \dfrac{\partial(S^{k'_2}_{0,0}\tilde{\varphi}_2)_+}{\partial\nu} - \dfrac{\partial(S^{k'_2}_{\delta,0}\tilde{\psi}_2)}{\partial\nu} = f_2,\\ S^{k'_2}_{0,\delta}\tilde{\varphi}_2 + S^{k'_2}_{\delta,\delta}\tilde{\psi}_2 - S^{k'_0}_{\delta,\delta}\tilde{\varphi}_0 = g_1,\\ \dfrac{\partial(S^{k'_2}_{0,\delta}\tilde{\varphi}_2)}{\partial\nu} + \dfrac{\partial(S^{k'_2}_{\delta,\delta}\tilde{\psi}_2)_-}{\partial\nu} - \dfrac{\partial(S^{k'_0}_{\delta,\delta}\tilde{\varphi}_0)_+}{\partial\nu} = g_2. \end{array}\right. \tag{2.8.38}$$

The proof of this theorem is basically the same as the one of Theorem 2.5.1. First, we define the operator T' from X^2 into Y^2 by $T'(\tilde{\Phi}) = (f_1, f_2, g_1, g_2)$ where (f_1, f_2, g_1, g_2) is given as in (2.8.38), and the operator T'_0 from X^2 into Y^2 by

$$T'_0(\tilde{\Phi}) = \left(\begin{array}{l} S^{k'_2}_{0,0}\tilde{\varphi}_1 - S^{k'_2}_{0,0}\tilde{\varphi}_2\\ \dfrac{\partial(S^{k'_2}_{0,0}\tilde{\varphi}_1)_-}{\partial\nu} - \dfrac{\partial(S^{k'_2}_{0,0}\tilde{\varphi}_2)_+}{\partial\nu}\\ S^{k'_2}_{\delta,\delta}\tilde{\psi}_2 - S^{k'_2}_{\delta,\delta}\tilde{\varphi}_0\\ \dfrac{\partial(S^{k'_2}_{\delta,\delta}\tilde{\psi}_2)_-}{\partial\nu} - \dfrac{\partial(S^{k'_2}_{\delta,\delta}\tilde{\varphi}_0)_+}{\partial\nu} \end{array}\right).$$

Then the following lemma holds.

Lemma 2.8.1 *The operator $T'_0 : X^2 \to Y^2$ is invertible.*

Proof. Let us solve the equation $T'_0(\tilde{\Phi}) = (f_1, f_2, g_1, g_2)$. Since the two first equations are decoupled from the two last ones, we start by solving the following system of integral equations

$$\left\{\begin{array}{l} S^{k'_2}_{0,0}\tilde{\varphi}_1 - S^{k'_2}_{0,0}\tilde{\varphi}_2 = f_1,\\ \dfrac{\partial(S^{k'_2}_{0,0}\tilde{\varphi}_1)_-}{\partial\nu} - \dfrac{\partial(S^{k'_2}_{0,0}\tilde{\varphi}_2)_+}{\partial\nu} = f_2. \end{array}\right.$$

Since ${k'_2}^2$ is not a Dirichlet eigenvalue of $-\Delta$ in Ω, the operator $S^{k'_2}_{0,0} : L^2(\partial\Omega) \to H^1(\partial\Omega)$ is invertible and we have

$$\tilde{\varphi}_1 = \tilde{\varphi}_2 + \left(S^{k'_2}_{0,0}\right)^{-1} f_1 \; .$$

Substituting this into the second equation, we readily get

$$\tilde{\varphi}_2 = -f_2 + \left(-\frac{1}{2} + \left(K^{k'_2}_0\right)^*\right)\left(S^{k'_2}_{0,0}\right)^{-1} f_1 \; .$$

The expression of $\tilde{\varphi}_1$ follows immediately. Analogously, we can easily express $(\tilde{\psi}_2, \tilde{\varphi}_0)$ in terms of (g_1, g_2). □

Lemma 2.8.2 *The operator $T' - T'_0 : X^2 \to Y^2$ is compact.*

Proof. The proof is exactly the same as the one of Lemma 2.5.2. □

Proof of Theorem 2.8.1. Since T'_0 is invertible and $T' - T'_0$ is compact, the Fredholm alternative holds and existence will follow from uniqueness.

Let $\tilde{\Phi} = (\tilde{\varphi}_1, \tilde{\varphi}_2, \tilde{\psi}_2, \tilde{\varphi}_0) \in X^2$ satisfy $T'\tilde{\Phi} = 0$. Consider the function v defined by

$$v(x) = \begin{cases} S_0^{k'_1} \tilde{\varphi}_1(x) & \text{for } x \in \Omega, \\ S_0^{k'_2} \tilde{\varphi}_2(x) + S_\delta^{k'_2} \tilde{\psi}_2(x) & \text{for } x \in \mathcal{O}_\delta, \\ S_\delta^{k'_0} \tilde{\varphi}_0 & \text{for } x \in \Omega_\delta^e. \end{cases} \tag{2.8.39}$$

This function satisfies the equations in (2.2.7) where the source term

$$\sum_{j,l=1,2} \chi_{jl} \partial_{x_j} u \partial_{x_l} u \equiv 0.$$

Moreover, we can easily prove in a similar way as for the fundamental field u that

$$\Im \int_{\partial\Omega_\delta} \frac{\partial v}{\partial \nu} v \, ds = 0 \, ,$$

from which we obtain, by using Lemma A.A.1.2, that $v \equiv 0$ in Ω_δ^e, since v satisfies the outgoing radiation condition. Thus, v satisfies the Helmholtz equation in $\mathcal{O}_\delta$ with $v = \partial v / \partial \nu = 0$ on $\partial \Omega_\delta$. By the unique continuation theorem, we deduce that $v \equiv 0$ in $\mathcal{O}_\delta$ and in the same way, we get $v \equiv 0$ in Ω.

Then, as for Theorem 2.5.1, there exists $\delta_0 > 0$ such that, for $0 \le \delta \le \delta_0$, $k_0^{'2}$ is not a Dirichlet eigenvalue for $-\Delta$ on Ω_δ^i, and, for such δ, we have necessarily $S_0^{k'_0} \tilde{\varphi}_0 \equiv 0$ in Ω_δ^i. From the jump of the normal derivative of $S_0^{k'_0} \tilde{\varphi}_0$ on $\partial\Omega_\delta$, we immediately deduce that $\tilde{\varphi}_0 = 0$.

Then we can easily find that $S_0^{k'_2} \tilde{\varphi}_2(x) + S_\delta^{k'_2} \tilde{\psi}_2 \equiv 0$ in Ω_δ^e. The jump of the normal derivative of this function on $\partial\Omega_\delta$ gives $\tilde{\psi}_2 = 0$. Since $k_2^{'2}$ is not a Dirichlet eigenvalue for $-\Delta$ on Ω, we arrive at $S_0^{k'_2} \tilde{\varphi}_2(x) + S_\delta^{k'_2} \tilde{\psi}_2 \equiv 0$ in Ω. From the jump of its normal derivative on $\partial\Omega$, we arrive at $\tilde{\varphi}_2 = 0$.

Finally, since $S_0^{k'_1} \tilde{\varphi}_1$ has a null trace on $\partial\Omega$, we obtain from Lemma A.A.1.2 that $S_0^{k'_1} \tilde{\varphi}_1 \equiv 0$ in $\mathbb{R}^2 \setminus \overline{\Omega}$ and from the jump of its normal derivative on $\partial\Omega$, we deduce that $\tilde{\varphi}_1 = 0$. The uniqueness of $\tilde{\Phi}$ is then proved which ends the proof of the theorem. □

Theorem 2.8.2 *Suppose $(k'_0)^2, (k'_2)^2$ are not Dirichlet eigenvalues for $-\Delta$ on Ω. Let V be the unique solution of*

$$\Delta V + k_2^{'2} V = \sum_{j,l=1,2} \chi_{jl} \partial_{x_j} u \partial_{x_l} u \, \mathrm{I}_{\mathcal{O}_\delta} \quad \text{in } \mathbb{R}^2 \, ,$$

with the outgoing radiation condition, and let $V_0 = V|_{\partial\Omega}$, $V_\delta = V|_{\partial\Omega_\delta}$, $V'_0 = \frac{\partial V}{\partial \nu}|_{\partial\Omega}$ and $V'_\delta = \frac{\partial V}{\partial \nu}|_{\partial\Omega_\delta}$.

Then, there exists $\delta_0 > 0$ such that for $0 < \delta < \delta_0$, if v is the solution of the problem (2.2.7) and $\tilde{\Phi} = (\tilde{\varphi}_1, \tilde{\varphi}_2, \tilde{\psi}_2, \tilde{\varphi}_0) \in X^2$ is the unique solution of

$$\begin{cases} S_{0,0}^{k_1'}\tilde{\varphi}_1 - S_{0,0}^{k_2'}\tilde{\varphi}_2 - S_{\delta,0}^{k_2'}\tilde{\psi}_2 = V_0, \\ \dfrac{\partial(S_{0,0}^{k_1'}\tilde{\varphi}_1)_-}{\partial\nu} - \dfrac{\partial(S_{0,0}^{k_2'}\tilde{\varphi}_2)_+}{\partial\nu} - \dfrac{\partial(S_{\delta,0}^{k_2'}\tilde{\psi}_2)}{\partial\nu} = V_0', \\ S_{0,\delta}^{k_2'}\tilde{\varphi}_2 + S_{\delta,\delta}^{k_2'}\tilde{\psi}_2 - S_{\delta,\delta}^{k_0'}\tilde{\varphi}_0 = -V_\delta, \\ \dfrac{\partial(S_{0,\delta}^{k_2'}\tilde{\varphi}_2)}{\partial\nu} + \dfrac{\partial(S_{\delta,\delta}^{k_2'}\tilde{\psi}_2)_-}{\partial\nu} - \dfrac{\partial(S_{\delta,\delta}^{k_0'}\tilde{\varphi}_0)_+}{\partial\nu} = -V_\delta', \end{cases} \tag{2.8.40}$$

then v can be represented as

$$v(x) = \begin{cases} S_0^{k_1'}\tilde{\varphi}_1(x) & \text{for } x \in \Omega\ , \\ V(x) + S_0^{k_2'}\tilde{\varphi}_2(x) + S_\delta^{k_2'}\tilde{\psi}_2(x) & \text{for } x \in \mathcal{O}_\delta\ , \\ S_\delta^{k_0'}\tilde{\varphi}_0(x) & \text{for } x \in \Omega_\delta^e\ . \end{cases} \tag{2.8.41}$$

Proof. Recalling Corollary 2.6.1, we can express explicitly V by setting

$$V(x) = \int_{\mathcal{O}_\delta} \Gamma_{k_2'}(x-y) \sum_{j,l=1,2} \chi_{jl}\partial_{x_j}u(y)\partial_{x_l}u(y)\, dy\ . \tag{2.8.42}$$

Then it is clear that the function defined as in (2.8.41) satisfies the Helmholtz equations, the transmission conditions and the radiation condition in (2.2.6).□

2.9 Asymptotic expansion of the second-harmonic field

We proceed as for the fundamental field u. We first define the operators $\tilde{Q}_\delta$, $\tilde{R}_\delta$ and $\tilde{W}_\delta$ from X into Y by

$$\begin{aligned}
\tilde{Q}_\delta(\tilde{\varphi},\tilde{\psi}) &:= \left(S_{0,0}^{k_1'}\tilde{\varphi} - S_{\delta,\delta}^{k_0'}\tilde{\psi}, \frac{\partial(S_{0,0}^{k_1'}\tilde{\varphi})_-}{\partial\nu} - \frac{\partial(S_{\delta,\delta}^{k_0'}\tilde{\psi})_+}{\partial\nu} \right), \\
\tilde{R}_\delta(\tilde{\varphi},\tilde{\psi}) &:= \Bigg((S_{0,\delta}^{k_2'} - S_{0,0}^{k_2'})\tilde{\varphi} + (S_{\delta,\delta}^{k_2'} - S_{\delta,0}^{k_2'})\tilde{\psi}, \\
&\qquad \frac{\partial}{\partial\nu}\Big((S_{0,\delta}^{k_2'}\tilde{\varphi}) - (S_{0,0}^{k_2'}\tilde{\varphi})_+ + (S_{\delta,\delta}^{k_2'}\tilde{\psi})_- - (S_{\delta,0}^{k_2'}\tilde{\psi}) \Big) \Bigg), \\
\tilde{W}_\delta(\tilde{\varphi},\tilde{\psi}) &:= \left(S_{0,0}^{k_2'}\tilde{\varphi} + S_{\delta,0}^{k_2'}\tilde{\psi}, \frac{\partial(S_{0,0}^{k_2'}\tilde{\varphi})_+}{\partial\nu} + \frac{\partial(S_{\delta,0}^{k_2'}\tilde{\psi})}{\partial\nu} \right), \\
\tilde{W}_0(\tilde{\varphi},\tilde{\psi}) &:= \left(S_{0,0}^{k_2'}\tilde{\varphi} + S_{0,0}^{k_2'}\tilde{\psi}, \frac{\partial(S_{0,0}^{k_2'}\tilde{\varphi})_+}{\partial\nu} + \frac{\partial(S_{0,0}^{k_2'}\tilde{\psi})_-}{\partial\nu} \right),
\end{aligned}$$

and the function $\tilde{V}^\delta$ on $\partial\Omega$ by

$$\tilde{V}_\delta := \left(V_\delta - V_0, V'_\delta - V'_0 \right) .$$

The following proposition holds.

Proposition 2.9.1 *Let $\tilde{\Phi} = (\tilde{\varphi}_1, \tilde{\varphi}_2, \tilde{\psi}_2, \tilde{\varphi}_0) \in X^2$ be the unique solution of (2.8.40), then $(\tilde{\varphi}_1, \tilde{\varphi}_0)$ and $(\tilde{\varphi}_2, \tilde{\psi}_2)$ are solutions of the following equations*

$$\tilde{Q}_\delta(\tilde{\varphi}_1, \tilde{\varphi}_0) = -\tilde{V}_\delta - \tilde{R}_\delta(\tilde{\varphi}_2, \tilde{\psi}_2) , \tag{2.9.43}$$

$$\tilde{W}_\delta(\tilde{\varphi}_2, \tilde{\psi}_2) = \left((S^{k'_1}_{0,0}\tilde{\varphi}_1), \frac{\partial (S^{k'_1}_{0,0}\tilde{\varphi}_1)_-}{\partial \nu} \right) - (V_0, V'_0) . \tag{2.9.44}$$

In order to expand $\tilde{\Phi}$, we need to prove its stability when δ goes to 0.

Proposition 2.9.2 *Let u be the solution to problem (2.2.6). Then, for δ small enough, there exists a constant $C > 0$ independent of δ and $0 < \eta < \delta$ such that*

$$\begin{aligned} \| u(x + \eta\nu(x)) - U(x) \|_{\mathcal{C}^1(\partial\Omega)} &\leq C\delta , \\ \left\| \frac{\partial u(x + \eta\nu(x))}{\partial \nu} - \frac{k_2^2}{k_0^2} \frac{\partial (U)_+}{\partial \nu}(x) \right\|_{\mathcal{C}^0(\partial\Omega)} &\leq C\delta . \end{aligned}$$

Proof. From the regularity of $\partial\Omega$, we can deduce, analogously to what was done in Proposition 2.7.1, that $(\varphi_1^0, \varphi_0^0)$ and (φ_2^0, ψ_2^0) belong to $(\mathcal{C}^1(\partial\Omega))^2$. Lemmas 2.4.4 and 2.6.2 are also true when replacing the spaces $L^2(\partial\Omega)$ and $H^1(\partial\Omega)$ by $\mathcal{C}^0(\partial\Omega)$ and $\mathcal{C}^1(\partial\Omega)$, respectively. See, for example, [19]. Then, it follows that

$$W_\delta = W_0 + O(\delta) , \tag{2.9.45}$$

where $O(\delta)$ is unform from $\mathcal{C}^1 \times \mathcal{C}^1$ into $\mathcal{C}^1 \times \mathcal{C}^0$. From (2.7.28) and (2.7.29), we get

$$\begin{aligned} \| \varphi_2 - \varphi_2^0 \|_{\mathcal{C}^0(\partial\Omega)} &\leq C\delta , \\ \| \psi_2 - \psi_2^0 \|_{\mathcal{C}^0(\partial\Omega)} &\leq C\delta , \end{aligned}$$

for some constant $C > 0$. It then follows that

$$\begin{aligned} u(x + \eta\nu(x)) &= S^{k_2}_{0,\eta}\varphi_2 + S^{k_2}_{\delta,\eta}\psi_2 \\ &= S^{k_2}_{0,0}(\varphi_2^0 + \psi_2^0) + O(\delta) \\ &= U(x) + O(\delta) , \end{aligned}$$

where $O(\delta)$ is in $\mathcal{C}^1(\partial\Omega)$. We also have

$$\begin{aligned} \frac{\partial u(x + \eta\nu(x))}{\partial \nu} &= \frac{\partial S^{k_2}_{0,\eta}\varphi_2}{\partial \nu} + \frac{\partial S^{k_2}_{\delta,\eta}\psi_2}{\partial \nu} \\ &= \frac{\partial (S^{k_2}_{0,0}\varphi_2^0)_+}{\partial \nu} + \frac{\partial (S^{k_2}_{0,0}\psi_2^0)_-}{\partial \nu} + O(\delta) \\ &= \frac{k_2^2}{k_0^2} \frac{\partial (U)_+}{\partial \nu}(x) + O(\delta) , \end{aligned}$$

where $O(\delta)$ is in $\mathcal{C}^0(\partial\Omega)$. The proposition is then proved. □

Now we give an expansion for the source term defined for $x + \eta\nu \in \mathcal{O}_\delta$ ($x \in \partial\Omega$ and $0 < \eta < \delta$) by

$$\Pi(x) = \sum_{j,l=1,2} \chi_{jl} \partial_{x_j} u(x) \partial_{x_l} u(x).$$

First, we recall our assumption on the susceptibility tensor

$$\chi_{jl}(x + \eta\nu) = \tilde{\chi}_{jl}\left(x, \frac{\eta}{\delta}\right), \qquad x \in \partial\Omega \, , \; 0 < \eta < \delta \, ,$$

where $\tilde{\chi}_{jl}$ are independent of δ. We define then Π_0 on $\partial\Omega$ by

$$\Pi_0(x) = \sum_{j,l=1,2} \left(\int_0^1 \tilde{\chi}_{jl}(x, \theta) \, d\theta \right) w_j^0(x) w_l^0(x) \, ,$$

where w^0 is given by

$$w^0(x) = \frac{\partial U}{\partial \tau}(x)\tau(x) + \frac{k_2^2}{k_0^2} \frac{\partial (U)_+}{\partial \nu}(x)\nu(x) \, .$$

The next proposition is a direct consequence of the expansion of the fundamental field u.

Proposition 2.9.3 *The following expansion holds.*

$$\partial_{x_j} u(x + \eta\nu(x)) \partial_{x_l} u(x + \eta\nu(x)) = w_j^0(x) w_l^0(x) + O(\delta) \, ,$$

where $x \in \partial\Omega$, $0 < \eta < \delta$, and $O(\delta)$ is in $\mathcal{C}^0(\partial\Omega)$.

Now, we give expansions of the function V defined by (2.8.42).

Proposition 2.9.4 *There exists $\varepsilon_\delta \to 0$ as $\delta \to 0$ such that*

$$\begin{aligned}
\|V_0 - \delta S_{0,0}^{k_2'} \Pi_0\|_{H^1(\partial\Omega)} &\leq \varepsilon_\delta \delta \, , \\
\|V_0' - \delta \frac{\partial (S_{0,0}^{k_2'} \Pi_0)_-}{\partial \nu}\|_{L^2(\partial\Omega)} &\leq \varepsilon_\delta \delta \, , \\
\|V_\delta - V_0\|_{H^1(\partial\Omega)} &\leq \varepsilon_\delta \delta \, , \\
\|V_\delta' - V_0' - \delta \Pi_0\|_{L^2(\partial\Omega)} &\leq \varepsilon_\delta \delta \, .
\end{aligned}$$

Proof. Recall that

$$V(x) = \int_0^\delta S_\eta^{k_2'} \Pi(x) \, d\eta \quad \text{for } x \in \mathcal{O}_\delta \, ,$$

to obtain that for $x \in \partial\Omega$,

$$\begin{aligned}
V_0(x) &= \int_0^\delta S_{\eta,0}^{k_2'} \Pi(x + \eta\nu(x)) \, d\eta \\
&= \delta S_{0,0}^{k_2'} \Pi_0(x) \\
&+ \int_0^\delta (S_{\eta,0}^{k_2'} - S_{0,0}^{k_2'}) \Pi(x + \eta\nu(x)) \, d\eta + S_{0,0}^{k_2'} \left(\int_0^\delta \left(\Pi(x + \eta\nu(x)) - \Pi_0(x) \right) d\eta \right).
\end{aligned}$$

But Π is uniformly bounded in $L^2(\mathcal{O}_\delta)$. Therefore, as an application of Lemma 2.4.4, the argument of the integral in the second term can be bounded in $H^1(\partial\Omega)$ by ε_δ and the second term is bounded by $\delta\varepsilon_\delta$. Concerning the third term, we notice that

$$\begin{aligned}
&\int_0^\delta \big(\Pi(x+\eta\nu(x)) - \Pi_0(x)\big)\, d\eta \\
&\quad = \sum_{j,l} \int_0^\delta \chi_{jl}(x+\eta\nu(x))\partial_{x_j} u(x+\eta\nu(x))\partial_{x_l} u(x+\eta\nu(x))\, d\eta \\
&\quad\quad - \sum_{j,l} \delta \left(\int_0^1 \tilde{\chi}_{jl}(x,\theta)\, d\theta \right) w_j^0(x) w_l^0(x)\, d\eta \\
&\quad = \sum_{j,l} \int_0^\delta \chi_{jl}(x+\eta\nu(x)) \\
&\quad\quad \Big(\partial_{x_j} u(x+\eta\nu(x))\partial_{x_l} u(x+\eta\nu(x)) - w_j^0(x) w_l^0(x)\Big)\, d\eta.
\end{aligned}$$

Therefore, it follows from Proposition 2.9.3 that

$$\left\| \int_0^\delta \big(\Pi(x+\eta\nu(x)) - \Pi_0(x)\big)\, d\eta \right\|_{L^2(\partial\Omega)} \leq C\delta^2 ,$$

for some constant C. Hence, the third term in the previous expression of V_0 is bounded in $H^1(\partial\Omega)$ by $C\delta^2$. The first inequality is then proved. The second inequality can be proved in exactly the same way.

Now we turn to the last two inequalities

$$\begin{aligned}
V_\delta(x) - V_0(x) &= \int_0^\delta (S_{\eta,\delta}^{k_2'} - S_{\eta,0}^{k_2'})\Pi(x+\eta\nu(x))\, d\eta \\
&= \int_0^\delta (S_{\eta,\delta}^{k_2'} - S_{\eta,\eta}^{k_2'})\Pi(x+\eta\nu(x))\, d\eta + \int_0^\delta (S_{\eta,\eta}^{k_2'} - S_{\eta,0}^{k_2'})\Pi(x+\eta\nu(x))\, d\eta.
\end{aligned}$$

Since $\Pi(x+\eta\nu(x))$ is bounded in $L^2(\partial\Omega)$, it follows that the arguments of each integral is bounded in $H^1(\partial\Omega)$ by ε_δ and $V_\delta - V_0$ is bounded by $\delta\varepsilon_\delta$. Thus

$$\begin{aligned}
V_\delta'(x) - V_0'(x) &= \int_0^\delta \left(\frac{\partial S_{\eta,\delta}^{k_2'}}{\partial\nu} - \frac{\partial S_{\eta,0}^{k_2'}}{\partial\nu} \right) \Pi(x+\eta\nu(x))\, d\eta \\
&= \int_0^\delta \left(\frac{\partial S_{\eta,\delta}^{k_2'}}{\partial\nu} - \frac{\partial (S_{\eta,\eta}^{k_2'})_+}{\partial\nu} \right) \Pi(x+\eta\nu(x))\, d\eta \\
&\quad + \int_0^\delta \left(\frac{\partial (S_{\eta,\eta}^{k_2'})_-}{\partial\nu} - \frac{\partial S_{\eta,0}^{k_2'}}{\partial\nu} \right) \Pi(x+\eta\nu(x))\, d\eta \\
&\quad + \int_0^\delta \Big(\Pi(x+\eta\nu(x)) - \Pi_0(x) \Big)\, d\eta + \delta\Pi_0(x).
\end{aligned}$$

Again, since $\Pi(x+\eta\nu(x))$ is bounded in $L^2(\partial\Omega)$, the argument of the first and second integrals are bounded in $L^2(\partial\Omega)$ by ε_δ while we have already proved that the last integral is bounded in $L^2(\partial\Omega)$ by $C\delta^2$. This proves the last inequality in the proposition. □

Next, we state and prove the following convergence result for $\tilde{\Phi}$.

Proposition 2.9.5 *Let $\tilde{\Phi}^\delta = (\tilde{\varphi}_1^\delta, \tilde{\varphi}_2^\delta, \tilde{\psi}_2^\delta, \tilde{\varphi}_0^\delta) \in X^2$ be the unique solution of (2.8.40). Then $(\frac{\tilde{\varphi}_1^\delta}{\delta}, \frac{\tilde{\varphi}_0^\delta}{\delta})$ and $(\frac{\tilde{\varphi}_2^\delta}{\delta}, \frac{\tilde{\psi}_2^\delta}{\delta})$ converge in X to $(\tilde{\varphi}_1^1, \tilde{\varphi}_0^1)$ and $(\tilde{\varphi}_2^1, \tilde{\psi}_2^1)$, respectively, where*

$$\begin{aligned} &\tilde{Q}_0(\tilde{\varphi}_1^1, \tilde{\varphi}_0^1) = -(0, \Pi_0)\ , \\ &\tilde{W}_0(\tilde{\varphi}_2^1, \tilde{\psi}_2^1) = \left(S_{0,0}^{k_1'}\tilde{\varphi}_1^1, \frac{\partial (S_{0,0}^{k_1'}\tilde{\varphi}_1^1)_-}{\partial \nu}\right) - \left(S_{0,0}^{k_2'}\Pi_0, \frac{\partial (S_{0,0}^{k_2'}\Pi_0)_-}{\partial \nu}\right) . \end{aligned} \tag{2.9.46}$$

Proof. The proof is very similar to the one of Proposition 2.7.3. From Propositions 2.9.4 and (2.7.28) it follows that

$$\left\| \tilde{Q}_\delta \left(\frac{\tilde{\varphi}_1^\delta}{\delta}, \frac{\tilde{\varphi}_0^\delta}{\delta} \right) \right\|_Y \le C_1 + \varepsilon_\delta \left(\left\| \frac{\tilde{\varphi}_2^\delta}{\delta} \right\|_{L^2(\partial\Omega)} + \left\| \frac{\tilde{\psi}_2^\delta}{\delta} \right\|_{L^2(\partial\Omega)} \right) .$$

On the other hand, (2.9.44) yields

$$\left\| \tilde{W}_\delta \left(\frac{\tilde{\varphi}_2^\delta}{\delta}, \frac{\tilde{\psi}_0^\delta}{\delta} \right) \right\|_Y \le C_1' + C_2' \left\| \frac{\tilde{\varphi}_1^\delta}{\delta} \right\|_{L^2(\partial\Omega)} ,$$

where C_1, C_1' and C_2' are some positive constants independent of δ and ε_δ. It is then easy to see that $\frac{\tilde{\varphi}_1^\delta}{\delta}$, $\frac{\tilde{\varphi}_2^\delta}{\delta}$, $\frac{\tilde{\psi}_0^\delta}{\delta}$, and $\frac{\tilde{\varphi}_0^\delta}{\delta}$ are bounded in $L^2(\partial\Omega)$. Therefore

$$\lim_{\delta\to 0} \left\| \tilde{R}_\delta \left(\frac{\tilde{\varphi}_2^\delta}{\delta}, \frac{\tilde{\psi}_0^\delta}{\delta} \right) \right\|_Y = 0,$$

and (2.9.46) is straightforward. □

Now we can give an expansion of the second-harmonic field away from the thin layer of nonlinear material $\mathcal{O}_\delta$.

Theorem 2.9.1 *Let v be the solution to problem (2.2.7). Then, the following expansion holds uniformly in $H^1_{\mathrm{loc}}(\mathbb{R}^2 \setminus \partial\Omega)$:*

$$v(x) = \delta v_0(x) + o(\delta)\ , \tag{2.9.47}$$

where v_0 is given by

$$v_0(x) = \begin{cases} S_0^{k_1'}\tilde{\varphi}_1^1(x) & \textit{for } x \in \Omega\ , \\ S_0^{k_0'}\tilde{\varphi}_0^1(x) & \textit{for } x \in \mathbb{R}^2 \setminus \overline{\Omega}\ . \end{cases} \tag{2.9.48}$$

Proof. From the representation formula (2.8.41), we have

$$v(x) = \begin{cases} S_0^{k_1'}\tilde{\varphi}_1(x) & \text{for } x \in \Omega\ , \\ S_\delta^{k_0'}\tilde{\varphi}_0(x) & \text{for } x \in \Omega_\delta^e\ . \end{cases}$$

Recalling (2.9.46) we immediately obtain (2.9.47). □

The proof of the asymptotic expansion (2.2.12) is now immediate.

Chapter 3

Convergence of the supercell method for defect modes calculations in photonic crystals

3.1 Introduction

Photonic crystals are periodic structures composed of dielectric materials and designed to exhibit interesting properties, such as spectral band gaps, in the propagation of classical electromagnetic waves. In other words, monochromatic electromagnetic waves of certain frequencies do not exist in these structures. Media with band gaps have many potential applications, for example, in optical communications, filters, lasers, and microwaves. See [37, 38, 60, 47] for an introduction to photonic crystals. While necessary conditions under which band gaps exist in general are not known, Figotin and Kuchment have produced an example of high-contrast periodic medium where band gaps exist and can be characterized [34, 35]. Other band gap structures have been found through computational and physical experiments. See [24, 22, 25, 9, 28].

In order to achieve lasers, filters, fibers, or waveguides, allowed modes are required in the band gaps. These modes are obtained by creating localized defects in the periodicity and correspond to isolated eigenvalues with finite multiplicity inside the gaps. The defect mode frequency strongly depends on the defect nature. Figotin and Klein rigorously proved that when a defect is introduced into the periodic structure, *i.e.*, a perturbation with compact support, it is possible to create a defect mode, which is an exponentially confined standing wave whose frequency lies in the band gap [30, 31, 29]. See also Ammari and Santosa [6] and Kuchment and Ong [48] for the issue of existence of exponentially confined modes guided by line defects in photonic crystals.

The defect modes as well as the guided modes associated with compact and line defects, respectively, are computed via the supercell technique. This technique consists in restricting the computation on a domain surrounding the defect with sufficient bulk crystal, called the *supercell*, with periodic conditions on its boundary. The boundary conditions on the supercell are, in principle, irrelevant if the mode is sufficiently confined. Since one would like to compute only the defect or the guided modes in the band gap, without the waste of computation and memory of finding all the eigenvalues associated with the supercell belonging to the continuous spectrum, one states the problem as one of finding the eigenvalues and eigenvectors closest to the mid-gap frequency.

The supercell method demonstrates very good concordance with experimental results and seems to be very accurate. However, analytic studies and rigorous proofs of convergence of this technique are essentially absent.

In this chapter we address some of the basic issues of the supercell method and prove the convergence of this technique. Although one can obtain analogous results for the case of full Maxwell equations, we only address the cases of transverse electric (TE) and transverse magnetic (TM) polarized electromagnetic waves in two-dimensional photonic structures.

The outline of this chapter is as follows. In the next section we review some basic facts on the spectra of periodic elliptic operators, emphasizing the Floquet-Bloch theory. We then describe in Section 3.3 the supercell method and investigate its mathematical foundations in the TM case. Section 3.4 is devoted to the TE case. Finally in Section 3.5 the results of numerical experiments are presented to illustrate our main findings.

3.2 Notation and preliminary results

Consider a photonic crystal characterized by its dielectric permittivity $\varepsilon_{\rm p}$ that is a real valued, piecewise constant and periodic function belonging to the set $\{\varepsilon_{\rm p} \in L^\infty(\mathbb{R}^2/\mathbb{Z}^2) : \ 0 < \varepsilon_1 \leq \varepsilon_{\rm p} \leq \varepsilon_2 \text{ a.e.}\}$ where ε_1 and ε_2 are constants. The magnetic permeability is supposed constant and equal to unity in all this chapter.

We assume that the crystal is periodic with period $[0,1]^2$, *i.e.*, that $\varepsilon_{\rm p}(x+n) = \varepsilon_{\rm p}(x)$ for almost all $x \in \mathbb{R}^2$ and all $n \in \mathbb{Z}^2$.

The propagation of electromagnetic waves is governed by the Maxwell's equations. It is common to reduce these equations in a 2-D medium to two sets of scalar equations in the transverse magnetic (TM) and the transverse electric (TE) cases. Each one can be solved by solving a scalar partial differential equation and the other scalar functions follow immediately from that solution.

These equations are the Helmholtz equation:

$$\Delta u + \omega^2 \varepsilon_{\rm p} u = 0 \ , \tag{3.2.1}$$

for the TM polarization, and the acoustic equation:

$$\nabla \cdot \frac{1}{\varepsilon_{\rm p}} \nabla u + \omega^2 u = 0 \ , \tag{3.2.2}$$

for the TE polarization.

We now recall some well-known results on the spectrum of the TM and TE operators in a periodic medium. Since we deal with a partial differential equation with periodic coefficients, it is natural to use a Floquet transform and apply the Floquet-Bloch theory.

Firstly, we briefly present the Floquet-Bloch theory applied to the TM and TE operators in periodic media. More details can be found in [47] where P. Kuchment presents a survey on mathematics of photonic crystals.

Let $A(x, D)$ denote the TM or TE operator on $L^2(\mathbb{R}^2)$ in a periodic medium characterized by ε_{p}, where $D = -i\nabla$. This operator is invariant with respect to the discrete group of translations $\mathbb{Z}^2$ acting on $\mathbb{R}^2$. It is then natural to apply the Fourier transform on $\mathbb{Z}^2$, which to a sufficiently decaying function $h(n)$ on $\mathbb{Z}^2$ assigns the Fourier series

$$\widehat{h}(\xi) = \sum_{j \in \mathbb{Z}^2} h(j) e^{i\xi \cdot j} ,$$

where $\xi \in \mathbb{R}^2$. However, since we deal with functions defined on $\mathbb{R}^2$, we use the Floquet transform.

Consider a function v defined on $\mathbb{R}^2$, sufficiently decaying at infinity. We can then define its Floquet transform by

$$\mathcal{F}v(x, \xi) = \sum_{j \in \mathbb{Z}^2} v(x - j) e^{i\xi \cdot j} = \widehat{v(x - \cdot)} . \tag{3.2.3}$$

It is easy to check that $\mathcal{F}v(\cdot, \xi)$ is ξ-quasi-periodic with respect to the first variable, that is:

$$(\mathcal{F}v)(x + n, \xi) = (\mathcal{F}v)(x, \xi) e^{i\xi \cdot n} , \quad \forall x \in \mathbb{R}^2 , n \in \mathbb{Z}^2 .$$

Moreover, it is periodic with respect to the variable ξ, called quasi-momentum, with period lattice $[0, 2\pi]^2$. It is then sufficient to know the function $\mathcal{F}v$ for $(x, \xi) \in Y \times \mathcal{B}$, where $Y = [0, 1[^2$ and $\mathcal{B} = [-\pi, \pi[^2$ (called in the literature the first Brillouin zone), to recover it on $\mathbb{R}^2 \times \mathbb{R}^2$.

It turns out that the Floquet transform commutes with partial differential operators with periodic coefficients. In particular, we notice that

$$\mathcal{F}(A(x, D)u) = A(x, D)(\mathcal{F}u) .$$

The Floquet transform allows us to represent a function on $L^2(\mathbb{R}^2)$ as a continuous sum of quasi-periodic functions. In fact, the Floquet theory defines an isometric mapping between $L^2(\mathbb{R}^2)$ and $L^2(\mathcal{B}, L^2_\xi(\mathbb{R}^2))$, $L^2_\xi(\mathbb{R}^2)$ being the space of ξ-quasi-periodic L^2- functions. The inverse of the Floquet transform is given by the following formula:

$$(\mathcal{F}^{-1}v)(x) = \frac{1}{|\mathcal{B}|} \int_B v(x, \xi) d\xi , \tag{3.2.4}$$

for any v in $L^2(\mathcal{B}, L^2_\xi(\mathbb{R}^2))$.

The isometric character of the Floquet transform, together with its commutation properties on partial differential operators with periodic coefficients make it very useful to study spectral problems. Indeed, the spectral problem for the operator $A(x, D)$ becomes a family of spectral problems for operators $A_\xi(x, D)$ (having formally the same expression but with domains depending on ξ), acting on functions defined on a bounded set (the period lattice of the photonic crystal), with ξ-quasi-periodicity.

An alternative version to the Floquet transform is the transform Φ defined as

$$\Phi v(x, \xi) = \sum_{j \in \mathbb{Z}^2} v(x - j) e^{-i\xi \cdot (x-j)} = e^{-i\xi \cdot x} \mathcal{F} v(x, \xi) \ .$$

The function Φv is periodic with respect to x and $(-x)$-quasi-periodic with respect to ξ with 2π-quasi-period:

$$\begin{cases} \Phi v(x + n, \xi) = \Phi v(x, \xi) \ , & n \in \mathbb{Z}^2 \ , \\ \Phi v(x, \xi + \zeta) = e^{-i\zeta \cdot x} \Phi v(x, \xi) \ , & \zeta \in 2\pi \mathbb{Z}^2 \ . \end{cases} \tag{3.2.5}$$

With this transform, we deal now with functions defined on a fixed space $L^2(\mathcal{B}, L^2(\mathbb{R}^2/\mathbb{Z}^2))$, while the operator $A(x, D)$ is splitted into a sum of operators $A(x, D - \xi)$, depending on ξ:

$$\Phi(A(x.D)u)(x, \xi) = A(x, D - \xi)(\Phi u)(x, \xi) \ .$$

The transform Φ is still an isometric mapping between $L^2(\mathbb{R}^2)$ and $L^2(\mathcal{B}, L^2(\mathbb{R}^2/\mathbb{Z}^2))$, and its inverse transform is:

$$(\Phi^{-1} v)(x) = \frac{1}{|\mathcal{B}|} \int_{\mathcal{B}} e^{ix \cdot \xi} v(x, \xi) d\xi \ .$$

Let Σ be the spectrum of $A(x, D)$ on $L^2(\mathbb{R}^2)$ and Σ^ξ the spectrum of $A(x, D - \xi)$ on $L^2(\mathbb{R}^2/\mathbb{Z}^2)$, then we can deduce immediately the following identity:

$$\Sigma = \cup_{\xi \in \mathcal{B}} \Sigma^\xi \ . \tag{3.2.6}$$

Now, with these tools, we are in the position to explore the spectrum of the TM and TE operators in periodic media.

In the case of the TE polarization, the operator we are studying is:

$$A(x, D) = -\nabla \cdot \frac{1}{\varepsilon_{\mathrm{p}}} \nabla \ .$$

After the transform Φ, we get the following spectral problem:

$$-(\nabla_x - i\xi) \cdot \frac{1}{\varepsilon_{\mathrm{p}}} (\nabla_x - i\xi) v(x, \xi) = \omega^2 v(x, \xi) \ , \quad v(\cdot, \xi) \in L^2(\mathbb{R}^2/\mathbb{Z}^2) \ . \tag{3.2.7}$$

We remark that $A(x, D - \xi)$ is an elliptic self-adjoint operator on $L^2(\mathbb{R}^2/\mathbb{Z}^2)$ with compact resolvent. It follows that its spectrum is discrete with countably many positive eigenvalues denoted $\lambda_n(\xi)$ and ordered increasingly. It is easy to prove the continuity of $\lambda_n(\xi)$ on $\xi \in \mathcal{B}$. Finally, defining the intervals I_n by

$$I_n = [\min_{\xi \in \mathcal{B}} \lambda_n(\xi), \max_{\xi \in \mathcal{B}} \lambda_n(\xi)] \ ,$$

we deduce the spectrum of the TE operator:

$$\Sigma_{\mathrm{TE}} = \cup_{n \in \mathbb{N}} I_n \ .$$

We then see clearly the band structure of the spectrum since it is a union of the intervals formed by the values of each eigenvalue when the quasimomentum varies in the Brillouin zone. In fact, if two successive intervals are disjoint, which means that the maximal value of an eigenvalue is smaller than the minimal value of the following one, then there is a gap in the spectrum Σ_{TE} and no propagation is possible for TE waves at the corresponding frequencies. This makes all the interest of photonic crystals.

Here, we introduce the following assumption.

Assumption : *In all what follows, we assume that the spectra the TM and TE operators are absolutely continuous.*

A. Morame proved this assumption for Maxwell operator in [53] in the case of C^∞ periodic coefficients and for Schrödinger operator in the case of C^∞ periodic metric. This assumption means that the eigenvalus $\lambda_n(\xi)$ can not be constant on a subset of $\mathcal{B}$ of positive measure. Numerical simulations and physical experiments agree with this assumption which we believe is true.

Another important property of photonic crystals is a consequence of the characterization of the decay of functions in $L^2(\mathbb{R}^2)$ in terms of the smoothness of their Floquet transform in the same spirit as the Paley-Wiener theorem. Suppose that the spectrum contains some gaps, that is $\Sigma_{TE} \neq \mathbb{R}^+$ and let ω be a frequency lying in a band gap. Let G_{p} be the Green's function of the TE operator defined by

$$\nabla \cdot \frac{1}{\varepsilon_{\mathrm{p}}} \nabla G_{\mathrm{p}}(\omega; x, y) + \omega^2 G_{\mathrm{p}}(\omega; x, y) = \delta(x - y) \ , \quad x \in \mathbb{R}^2 \ . \tag{3.2.8}$$

It has been established in [21, 13] that, for ε_{p} measurable, in L^∞, bounded and away from 0, the Floquet transform of G_{p} is analytic with respect to ω in a complex neighborhood of the real axis. In view of Paley-Wiener-type theorems, the analyticity of $\mathcal{F}G_{\mathrm{p}}$ is the key ingredient of the proof of the following result [32, 33, 29, 31].

Lemma 3.2.1 *There exist two positive constants C_1 and C_2 depending only on $\omega_0^2 > 0$ such that for any $\omega^2 \notin \Sigma_{\mathrm{TE}}$,*

$$|G_{\mathrm{p}}(\omega; x, y)| \leq C_1 e^{-C_2 dist(\omega^2, \Sigma_{\mathrm{TE}})|x-y|} \ , \quad \textit{for } |x - y| \to +\infty \ . \tag{3.2.9}$$

Remark 3.2.1 *The behaviour of the Green's function at infinity is the essential feature of PBG materials: it explains why localized defects in photonic crystals may act as perfect cavities, when the frequency lies in a band gap. Electromagnetic waves can be represented in terms of G_{p} and thus inherit the exponential decay property.*

In the case of the TM polarization, the operator we are studying is:

$$A(x, D) = -\frac{1}{\varepsilon_{\mathrm{p}}} \Delta \ .$$

Taking the transform Φ, we get the following spectral problem:

$$-\frac{1}{\varepsilon_{\mathrm{p}}} (\nabla_x - i\xi) \cdot (\nabla_x - i\xi) v(x, \xi) = \omega^2 v(x, \xi) \ , \quad v(\cdot, \xi) \in L^2(\mathbb{R}^2/\mathbb{Z}^2) \ . \tag{3.2.10}$$

The difference with the TE case is that this operator is elliptic, self-adjoint with compact resolvent on the weighted space $L^2(\mathbb{R}^2, \varepsilon_{\mathrm{p}}(x) \, dx)$.

The results are therefore the same as for the TE case, and we get a spectrum with band structure:

$$\Sigma_{\mathrm{TM}} = \cup_{n\in\mathbb{N}} I_n \ ,$$

where $(I_n)_{n\in\mathbb{N}}$ are defined in the same way as for the TE case.

Analogous properties to the TE case hold. In particular, Lemma 3.2.1 holds with the Green's function associated with the TM polarization.

From now on and until otherwise mentioned, we deal with TM-polarized electromagnetic waves. We consider a background medium characterized by its dielectric permittivity ε_{p}.

First, we introduce some simplified notations.

Definition 3.2.1 *We define the operator A_{p} by*

$$A_{\mathrm{p}} = -\frac{1}{\varepsilon_{\mathrm{p}}}\Delta \ , \quad \text{on } L^2(\mathbb{R}^2) \ ,$$

and denote by Σ_{p} its spectrum.

For $\xi \in [0, 2\pi[^2$ we define A_{p}^{ξ} on $L^2(\mathbb{R}^2/\mathbb{Z}^2)$ by

$$A_{\mathrm{p}}^{\xi} = -\frac{1}{\varepsilon_{\mathrm{p}}}(\nabla_x - i\xi)\cdot(\nabla_x - i\xi) \ ,$$

and denote by $\Sigma_{\mathrm{p}}^{\xi}$ its spectrum.

We create a perturbation of the background medium by modifying its dielectric permittivity into ε as follows:

$$\varepsilon(x) = \varepsilon_{\mathrm{p}}(x) - (\delta\varepsilon)\chi_{\Omega}(x) \ , \tag{3.2.11}$$

where $(\delta\varepsilon)$ is a real constant and Ω is a bounded domain in $\mathbb{R}^2$.

The perturbation of the dielectric permittivity induces a modification of the TM operator into

$$A = -\frac{1}{\varepsilon}\Delta \ , \tag{3.2.12}$$

and, consequently, the spectrum Σ of A is different from the spectrum Σ_{p} of A_{p}. However, it has been proved that the perturbation of the TM operator is relatively compact and therefore it keeps unchanged the essential spectrum of A_{p}. See [30]. Since the spectrum Σ_{p} is purely continuous, the perturbation will result in the addition of eigenvalues of finite multiplicity to Σ_{p}.

The following theorem from [30] is of importance to us.

Theorem 3.2.1 *Suppose that the spectrum Σ_{p} of the operator A_{p} has a gap and suppose that the defect $(\Omega, (\delta\varepsilon))$ has created an isolated eigenvalue ω^2 in the gap. Let u be an associated eigenvector. Then, there exist two constants C_1 and C_2, depending only on the distance of ω^2 to the spectrum Σ_{p}, such that*

$$\|u\|_{L^2(B_x)} \leq C_1 e^{-C_2 dist(x,\Omega)} \|u\|_{L^2(\Omega)} \ , \quad \forall x \in \mathbb{R}^2 \ ,$$

where B_x is the ball of center x and radius one.

Proof. The eigenmode u is solution of the following equation:

$$\Delta u + \omega^2 \varepsilon(x) u = 0 \,. \tag{3.2.13}$$

It is easy then to see that u is solution of the following integral equation:

$$u(x) = (\delta\varepsilon)\omega^2 \int_\Omega G_{\mathrm{p}}(\omega; x, y) u(y) \, dy \,. \tag{3.2.14}$$

The proof of the theorem is then a direct consequence of the exponential decay of the Green's function in Lemma 3.2.1. □

Remark 3.2.2 *This theorem has very important consequences. It explains why we can confine electromagnetic waves in defects or guide them along a defect. The use of dielectric material that has very low loss and the exponential decrease of the electromagnetic field away from the defect ensures a very efficient confinement with a cladding of few periods of the photonic crystal.*

3.3 The supercell method

We start this section by giving a mathematical description of the supercell method.

3.3.1 Definitions and preliminary results

We consider the background and perturbed media introduced in the previous section with their corresponding TM operators and spectra. Since the perturbed medium is not periodic, the Floquet's theory does not apply.

To recover a periodic medium, we define an artificial medium in the following way. Without loss of generalization, we can suppose that the defect support Ω is centered at 0. For $N \in \mathbb{N}$ large enough to have $\Omega \in]-N, N[^2$, we define the $(2N)$-periodic L^∞-function ε_N by:

$$\begin{cases} \varepsilon_N(x) = \varepsilon(x) \,, \quad \forall x \in]-N, N[^2 \,, \\ \varepsilon_N(x + 2Nj) = \varepsilon_N(x) \,, \quad \forall x \in \mathbb{R}^2 \,, \forall j \in \mathbb{N}^2 \,. \end{cases} \tag{3.3.15}$$

Definition 3.3.1 *We define the operator A_N on $L^2(\mathbb{R}^2)$ by:*

$$A_N = -\frac{1}{\varepsilon_N}\Delta \,, \tag{3.3.16}$$

and let Σ_N be its spectrum.

For $\xi \in \mathcal{B}_N = [-\frac{\pi}{2N}, \frac{\pi}{2N}[^2$, we define the operator A_N^ξ on $L^2(\mathbb{R}^2/2N\mathbb{Z}^2)$ by:

$$A_N^\xi = -\frac{1}{\varepsilon_N}(\nabla - i\xi)\cdot(\nabla - i\xi) \,,$$

and denote by Σ_N^ξ its spectrum.

The function ε_N defines a photonic crystal formed by the defect repeated with a $2N$-period inside the original photonic crystal. It is therefore obvious that the spectrum Σ_N is an absolutely continuous spectrum. The question is: what does it happen when N goes to infinity?

A natural answer is that since the repeated defects will be away from each other, they will not interact and, in the neighborhood of one defect, the operator will see almost an infinite crystal. We expect then a kind of convergence of Σ_N to the spectrum Σ corresponding to one defect in the infinite photonic crystal. So for N large enough, after taking the Floquet transform in the supercell and computing the spectrum, we will find a spectrum divided into wide bands very close to those corresponding to the background medium and very narrow bands (almost a horizontal line when plotted against the quasi-momentum) that should correspond to the defect modes of the perturbed crystal. This is what will be proved in the following subsections.

To give a characterization of the convergence of the spectrum of the supercell, we will use the Hausdorff distance denoted $\mathrm{dist}_{\mathcal{H}}$, that is a measure of the resemblance of two (fixed) sets.

Definition 3.3.2 *Let E and F be two non empty subsets of a metric set. We define the Hausdorff distance denoted $dist_{\mathcal{H}}$ between E and F as*

$$dist_{\mathcal{H}}(E,F) = \inf\{d \geq 0 \; ; \; \forall (x,y) \in E \times F, \; dist(x,F) < d \text{ and } dist(y,E) < d\}\,.$$

This means that if $\mathrm{dist}_{\mathcal{H}}(E,F) = d$, then any point of one of the two sets is within distance d from some point of the other set.

Finally, we give in the following proposition an important result from the spectral theory, see [58], that will be useful for the convergence results.

Proposition 3.3.1 *Let A be a self-adjoint operator with a domain $\mathcal{D}(A)$ and a spectrum $\sigma(A)$, then, for $\mu \in \mathbb{R}$:*

$$dist(\mu, \sigma(A)) = \min_{\phi \in \mathcal{D}(A)} \frac{\|(A-\mu I)\phi\|}{\|\phi\|} \tag{3.3.17}$$

3.3.2 Convergence of the "continuous spectrum"

Here we give a characterization of the convergence of the part corresponding to the spectrum of the unperturbed crystal.

Theorem 3.3.1 *For any $\omega_0 > 0$ and $N_0 \in \mathbb{N}$, there exists $C > 0$, depending only on ω_0, N_0 and Ω, such that*

$$\max_{\omega^2 \in \cup_{k \in [-N+1, N-1[^2 \cap \mathbb{N}^2} \Sigma_{\mathrm{p}}^{\xi + k\pi/N} \cap [0,\omega_0^2]} dist(\omega^2, \Sigma_N^{\xi}) \leq \frac{C}{N^2}\,, \tag{3.3.18}$$

for any $N \geq N_0$ and any $\xi \in \mathcal{B}_N$.

Proof. Let $k \in [-N+1, N-1[^2 \cap \mathbb{N}^2$ and $\xi \in \mathcal{B}_N$. Let ω^2 be in $\Sigma_{\mathrm{p}}^{\xi+k\pi/N} \cap [0,\omega_0^2]$. Since $\xi + k\pi/N \in \mathcal{B}$, there exists $\phi \in L^2(\mathbb{R}^2/\mathbb{Z}^2)$ with unit norm such that

$$\Big(\nabla - i\big(\xi + \frac{k\pi}{N}\big)\Big) \cdot \Big(\nabla - i\big(\xi + \frac{k\pi}{N}\big)\Big)\phi + \omega^2 \varepsilon_{\mathrm{p}}\phi = 0\,. \tag{3.3.19}$$

Let $\tilde{\phi}$ be defined in $L^2(\mathbb{R}^2/2N\mathbb{Z}^2)$ as

$$\tilde{\phi}(x) = \phi(x)e^{-i\frac{\pi}{N}k\cdot x} \; . \tag{3.3.20}$$

We have $\|\tilde{\phi}\|_{L^2(\mathbb{R}^2/2N\mathbb{Z}^2)} = 4N^2$, and it satisfies the following equation.

$$(\nabla - i\xi)\cdot(\nabla - i\xi)\tilde{\phi} + \omega^2\varepsilon_{\rm p}\tilde{\phi} = 0 \; , \tag{3.3.21}$$

which can be rewritten as follows

$$(\nabla - i\xi)\cdot(\nabla - i\xi)\tilde{\phi} + \omega^2\varepsilon\tilde{\phi} = -\chi_\Omega(\delta\varepsilon)\omega^2\tilde{\phi} \; . \tag{3.3.22}$$

Let C_1 be the minimal number of unit squares in which Ω can be strictly included. Since the L^2-norm of $\tilde{\phi}$ in a unit square is 1, we have:

$$\|\tilde{\phi}\|_{L^2(\Omega)} \leq C_1 \; .$$

Thus

$$\begin{aligned}
\frac{\|(\nabla - i\xi)\cdot(\nabla - i\xi)\tilde{\phi} + \omega^2\varepsilon\tilde{\phi}\|_{L^2(\mathbb{R}^2/(2N)\mathbb{Z}^2)}}{\|\tilde{\phi}\|_{L^2(\mathbb{R}^2/2N\mathbb{Z}^2)}} &= (\delta\varepsilon)\omega^2\frac{\|\tilde{\phi}\|_{L^2(\Omega)}}{\|\tilde{\phi}\|_{L^2(\mathbb{R}^2/2N\mathbb{Z}^2)}} \\
&\leq \frac{C_2}{N^2} \; ,
\end{aligned}$$

where $C_2 = |(\delta\varepsilon)|\omega_0^2 C_1$.

The operator $-\frac{1}{\varepsilon}(\nabla - i\xi)\cdot(\nabla - i\xi)$ is self-adjoint in $\big(L^2(\mathbb{R}^2/2N\mathbb{Z}^2), \varepsilon(x)dx\big)$. Then, from Proposition 3.3.1, the distance of ω^2 to Σ_N^ξ is at most equal to the following expression divided by the norm of $\tilde{\phi}$ in $L^2(\mathbb{R}^2/2N\mathbb{Z}^2)$. We have

$$\begin{aligned}
\int_{]-N,N[^2} \left| -\frac{1}{\varepsilon}(\nabla - i\xi)\cdot(\nabla - i\xi)\tilde{\phi} - \omega^2\tilde{\phi}\right|^2 \varepsilon\, dx \\
&= \int_{]-N,N[^2} \left|(\nabla - i\xi)\cdot(\nabla - i\xi)\tilde{\phi} + \omega^2\varepsilon\tilde{\phi}\right|^2 \frac{dx}{\varepsilon} \\
&\leq \frac{C}{N^2}\|\tilde{\phi}\|_{L^2(\mathbb{R}^2/2N\mathbb{Z}^2)} \; ,
\end{aligned}$$

where $C = \frac{C_2}{\min_{x\in]-N,N[^2}\varepsilon(x)}$.

It follows from Proposition 3.3.1 that there exists an eigenvalue ω_ξ^2 belonging to the spectrum Σ_N^ξ of the operator A_N^ξ such that

$$|\omega^2 - \omega_\xi^2| \leq \frac{C}{N^2} \; ,$$

which ends the proof. □

Remark 3.3.1 *This theorem tells us that card*$\big(\Sigma_N^\xi \cap [0,\omega_0^2]\big)$ *for* $\xi \in \mathcal{B}_N$ *will grow at least as fast as* N^2*card*$\big(\Sigma_p^{\xi'} \cap [0,\omega_0^2]\big)$ *for any* $\xi' \in \mathcal{B}$*. So when we use the supercell method to determine the defects modes, we are in front of a dilemma. The larger is the size of the supercell, the better is the approximation of the defect eigenvalues. But this will take much more time and require greater* *memory size because of the size of the computational domain and the growing number of useless (in the sense that they do not correspond to the defect) eigenvalues. It is important then to determine the convergence rate of the eigenvalues corresponding to the defect.*

Since we know that the spectrum $\Sigma_N = \cup_{\xi \in \mathcal{B}_{\mathcal{N}}} \Sigma_N^\xi$ *is absolutely continuous, we deduce that each connected component of* $(\mathbb{R}^2 \setminus \Sigma_N) \cap \Sigma_\mathrm{p} \cap [0, \omega_0]$ *has a width smaller than* $\frac{2C}{N^2}$.

In practice, because of the growth of degeneracy of the eigenvalues located in Σ_p *with* N*, there will be almost no visible gap inside the bands of* Σ_N *but the remark remains useful for the perturbation brought to the edges of the bands. In particular, it is useful to check if a perturbation of the edges of a band in* Σ_p *is due to the presence of a defect eigenvalue in* Σ *close to the band or not.*

3.3.3 Convergence of the defect eigenvalues

Here we are concerned with the behaviour of the part of the spectrum Σ_N that will give us an approximation of the defect modes (eigenvalues with finite multiplicity in Σ). Let us first try to give a characterization of this part.

Definition 3.3.3 *For* $\eta > 0$*, we define* $\Sigma_{\mathrm{d},N}^\eta$ *as the union of the connected components of* Σ_N *that are at least* η*-distant from* Σ_p.

We also define Σ_d *as the set of the defect eigenvalues of the perturbed photonic crystal:*

$$\Sigma_\mathrm{d} = \Sigma \setminus \Sigma_\mathrm{p} \ .$$

Finally, we introduce $\Sigma_{\mathrm{d},N}^{\xi,\eta}$ *and* Σ_d^η *as*

$$\Sigma_{\mathrm{d},N}^{\xi,\eta} = \{\omega^2 \in \Sigma_N^\xi : \mathit{dist}(\omega^2, \Sigma_\mathrm{p}) \geq \eta\} \ .$$

$$\Sigma_\mathrm{d}^\eta = \{\omega_\mathrm{d}^2 \in \Sigma_\mathrm{d} : \mathit{dist}(\omega_\mathrm{d}^2, \Sigma_\mathrm{p}) \geq \eta\} \ .$$

The following proposition holds.

Proposition 3.3.2 *For every gap* $]a, b[$ *in* Σ_p $(0 < a < b)$ *satisfying* $[a, b] \cap \Sigma = \emptyset$*, there exists* $N_1 \in \mathbb{N}$ *such that, for* $N \geq N_1$*,* $\Sigma_N \cap [a, b] = \emptyset$.

Proof. Suppose that the proposition is false. Then for any $N_0 \in \mathbb{N}$ there exists $N \geq N_0$ and $\omega_N^2 \in]a, b[\cap \Sigma_N$. This means that there exist $\xi_N \in \mathcal{B}_\mathcal{N}$ and $\phi_N \in L^2(\mathbb{R}^2/2N\mathbb{Z}^2)$ with unit norm such that

$$(\nabla - i\xi_N) \cdot (\nabla - i\xi_N)\phi_N + \omega_N^2 \varepsilon_N \phi_N = 0 \quad \text{in } L^2(\mathbb{R}^2/2N\mathbb{Z}^2) \ . \tag{3.3.23}$$

Now, we define $\tilde{\phi}_N$ in $L^2(\mathbb{R}^2)$ by

$$\tilde{\phi}_N(x) = \int_\Omega G(\omega_N^2; x, y) e^{-i\xi_N \cdot y} \phi_N(y) \, dy \ , \tag{3.3.24}$$

where $G(\omega^2; x, y)$ is the Green's kernel defined for $\omega^2 \notin \Sigma_\mathrm{p}$ by

$$\Delta G(\omega^2; x, y) + \omega^2 \varepsilon_\mathrm{p} G(\omega^2; x, y) = \delta(x - y) \ .$$

The following lemma is needed.

Lemma 3.3.1 *There exist $N_0 > 0$ depending only on a, b and Σ_{p}, such that for $N \geq N_0$, we have:*

$$\|\tilde{\phi}_N\|_{L^2(\mathbb{R}^2)} \geq \frac{1}{2} .$$

Proof. From the expression of $\tilde{\phi}_N$ we deduce:

$$\begin{aligned}
(\delta\varepsilon)\omega_N^2\tilde{\phi}_N(x) &= (\delta\varepsilon)\omega_N^2 \int_\Omega G(\omega_N^2; x, y) e^{-i\xi_N\cdot y}\phi_N(y)\, dy \\
&= \int_{\mathbb{R}^2} G(\omega_N^2; x, y)(\Delta + \omega_N^2\varepsilon_{\mathrm{p}})\big(e^{-i\xi_N\cdot y}\phi_N(y)\big)\, dy \\
&\quad - \int_{\mathbb{R}^2} G(\omega_N^2; x, y)(\Delta + \omega_N^2\varepsilon)\big(e^{-i\xi_N\cdot y}\phi_N(y)\big)\, dy \\
&= \int_{\mathbb{R}^2} (\Delta + \omega_N^2\varepsilon_{\mathrm{p}}) G(\omega_N^2; x, y) e^{-i\xi_N\cdot y}\phi_N(y)\, dy \\
&\quad - \int_{\mathbb{R}^2} G(\omega_N^2; x, y) e^{-i\xi_N\cdot y} \\
&\qquad \Big((\nabla - i\xi_N)\cdot(\nabla - i\xi_N) + \omega_N^2\varepsilon\Big)\phi_N(y)\, dy \\
&= e^{-i\xi_N\cdot x}\phi_N(x) \\
&\quad - \int_\Omega \sum_{j\in\mathbb{Z}^2, j\neq 0} \Big(G(\omega_N^2; x, y + 2Nj) e^{-i2N\xi_N\cdot j}\Big) e^{-i\xi_N\cdot y}\phi_N(y) dy.
\end{aligned}$$

Let us now prove that the L^2-norm of the last term in $]-N,N[^2$ converges to 0. From the exponential decay of the Green's function, we deduce that there exist positive constants C_1 and C_2 depending only on the distance of a and b to Σ_{p} such that, for any $\omega^2 \in]a,b[$, we have [6]:

$$\sum_{j\in\mathbb{Z}^2, j\neq 0} \big|G(\omega^2; x, y + Nj)\big| \leq C_1 e^{-C_2 N}, \qquad \forall x \in]-N,N[^2, \ \forall y \in \Omega . \tag{3.3.25}$$

It follows then, since $\|\phi_N\|_{L^2(]-N,N[^2)} = 1$, that for any $x \in]-N,N[^2$, we have:

$$\begin{aligned}
&\left|\int_\Omega \sum_{j\in\mathbb{Z}^2, j\neq 0} \Big(G(\omega_N^2; x, y + Nj) e^{-iN\xi_N\cdot j}\Big) e^{-i\xi_N\cdot y}\phi_N(y) dy\right| \\
&\qquad \leq C_1 e^{-C_2 N} \int_\Omega |\phi_N(y)|\, dy \\
&\qquad \leq C_1 e^{-C_2 N} |\Omega|^{\frac{1}{2}} \|\phi_N\|_{L^2(\Omega)} \\
&\qquad \leq C_1 e^{-C_2 N} |\Omega|^{\frac{1}{2}} .
\end{aligned}$$

We then deduce that:

$$\begin{aligned}
&\left\|\int_\Omega \sum_{j\in\mathbb{Z}^2, j\neq 0} \Big(G(\omega_N^2; x, y + Nj) e^{-iN\xi_N\cdot j}\Big) e^{-i\xi_N\cdot y}\phi_N(y) dy\right\|_{L^2(]-N,N[^2)} \\
&\qquad \leq |\Omega|^{\frac{1}{2}} N C_1 e^{-C_2 N} .
\end{aligned}$$

Hence, recalling that $\|e^{-i\xi_N\cdot x}\phi_N(x)\|_{L^2(]-N,N[^2)} = 1$, there exists $N_0 > 0$ such that for any $N \geq N_0$, we have:

$$\|\tilde{\phi}_N\|_{L^2(\mathbb{R}^2)} \geq \|\tilde{\phi}_N\|_{L^2(]-N,N[^2)} \geq \frac{1}{2} \, . \tag{3.3.26}$$

Lemma 3.3.1 is then proved. □

We now turn to the proof of Proposition 3.3.2. We have

$$\begin{aligned}
\Delta\tilde{\phi}_N + \omega_N^2\varepsilon\tilde{\phi}_N &= \int_\Omega (\Delta_x + \omega_N^2\varepsilon)G(\omega_N^2; x, y)e^{-i\xi_N\cdot y}\phi_N(y)\, dy \\
&= \int_\Omega (\Delta_x + \omega_N^2\varepsilon_{\mathrm{p}})G(\omega_N^2; x, y)e^{-i\xi_N\cdot y}\phi_N(y)\, dy \\
&\quad -(\delta\varepsilon)\chi_\Omega(x)\omega_N^2 \int_\Omega G(\omega_N^2; x, y)e^{-i\xi_N\cdot y}\phi_N(y)\, dy \\
&= \chi_\Omega(x)e^{-i\xi_N\cdot x}\phi_N(x) \\
&\quad -\chi_\Omega(x)\int_{\mathbb{R}^2} G(\omega_N^2; x, y)(\Delta_y + \omega_N^2\varepsilon_{\mathrm{p}})(e^{-i\xi_N\cdot y}\phi_N(y))\, dy \\
&\quad +\chi_\Omega(x)\int_{\mathbb{R}^2} G(\omega_N^2; x, y)(\Delta_y + \omega_N^2\varepsilon)(e^{-i\xi_N\cdot y}\phi_N(y))\, dy \\
&= \chi_\Omega(x)e^{-i\xi_N\cdot x}\phi_N(x) \\
&\quad -\chi_\Omega(x)\int_{\mathbb{R}^2} (\Delta_y + \omega_N^2\varepsilon_{\mathrm{p}})G(\omega_N^2; x, y)e^{-i\xi_N\cdot y}\phi_N(y)\, dy \\
&\quad +\chi_\Omega(x)\int_{\mathbb{R}^2} G(\omega_N^2; x, y)e^{-i\xi_N\cdot y} \\
&\qquad\qquad \Big((\nabla - i\xi_N)\cdot(\nabla - i\xi_N) + \omega_N^2\varepsilon\Big)\phi_N(y)\, dy \\
&= (\delta\varepsilon)\omega_N^2\chi_\Omega(x) \\
&\qquad \int_\Omega \Big(\sum_{j\in\mathbb{Z}^2, j\neq 0} G(\omega_N^2; x, y + Nj)e^{-i\xi_N\cdot(y+Nj)}\Big)\phi_N(y)\, dy \, .
\end{aligned}$$

Using estimate (3.3.25), we deduce the existence of positive constants C_1 and C_2 depending only on the distance of a and b to Σ_{p} such that

$$\Big|\sum_{j\in\mathbb{Z}^2, j\neq 0} G(\omega_N^2; x, y + Nj)e^{-i\xi_N\cdot(y+Nj)}\Big| \leq C_1 e^{-C_2 N} \, , \tag{3.3.27}$$

for any $x, y \in \Omega$. We then obtain that

$$\begin{aligned}
&\Big|\int_\Omega \Big(\sum_{j\in\mathbb{Z}^2, j\neq 0} G(\omega_N^2; x, y + Nj)e^{-i\xi_N\cdot(y+Nj)}\Big)\phi_N(y)\, dy\Big| \\
&\qquad\qquad \leq C_1 e^{-C_2 N}|\Omega|^{\frac{1}{2}}\|\phi_N\|_{L^2(\Omega)} \\
&\qquad\qquad \leq C_1 e^{-C_2 N}|\Omega|^{\frac{1}{2}} \, .
\end{aligned}$$

This yields the following result:

$$\|\Delta\tilde{\phi}_N + \omega_N^2\varepsilon\tilde{\phi}_N\|_{L^2(\mathbb{R}^2)} \leq |(\delta\varepsilon)|\omega_N^2|\Omega|C_1 e^{-C_2 N} \, . \tag{3.3.28}$$

Lemma 3.3.1 yields the estimate

$$\mathrm{dist}(\omega_N^2, \Sigma) \leq \frac{|(\delta\varepsilon)|\, b\, |\Omega|}{\min_{x\in]-N,N[^2} \varepsilon(x)} C_1 e^{-C_2 N} .$$

from which we conclude that $\mathrm{dist}(]a,b[,\Sigma) = 0$. This is a contradiction with the assumption. The proof of the proposition is complete. $\square$

Now we can prove the following result concerning the convergence to the defect modes.

Theorem 3.3.2 *Suppose that the perturbation has created defect eigenvalues. Then, there exist $\eta_0 > 0$ and $N_0 \in \mathbb{N}$ such that for any $\eta \leq \eta_0$ and $N \geq N_0$,*

$$\Sigma_{\mathrm{d},N}^{\xi,\eta} \neq \emptyset\ , \quad \forall \xi \in \mathcal{B}_{\mathcal{N}}\ .$$

Moreover, for any $\omega_0^2 > 0$ and $\eta \leq \eta_0$, there exist two positive constants C_1 and C_2 depending only on ω_0^2 and η such that for any $\xi \in \mathcal{B}_{\mathcal{N}}$:

$$dist_{\mathcal{H}}\left(\Sigma_{\mathrm{d},N}^{\xi,\eta} \cap [0,\omega_0^2], \Sigma_{\mathrm{d}}^{\eta} \cap [0,\omega_0^2]\right) \leq C_1 e^{-C_2 N}. \tag{3.3.29}$$

Proof. Let ω_{d}^2 be a defect eigenvalue in Σ_{d}. It follows that there exists a function u in $L^2(\mathbb{R}^2)$ with unit norm such that

$$\Delta u + \omega_{\mathrm{d}}^2 \varepsilon u = 0 \quad \text{in } \mathbb{R}^2\ . \tag{3.3.30}$$

Let ξ be in $\mathcal{B}_{\mathcal{N}}$. We define u^ξ in $L^2(\mathbb{R}^2/2N\mathbb{Z}^2)$ by

$$u^\xi(x) = \sum_{j\in\mathbb{Z}^2} u(x+Nj) e^{i\xi\cdot(x+Nj)}\ .$$

Then for $x \in]-N,N[^2$, we have

$$\begin{aligned}
&\Big((\nabla - i\xi)\cdot(\nabla - i\xi) + \omega_{\mathrm{d}}^2 \varepsilon_N\Big) u^\xi(x) \\
&\quad= \sum_{j\in\mathbb{Z}^2} e^{i\xi\cdot(x+Nj)} (\Delta + \omega_{\mathrm{d}}^2 \varepsilon_N) u(x+Nj) \\
&\quad= \sum_{j\in\mathbb{Z}^2} e^{i\xi\cdot(x+Nj)} \Big(\Delta + \omega_{\mathrm{d}}^2 \varepsilon(x+Nj)\Big) u(x+Nj) \\
&\qquad + (\delta\varepsilon)\omega_{\mathrm{d}}^2 \sum_{j\in\mathbb{Z}^2} e^{i\xi\cdot(x+Nj)} \Big(\varepsilon_N(x) - \varepsilon(x+Nj)\Big) u(x+Nj) \\
&\quad= -(\delta\varepsilon)\omega_{\mathrm{d}}^2 \chi_\Omega(x) \sum_{j\in\mathbb{Z}^2, j\neq 0} e^{i\xi\cdot(x+Nj)} u(x+Nj)\ .
\end{aligned}$$

On the other hand, for $x \in \mathbb{R}^2$,

$$\begin{aligned}
u(x) &= \int_{\mathbb{R}^2} \delta(x-y) u(y)\, dy \\
&= \int_{\mathbb{R}^2} (\Delta + \varepsilon_{\mathrm{p}} \omega_{\mathrm{d}}^2) G(\omega_{\mathrm{d}}^2; x, y) u(y)\, dy \\
&= \int_{\mathbb{R}^2} G(\omega_{\mathrm{d}}^2; x, y)(\Delta + \varepsilon_{\mathrm{p}} \omega_{\mathrm{d}}^2) u(y)\, dy \\
&= (\delta\varepsilon)\omega_{\mathrm{d}}^2 \int_\Omega G(\omega_{\mathrm{d}}^2; x, y) u(y)\, dy.
\end{aligned}$$

Therefore

$$\Big((\nabla - i\xi)\cdot(\nabla - i\xi) + \omega_{\mathrm{d}}^2 \varepsilon_N\Big) u^\xi(x)$$
$$= -(\delta\varepsilon)^2 \omega_{\mathrm{d}}^4 \chi_\Omega(x) \int_\Omega \Big(\sum_{j\in\mathbb{Z}^2, j\neq 0} G(\omega_{\mathrm{d}}^2; x+Nj, y) e^{i\xi\cdot(x+Nj)} \Big) u(y)\, dy.$$

From (3.3.25), it follows that there exist two positive constants C_1 and C_2, depending only on ω_{d}^2, such that

$$\begin{aligned}
\left| \int_\Omega \Big(\sum_{j\in\mathbb{Z}^2, j\neq 0} G(\omega_{\mathrm{d}}^2; x+Nj, y) e^{i\xi\cdot(x+Nj)} \Big) u(y)\, dy \right| &\leq C_1 e^{-C_2 N} \int_\Omega |u(y)|\, dy \\
&\leq C_1 e^{-C_2 N} |\Omega|^{\frac{1}{2}} \|u\|_{L^2(\Omega)} \\
&\leq |\Omega|^{\frac{1}{2}} C_1 e^{-C_2 N} .
\end{aligned}$$

Therefore

$$\left\| (\nabla - i\xi)\cdot(\nabla - i\xi) u^\xi(x) + \omega_{\mathrm{d}}^2 \varepsilon_N u^\xi(x) \right\|_{L^2(]-N,N[^2)} \leq (\delta\varepsilon)^2 \omega_{\mathrm{d}}^4 |\Omega| C_1 e^{-C_2 N} . \tag{3.3.31}$$

Since

$$u^\xi(x) = u(x) e^{i\xi\cdot x} + \sum_{j\in\mathbb{Z}^2, j\neq 0} u(x+Nj) e^{i\xi\cdot(x+Nj)} \ , x\in]-N,N[^2,$$

$$\lim_{N\to+\infty} \|u(x) e^{i\xi\cdot x}\|_{L^2(]-N,N[^2)} = 1 \ ,$$

and

$$\| \sum_{j\in\mathbb{Z}^2, j\neq 0} u(x+Nj) e^{i\xi\cdot(x+Nj)} \|_{L^2(]-N,N[^2)} \leq |\Omega|^{\frac{1}{2}} N C_1 e^{-C_2 N} \ ,$$

we deduce that for N large enough,

$$\|u^\xi\|_{L^2(]-N,N[^2)} \geq \frac{1}{2} \ .$$

Thus, we conclude that

$$\mathrm{dist}(\omega_{\mathrm{d}}^2, \Sigma_N^\xi) \leq C_1 e^{-C_2 N} \ ,$$

for two positive constants C_1 and C_2, depending only on ω_{d}^2.

It is clear that we can choose these constants such that

$$\max_{\omega_{\mathrm{d}} \in \Sigma_{\mathrm{d}}^\eta \cap [0,\omega_0^2]} \mathrm{dist}(\omega_{\mathrm{d}}^2, \Sigma_N^\xi) \leq C_1 e^{-C_2 N} \ , \tag{3.3.32}$$

uniformly for $\xi \in \mathcal{B}_{\mathcal{N}}$. Hence, any defect eigenvalue $\omega_{\mathrm{d}}^2 \in \Sigma_{\mathrm{d}}$ is a limit point of $\left(\Sigma_N^\xi\right)_{N\in\mathbb{N}}$.

Let $\eta > 0$ be small enough to get $\Sigma_{\mathrm{d}}^\eta \neq \emptyset$. Applying Proposition 3.3.2, we may see that there exists $N_0 \in \mathbb{N}$ depending only on ω_0^2 and η such that $\Sigma_{\mathrm{d},N}^{\xi,\eta} \cap [0,\omega_0^2]$ has at least as many connected components as $\mathrm{card}(\Sigma_{\mathrm{d}}^\eta \cap [0,\omega_0^2])$

for $N \geq N_0$. To prove this, we take a neighborhood of $\Sigma_{\mathrm{d}}^{\eta} \cap [0, \omega_0^2]$ formed by disjoint intervals and that are away from Σ_{p}, each one of them containing exactly one defect eigenvalue. Then from Proposition 3.3.2, we deduce that for N large enough, the edges of these intervals will be strictly distant from Σ_N. On the other hand, we have proved here that for N large enough, the intersection of every interval with Σ_N^{ξ} is not empty. This means that $\Sigma_{\mathrm{d},N}^{\xi,\eta}$ is not empty if we take η small enough and then let N be large enough. By the same way, (3.3.32) can be written as

$$\max_{\omega_{\mathrm{d}} \in \Sigma_{\mathrm{d}}^{\eta} \cap [0,\omega_0^2]} \mathrm{dist}(\omega_{\mathrm{d}}^2, \Sigma_{\mathrm{d},N}^{\xi,\eta}) \leq C_1 e^{-C_2 N} , \tag{3.3.33}$$

uniformly for $\xi \in \mathcal{B}_{\mathcal{N}}$. The proof of the first part of the theorem is then done.

Now, let $\xi \in \mathcal{B}_{\mathcal{N}}$ and let $\omega^2 \in \Sigma_{\mathrm{d},N}^{\xi,\eta}$. There exists $\phi \in L^2(\mathbb{R}^2/2N\mathbb{Z}^2)$ with unit norm such that

$$(\nabla - i\xi) \cdot (\nabla - i\xi)\phi + \omega^2 \varepsilon_N \phi = 0 .$$

Then, we define u in $L^2(\mathbb{R}^2)$ by

$$u(x) = \int_\Omega G(\omega^2; x, y)\phi(y) e^{-i\xi\cdot y}\, dy .$$

Let us now find a lower bound for $\|u\|_{L^2(\mathbb{R}^2)}$. We compute

$$\begin{aligned}
(\delta\varepsilon)\omega^2 u(x) &= \int_{\mathbb{R}^2} G(\omega^2; x, y)\big(\Delta + \omega^2 \varepsilon_{\mathrm{p}}\big)\big(\phi(y)e^{-i\xi\cdot y}\big)\, dy \\
&\quad - \int_{\mathbb{R}^2} G(\omega^2; x, y)\big(\Delta + \omega^2 \varepsilon\big)\big(\phi(y)e^{-i\xi\cdot y}\big)\, dy \\
&= \phi(x)e^{-i\xi\cdot x} \\
&\quad - \int_{\mathbb{R}^2} G(\omega^2; x, y)e^{-i\xi\cdot y}\big((\nabla - i\xi)\cdot(\nabla - i\xi) + \omega^2\varepsilon\big)\phi(y)\, dy \\
&= \phi(x)e^{-i\xi\cdot x} \\
&\quad -(\delta\varepsilon)\omega^2 \int_\Omega \sum_{j\in\mathbb{Z}^2, j\neq 0} \left(G(\omega^2; x, y + Nj)e^{-i\xi\cdot(y+Nj)}\right)\phi(y)\, dy .
\end{aligned}$$

Since there exist positive constants C_1 and C_2, depending only on η and ω_0^2, such that

$$\left| \sum_{j\in\mathbb{Z}^2, j\neq 0} \left(G(\omega^2; x, y+Nj)e^{-i\xi\cdot(y+Nj)}\right)\right| \leq C_1 e^{-C_2 N} \ , \ \forall x \in]-N, N[^2 \ , \forall y \in \Omega \ , \tag{3.3.34}$$

for any $\omega^2 \in [0, \omega_0^2]$ such that $\mathrm{dist}(\omega^2, \Sigma_{\mathrm{p}}) \geq \eta$, we deduce that

$$\left\| \int_\Omega \sum_{j\in\mathbb{Z}^2, j\neq 0} \left(G(\omega^2; x, y + Nj)e^{-i\xi\cdot(y+Nj)}\right)\phi(y)\, dy \right\|_{L^2(]-N,N[^2)} \leq N C_1 e^{-C_2 N} , \tag{3.3.35}$$

where the constants C_1 and C_2 are different from the previous ones but have the same dependence. Recalling that $\|\phi\|_{L^2(]-N,N[^2)} = 1$, we deduce the existence of $N_0 > 0$ such that

$$\|\phi\|_{L^2(\mathbb{R}^2)} \geq \|\phi\|_{L^2(]-N,N[^2)} \geq \frac{1}{2} . \tag{3.3.36}$$

On the other hand,

$$
\begin{aligned}
(\Delta+\omega^2\varepsilon)u(x) &= \int_\Omega (\Delta_x+\omega^2\varepsilon)G(\omega^2;x,y)\phi(y)e^{-i\xi\cdot y}\,dy \\
&= \chi_\Omega(x)\phi(x)e^{-i\xi\cdot x} - (\varepsilon_{\mathrm{p}}(x)-\varepsilon(x))\,\omega^2\int_\Omega G(\omega^2;x,y)\phi(y)e^{-i\xi\cdot y}\,dy \\
&= \chi_\Omega(x)\phi(x)e^{-i\xi\cdot x} - \chi_\Omega(x)(\delta\varepsilon)\omega^2\int_\Omega G(\omega^2;x,y)\phi(y)e^{-i\xi\cdot y}\,dy \\
&= \chi_\Omega(x)\phi(x)e^{-i\xi\cdot x} \\
&\quad -\chi_\Omega(x)\int_{\mathbb{R}^2} G(\omega^2;x,y)\left(\Delta+\omega^2\varepsilon_{\mathrm{p}}\right)\left(\phi(y)e^{-i\xi\cdot y}\right)\,dy \\
&\quad +\chi_\Omega(x)\int_{\mathbb{R}^2} G(\omega^2;x,y)\left(\Delta+\omega^2\varepsilon\right)\left(\phi(y)e^{-i\xi\cdot y}\right)\,dy \\
&= \chi_\Omega(x)\phi(x)e^{-i\xi\cdot x} \\
&\quad -\chi_\Omega(x)\int_{\mathbb{R}^2} \left(\Delta_y+\omega^2\varepsilon_{\mathrm{p}}\right)G(\omega^2;x,y)\phi(y)e^{-i\xi\cdot y}\,dy \\
&\quad +\chi_\Omega(x)\int_{\mathbb{R}^2} G(\omega^2;x,y)e^{-i\xi\cdot y}\left((\nabla-i\xi)\cdot(\nabla-i\xi)+\omega^2\varepsilon\right)\phi(y)\,dy \\
&= \chi_\Omega(x)(\delta\varepsilon)\omega^2\int_{\mathbb{R}^2} G(\omega^2;x,y)e^{-i\xi\cdot y}\phi(y)\left(\sum_{j\in\mathbb{Z}^2,j\neq 0}\chi_\Omega(y-Nj)\right)\,dy \\
&= \chi_\Omega(x)(\delta\varepsilon)\omega^2\int_\Omega \sum_{j\in\mathbb{Z}^2,j\neq 0}\left(G(\omega^2;x,y+Nj)e^{-i\xi\cdot(y+Nj)}\right)\phi(y)\,dy\,.
\end{aligned}
$$

Therefore, it follows from (3.3.34) that

$$
\left|\Delta u(x)+\omega^2\varepsilon u(x)\right| \leq |(\delta\varepsilon)|\omega_0^2|\Omega|^{\frac{1}{2}}C_1e^{-C_2N}\,,
$$

for any $x\in\Omega$. Consequently,

$$
||\Delta u+\omega^2\varepsilon u||_{L^2(\mathbb{R}^2)} \leq |(\delta\varepsilon)|\omega_0^2|\Omega|C_1e^{-C_2N}\,. \tag{3.3.37}
$$

From (3.3.36), we readily get

$$
\mathrm{dist}(\omega^2,\Sigma) \leq C_1e^{-C_2N}\,,
$$

where C_1 and C_2 are different from the previous ones but have the same dependence.

Since $\mathrm{dist}(\omega^2,\Sigma_{\mathrm{p}})\geq\eta$, we easily arrive at

$$
\mathrm{dist}(\omega^2,\Sigma_{\mathrm{d}}^\eta) \leq C_1e^{-C_2N}\,,
$$

which ends the proof of the theorem. □

An immediate consequence of this theorem is the following.

Corollary 3.3.1 *Suppose that the perturbation has created defect eigenvalues. Then, there exists $\eta_0>0$ and $N_0\in\mathbb{N}$ such that $\Sigma_{\mathrm{d},N}^\eta\neq\emptyset$ for $\eta\leq\eta_0$ and $N\geq N_0$.*

Moreover, there exists $N_1\in\mathbb{N}$ depending only on η such that the number of connected components of $\Sigma_{\mathrm{d},N}^\eta\cap[0,\omega_0^2]$ is at least equal to card $\left(\Sigma_{\mathrm{d}}^\eta\cap[0,\omega_0^2]\right)$ and the width of each component decays exponentially with N.

Proof. The proof follows immediately from the facts that each eigenvalue in $\Sigma_{\mathrm{d},N}^{\xi,\eta}$ is continuous with respect to ξ, and

$$\Sigma_N = \cup_{\xi \in \mathcal{B}_{\mathcal{N}}} \Sigma_N^{\xi} \, .$$

□

Remark 3.3.2 *These results are very important in practice for determining the defect modes of 2D-photonic crystals. Indeed, after identifying the background continuous spectrum by computing numerically $\Sigma_{\mathrm{p}}^{\xi}$ for $\xi \in \mathcal{B}$, we have the gaps and we can have constants C_1 and C_2 depending on $dist(\omega^2, \Sigma_{\mathrm{p}})$ such that*

$$\left| G(\omega^2; x, y) \right| \leq C_1 e^{-C_2 N} \, .$$

Then we compute Σ_N^{ξ} for some $\xi \in \mathcal{B}_{\mathcal{N}}$, and from the eigenvalues that are not located in Σ_{p} we deduce an approximation of the defect eigenvalues.

3.4 The TE polarization

In this section we deal with the TE polarization. The same results hold, but the proofs are slightly different. This is a consequence of the dependence of the domain of the acoustic operator on the inverse of the dielectric function. So when we perturb ε_{p} into ε, the operator $-\nabla . \frac{1}{\varepsilon_{\mathrm{p}}} \nabla$ is transformed into $-\nabla . \frac{1}{\varepsilon} \nabla$ and we see clearly that, in general, these operators do not have the same domain. So the proofs have to be adjusted.

3.4.1 Definition and preliminary results

First we introduce some analogous notations to those in Definition 3.2.1.

Definition 3.4.1 *Let A_{p} be the operator defined by*

$$A_{\mathrm{p}} = -\nabla . \frac{1}{\varepsilon_{\mathrm{p}}} \nabla \, , \quad on \ L^2(\mathbb{R}^2) \, ,$$

and let Σ_p denote its spectrum.

For $\xi \in [0, 2\pi[^2$ we define A_{p}^{ξ} on $L^2(\mathbb{R}^2/\mathbb{Z}^2)$ by

$$A_{\mathrm{p}}^{\xi} = -(\nabla_x - i\xi) \cdot \frac{1}{\varepsilon_{\mathrm{p}}} (\nabla_x - i\xi) \, ,$$

and denote by $\Sigma_{\mathrm{p}}^{\xi}$ its spectrum.

We perturb the background periodic medium on a bounded domain as done in (3.2.11).

It has been proved that the perturbation is relatively compact and so does not affect the essential spectrum of A_{p}. Recalling our assumption on the absolute continuity of the spectrum of A_{p}, we deduce that the perturbation will result in the addition of eigenvalues of finite multiplicity to Σ_{p}.

We define ε_N, A_N, A_N^{ξ}, Σ_N, and Σ_N^{ξ} in the same way as in Section 3.3.1. To avoid the problem of the dependence of the domain on ε, we introduce a new operator that will have the same spectral properties as those of A_{p}.

Definition 3.4.2 *Let B_{p} be the operator defined on $L^2(\mathbb{R}^2)^2$ by*

$$B_{\mathrm{p}} = -\frac{1}{\varepsilon_{\mathrm{p}}}\nabla\nabla\cdot\ .$$

For $\xi \in [0, 2\pi[^2$ we define B_{p}^{ξ} on $L^2(\mathbb{R}^2/\mathbb{Z}^2)^2$ by

$$B_{\mathrm{p}}^{\xi} = -\frac{1}{\varepsilon_{\mathrm{p}}}(\nabla - i\xi)(\nabla - i\xi)\cdot\ .$$

We also define B_N and B_N^{ξ} analogously as done for A_{p}.

The operator B_{p} is a self-adjoint periodic differential operator on

$$\left(L^2(\mathbb{R}^2/\mathbb{Z}^2)^2, \varepsilon_{\mathrm{p}}\, dx\right).$$

However, since its kernel has infinite dimension it is not elliptic. Actually, the kernel is the subspace of divergence free vectors. We can not apply the same technique as for A_{p} to prove that the spectrum of B_{p}^{ξ} is a set of positive eigenvalues that accumulate at infinity and that the spectrum of B_{p} is an absolutely continuous spectrum with band structure located in $\mathbb{R}^+$. It is however possible to extend this operator into a larger elliptic self-adjoint operator that will coincide with B_{p} on a subspace that is complementary with the kernel of B_{p} (see [47]). We can deduce then that the spectrum of B_{p} in $\mathbb{R}^+ \setminus \{0\}$ is absolutely continuous and that 0 is an eigenvalue with infinite multiplicity. This technique is used to prove the band structure of the Maxwell operator. Another way to characterize the structure of the spectrum of B_{p} is to relate it to the spectrum of A_{p}. This is given by the following theorem.

Theorem 3.4.1 *For any $\xi \in [0, 2\pi[^2$, the spectra of B_{p}^{ξ}, B_{p}, B_N^{ξ}, B_N and B are $\Sigma_{\mathrm{p}}^{\xi} \cup \{0\}$, Σ_{p}, $\Sigma_N^{\xi} \cup \{0\}$, Σ_N, and Σ, respectively. Moreover,*

(i) *The operators B_{p}^{ξ} and B_N^{ξ} have exactly the same eigenvalues as A_{p}^{ξ} and A_N^{ξ} respectively, except for 0 which is an eigenvalue of A_{p}^0 and A_N^0 of multiplicity 1 and is not an eigenvalue of A_{p}^{ξ} and A_N^{ξ} when $\xi \neq 0$ while it is an eigenvalue of B_{p}^{ξ} and B_N^{ξ} for any ξ with infinite multiplicity.*

(ii) *The spectra of B_{p} and B_N are absolutely continuous spectra in $\mathbb{R}^+ \setminus \{0\}$ and 0 is an eigenvalue of infinite multiplicity.*

(iii) *The operators A and B have the same absolutely continuous spectrum and the eigenvalues have exactly the same multiplicity for A and B except for 0 that is an eigenvalue of B with infinite multiplicity.*

Proof. Let $\xi \in [0, 2\pi[^2$ and $\omega^2 \geq 0$. Suppose that either $\xi \neq 0$ or $\omega^2 \neq 0$ and that ω^2 is in the spectrum of A_{p}^{ξ}. Then there exists $\phi \in L^2(\mathbb{R}^2/\mathbb{Z}^2)$ such that $\phi \neq 0$ and

$$(\nabla - i\xi)\cdot\frac{1}{\varepsilon_{\mathrm{p}}}(\nabla - i\xi)\phi + \omega^2\phi = 0\ .$$

We can easily see that since ξ and ω^2 are not simultaneously equal to 0, $(\nabla - i\xi)\phi \neq 0$. Let $\psi = \frac{1}{\varepsilon_{\mathrm{p}}}(\nabla - i\xi)\phi \in L^2(\mathbb{R}^2/\mathbb{Z}^2)^2$. Then

$$(\nabla - i\xi)(\nabla - i\xi) \cdot \psi + \omega^2 \varepsilon_{\mathrm{p}} \psi = 0 ,$$

which means that ω^2 is an eigenvalue of B^ξ_{p}. Moreover, if ϕ_1 and ϕ_2 are two linearly independent eigenvectors related to the same eigenvalue $\omega^2 \neq 0$, then $\psi_1 = \frac{1}{\varepsilon_{\mathrm{p}}}(\nabla - i\xi)\phi_1$ and $\psi_2 = \frac{1}{\varepsilon_{\mathrm{p}}}(\nabla - i\xi)\phi_2$ are linearly independent.

We conclude that all the eigenvalues of A^ξ_{p} except for the eigenvalue 0 of A^0_{p} are eigenvalues of B^ξ_{p}. We will see that 0 is an infinite multiplicity eigenvalue of A^0_{p}.

Conversely, let ω^2 be an eigenvalue of B^ξ_{p} and let $\psi \in L^2(\mathbb{R}^2/\mathbb{Z}^2)^2$ be such that $\psi \neq 0$ and satisfies

$$(\nabla - i\xi)(\nabla - i\xi) \cdot \psi + \omega^2 \varepsilon_{\mathrm{p}} \psi = 0 .$$

Suppose that $(\nabla - i\xi) \cdot \psi = 0$. Then, since $\psi \neq 0$, we have $\omega^2 = 0$. We also obtain that $\nabla.(e^{-i\xi\cdot x}\psi) = 0$, or equivalently, that there exists $\alpha \in L^2(\mathbb{R}^2/\mathbb{Z}^2)$ such that

$$e^{-i\xi\cdot x}\psi = \nabla \times (\alpha e^{-i\xi\cdot x}) ,$$

where $\nabla \times \alpha = (\partial_2\alpha, -\partial_1\alpha)$. It follows that

$$\psi = \nabla \times \alpha - i \begin{pmatrix} \xi_2 \\ -\xi_1 \end{pmatrix} \alpha .$$

Hence, 0 is an eigenvalue of B^ξ_{p} with infinite multiplicity.

In the case where $(\nabla - i\xi) \cdot \psi \neq 0$, let $\phi = (\nabla - i\xi) \cdot \psi \in L^2(\mathbb{R}^2/\mathbb{Z}^2)$. Then,

$$(\nabla - i\xi) \cdot \frac{1}{\varepsilon_{\mathrm{p}}}(\nabla - i\xi)\phi + \omega^2\phi = 0 ,$$

which means that ω^2 is an eigenvalue of A^ξ_{p}. We can also show that if ψ_1 and ψ_2 are two linearly independent eigenvectors of B^ξ_{p} related to the same eigenvalue $\omega^2 \neq 0$, then $\phi_1 = (\nabla - i\xi) \cdot \psi_1$ and $\phi_2 = (\nabla - i\xi) \cdot \psi_2$ are linearly independent.

The same proof holds for the operators A^ξ_N and B^ξ_N and for the eigenvalues of A and B. □

As a consequence of the above theorem, we can recover the properties of the spectra of A^ξ_N and A_N by studying those of B^ξ_N and B_N to which we can apply mainly the same technique as in the TM case since their domain does not depend on ε.

To this end we need to give an analogous result to Lemma 3.2.1 for the operator B_{p}. We define the resolvent $R(z) = (B_{\mathrm{p}} - z)^{-1}$.

Lemma 3.4.1 *For any $z \notin \Sigma_{\mathrm{p}}$ and $l > 0$ we have*

$$\|\chi_{x,l} R(z) \chi_{y,l}\| \leq \left(\frac{9}{\eta}\right) e^{(\sqrt{2}l/4)} e^{-m_z|x-y|} \quad \textit{for all } x, y \in \mathbb{R}^2 , \tag{3.4.38}$$

with

$$m_z = \frac{\eta}{4(2\varepsilon_-^{-1} + |z| + \eta)} , \tag{3.4.39}$$

where $\|\cdot\|$ *denotes the* L^2*-norm on* $\mathbb{R}^2$, $\eta = \mathit{dist}(z, \Sigma_{\mathrm{p}})$, $\varepsilon_- = \min_{x\in\mathbb{R}^2} \varepsilon_{\mathrm{p}}(x)$, *and* $\chi_{x,l}$ *is the characteristic function of the cube* $\{y = (y_1, y_2) \in \mathbb{R}^2 : |y_1 - x_1| < \frac{l}{2}$ *and* $|y_2 - x_2| < \frac{l}{2}\}$.

Proof. The proof is exactly the same as the one for the Helmholtz operator which uses a Combes-Thomas argument and is given by A. Figotin and A. Klein in [30, 31, 29].

Let B_a denote the operators formally given by

$$B_a = e^{a\cdot x} B_p e^{-a\cdot x}\ , \quad a \in \mathbb{R}^2\ , \tag{3.4.40}$$

as the closed densely defined operators (uniquely) introduced by the corresponding quadratic forms defined on $C_0^1(\mathbb{R}^2)$ by

$$\mathcal{B}_a[\psi] = \langle \nabla\cdot(e^{a\cdot x}\psi), \frac{1}{\varepsilon_{\mathrm{p}}(x)}\nabla\cdot(e^{-a\cdot x}\psi)\rangle = \langle(\nabla+a)\cdot\psi, \frac{1}{\varepsilon_{\mathrm{p}}(x)}(\nabla-a)\cdot\psi\rangle\ . \tag{3.4.41}$$

We also introduce the quadratic form $\mathcal{Q}_a$ as

$$\begin{aligned}\mathcal{Q}_a[\psi] &= \mathcal{B}_a[\psi] - \mathcal{B}_0[\psi] \\ &= \langle a\cdot\psi, \frac{1}{\varepsilon_{\mathrm{p}}(x)}\nabla\cdot\psi\rangle - \langle\nabla\cdot\psi, \frac{1}{\varepsilon_{\mathrm{p}}(x)}a\cdot\psi\rangle \\ &\quad -\langle a\cdot\psi, \frac{1}{\varepsilon_{\mathrm{p}}(x)}a\cdot\psi\rangle\end{aligned}$$

Since

$$\left|\langle a\cdot\psi, \frac{1}{\varepsilon_{\mathrm{p}}(x)}\nabla\cdot\psi\rangle\right| \le \frac{1}{2}|a|\left(\langle\psi, \frac{1}{\varepsilon_{\mathrm{p}}(x)}\psi\rangle + \langle\nabla\cdot\psi, \frac{1}{\varepsilon_{\mathrm{p}}(x)}\nabla\cdot\psi\rangle\right)\ , \tag{3.4.42}$$

we have

$$|\mathcal{Q}_a[\psi]| \le |a|\mathcal{B}_0[\psi] + |a|(1+|a|)\varepsilon_-^{-1}\|\psi\|^2 \quad \text{for all } \psi \in C_0^1(\mathbb{R}^2)\ . \tag{3.4.43}$$

Then we require $|a| < 1$ and use Theorem VI.3.9 in [43] to conclude that $\mathcal{B}_a$ is a closable sectorial form and define B_a as the unique m-sectorial operator associated with it. If in addition $z \notin \Sigma_p$ and

$$\Lambda \equiv 2\left\|(|a|(1+|a|)\varepsilon_-^{-1} + |a|B_{\mathrm{p}})(B_{\mathrm{p}} - zI)^{-1}\right\| < 1\ , \tag{3.4.44}$$

we can conclude that $z \notin \Sigma_a$ (the spectrum of B_a) and

$$\|R_a(z) - R_0(z)\| \le \frac{4\Lambda}{(1-\Lambda)^2}\|R_0(z)\|\ , \tag{3.4.45}$$

where $R_a(z) = (B_a - zI)^{-1}$.

Since

$$\begin{aligned}\Lambda &= 2\left\|(|a|(1+|a|)\varepsilon_-^{-1} + |a|z)(B_{\mathrm{p}} - zI)^{-1} + |a|\right\| \\ &\le 2|a|\Big(\big((1+|a|)\varepsilon_-^{-1} + |z|\big)\eta^{-1} + 1\Big) \\ &\le 2|a|\Big((2\varepsilon_-^{-1} + |z|)\eta^{-1} + 1\Big)\ ,\end{aligned}$$

it is sufficient to take

$$|a| < \frac{\eta}{2(2\varepsilon_-^{-1} + |z| + \eta)} , \tag{3.4.46}$$

to ensure $\Lambda < 1$. In fact, we take

$$|a| < m_z = \frac{\eta}{4(2\varepsilon_-^{-1} + |z| + \eta)} , \tag{3.4.47}$$

so that we get $\Lambda < \frac{1}{2}$. It follows that

$$\|R_a(z)\| \le \left(1 + \frac{4\Lambda}{(1-\Lambda)^2}\right) \|R_0(z)\| \le \frac{9}{\eta} . \tag{3.4.48}$$

Now, let $x_0, y_0 \in \mathbb{R}^2$, $l > 0$, and take

$$a = \frac{m_z}{|x_0 - y_0|}(x_0 - y_0) .$$

We have

$$\begin{aligned} \|\chi_{x_0,l} R_0(z) \chi_{y_0,l}\| &= \|\chi_{x_0,l} e^{-a\cdot x} R_a(z) e^{a\cdot x} \chi_{y_0,l}\| \\ &= e^{-m_z\cdot|x_0-y_0|} \|\chi_{x_0,l} e^{-a\cdot(x-x_0)} R_a(z) e^{a\cdot(x-y_0)} \chi_{y_0,l}\| \\ &\le \frac{9}{\eta} e^{-m_z\cdot|x_0-y_0|} \|\chi_{x_0,l} e^{-a\cdot(x-x_0)}\|_\infty \|\chi_{y_0,l} e^{-a\cdot(x-y_0)}\|_\infty . \end{aligned}$$

We also notice that

$$\|\chi_{x_0,l} e^{\pm a\cdot(x-x_0)}\|_\infty \le e^{\frac{l}{\sqrt{2}} m_z} ,$$

and since $m_z \le \frac{1}{4}$, the theorem is proved. □

As a consequence, the matricial Green's kernel of B_{p} has a similar exponential decay as the Green's kernel of A_{p}. Let $\omega^2 \notin \Sigma_p$, we define the matricial Green's kernel $K(\omega^2; x, y)$ as the solution to

$$\nabla\nabla \cdot K(\omega^2; x, y) + \omega^2 \varepsilon_{\mathrm{p}} K(\omega^2; x, y) = \delta(x-y) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} . \tag{3.4.49}$$

Here we shall impose an outgoing radiation condition on $\nabla \cdot K$ in order to ensure uniqueness. As a direct consequence of the previous lemma the following result holds.

Corollary 3.4.1 *There exist two positive constants C_1 and C_2 depending only on $\omega_0^2 > 0$ such that for any $\omega^2 \notin \Sigma_{\mathrm{p}}$,*

$$|K(\omega^2; x, y)| \le C_1 e^{-C_2 \, dist(\omega^2, \Sigma_{\mathrm{p}})|x-y|} , \quad \textit{for } |x-y| \to +\infty . \tag{3.4.50}$$

Now we are ready to prove the analogous results to those concerning the TM polarization.

3.4.2 Convergence of the "continuous spectrum"

As done for the TM polarization, we give an estimate of the perturbation brought to the continuous spectrum of A_{p} by the supercell method.

Theorem 3.4.2 *For any $\omega_0 > 0$ and $N_0 \in \mathbb{N}$, there exists $C > 0$, depending only on ω_0, N_0 and Ω, such that*

$$\max_{\omega^2 \in \cup_{k\in[-N+1,N-1[^2\cap\mathbb{N}^2}\Sigma_{\mathrm{p}}^{\xi+k\pi/N}\cap[0,\omega_0^2]} dist(\omega^2, \Sigma_N^\xi) \le \frac{C}{N^2} , \tag{3.4.51}$$

for any $N \ge N_0$ and any $\xi \in \mathcal{B}_{\mathcal{N}}$.

Proof. Let $k \in [-N+1, N-1[^2\cap\mathbb{N}^2$ and $\xi \in \mathcal{B}_{\mathcal{N}}$. Let ω^2 be in $\Sigma_{\mathrm{p}}^{\xi+k\pi/N}\cap[0,\omega_0^2]$. If $\omega^2 = 0$, then necessarily $\xi = 0$ and $k = 0$ and in that case we now that $0 \in \Sigma_N^\xi$.

Let us consider now $\omega^2 \ne 0$. From Theorem 3.4.1, we deduce that ω^2 is in the spectrum of $B_{\mathrm{p}}^{\xi+k\pi/N}$.

Since $\xi + k\pi/N \in \mathcal{B}$, there exists $\phi \in L^2(\mathbb{R}^2/\mathbb{Z}^2)^2$ with unit norm such that

$$\left(\nabla - i(\xi + \frac{k\pi}{N})\right)\left(\nabla - i(\xi + \frac{k\pi}{N})\right) \cdot \phi + \omega^2\varepsilon_{\mathrm{p}}\phi = 0 . \tag{3.4.52}$$

Let $\tilde\phi$ be defined in $L^2(\mathbb{R}^2/2N\mathbb{Z}^2)^2$ as

$$\tilde\phi(x) = \phi(x)e^{-i\frac{\pi}{N}k\cdot x} . \tag{3.4.53}$$

We have $||\tilde\phi||_{L^2(\mathbb{R}^2/2N\mathbb{Z}^2)^2} = 4N^2$, and it satisfies the following equation.

$$(\nabla - i\xi)(\nabla - i\xi)\cdot\tilde\phi + \omega^2\varepsilon_{\mathrm{p}}\tilde\phi = 0 , \tag{3.4.54}$$

which can be written as

$$(\nabla - i\xi)(\nabla - i\xi)\cdot\tilde\phi + \omega^2\varepsilon\tilde\phi = -\chi_\Omega(\delta\varepsilon)\omega^2\tilde\phi . \tag{3.4.55}$$

We prove then in the same way as done for the TM case that there exists an eigenvalue ω_ξ^2 belonging to the spectrum of B_N^ξ, that is $\Sigma_N^\xi \cup \{0\}$, satisfying

$$|\omega^2 - \omega_\xi^2| \le \frac{C}{N^2} .$$

Since we considered $\omega^2 \ne 0$, for N large enough $\omega_\xi^2 \ne 0$ and then $\omega_\xi^2 \in \Sigma_N^\xi$. This means that

$$\mathrm{dist}(\omega^2, \Sigma_N^\xi) \le \frac{C}{N^2} .$$

The theorem is then proved. □

3.4.3 Convergence of the defect eigenvalues

Analogously to the TM polarization, we give a characterization of the part of the spectrum Σ_N corresponding to the defect eigenvalues of Σ. We use the notations introduced in Definition 3.3.3. The following proposition holds.

Proposition 3.4.1 *For every gap* $]a,b[$ *in* $\Sigma_{\rm p}$ $(0 < a < b)$ *satisfying* $]a,b[\cap\Sigma = \emptyset$, *there exists* $N_1 \in \mathbb{N}$ *such that, for* $N \geq N_1$, $\Sigma_N \cap]a,b[= \emptyset$.

Proof. Suppose that the proposition is false. Then for any $N_0 \in \mathbb{N}$ there exists $N \geq N_0$ and $\omega_N^2 \in]a,b[\cap\Sigma_N$. This means that ω_N^2 is in the spectrum of B_N. Then there exist $\xi_N \in \mathcal{B}_\mathcal{N}$ and $\phi_N \in L^2(\mathbb{R}^2/2N\mathbb{Z}^2)^2$ with unit norm such that

$$(\nabla - i\xi_N)(\nabla - i\xi_N)\cdot\phi_N + \omega_N^2\varepsilon_N\phi_N = 0\ , \quad \text{in } L^2(\mathbb{R}^2/2N\mathbb{Z}^2)^2\ . \qquad (3.4.56)$$

Now, define $\tilde{\phi}_N$ in $L^2(\mathbb{R}^2)$ as

$$\tilde{\phi}_N(x) = \int_\Omega K(\omega_N^2; x, y)e^{-i\xi_N\cdot y}\phi_N(y)\,dy\ . \qquad (3.4.57)$$

Using $\tilde{\phi}_N$, we prove in a similar way as for Proposition 3.3.2 that

$$\frac{\|\nabla\nabla\cdot\tilde{\phi}_N + \omega_N^2\varepsilon\tilde{\phi}_N\|_{L^2(\mathbb{R}^2)^2}}{\|\tilde{\phi}_N\|_{L^2(\mathbb{R}^2)^2}} \leq C_1e^{-C_2N}\ , \qquad (3.4.58)$$

for some positive constants C_1 and C_2. Since ω_N^2 is away form 0 then

$$\mathrm{dist}(\omega_N^2, \Sigma) \leq C_1e^{-C_2N}\ , \qquad (3.4.59)$$

which leads to a contradiction. □

Now we give the main result for the TE case about the convergence of the eigenvalues of the supercell corresponding to the defect.

Theorem 3.4.3 *Suppose that the perturbation has created defect eigenvalues. Then, there exists* $\eta_0 > 0$ *and* $N_0 \in \mathbb{N}$ *such that for any* $\eta \leq \eta_0$ *and* $N \geq N_0$,

$$\Sigma_{\mathrm{d},N}^{\xi,\eta} \neq \emptyset\ , \quad \forall\xi \in \mathcal{B}_\mathcal{N}\ .$$

Moreover, for any $\omega_0^2 > 0$ *and* $\eta \leq \eta_0$, *there exists two positive constants* C_1 *and* C_2 *depending only on* ω_0^2 *and* η *such that for any* $\xi \in \mathcal{B}_\mathcal{N}$:

$$dist_\mathcal{H}\left(\Sigma_{\mathrm{d},N}^{\xi,\eta}\cap[0,\omega_0^2], \Sigma_\mathrm{d}^\eta\cap[0,\omega_0^2]\right) \leq C_1e^{-C_2N}\ . \qquad (3.4.60)$$

Proof. Since we deal with a part of the spectrum that is away from 0, the statements are exactly the same when considering the spectra related to $B_{\rm p}$ instead of $A_{\rm p}$. The proof becomes then similar to the one of Theorem 3.3.2. □

Note that the Corollary 3.3.1 holds for the TE polarization.

3.5 Numerical experiments

The numerical simulations presented in this section are computed with the *MIT Photonic-Bands* (MPB) package [42]. We consider a 2-D photonic crystal in which the dielectric permittivity takes the values of 1 and 12. The structure of the crystal is shown in Figure 3.1 where the dark area corresponds to dielectric permittivity 12.

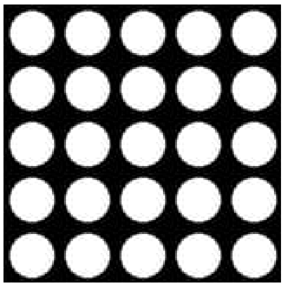


Figure 3.1: The periodic structure.

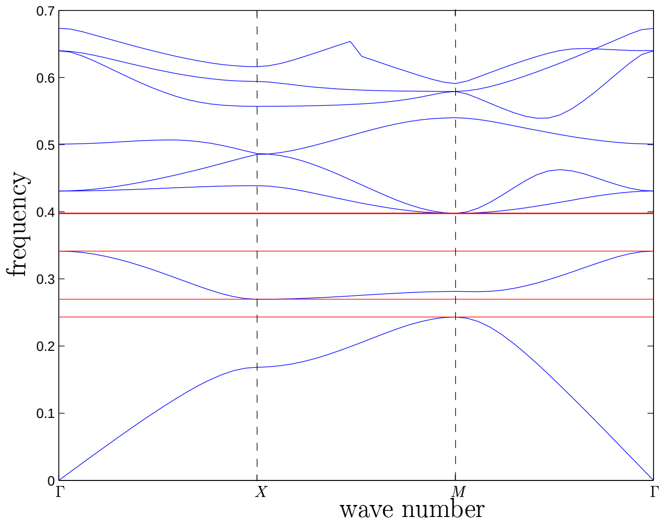


Figure 3.2: TE-spectrum of the periodic structure.

We investigate only the TE polarization. We compute the TE-spectrum of this structure for the first 8 bands. This is shown in Figure 3.2 where we notice the presence of two gaps between the first and the second bands and between the second and the third bands. The singularities of the last band come from the fact that it crosses the following band which is not represented on the diagram.

Then we introduce a defect to this periodic structure by changing the dielectric permittivity in one disc from 1 into 12. The corresponding 7x7 supercell is represented in Figure 3.3. We compute the TE-spectrum in the supercell for a fixed wave number and for different sizes of the supercell (3,5,7). The results are shown in Figure 3.4. The horizontal dashed lines delimit the gaps of the periodic medium.

We notice clearly the presence of two defect eigenvalues in the second gap. The values of the defect frequencies and the relative difference with the 7x7 supercell results are shown in table 3.1.

The convergence of the continuous spectrum is in $1/N^2$ but the multiplicative constant depends on the dispersion of the band considered (the differential of the frequency with respect to the wave vector). This explains why the convergence in the first band (the most dispersive) is the lowest.

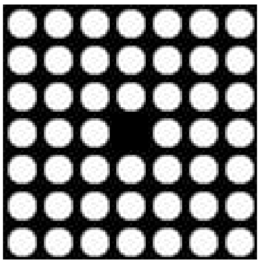


Figure 3.3: The 7x7 supercell.

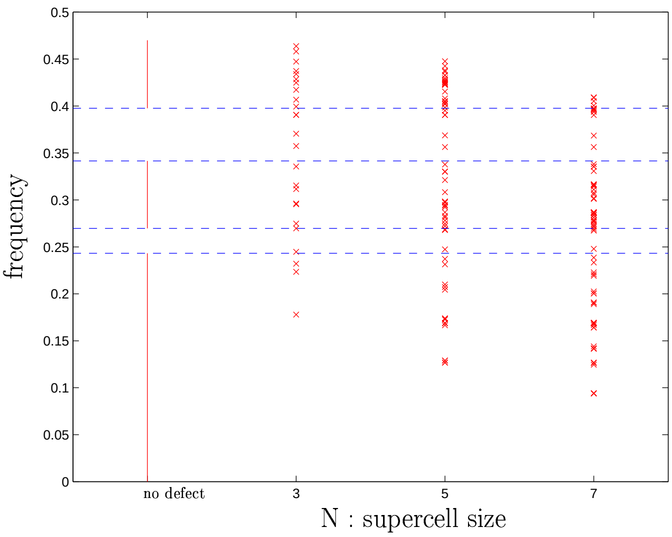


Figure 3.4: TE-spectrum of the supercell.

In Figure 3.5 we plotted the defect frequencies against the wave number. In the 3x3 supercell, the defect frequencies oscillate with an amplitude about 1% while the oscillation is about 0.1% in the 5x5 supercell and about 0.05% in the 7x7 supercell.

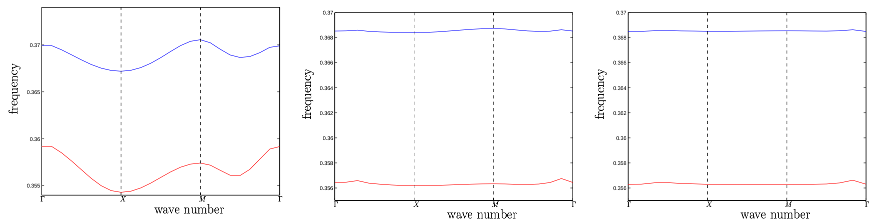
Finally, in Figures 3.6-3.8 we represent the energy distribution and the magnetic field for the defect modes in the case of the 7x7 supercell.

3.6 Conclusion

We presented in this chapter a rigorous proof of the convergence of the supercell method. The convergence speed is related to the exponential decay of the

Supercell size	3x3	5x5	7x7
Defect frequency 1	0.3574 0.3%	0.3563 $\leq$00.3%	0.3563
Defect frequency 2	0.3706 0.6%	0.3687 0.05%	0.3685

Table 3.1: Defect frequencies and relative difference with the 7x7 supercell.



(a) 3x3 (b) 5x5 (c) 7x7

Figure 3.5: Dependence of the defect frequencies on the wave number.

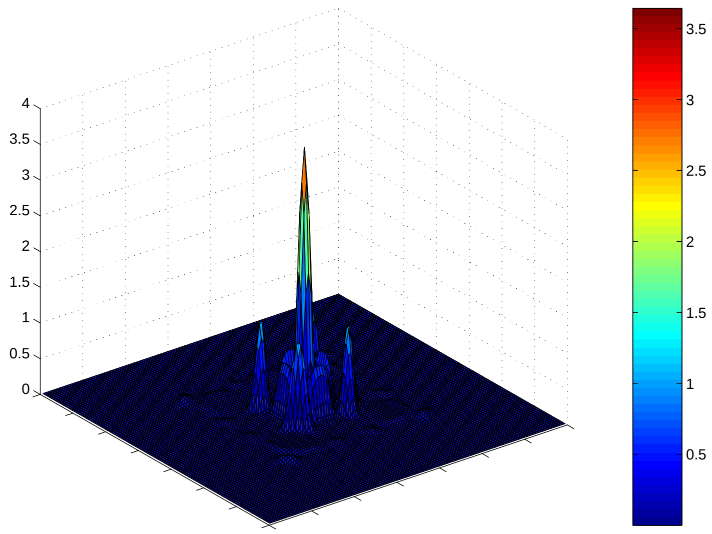


Figure 3.6: Energy distribution in the first defect mode.

Green's function. If (ω_a^2, ω_b^2) is a gap of the photonic crystal (ω_a^2, ω_b^2 belong to the spectrum), then it was proved that for $\omega^2 \in (\omega_a^2, \omega_b^2)$, the exponential decay of the Green's function is of the form

$$O(\exp(-C\sqrt{|\omega^2 - \omega_a^2||\omega^2 - \omega_b^2|}\ |x|)). \tag{3.6.61}$$

It follows that the convergence of the defect eigenvalues will be slower when they are closer to the edges of the gap. This is not an important problem since these modes are useless. Actually, we are interested in the localization property of the defect modes which is weak for such eigenvalues.

Finally, we remark that this method becomes very costly when looking for defects lying over few bands. For example, if we look for a defect eigenvalue lying in a gap between the fourth and the fifth band, when computing the spectrum of the 5×5 supercell, every band will contribute with 5^2 eigenvalues and the defect eigenvalue will be the 101^{st} eigenvalue which costs a lot of calculations.

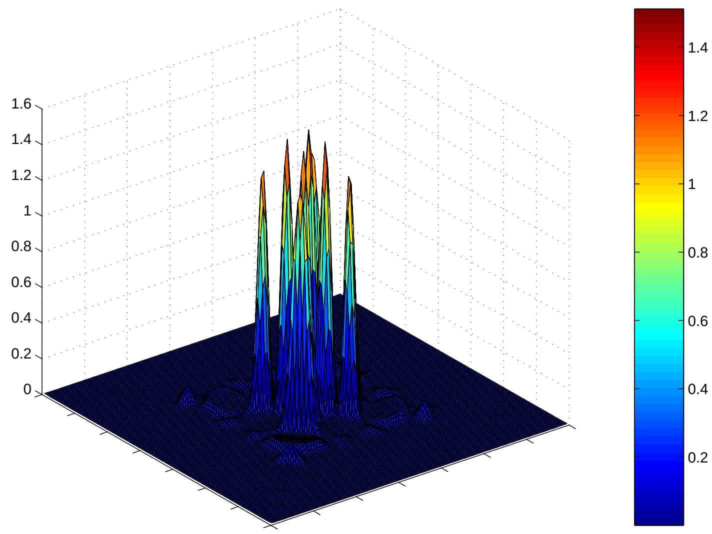


Figure 3.7: Energy distribution in the second defect mode.

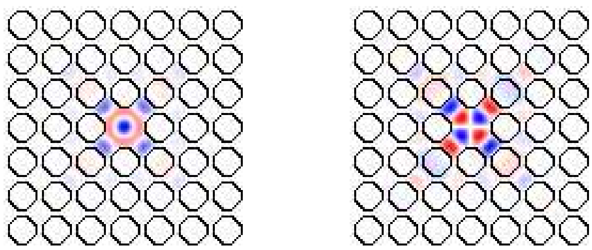


Figure 3.8: Magnetic field distribution in the first and second defect modes.

We believe that it should be possible to determine such eigenvalues in a faster way with integral operator methods.

Chapter 4

Modeling photonic crystal fibers

4.1 Introduction

Optical fibers are today finding wide use in areas covering telecommunications, sensor technologies, spectroscopy, and medicine [17].

Ordinary optical fibers guide light by total internal reflection, which relies on the refractive index of the central core being greater than that of the surrounding cladding. This physical mechanism has been known and exploited technologically for many years. However, within the past decade the research in new purpose-built materials has opened up the possibilities of localizing and controlling light in cavities and waveguides by a new physical mechanism, namely the photonic band gap effect (PBG).

The PBG effect may be achieved in periodically structured materials having a periodicity on the scale of the optical wavelength. Such periodic structures are usually referred to as photonic crystals, or photonic band gap structures. By appropriate choice of crystal structure, the dimensions of the periodic lattice, and the properties of the component materials, propagation of electromagnetic waves in certain frequency bands (the photonic band gaps) may be forbidden within the crystal [69].

In [46], Knight and colleagues describe a fundamentally different type of optical fiber, one that has a core with a lower refractive index than the cladding and so rules out the possibility of internal reflection. Instead, light is guided by a mechanism which allows it to be piped through air.

The core of the new fiber is essentially a defect surrounded by a periodic array of air holes running along the entire length of the fiber. The defect acts like the core of an optical fiber. Light, which is expelled from the periodic structure surrounding the core, can only propagate along it. The new fiber operates truly by the photonic band gap effect. We refer to such a structure as a photonic crystal fiber (PCF).

In this chapter we model the propagation of electromagnetic waves in photonic crystal fibers. We give a mathematical framework for understanding their very unusual properties compared with the conventional fibers, attributed to an operation of the well-known mechanism of total reflection, and develop theoretical tools for the modeling of these photonic crystal fibers. We find conditions under which guided modes exist, and the nature of such modes. We study their dispersion properties and verify their exponential confinement. In particular, we show that there exists a discrete set of these modes parameterized by a wave-number parameter. We illustrate the main findings of the investigation in numerical examples.

4.2 Problem statement

We consider a 2-D photonic crystal, that is a medium characterized by a dielectric permittivity being periodic in two normal directions and invariant in the third normal direction. More precisely, the dielectric permittivity is given by a piecewise constant L^∞ and away from 0 function $\varepsilon_{\mathrm{p}}(x)$. This means that there exist ε_- and ε_+ positive constants such that:

$$0 < \varepsilon_- \leq \varepsilon_{\mathrm{p}}(x) \leq \varepsilon_+ < \infty \ , \ \text{a.e. } x \in \mathbb{R}^2 \ . \tag{4.2.1}$$

The bounds $\varepsilon-$ and ε_+ are supposed to be reached. The function ε_{p} is assumed to be independent of x_3 and unit-periodic in the $x_3 = 0$ plane:

$$\varepsilon_{\mathrm{p}}(x_1+1, x_2) = \varepsilon_{\mathrm{p}}(x_1, x_2), \quad \varepsilon_{\mathrm{p}}(x_1, x_2+1) = \varepsilon_{\mathrm{p}}(x_1, x_2) \ . \tag{4.2.2}$$

To this perfect 2-D photonic crystal, we introduce a line defect which is represented by a perturbation to the dielectric function $(\delta\varepsilon)(x_1, x_2)$. The perturbation is confined to the domain Ω:

$$(\delta\varepsilon)(x_1, x_2) = 0, \quad x \in \Omega^c \ .$$

Then the medium with defect has the dielectric function

$$\varepsilon_{\mathrm{p}}(x_1, x_2) = \varepsilon(x_1, x_2) + (\delta\varepsilon)(x_1, x_2) \ . \tag{4.2.3}$$

Our goal is to find the guided modes in this structure, *i.e.*, frequencies for which there exist solutions to the time-harmonic Maxwell equations that are propagating along the defect and the energy of which is confined to the defect area.

4.3 Maxwell equations

The electromagnetic fields (E, H) satisfy the following time-harmonic Maxwell equations:

$$\left\{ \begin{array}{lcl} \nabla \times H & = & -i\omega\varepsilon(x)E \ , \\ \nabla \times E & = & i\omega H \ . \end{array} \right. \tag{4.3.4}$$

However, this system can be studied from two scalar equations. Actually, the geometry of the medium and its dielectric function are independent of the third space coordinate x_3. Since we are looking for guided waves along the third direction, we take E and H with fixed exponential variation in the coordinate x_3 of the form $e^{i\beta x_3}$. This means that the electromagnetic field have the expression

$(Ee^{i\beta x_3}, He^{i\beta x_3})$, where E and H only depend on (x_1, x_2). As we can see under such assumption, the curl operator reduces to

$$\nabla \times (He^{i\beta x_3}) = e^{i\beta x_3} \begin{pmatrix} \dfrac{\partial H_3}{\partial x_2} - i\beta H_2 \\ i\beta H_1 - \dfrac{\partial H_3}{\partial x_1} \\ \dfrac{\partial H_2}{\partial x_1} - \dfrac{\partial H_1}{\partial x_2} \end{pmatrix} . \tag{4.3.5}$$

Consequently, the harmonic Maxwell system is now decoupled in two independent subsystems. The solutions to the first one:

$$\left\{ \begin{array}{lcl} i\omega \left(\varepsilon(x) - \dfrac{\beta^2}{\omega^2} \right) E_1 + \dfrac{\partial H_3}{\partial x_2} & = & 0 \, , \\ i\omega \left(\varepsilon(x) - \dfrac{\beta^2}{\omega^2} \right) E_2 - \dfrac{\partial H_3}{\partial x_1} & = & 0 \, , \\ -i\omega H_3 + \dfrac{\partial E_2}{\partial x_1} - \dfrac{\partial E_1}{\partial x_2} & = & 0 \, , \end{array} \right. \tag{4.3.6}$$

are called transverse electric (TE) and have the property $E_3 \equiv 0$. The solutions to the second one:

$$\left\{ \begin{array}{lcl} i\omega\varepsilon(x) E_3 + \dfrac{\partial H_2}{\partial x_1} - \dfrac{\partial H_1}{\partial x_2} & = & 0 \, , \\ -i\omega \left(1 - \dfrac{\beta^2}{\omega^2 \varepsilon(x)} \right) H_1 + \dfrac{\partial E_3}{\partial x_2} & = & 0 \, , \\ -i\omega \left(1 - \dfrac{\beta^2}{\omega^2 \varepsilon(x)} \right) H_2 - \dfrac{\partial E_3}{\partial x_1} & = & 0 \, , \end{array} \right. \tag{4.3.7}$$

are called transverse magnetic (TM) and have the property $H_3 \equiv 0$. In both cases, solutions can be computed from a unique scalar function (resp. H_3 or E_3) which satisfies one of the following equations:

$$\left\{ \begin{array}{lcl} \nabla \cdot \dfrac{1}{\varepsilon(x) - \frac{\beta^2}{\omega^2}} \nabla H_3 + \omega^2 H_3 & = & 0 \, , \\ \nabla \cdot \dfrac{\varepsilon(x)}{\varepsilon(x) - \frac{\beta^2}{\omega^2}} \nabla E_3 + \omega^2 \varepsilon(x) E_3 & = & 0 \, . \end{array} \right. \tag{4.3.8}$$

The problem consists then in finding $(\omega^2, \beta^2, u) \in \mathbb{R}^+ \times \mathbb{R}^+ \times L^2(\mathbb{R}^2)$ such that $\beta^2 < \omega^2 \varepsilon_-$ and u is solution of

$$\nabla \cdot \frac{1}{\varepsilon(x) - \frac{\beta^2}{\omega^2}} \nabla u + \omega^2 u = 0 \, , \tag{4.3.9}$$

in the TE case and of

$$\nabla \cdot \frac{\varepsilon(x)}{\varepsilon(x) - \frac{\beta^2}{\omega^2}} \nabla u + \omega^2 \varepsilon(x) u = 0 \, , \tag{4.3.10}$$

in the TM case.

4.4 Periodic operators and Floquet theory

As we look into the equations (4.3.9) and (4.3.10), we notice that they are partial differential equations with almost periodic coefficients. More precisely, these are spectral problems of partial differential operators with coefficients that are compactly supported perturbations of periodic functions. Let us then consider the periodic operators.

For $\alpha^2 < \varepsilon_-$, we define the unbounded operators A^{p}_α and B^{p}_α as

$$\begin{array}{rcl} A^{\mathrm{p}}_\alpha : L^2(\mathbb{R}^2) & \to & L^2(\mathbb{R}^2) \\ u & \mapsto & A^{\mathrm{p}}_\alpha u = -\nabla \cdot \dfrac{1}{\varepsilon_{\mathrm{p}}(x) - \alpha^2} \nabla u \,, \end{array} \tag{4.4.11}$$

and

$$\begin{array}{rcl} B^{\mathrm{p}}_\alpha : L^2(\mathbb{R}^2) & \to & L^2(\mathbb{R}^2) \\ u & \mapsto & B^{\mathrm{p}}_\alpha u = -\dfrac{1}{\varepsilon_{\mathrm{p}}(x)} \nabla \cdot \dfrac{\varepsilon_{\mathrm{p}}(x)}{\varepsilon_{\mathrm{p}}(x) - \alpha^2} \nabla u \,. \end{array} \tag{4.4.12}$$

These are self-adjoint partial differential operators with periodic coefficients. The self-adjointness character of B^{p}_α is seen in the weighted Sobolev space $L^2(\mathbb{R}^2, \varepsilon_{\mathrm{p}}(x)dx)$.

Let us start by considering A^{p}_α. This is an acoustic operator. It is also the operator governing the propagation of TE-polarized electromagnetic waves in a 2-D medium with a virtual dielectric permittivity $\varepsilon_{\mathrm{p}} - \alpha^2$. Its spectrum has a band structure depending on the parameter α and it is well known that such operators can have band gaps, *i.e.*, intervals of values of ω that do not belong to the spectrum of A^{p}_α and so propagating waves at frequencies ω can not exist in the virtual 2-D photonic crystal with dielectric permittivity $\varepsilon_{\mathrm{p}} - \alpha^2$.

The case of B^{p}_α is slightly different. This is not an operator governing the propagation of TM-polarized in some dielectric medium since it is not a Helmholtz operator. However, it still has band-structure spectrum. Actually, since it is elliptic and self-adjoint, when applying the Floquet transform we find a collection of operators defined on the unit cell, depending continuously on the dual variable and with point spectrum in the positive half-real axis accumulating at infinity. Then it is clear that the spectrum of B^{p}_α has a band-structure. The other question that we can ask is: Can it have gaps?

The answer is yes. First, we notice that when $\alpha = 0$, B^{p}_0 is a Helmholtz operator. It is well known that for suitable periodic dielectric function ε_{p}, the Helmholtz operator

$$\begin{array}{rcl} B^{\mathrm{p}}_0 : L^2(\mathbb{R}^2) & \to & L^2(\mathbb{R}^2) \\ u & \mapsto & B^{\mathrm{p}}_0 u = -\dfrac{1}{\varepsilon_{\mathrm{p}}(x)} \Delta u \,, \end{array} \tag{4.4.13}$$

can exhibit band gaps. It remains to prove the continuous dependence of the spectrum of B^{p}_α on α to conclude that, at least for α close to 0, B^{p}_α has gaps in its spectrum. The continuity can be seen with the dependence on α of the point spectrum of the Floquet transformed operators.

In what follows, we suppose that ε_{p} is such that A^{p}_α or B^{p}_α (depending on which polarization is considered) has a gap for α^2 belonging to a non-empty open subset of $(0, \varepsilon_-)$.

4.5 The Green's kernel

Here we define the Green's kernel for the operators A_α^{p} and B_α^{p} when they have gaps.

4.5.1 The TE polarization

Let us suppose that for some $\alpha \in (0, \varepsilon_-)$, the operator A_α^{p} has gaps in its spectrum. We denote by Σ_α the spectrum of A_α^{p}. Let ω^2 be in $\mathbb{R}^+ \setminus \Sigma_\alpha$. We can then define the Green's kernel $G_\alpha(\omega^2; x, y)$ as the solution to

$$\nabla \cdot \frac{1}{\varepsilon_{\mathrm{p}}(x) - \alpha^2} \nabla G_\alpha(\omega^2; x, y) + \omega^2 G_\alpha(\omega^2; x, y) = \delta(x - y) \ . \tag{4.5.14}$$

One of the main properties of the Green's kernel is stated in the following lemma.

Lemma 4.5.1 *There exist positive constants C_1 and C_2 depending on α and ω_0^2 such that for any $\omega^2 \in]0, \omega_0^2[\setminus \Sigma_\alpha$:*

$$|G_\alpha(\omega^2; x, y)| \leq C_1 e^{C_2 \, dist(\omega^2, \Sigma_\alpha)|x-y|} \ , \quad |x - y| \to +\infty \ . \tag{4.5.15}$$

This explains why an incident wave with frequency lying in the gap is reflected by the photonic crystal and decays exponentially inside it. It also gives a justification to the exponential localization of modes created by adding a compactly supported defect in the crystal.

The exponential decay is obtained by using a Combes-Thomas [21] argument to get the appropriate estimates on the resolvent. It is known however that the radius of localization

$$\frac{1}{C_2 \mathrm{dist}(\omega^2, \Sigma_\alpha)}$$

is not optimal close to the spectrum. More precisely, let $]a, b[$ be a gap of A_α^{p}, *i.e.*,

$$]a, b[\cap \Sigma_\alpha = \emptyset \quad \text{and} \quad a, b \in \Sigma_\alpha \ ,$$

then it has been proved that we have a decay estimate of the form:

$$e^{-C\sqrt{|\omega^2 - a||\omega^2 - b|}|x-y|} \ .$$

This is obtained by a general operator-theoretic approach. The main idea consists in using the Paley-Wiener theorems for the Floquet transform and the exponential decay of functions for which the Floquet transform has analytic dependence on the dual variable in a neighborhood of the real axis.

Another property of the Green's function is its weak singularity when $x = y$.

Lemma 4.5.2 *Let D be a bounded domain in which ε_{p} is constant. Then the function*

$$G_\alpha(\omega^2; x, y) - \frac{\varepsilon_{\mathrm{p}} - \alpha^2}{2\pi} \log |x - y| \tag{4.5.16}$$

is continuous for x, y in D when $|x - y| \to 0$.

Proof. We recall that

$$\Delta\left(\frac{1}{2\pi}\log|x-y|\right)=\delta(x-y)\ . \tag{4.5.17}$$

Let us define K by

$$K(x,y)=G_\alpha(\omega^2;x,y)-\frac{\varepsilon_{\rm p}-\alpha^2}{2\pi}\log|x-y|\ .$$

We remark that K satisfies the following Helmholtz equation:

$$\Delta K(x,y)+\omega^2(\varepsilon_{\rm p}-\alpha^2)K(x,y)=-\omega^2\frac{(\varepsilon_{\rm p}-\alpha^2)^2}{2\pi}\log|x-y|\ . \tag{4.5.18}$$

Since $\log|x-y|$ is L^2_y-integrable, we deduce that K, considered as a function of y for a fixed x, is in $H^2(D)$ and is continuous when $|x-y|\to 0$. □

4.5.2 The TM polarization

Again, the case of the TM polarization is not exactly similar to the TE polarization. Since the operator $B^{\rm p}_\alpha$ is not a Helmholtz operator, the Green's kernel is different from the one of $B^{\rm p}_0$. We use the same notations as done in the previous section calling Σ_α the spectrum of $B^{\rm p}_\alpha$ and $G_\alpha(\omega^2;x,y)$ the solution to

$$\nabla\cdot\frac{\varepsilon_{\rm p}(x)}{\varepsilon_{\rm p}(x)-\alpha^2}\nabla G_\alpha(\omega^2;x,y)+\omega^2\varepsilon_{\rm p}(x)G_\alpha(\omega^2;x,y)=\delta(x-y)\ . \tag{4.5.19}$$

Nevertheless, the analogous results to the ones cited in the previous section hold. Actually, Lemma 4.5.1 relies on a Combes-Thomas argument [21] that can still be used. We have just to modify the duality in $L^2(\mathbb{R}^2)$ defining it as

$$\langle u,v\rangle=\int_{\mathbb{R}^2}u(x)\,\overline{v}(x)\,\varepsilon_{\rm p}(x)\,dx\ .$$

The analogous result to the one in Lemma 4.5.2 is that the function

$$G_\alpha(\omega^2;x,y)-\frac{\varepsilon_{\rm p}-\alpha^2}{2\pi\varepsilon_{\rm p}}\log|x-y| \tag{4.5.20}$$

is continuous for x,y in D when $|x-y|\to 0$.

4.6 An integral formulation of the photonic fiber problem

Now we introduce a compactly supported perturbation to the dielectric function of the medium which is transformed into $\varepsilon(x)$ defined in (4.2.3) and we look for guided modes $(\omega^2,\beta^2,u)\in\mathbb{R}^+\times\mathbb{R}^+\times L^2(\mathbb{R}^2)$ solutions of (4.3.9) or (4.3.10).

4.6.1 The TE polarization

We consider here the TE polarization. Suppose that we have a guided mode. This clearly means that u is an eigenfunction of $A_{\frac{\beta}{\omega}}$ for the eigenvalue ω^2 where A_α is the operator defined for $\alpha^2 < \varepsilon_-$ as

$$\begin{array}{rcl} A_\alpha : L^2(\mathbb{R}^2) & \to & L^2(\mathbb{R}^2) \\ u & \mapsto & A_\alpha u = -\nabla \cdot \dfrac{1}{\varepsilon(x) - \alpha^2} \nabla u \; . \end{array} \tag{4.6.21}$$

It is then interesting to look for the spectral properties of the operator A_α and for a practical characterization of its eigenvalues when they exist. The following proposition is a consequence of a classical result in spectral theory.

Proposition 4.6.1 *For any $\alpha \in]0, \varepsilon_-[$, the operators A^{p}_α and A_α have the same essential spectrum.*

This is a consequence of the Weyl's theorem since it can be proved that $A_\alpha - A^{\mathrm{p}}_\alpha$ is a relatively compact perturbation of A^{p}_α.

Then the spectrum of A_α lying in the gaps of A^{p}_α will consist in eigenvalues of finite multiplicity that can accumulate only at the edges of the gaps. Moreover, A_α has the same continuous spectrum as A^{p}_α. An interesting question is: what about the existence of eigenvalues of A_α in the continuous spectrum? There is no result for the moment answering whether such eigenvalues can appear or not. In the case that such eigenvalues exist, the behaviour of the corresponding eigenfunctions is not obvious. On one hand, they should be localized due to the local character of the perturbation and on the other hand, it has enough energy to propagate along the medium.

We suppose here that the guided mode we consider is such that $\omega^2 \notin \Sigma_{\frac{\beta}{\omega}}$.

Recalling that ε_{p} and ε are piecewise constant, we define the finite partition $(D_i)_{i\in I}$ of Ω as the disjoint subdomains of Ω in which ε_{p}, ε and thus $(\delta\varepsilon)$ are constant. We also define $\Pi = \cup_{i\in I} \partial D_i$. We suppose that the curves $\overline{D_i} \cap \overline{D_j}$ and $\overline{D_i} \cap \Omega^c$ are smooth.

The following proposition holds.

Proposition 4.6.2 *The guided modes $(\omega^2, \beta^2, u) \in \mathbb{R}^+ \times \mathbb{R}^+ \times L^2(\mathbb{R}^2)$ satisfying $\omega^2 \notin \Sigma_{\frac{\beta}{\omega}}$ are exactly the functions u satisfying*

$$\left[\frac{1}{\varepsilon - \frac{\beta^2}{\omega^2}} \partial_\nu u \right] = 0 \; ,$$

and are solutions of the following integral equation:

$$\begin{aligned} u(x) &= \omega^2 \int_\Omega \frac{(\delta\varepsilon)}{(\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2})} G_{\frac{\beta}{\omega}}(\omega^2; x, y) u(y)\, dy \\ &\quad + \int_\Pi G_{\frac{\beta}{\omega}}(\omega^2; x, y) \left[\frac{(\delta\varepsilon)}{(\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2})} \right] \frac{1}{(\varepsilon - \frac{\beta^2}{\omega^2})} \partial_\nu u(y)\, dl_y \; , \end{aligned} \tag{4.6.22}$$

where $\partial_\nu u$ is the normal derivative of u on Π and $[f]$ represents the jump of f across Π in the ν direction.

Proof. Suppose that u satisfies the conditions above. It is clear then that u satisfies (4.3.9) in Ω^c. Now let us consider u in a domain D_i. Since $\varepsilon_{\rm p}$, ε and $(\delta\varepsilon)$ are constant in D_i, we have:

$$\begin{aligned}\left(\frac{1}{\varepsilon(x)-\frac{\beta^2}{\omega^2}}\Delta_x+\omega^2\right)G_{\frac{\beta}{\omega}}(\omega^2;x,y) &= \frac{\varepsilon_{\rm p}(x)-\frac{\beta^2}{\omega^2}}{\varepsilon(x)-\frac{\beta^2}{\omega^2}}\delta(x-y) \\ &\quad -\omega^2\frac{(\delta\varepsilon)(x)}{\varepsilon(x)-\frac{\beta^2}{\omega^2}}G_{\frac{\beta}{\omega}}(\omega^2;x,y)\ ,\end{aligned} \tag{4.6.23}$$

for any $x\in\Omega\setminus\Pi$ and any $y\in\mathbb{R}^2$. It follows that for any $i\in I$ and any $x\in D_i$, we have:

$$\begin{aligned}\left(\nabla\cdot\frac{1}{\varepsilon(x)-\frac{\beta^2}{\omega^2}}\nabla+\omega^2\right)u(x) \ &= \ \omega^2\frac{(\delta\varepsilon)(x)}{\varepsilon(x)-\frac{\beta^2}{\omega^2}}u(x) \\ &\quad -\omega^4\frac{(\delta\varepsilon)(x)}{\varepsilon(x)-\frac{\beta^2}{\omega^2}}\int_\Omega\frac{(\delta\varepsilon)}{(\varepsilon_{\rm p}-\frac{\beta^2}{\omega^2})}G_{\frac{\beta}{\omega}}(\omega^2;x,y)u(y)\,dy \\ &\quad -\omega^2\frac{(\delta\varepsilon)(x)}{\varepsilon(x)-\frac{\beta^2}{\omega^2}}\int_\Pi G_{\frac{\beta}{\omega}}(\omega^2;x,y)\left[\frac{(\delta\varepsilon)}{(\varepsilon_{\rm p}-\frac{\beta^2}{\omega^2})}\right]\frac{1}{(\varepsilon-\frac{\beta^2}{\omega^2})}\partial_\nu u(y)\,dl_y \\ &\quad =0\ .\end{aligned}$$

Then u solves equation (4.3.9) in $\mathbb{R}^2\setminus\Pi$. Recalling the jump relation it satisfies, we conclude that u solves (4.3.9) in $\mathbb{R}^2$.

Conversely, let us suppose that u solves equation (4.3.9). Then u satisfies the jump relation

$$\left[\frac{1}{(\varepsilon-\frac{\beta^2}{\omega^2})}\partial_\nu u\right]=0$$

on Π.

Moreover, we have:

$$\begin{aligned}u(x) \ &= \ \int_{\mathbb{R}^2}\left(\nabla\cdot\frac{1}{\varepsilon_{\rm p}(y)-\frac{\beta^2}{\omega^2}}\nabla+\omega^2\right)G_{\frac{\beta}{\omega}}(\omega^2;x,y)u(y)\,dy \\ &= \ -\int_{\mathbb{R}^2}\frac{1}{\varepsilon_{\rm p}(y)-\frac{\beta^2}{\omega^2}}\nabla G_{\frac{\beta}{\omega}}(\omega^2;x,y)\cdot\nabla u(y)\,dy \\ &\quad +\omega^2\int_{\mathbb{R}^2}G_{\frac{\beta}{\omega}}(\omega^2;x,y)u(y)\,dy \\ &= \ \int_\Omega\frac{(\delta\varepsilon)(y)}{(\varepsilon_{\rm p}(y)-\frac{\beta^2}{\omega^2})(\varepsilon(y)-\frac{\beta^2}{\omega^2})}\nabla G_{\frac{\beta}{\omega}}(\omega^2;x,y)\cdot\nabla u(y)\,dy \\ &\quad +\int_{\mathbb{R}^2}G_{\frac{\beta}{\omega}}(\omega^2;x,y)\nabla\cdot\frac{1}{\varepsilon(y)-\frac{\beta^2}{\omega^2}}\nabla u(y)\,dy \\ &\quad +\omega^2\int_{\mathbb{R}^2}G_{\frac{\beta}{\omega}}(\omega^2;x,y)u(y)\,dy \\ &= \ \sum_{i\in I}\int_{D_i}\frac{(\delta\varepsilon)(y)}{(\varepsilon_{\rm p}(y)-\frac{\beta^2}{\omega^2})(\varepsilon(y)-\frac{\beta^2}{\omega^2})}\nabla G_{\frac{\beta}{\omega}}(\omega^2;x,y)\cdot\nabla u(y)\,dy\ .\end{aligned}$$

Denoting by $\varepsilon_{\mathrm{p}}^i$, ε^i and $(\delta\varepsilon)^i$ the values of ε_{p}, ε and $(\delta\varepsilon)$ in D_i, we get

$$\begin{aligned}
u(x) &= -\sum_{i\in I}\int_{D_i} \frac{(\delta\varepsilon)^i}{(\varepsilon_{\mathrm{p}}^i - \frac{\beta^2}{\omega^2})} G_{\frac{\beta}{\omega}}(\omega^2;x,y)\nabla\cdot\frac{1}{\varepsilon^i - \frac{\beta^2}{\omega^2}}\nabla u(y)\,dy \\
&\quad + \sum_{i\in I}\int_{\partial D_i} G_{\frac{\beta}{\omega}}(\omega^2;x,y)\frac{(\delta\varepsilon)^i}{(\varepsilon_{\mathrm{p}}^i - \frac{\beta^2}{\omega^2})(\varepsilon^i - \frac{\beta^2}{\omega^2})}\partial_\nu u(y)\,dl_y \\
&= \omega^2\int_\Omega \frac{(\delta\varepsilon)(y)}{(\varepsilon_{\mathrm{p}}(y) - \frac{\beta^2}{\omega^2})} G_{\frac{\beta}{\omega}}(\omega^2;x,y)u(y)\,dy \\
&\quad + \int_\Pi G_{\frac{\beta}{\omega}}(\omega^2;x,y)\left[\frac{(\delta\varepsilon)}{(\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2})}\right]\frac{1}{(\varepsilon(y) - \frac{\beta^2}{\omega^2})}\partial_\nu u(y)\,dl_y\ ,
\end{aligned}$$

which ends the proof. □

4.6.2 The TM polarization

Now we consider the TM polarization for which the results are mainly the same. Suppose that we have a guided mode. Then u is an eigenfunction of $B_{\frac{\beta}{\omega}}$ for the eigenvalue ω^2 where B_α is the operator defined for $\alpha^2 < \varepsilon_-$ as

$$\begin{aligned}
B_\alpha : L^2(\mathbb{R}^2) &\to L^2(\mathbb{R}^2) \\
u &\mapsto B_\alpha u = -\frac{1}{\varepsilon}\nabla\cdot\frac{\varepsilon}{\varepsilon(x)-\alpha^2}\nabla u\ .
\end{aligned} \tag{4.6.24}$$

The counterpart of Proposition 4.6.1 is the following.

Proposition 4.6.3 *For any $\alpha \in]0,\varepsilon_-[$, the operators B_α^{p} and B_α have the same essential spectrum.*

We consider only guided modes for which $\omega^2 \notin \Sigma_{\frac{\beta}{\omega}}$. The following proposition holds.

Proposition 4.6.4 *The guided modes $(\omega^2,\beta^2,u) \in \mathbb{R}^+\times\mathbb{R}^+\times L^2(\mathbb{R}^2)$ satisfying $\omega^2 \notin \Sigma_{\frac{\beta}{\omega}}$ are exactly the functions u satisfying*

$$\left[\frac{\varepsilon}{\varepsilon - \frac{\beta^2}{\omega^2}}\partial_\nu u\right] = 0\ ,$$

and are solutions of the following integral equation:

$$\begin{aligned}
u(x) &= \omega^2\int_\Omega \frac{\varepsilon_{\mathrm{p}}(\delta\varepsilon)}{(\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2})} G_{\frac{\beta}{\omega}}(\omega^2;x,y)u(y)\,dy \\
&\quad + \frac{\beta^2}{\omega^2}\int_\Pi G_{\frac{\beta}{\omega}}(\omega^2;x,y)\left[\frac{(\delta\varepsilon)}{\varepsilon(\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2})}\right]\frac{\varepsilon}{(\varepsilon - \frac{\beta^2}{\omega^2})}\partial_\nu u(y)\,dl_y\ ,
\end{aligned} \tag{4.6.25}$$

where $\partial_\nu u$ is the normal derivative of u on Π and $[f]$ represents the jump of f across Π in the ν direction.

Proof. Suppose that u satisfies the conditions above. Then it is clear that u satisfies (4.3.10) in Ω^c. Now let us consider u in a domain D_i. Since ε_{p}, ε, and $(\delta\varepsilon)$ are constant in D_i, we have for any $x \in D_i$ and any $y \in \mathbb{R}^2$:

$$\begin{aligned}\left(\frac{\varepsilon(x)}{\varepsilon(x)-\frac{\beta^2}{\omega^2}}\Delta_x+\omega^2\varepsilon(x)\right)G_{\frac{\beta}{\omega}}(\omega^2;x,y) &= \frac{(\varepsilon_{\mathrm{p}}(x)-\frac{\beta^2}{\omega^2})\varepsilon(x)}{(\varepsilon(x)-\frac{\beta^2}{\omega^2})\varepsilon_{\mathrm{p}}(x)}\delta(x-y) \\ &\quad -\omega^2\frac{\varepsilon(x)(\delta\varepsilon)(x)}{(\varepsilon(x)-\frac{\beta^2}{\omega^2})}G_{\frac{\beta}{\omega}}(\omega^2;x,y)\ ,\end{aligned} \tag{4.6.26}$$

from which we deduce in a similar way as done in the TE case that u satisfies equation (4.3.10) in $\Omega\setminus\Pi$. Recalling the jump relation it satisfies, we deduce that u satisfies (4.3.10) in $\mathbb{R}^2$.

Conversely, suppose that u solves equation (4.3.10). Then u satisfies the jump relation

$$\left[\frac{\varepsilon}{(\varepsilon-\frac{\beta}{\omega})}\partial_\nu u\right]=0$$

on Π.

Moreover, we have:

$$\begin{aligned}
u(x) &= \int_{\mathbb{R}^2}\left(\nabla\cdot\frac{\varepsilon_{\mathrm{p}}(y)}{\varepsilon_{\mathrm{p}}(y)-\frac{\beta^2}{\omega^2}}\nabla+\omega^2\varepsilon_{\mathrm{p}}(y)\right)G_{\frac{\beta}{\omega}}(\omega^2;x,y)u(y)\,dy \\
&= -\int_{\mathbb{R}^2}\frac{\varepsilon_{\mathrm{p}}(y)}{\varepsilon_{\mathrm{p}}(y)-\frac{\beta^2}{\omega^2}}\nabla G_{\frac{\beta}{\omega}}(\omega^2;x,y)\cdot\nabla u(y)\,dy \\
&\quad +\omega^2\int_{\mathbb{R}^2}G_{\frac{\beta}{\omega}}(\omega^2;x,y)u(y)\varepsilon_{\mathrm{p}}(y)\,dy \\
&= \frac{\beta^2}{\omega^2}\int_{\Omega}\frac{(\delta\varepsilon)(y)}{(\varepsilon_{\mathrm{p}}(y)-\frac{\beta^2}{\omega^2})(\varepsilon(y)-\frac{\beta^2}{\omega^2})}\nabla G_{\frac{\beta}{\omega}}(\omega^2;x,y)\cdot\nabla u(y)\,dy \\
&\quad +\omega^2\int_{\Omega}G_{\frac{\beta}{\omega}}(\omega^2;x,y)u(y)(\delta\varepsilon)(y)\,dy \\
&\quad +\int_{\mathbb{R}^2}G_{\frac{\beta}{\omega}}(\omega^2;x,y)\nabla\cdot\frac{\varepsilon_{\mathrm{p}}(y)}{\varepsilon(y)-\frac{\beta^2}{\omega^2}}\nabla u(y)\,dy \\
&\quad +\omega^2\int_{\mathbb{R}^2}G_{\frac{\beta}{\omega}}(\omega^2;x,y)u(y)\varepsilon_{\mathrm{p}}(y)\,dy \\
&= -\frac{\beta^2}{\omega^2}\sum_{i\in I}\int_{D_i}\frac{(\delta\varepsilon)^i}{\varepsilon^i(\varepsilon^i_{\mathrm{p}}-\frac{\beta^2}{\omega^2})}G_{\frac{\beta}{\omega}}(\omega^2;x,y)\nabla\cdot\frac{\varepsilon^i}{(\varepsilon^i-\frac{\beta^2}{\omega^2})}\nabla u(y)\,dy \\
&\quad +\frac{\beta^2}{\omega^2}\sum_{i\in I}\int_{\partial D_i}\frac{(\delta\varepsilon)^i}{(\varepsilon^i_{\mathrm{p}}-\frac{\beta^2}{\omega^2})(\varepsilon^i-\frac{\beta^2}{\omega^2})}G_{\frac{\beta}{\omega}}(\omega^2;x,y)\partial_\nu u(y)\,dy \\
&\quad +\omega^2\int_{\Omega}G_{\frac{\beta}{\omega}}(\omega^2;x,y)u(y)(\delta\varepsilon)(y)\,dy\ ,
\end{aligned}$$

and therefore

$$\begin{aligned} u(x) &= \beta^2 \sum_{i\in I} \int_{D_i} \frac{(\delta\varepsilon)^i}{(\varepsilon_{\mathrm{p}}^i - \frac{\beta^2}{\omega^2})} G_{\frac{\beta}{\omega}}(\omega^2; x, y) u(y)\, dy \\ &+ \frac{\beta^2}{\omega^2} \sum_{i\in I} \int_{\partial D_i} \frac{(\delta\varepsilon)^i}{(\varepsilon_{\mathrm{p}}^i - \frac{\beta^2}{\omega^2})(\varepsilon^i - \frac{\beta^2}{\omega^2})} G_{\frac{\beta}{\omega}}(\omega^2; x, y) \partial_\nu u(y)\, dy \\ &+ \omega^2 \int_\Omega G_{\frac{\beta}{\omega}}(\omega^2; x, y) u(y) (\delta\varepsilon)(y)\, dy \\ &= \omega^2 \int_\Omega \frac{\varepsilon_{\mathrm{p}}(y)}{(\varepsilon_{\mathrm{p}}(y) - \frac{\beta^2}{\omega^2})} G_{\frac{\beta}{\omega}}(\omega^2; x, y) u(y) (\delta\varepsilon)(y)\, dy \\ &+ \frac{\beta^2}{\omega^2} \int_\Pi G_{\frac{\beta}{\omega}}(\omega^2; x, y) \left[\frac{(\delta\varepsilon)}{(\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2})\varepsilon} \right] \frac{\varepsilon(y)}{(\varepsilon(y) - \frac{\beta^2}{\omega^2})} \partial_\nu u(y)\, dy \,. \end{aligned}$$

The proposition is then proved. □

4.7 Preliminary results

We introduce in this section new integral operators that will be useful for finding guided modes. We start by orienting the curves $\overline{D_i} \cap \overline{D_j}$ and $\overline{D_i} \cap \Omega^c$ and define a normal vector ν on each one.

Definition 4.7.1 *We define the operator $\mathcal{A}_{\omega,\beta}$ for $\omega^2 \notin \Sigma_{\frac{\beta}{\omega}}$ by*

$$\begin{aligned} \mathcal{A}_{\omega,\beta} : L^2(\Omega) \times L^2(\Pi) &\to L^2(\Omega) \times L^2(\Pi) \\ (u, \varphi) &\mapsto \mathcal{A}_{\omega,\beta}(u, \varphi) = (v, \psi) \,, \end{aligned}$$

such that

$$\begin{aligned} v(x) &= \omega^2 \int_\Omega \frac{(\delta\varepsilon)}{(\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2})} G_{\frac{\beta}{\omega}}(\omega^2; x, y) u(y)\, dy \\ &+ \int_\Pi G_{\frac{\beta}{\omega}}(\omega^2; x, y) \left[\frac{(\delta\varepsilon)}{(\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2})} \right] \varphi(y)\, dl_y \,, \quad x \in \Omega \,, \end{aligned} \tag{4.7.27}$$

and

$$\psi(x) = \frac{1}{\varepsilon(x)^\mu - \frac{\beta^2}{\omega^2}} \partial_\nu^\mu v(x) \,, \quad x \in \Pi \,, \tag{4.7.28}$$

for some $\mu \in \{+, -\}$, where for $x \in \Pi$ and f defined on a neighborhood of Π, $f^\pm(x) = \lim_{\tau \to 0^\pm} f(x + \tau\nu_x)$.

In fact, the parameter μ has just to take a fixed value $+$ or $-$ on each component $\overline{D_i} \cap \overline{D_j}$ and $\overline{D_i} \cap \Omega^c$, i, j in I. The following proposition holds.

Proposition 4.7.1 *The operator $\mathcal{A}_{\omega,\beta}$ is compact.*

Proof. Let $(v, \psi) = \mathcal{A}_{\omega,\beta}(u, \varphi)$. It is obvious that in each subdomain D_i, v solves a Helmholtz equation with an L^2 right hand side. It follows that $v \in$

$\prod_{i\in I} H^2(D_i)$ and $\psi \in \prod_{i,j\in I} H^{1/2}(\overline{D_i}\cap\overline{D_j})\times\prod_{i\in I} H^{1/2}(\overline{D_i}\cap\Omega^c)$. The compactness of $\mathcal{A}_{\omega,\beta}$ is then a consequence of the compact embedding of $\prod_{i\in I} H^2(D_i)$ in $L^2(\Omega)$ and of $\prod_{i,j\in I} H^{1/2}(\overline{D_i}\cap\overline{D_j})\times\prod_{i\in I} H^{1/2}(\overline{D_i}\cap\Omega^c)$ in $L^2(\Pi)$. □

Now we define the analogous operator that will be useful in the TM polarization.

Definition 4.7.2 *We define the operator $\mathcal{B}_{\omega,\beta}$ for $\omega^2 \notin \Sigma_{\frac{\beta}{\omega}}$ by*

$$\begin{array}{rcl}\mathcal{B}_{\omega,\beta} : L^2(\Omega)\times L^2(\Pi) & \to & L^2(\Omega)\times L^2(\Pi) \\ (u,\varphi) & \mapsto & \mathcal{B}_{\omega,\beta}(u,\varphi) = (v,\psi)\ ,\end{array}$$

such that

$$\begin{aligned} v(x) \ &= \ \omega^2 \int_\Omega \frac{\varepsilon_{\mathrm{p}}(\delta\varepsilon)}{(\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2})} G_{\frac{\beta}{\omega}}(\omega^2;x,y)u(y)\,dy \\ &+\frac{\beta^2}{\omega^2}\int_\Pi G_{\frac{\beta}{\omega}}(\omega^2;x,y)\left[\frac{(\delta\varepsilon)}{\varepsilon(\varepsilon_{\mathrm{p}}-\frac{\beta^2}{\omega^2})}\right]\varphi(y)\,dl_y\ , \quad x\in\Omega\ , \end{aligned} \tag{4.7.29}$$

and

$$\psi(x) = \frac{\varepsilon(x)^\mu}{\varepsilon(x)^\mu - \frac{\beta^2}{\omega^2}}\partial^\mu_\nu v(x)\ , \quad x\in\Pi\ , \tag{4.7.30}$$

for some $\mu \in \{+,-\}$.

The following proposition holds.

Proposition 4.7.2 *The operator $\mathcal{B}_{\omega,\beta}$ is compact.*

The proof is exactly the same as for $\mathcal{A}_{\omega,\beta}$.

4.8 Guided modes in the photonic fiber

Now we are going to give the main result of this chapter. Actually, we characterize the guided modes in the photonic fiber as a spectral problem on a compact operator.

Theorem 4.8.1 *The guided modes (ω^2,β^2,u) in the TE-polarization satisfying $\omega^2 \notin \Sigma_{\frac{\beta^2}{\omega^2}}$ are exactly the solutions to the following spectral problem:*

$$\mathcal{A}_{\omega,\beta}(u,\varphi) = (u,\varphi) \tag{4.8.31}$$

for some $\varphi \in L^2(\mathbb{R}^2)$.

Proof. Suppose that (ω^2,β^2,u) is a guided mode and that $\omega^2 \notin \Sigma_{\frac{\beta^2}{\omega^2}}$. Then from Proposition 4.6.2, we have

$$\mathcal{A}_{\omega,\beta}(u, \frac{1}{\varepsilon(x)^\mu - \frac{\beta^2}{\omega^2}}\partial^\mu_\nu u) = (u, \frac{1}{\varepsilon(x)^\mu - \frac{\beta^2}{\omega^2}}\partial^\mu_\nu u)\ . \tag{4.8.32}$$

Conversely, suppose that (u, φ) is an eigenfunction of $\mathcal{A}_{\omega,\beta}$ for the eigenvalue 1. Then, recalling Proposition 4.6.2, we need only to prove that

$$\left[\frac{1}{\varepsilon - \frac{\beta^2}{\omega^2}} \partial_\nu u\right] = 0 \,.$$

to establish that (ω^2, β^2, u) is a guided mode.

From the equation satisfied by $G_{\frac{\beta}{\omega}}(\omega^2; x, y)$ we deduce that for any $x \in \Pi$ and any $y \in \Omega \setminus \Pi$ we have

$$\left[\frac{1}{\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2}} \partial_\nu G_{\frac{\beta}{\omega}}(\omega^2; x, y)\right] = 0 \,. \tag{4.8.33}$$

It follows that

$$\left[\frac{1}{\varepsilon - \frac{\beta^2}{\omega^2}} \partial_\nu G_{\frac{\beta}{\omega}}(\omega^2; x, y)\right] = \left[\frac{\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2}}{\varepsilon - \frac{\beta^2}{\omega^2}}\right] \frac{1}{\varepsilon_{\mathrm{p}}^\mu - \frac{\beta^2}{\omega^2}} \partial_\nu^\mu G_{\frac{\beta}{\omega}}(\omega^2; x, y) \,. \tag{4.8.34}$$

Let us consider

$$\frac{1}{\varepsilon^\mu - \frac{\beta^2}{\omega^2}} \partial_\nu^\mu \int_\Pi G_{\frac{\beta}{\omega}}(\omega^2; x, y) \left[\frac{(\delta\varepsilon)}{(\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2})}\right] \varphi(y)\, dl_y \,.$$

From Lemma 4.5.2 we deduce that

$$\begin{aligned}
&\frac{1}{\varepsilon^\mu - \frac{\beta^2}{\omega^2}} \partial_\nu^\mu \int_\Pi G_{\frac{\beta}{\omega}}(\omega^2; x, y) \left[\frac{(\delta\varepsilon)}{(\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2})}\right] \varphi(y)\, dl_y \\
&= \int_\Pi \frac{1}{\varepsilon^\mu - \frac{\beta^2}{\omega^2}} \partial_\nu^\mu \left(G_{\frac{\beta}{\omega}}(\omega^2; x, y) - \frac{\varepsilon_{\mathrm{p}}^\mu - \frac{\beta^2}{\omega^2}}{2\pi} \log|x-y| \right) \left[\frac{(\delta\varepsilon)}{(\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2})}\right] \varphi(y)\, dl_y \\
&\quad + \frac{1}{\varepsilon^\mu - \frac{\beta^2}{\omega^2}} \partial_\nu^\mu \int_\Pi \frac{\varepsilon_{\mathrm{p}}^\mu - \frac{\beta^2}{\omega^2}}{2\pi} \log|x-y| \left[\frac{(\delta\varepsilon)}{(\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2})}\right] \varphi(y)\, dl_y \,.
\end{aligned}$$

The following identity is a classical result in the potential theory:

$$\partial_\nu^\mu \int_\Pi \frac{1}{2\pi} \log|x-y| \varphi(y)\, dl_y = \mu \frac{1}{2} \varphi(x) + \int_\Pi \frac{1}{2\pi} \partial_\nu^\mu \log|x-y| \varphi(y) dl_y \,. \tag{4.8.35}$$

Therefore

$$\begin{aligned}
&\frac{1}{\varepsilon^\mu - \frac{\beta^2}{\omega^2}} \partial_\nu^\mu \int_\Pi G_{\frac{\beta}{\omega}}(\omega^2; x, y) \left[\frac{(\delta\varepsilon)}{(\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2})}\right] \varphi(y)\, dl_y \\
&\qquad = \int_\Pi \frac{1}{\varepsilon^\mu - \frac{\beta^2}{\omega^2}} \partial_\nu^\mu G_{\frac{\beta}{\omega}}(\omega^2; x, y) \left[\frac{(\delta\varepsilon)}{(\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2})}\right] \varphi(y)\, dl_y \\
&\qquad\quad + \mu \frac{1}{2} \frac{\varepsilon_{\mathrm{p}}^\mu - \frac{\beta^2}{\omega^2}}{\varepsilon^\mu - \frac{\beta^2}{\omega^2}} \left[\frac{(\delta\varepsilon)}{\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2}}\right] \varphi(x) \,.
\end{aligned}$$

We then deduce the expression of the jump we are looking for:

$$\begin{aligned}
\left[\frac{1}{\varepsilon - \frac{\beta^2}{\omega^2}} \partial_\nu u\right] &= \left[\frac{\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2}}{\varepsilon - \frac{\beta^2}{\omega^2}}\right] \frac{1}{\varepsilon_{\mathrm{p}}^\mu - \frac{\beta^2}{\omega^2}} \partial_\nu^\mu u \\
&\quad + \left(\left[\mu \frac{1}{2} \frac{\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2}}{\varepsilon - \frac{\beta^2}{\omega^2}}\right] - \mu \frac{1}{2} \left[\frac{\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2}}{\varepsilon - \frac{\beta^2}{\omega^2}}\right] \right) \left[\frac{(\delta\varepsilon)}{\varepsilon_{\mathrm{p}} - \frac{\beta^2}{\omega^2}}\right] \varphi \,.
\end{aligned}$$

After making the necessary simplifications, we get

$$\left[\frac{1}{\varepsilon - \frac{\beta^2}{\omega^2}}\partial_\nu u\right] = \left[\frac{\varepsilon_{\rm p} - \frac{\beta^2}{\omega^2}}{\varepsilon - \frac{\beta^2}{\omega^2}}\right]\frac{\varepsilon^\mu - \frac{\beta^2}{\omega^2}}{\varepsilon_{\rm p}^\mu - \frac{\beta^2}{\omega^2}}\left(\frac{1}{\varepsilon^\mu - \frac{\beta^2}{\omega^2}}\partial_\nu^\mu u - \varphi\right) . \tag{4.8.36}$$

The second identity in $\mathcal{A}_{\omega,\beta}(u,\varphi) = (u,\varphi)$ gives the desired result. $\square$

Here is the analogous result concerning the TM polarization.

Theorem 4.8.2 *The guided modes (ω^2, β^2, u) in the TM-polarization satisfying $\omega^2 \notin \Sigma_{\frac{\beta^2}{\omega^2}}$ are exactly the solutions to the following spectral problem.*

$$\mathcal{B}_{\omega,\beta}(u,\varphi) = (u,\varphi) \ , \tag{4.8.37}$$

for some $\varphi \in L^2(\mathbb{R}^2)$.

Proof. If (ω^2, β^2, u) is a guided mode and $\omega^2 \notin \Sigma_{\frac{\beta^2}{\omega^2}}$, then from Proposition 4.6.4, we have clearly

$$\mathcal{B}_{\omega,\beta}(u, \frac{1}{\varepsilon(x)^\mu - \frac{\beta^2}{\omega^2}}\partial_\nu^\mu u) = (u, \frac{1}{\varepsilon(x)^\mu - \frac{\beta^2}{\omega^2}}\partial_\nu^\mu u) \ . \tag{4.8.38}$$

Conversely, suppose that (u,φ) is an eigenfunction of $\mathcal{B}_{\omega,\beta}$ for the eigenvalue 1. Recalling Proposition 4.6.4, we just have to prove that

$$\left[\frac{\varepsilon}{\varepsilon - \frac{\beta^2}{\omega^2}}\partial_\nu u\right] = 0 \ .$$

From the equation satisfied by $G_{\frac{\beta}{\omega}}(\omega^2; x, y)$ we deduce that for any $x \in \Pi$ and any $y \in \Omega \setminus \Pi$ we have

$$\left[\frac{\varepsilon_{\rm p}}{\varepsilon_{\rm p} - \frac{\beta^2}{\omega^2}}\partial_\nu G_{\frac{\beta}{\omega}}(\omega^2; x, y)\right] = 0 \ . \tag{4.8.39}$$

As a consequence, we have

$$\left[\frac{\varepsilon}{\varepsilon - \frac{\beta^2}{\omega^2}}\partial_\nu G_{\frac{\beta}{\omega}}(\omega^2; x, y)\right] = \left[\frac{\varepsilon(\varepsilon_{\rm p} - \frac{\beta^2}{\omega^2})}{\varepsilon_{\rm p}(\varepsilon - \frac{\beta^2}{\omega^2})}\right]\frac{\varepsilon_{\rm p}}{\varepsilon_{\rm p}^\mu - \frac{\beta^2}{\omega^2}}\partial_\nu^\mu G_{\frac{\beta}{\omega}}(\omega^2; x, y) \ . \tag{4.8.40}$$

Using again the classical potential theory result mentioned in the previous proof, we get

$$\begin{aligned}
&\frac{\varepsilon^\mu}{\varepsilon^\mu - \frac{\beta^2}{\omega^2}}\partial_\nu^\mu \int_\Pi G_{\frac{\beta}{\omega}}(\omega^2; x, y)\left[\frac{(\delta\varepsilon)}{\varepsilon(\varepsilon_{\rm p} - \frac{\beta^2}{\omega^2})}\right]\varphi(y)\, dl_y \\
&\qquad = \int_\Pi \frac{\varepsilon^\mu}{\varepsilon^\mu - \frac{\beta^2}{\omega^2}}\partial_\nu^\mu G_{\frac{\beta}{\omega}}(\omega^2; x, y)\left[\frac{(\delta\varepsilon)}{\varepsilon(\varepsilon_{\rm p} - \frac{\beta^2}{\omega^2})}\right]\varphi(y)\, dl_y \\
&\qquad\quad + \mu\frac{1}{2}\frac{\varepsilon^\mu(\varepsilon_{\rm p}^\mu - \frac{\beta^2}{\omega^2})}{\varepsilon_{\rm p}^\mu(\varepsilon^\mu - \frac{\beta^2}{\omega^2})}\left[\frac{(\delta\varepsilon)}{\varepsilon(\varepsilon_{\rm p} - \frac{\beta^2}{\omega^2})}\right]\varphi(x) \ .
\end{aligned}$$

We deduce the expression of the jump we are looking for:

$$\begin{aligned}\left[\frac{\varepsilon}{\varepsilon-\frac{\beta^2}{\omega^2}}\partial_\nu u\right] &= \left[\frac{\varepsilon(\varepsilon_{\mathrm{p}}-\frac{\beta^2}{\omega^2})}{\varepsilon_{\mathrm{p}}(\varepsilon-\frac{\beta^2}{\omega^2})}\right]\frac{\varepsilon_{\mathrm{p}}^\mu}{\varepsilon_{\mathrm{p}}^\mu-\frac{\beta^2}{\omega^2}}\partial_\nu^\mu u\\ &+\left(\left[\mu\frac{1}{2}\frac{\varepsilon(\varepsilon_{\mathrm{p}}-\frac{\beta^2}{\omega^2})}{\varepsilon_{\mathrm{p}}(\varepsilon-\frac{\beta^2}{\omega^2})}\right]-\mu\frac{1}{2}\left[\frac{\varepsilon(\varepsilon_{\mathrm{p}}-\frac{\beta^2}{\omega^2})}{\varepsilon_{\mathrm{p}}(\varepsilon-\frac{\beta^2}{\omega^2})}\right]\right)\left[\frac{(\delta\varepsilon)}{\varepsilon_{\mathrm{p}}-\frac{\beta^2}{\omega^2}}\right]\varphi\,,\end{aligned}$$

and therefore we get

$$\left[\frac{\varepsilon}{\varepsilon-\frac{\beta^2}{\omega^2}}\partial_\nu u\right] = \left[\frac{\varepsilon(\varepsilon_{\mathrm{p}}-\frac{\beta^2}{\omega^2})}{\varepsilon_{\mathrm{p}}(\varepsilon-\frac{\beta^2}{\omega^2})}\right]\frac{\varepsilon_{\mathrm{p}}^\mu(\varepsilon^\mu-\frac{\beta^2}{\omega^2})}{\varepsilon^\mu(\varepsilon_{\mathrm{p}}^\mu-\frac{\beta^2}{\omega^2})}\left(\frac{\varepsilon^\mu}{\varepsilon^\mu-\frac{\beta^2}{\omega^2}}\partial_\nu^\mu u-\varphi\right). \tag{4.8.41}$$

The second identity in $\mathcal{B}_{\omega,\beta}(u,\varphi)=(u,\varphi)$ gives the desired result. □

In both cases, because of the exponential decay of the corresponding Green's function, it is clear that the guided modes are exponentially confined.

4.9 Gaps opening in Σ_α: TE polarization

In this section we are interested in the existence of gaps in the spectrum of the operator A_α^{p} and especially in the asymptotic behaviour under some limit conditions on α.

Our approach is inspired by the work of Hempel and Lienau in [41] where almost all the results of this section can be found with weaker conditions on the smoothness of what will be denoted the domain Ω. We give here all the proofs adapting them to our problem for the sake of clarity.

The structure of the 2D-photonic crystal considered here is simple, but the results could be generalized to many other structures.

4.9.1 Medium description

For $\mathbf{n}=(n_1,n_2)\in\mathbb{Z}^2$ we define $Q_{\mathbf{n}}=(n_1,n_1+1)\times(n_2,n_2+1)$. Let Ω_0 be a connected open domain with smooth boundary such that $\Omega_0\subset\subset Q_0$. We define

$$\begin{aligned}\Omega_{\mathbf{n}} &= \Omega_0+\mathbf{n}\,,\\ \Omega &= \cup_{\mathbf{n}\in\mathbb{Z}^2}\Omega_{\mathbf{n}}\,,\\ \Omega_{\mathbf{n}}^c &= Q_{\mathbf{n}}\setminus\overline{\Omega_{\mathbf{n}}}\,,\end{aligned}$$

and

$$\Omega^c=\mathbb{R}^2\setminus\overline{\Omega}\,.$$

Finally, ∂D denotes the boundary of the domain D.

We consider the photonic crystal which dielectric permittivity is given by $\varepsilon_{\mathrm{p}}(x)$ that satisfies

$$\varepsilon_{\mathrm{p}}(x)=\begin{cases}1 & x\in\Omega^c\,,\\ \epsilon+1 & x\in\Omega\,,\end{cases} \tag{4.9.42}$$

where ϵ is a positive constant.

This dielectric function represents a photonic fiber made of rods of dielectric $1+\epsilon>1$ with section Ω_0 placed periodically in air or more generally in a homogeneous dielectric medium with permittivity strictly lower than that of the rods (after scaling, we come back to the problem with $\varepsilon_{\mathrm{p}}(x)$).

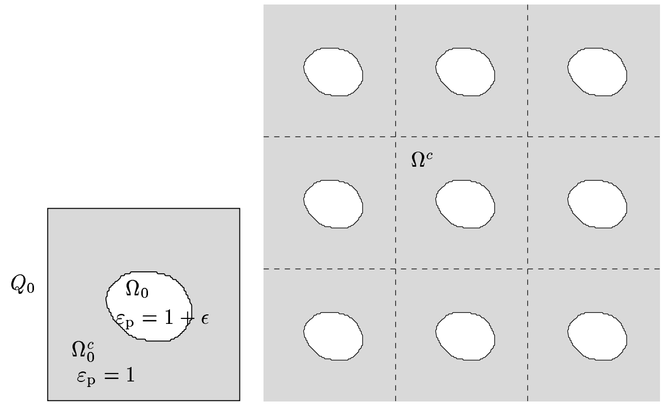


Figure 4.1: Section of the photonic fiber cladding.

4.9.2 The spectral problem

We are interested in the spectrum Σ_α of the operator A_α^{p} and more precisely in the existence of gaps in Σ_α. Our idea is the following: suppose that α^2 goes to 1, then the coefficient of A_α^{p} that takes the value $1-\alpha^2 \ll 1$ in Ω^c and $\epsilon + 1 - \alpha^2 \approx \epsilon > 0$ will have a very high contrast. It can then be expected to find gaps in the corresponding spectrum. Of course, this is very far from the final proof, since we do not even know where these gaps will appear. It can for example appear around values that diverge which will be useless since we look for gaps around finite values of ω^2.

Our original spectral problem is then

$$\nabla \cdot \frac{1}{\varepsilon_{\mathrm{p}}(x) - \alpha^2} \nabla u + \omega^2 u = 0 \; . \tag{4.9.43}$$

Since $\alpha^2 \to 1^-$, we introduce the small positive parameter $\eta = 1 - \alpha^2$. We also define the operator $\tilde{A}_\eta$ as

$$\tilde{A}_\eta = -\nabla \cdot (1 + \frac{\epsilon}{\eta}\chi_{\Omega^c})\nabla u \; , \tag{4.9.44}$$

and the new spectral parameter $\lambda = (\epsilon + \eta)\omega^2$. It can be easily seen that $\tilde{A}_\eta = (\epsilon + \eta) A_\alpha^{\mathrm{p}}$.

Our new spectral problem consists now in finding gaps in the spectrum $\tilde{\Sigma}_\eta$ of $\tilde{A}_\eta$ when η goes to 0^+.

4.9.3 Asymptotic behaviour of the spectrum

We introduce the quadratic form $\mathfrak{a}_\eta[u]$, also denoted $\mathfrak{a}_\eta[u,u]$, in the Hilbert space $L^2(\mathbb{R}^2)$ defined by

$$\mathfrak{a}_\eta[u] = \int_{\mathbb{R}^2} (1 + \frac{\epsilon}{\eta}\chi_{\Omega^c}) |\nabla u|^2 \, dx \; , \tag{4.9.45}$$

for $u \in D(\mathfrak{a}_\eta) = H^1(\mathbb{R}^2)$, the usual Sobolev space with the norm $\|u\|_1 = \|u\|_{L^2(\mathbb{R}^2)} + \|\nabla u\|_{L^2(\mathbb{R}^2)}$. It is obvious that this quadratic form is positive, densely defined and closed. It then defines a unique self-adjoint operator in $L^2(\mathbb{R}^2)$ that is $\tilde{A}_\eta$ since

$$(\tilde{A}_\eta u, v) = \mathfrak{a}_\eta[u,v] \ , \quad u \in D(\tilde{A}_\eta) \ , \quad v \in D(\mathfrak{a}_\eta) \ . \tag{4.9.46}$$

The operator $\tilde{A}_\eta$ is then uniquely determined by its quadratic form. This allows us to study the limit of the quadratic form $\mathfrak{a}_\eta$ in order to determine the limiting spectrum of $\tilde{A}_\eta$.

It is clear that the quadratic form $\mathfrak{a}_\eta$, whose domain is independent of η, increases monotonically when $\eta \to 0^+$. The monotone convergence theorem for an increasing sequence of quadratic forms [62] yields a closed quadratic form $\mathfrak{a}_0$ defined by

$$D(\mathfrak{a}_0) = \{u \in H^1(\mathbb{R}^2) \ ; \sup_{\eta>0} \mathfrak{a}_\eta[u] < \infty\} \ , \tag{4.9.47}$$

and

$$\mathfrak{a}_0[u] = \lim_{\eta\to 0^+} \mathfrak{a}_\eta[u] = \sup_{\eta>0} \mathfrak{a}_\eta[u] \ , \quad u \in D(\mathfrak{a}_0) \ . \tag{4.9.48}$$

Furthermore, this quadratic form defines a unique self-adjoint operator $\tilde{A}_0$ which satisfies

$$\tilde{A}_\eta \to \tilde{A}_0 \quad \text{in the strong resolvent sense,} \quad \eta \to 0^+ \ . \tag{4.9.49}$$

This operator acts in a (possibly smaller) Hilbert space given by the closure of $D(\mathfrak{a}_0)$ in $L^2(\mathbb{R}^2)$, and we think of the resolvent of $\tilde{A}_0$ as the zero operator on the orthogonal complement of $D(\mathfrak{a}_0)$ in $L^2(\mathbb{R}^2)$.

We recall that $\tilde{A}_\eta$ converges to $\tilde{A}_0$ in the strong resolvent sense if and only if:

$$(\tilde{A}_\eta + I)^{-1} f \to (\tilde{A}_0 + I)^{-1} f \ , \quad \forall f \in L^2(\mathbb{R}^2) \ . \tag{4.9.50}$$

Now let us prove that $\tilde{A}_0$ is the Dirichlet Laplacian on Ω.

Lemma 4.9.1 *Suppose $u \in H^1(\mathbb{R}^2)$ is such that $\mathfrak{a}_\eta[u] < C$ for all $\eta > 0$ and some positive constant C. Then $u = 0$ a.e. in Ω^c.*

Proof. Suppose that $u \in H^1(\mathbb{R}^2)$ is such that for any $\eta > 0$ and for some positive constant C we have $\mathfrak{a}_\eta[u] < C$. It follows that

$$\frac{\epsilon}{\eta} \int_{\Omega^c} |\nabla u|^2 \, dx < C \ , \quad \forall \eta > 0 \ . \tag{4.9.51}$$

This implies that $\nabla u = 0$ a.e. in Ω^c which is connected and so u is constant in Ω^c. Since $u \in L^2(\mathbb{R}^2)$, it follows that $u = 0$ a.e. in Ω^c. □

As a consequence, we have the following corollary.

Corollary 4.9.1 *The domain of $\mathfrak{a}_0$ is the space*

$$\tilde{H}^1_0(\Omega) = \{u \in H^1(\mathbb{R}^2) \ ; \ u(x) = 0 \ a.e. \ in \ \Omega^c\} \ , \tag{4.9.52}$$

which coincides with the classical space $H^1_0(\Omega)$ defined as the closure of $C^\infty_c(\Omega)$ in the $\|\cdot\|_1$-norm provided Ω is regular, which we suppose (note that an exterior cone condition is sufficient).

This determines the self-adjoint operator $\tilde{A}_0$.

Corollary 4.9.2 *The limiting operator $\tilde{A}_0$ is the Dirichlet Laplacian in the domain Ω denoted $-\Delta_\Omega$ with the domain given by the closure of $H^2(\Omega)$ in $H_0^1(\Omega)$.*

The following proposition holds.

Proposition 4.9.1 *The operator $\tilde{A}_\eta$ converges to $-\Delta_\Omega = \bigoplus_{\mathbf{n}\in\mathbb{Z}^2} (-\Delta_{\Omega_\mathbf{n}})$ in the strong resolvent sense.*

It is clear that the operator $-\Delta_{\Omega_0}$ has compact resolvent and then its spectrum consists in a sequence of discrete eigenvalues of finite multiplicity. We denote these (repeated) eigenvalues, ordered by min – max, as δ_k, $k \in \mathbb{N}^*$, or

$$0 < \delta_1 \leq \delta_2 \leq \cdots \leq \delta_k \leq \delta_{k+1} \leq \cdots \ , \quad k \in \mathbb{N}^* \ , \tag{4.9.53}$$

where $\delta_k \to +\infty$ as $k \to +\infty$. The spectrum of $-\Delta_\Omega$ is then the set $\{\delta_k \ , \ k \in \mathbb{N}^*\}$, each point in the spectrum being an eigenvalue of infinite multiplicity.

Determining the strong resolvent limit is however not sufficient to determine the limit of the spectrum of $\tilde{A}_\eta$. Actually we need a norm resolvent convergence to determine the uniform limit of any compactly supported part of the spectrum of $\tilde{A}_\eta$.

Let us now turn to the Floquet theory and look into the operator $\tilde{A}_\eta$ as the "direct integral" of the operators $\tilde{A}_\eta^\gamma$:

$$\tilde{A}_\eta = \int_{\gamma\in(-\pi,\pi]^2}^{\oplus} \tilde{A}_\eta^\gamma \, d\gamma, \tag{4.9.54}$$

where $\tilde{A}_\eta^\gamma$ denotes the operator $\nabla \cdot (1 + \frac{\epsilon}{\eta})\nabla$ acting on $L_\gamma^2(Q_0)$, the subspace of $L^2(Q_0)$ with γ-periodic boundary condition. We denote by $\mathfrak{a}_\eta^\gamma$ its associated quadratic form which domain is the space of γ-periodic functions in $H^1(Q_0)$.

It is obvious that each $\tilde{A}_\eta^\gamma$ has compact resolvent. Let $(\lambda_{\eta,k}^\gamma)_{k\in\mathbb{N}^*}$ be its (finite multiplicity) eigenvalues ordered by the min – max, *i.e.*, $\lambda_{\eta,k}^\gamma \leq \lambda_{\eta,k+1}^\gamma$. We recall that the (continuous) spectrum of $\tilde{A}_\eta$ consists in the union of the intervals corresponding to the range of each $\gamma \mapsto \lambda_{\eta,k}^\gamma$ when γ varies in $(-\pi,\pi]^2$, *i.e.*,

$$\tilde{\Sigma}_\eta = \cup_{k\in\mathbb{N}^*}\{\lambda_{\eta,k}^\gamma \mid \gamma \in (-\pi,\pi]^2\} \ . \tag{4.9.55}$$

Let us now introduce the Dirichlet and Neumann operators on Q_0, denoted by $\tilde{A}_\eta^{(D)}$ and $\tilde{A}_\eta^{(N)}$, respectively, acting like $-\nabla \cdot (1 + \frac{\epsilon}{\eta})\nabla$ on $L^2(Q_0)$ and their respective associated quadratic forms $\mathfrak{a}_\eta^{(D)}$ and $\mathfrak{a}_\eta^{(N)}$, with domains $H_0^1(Q_0)$ and $H^1(Q_0)$, respectively.

As for $\tilde{A}_\eta^\gamma$, the operators $\tilde{A}_\eta^{(D)}$ and $\tilde{A}_\eta^{(N)}$ have compact resolvent and we denote by $\lambda_{\eta,k}^{(D)}$ and $\lambda_{\eta,k}^{(N)}$ their respective ordered eigenvalues. From the min – max principle, we deduce that

$$\lambda_{\eta,k}^{(N)} \leq \lambda_{\eta,k}^\gamma \leq \lambda_{\eta,k}^{(D)} \ , \quad k \in \mathbb{N}^* \ , \ \ \gamma \in (-\pi,\pi]^2 \ , \ \ \eta > 0 \ . \tag{4.9.56}$$

It follows that

$$\tilde{\Sigma}_\eta \subset \bigcup_{k\in\mathbb{N}^*} [\lambda_{\eta,k}^{(N)}, \lambda_{\eta,k}^{(D)}] \ . \tag{4.9.57}$$

Again, we apply the monotone convergence theorem for quadratic forms to the forms $\mathfrak{a}_\eta^\gamma$, $\mathfrak{a}_\eta^{(N)}$, and $\mathfrak{a}_\eta^{(D)}$ and we obtain the limiting quadratic forms $\mathfrak{a}_0^\gamma$, $\mathfrak{a}_0^{(N)}$, and $\mathfrak{a}_0^{(D)}$, respectively. The self-adjoint operators associated to these quadratic forms are $\tilde{A}_0^\gamma$, $\tilde{A}_0^{(N)}$, and $\tilde{A}_0^{(D)}$, respectively.

The operator $\tilde{A}_0^{(D)}$ is a self-adjoint operator on $H_0^1(\Omega_0)$ and $\tilde{A}_0^{(N)}$ acts on the subspace $H_0^1(\Omega_0) \oplus \mathbf{1}_{Q_0}$ of the functions $u = \tilde{u} + c \in H^1(Q_0)$ where $\tilde{u} \in H_0^1(\Omega_0)$ and $c \in \mathbb{R}$ is a constant.

The operators $\tilde{A}_0^\gamma$, $\tilde{A}_0^{(N)}$, and $\tilde{A}_0^{(D)}$ are the strong resolvent limits of $\tilde{A}_\eta^\gamma$, $\tilde{A}_\eta^{(N)}$, and $\tilde{A}_\eta^{(D)}$, respectively. We recall that these operators have compact resolvent and then purely discrete spectrum. By a result of Kato [43] (cf. [Thm. VIII-3.5]), compactness implies the convergence in the norm resolvent sense. Then we have

$$\tilde{A}_\eta^\gamma \to \tilde{A}_0^\gamma \ , \quad \text{in norm resolvent sense,} \quad \eta \to 0 \ , \tag{4.9.58}$$

for each $\gamma \in (-\pi, \pi]^2$, and

$$\tilde{A}_\eta^{(D)} \to \tilde{A}_0^{(D)} \ , \quad \tilde{A}_\eta^{(N)} \to \tilde{A}_0^{(N)} \ , \quad \text{in norm resolvent sense,} \quad \eta \to 0 \ . \tag{4.9.59}$$

Let us denote by $(\nu_k)_{k\in\mathbb{N}}$ the eigenvalues of the operator $\tilde{A}_0^{(N)}$ ordered by the min $-$ max principle.

$$0 = \nu_1 < \nu_2 \leq \nu_3 \leq \cdots \leq \nu_k \leq \nu_k + 1 \leq \cdots \ , \qquad k \in \mathbb{N}^* \ . \tag{4.9.60}$$

From equation (4.9.59) we deduce that

$$\lambda_{\eta,k}^{(N)} \to \nu_k \ , \quad \eta \to 0 \ , \ k \in \mathbb{N}^* \ . \tag{4.9.61}$$

We recall that the domain of the form limit $\mathfrak{a}_0^{(N)}$ is the subspace of the functions in $H^1(\mathbb{R}^2)$ that are constant in $Q_0 \setminus \overline{\Omega_0}$ and then the operator $\tilde{A}_0^{(N)}$ is not the Neumann operator on Ω_0.

The following proposition gives the operator limit of $\tilde{A}_\eta^\gamma$.

Proposition 4.9.2 *(i) The limit of the Dirichlet operator $\tilde{A}_\eta^{(D)}$ is the Dirichlet operator $\tilde{A}_0^{(D)} = -\Delta_{\Omega_0}$. Moreover,*

$$\lambda_{\eta,k}^{(D)} \to \delta_k \ , \quad \eta \to 0 \ , \ k \in \mathbb{N}^* \ . \tag{4.9.62}$$

(ii) For any $\gamma \in (-\pi, \pi]^2 \setminus \{(0,0)\}$, we have $\tilde{A}_0^\gamma = \tilde{A}_0^{(D)} = -\Delta_{\Omega_0}$ and

$$\lambda_{\eta,k}^\gamma \to \delta_k \ , \quad \eta \to 0 \ , \ k \in \mathbb{N}^* \ , \ \gamma \neq (0,0) \ . \tag{4.9.63}$$

(iii) For $\gamma_0 = (0,0)$, we have $\tilde{A}_0^{\gamma_0} = \tilde{A}_0^{(N)}$ and

$$\lambda_{\eta,k}^{\gamma_0} \to \nu_k \ , \quad \eta \to 0 \ , \ k \in \mathbb{N}^* \ . \tag{4.9.64}$$

Proof. From (4.9.58) and (4.9.59) it follows that we only need to identify the limiting operators that is equivalent to identifying the corresponding quadratic forms.

It is obvious that, since all the quadratic forms considered are defined by the same expression

$$\int_{Q_0} (1+\frac{\epsilon}{\eta})|\nabla u|^2\, dx ,$$

we only need to determine the form domains of the limiting quadratic forms.

Concerning $\tilde{A}_0^{(D)}$, it is clear that it is defined for the subspace of $H_0^1(Q_0)$ of the functions with null gradient in $Q_0 \setminus \overline{\Omega_0}$, which corresponds to $H_0^1(\Omega_0)$. We deduce then that $\tilde{A}_0^{(D)} = -\Delta_{\Omega_0}$.

Now let us consider $\mathfrak{a}_\eta^\gamma$ for $\gamma \neq \gamma_0$. The form domain of $\mathfrak{a}_0^\gamma$ is the subspace of γ-periodic functions in $H^1(Q_0)$ that are constant in $Q_0 \setminus \overline{\Omega_0}$. Since $\gamma \neq (0,0)$, this constant is necessarily 0 and the form domain of $\mathfrak{a}_0^\gamma$ is then $H_0^1(Q_0)$. It follows that for $\gamma \neq \gamma_0$, $\tilde{A}_0^\gamma = \tilde{A}_0^{(D)} = -\Delta_{\Omega_0}$.

Finally the form domain of $\mathfrak{a}_0^{\gamma_0}$ is the subspace of periodic functions in $H^1(Q_0)$ that are constant in $Q_0 \setminus \overline{\Omega_0}$ or simply the subspace of functions in $H^1(Q_0)$ that are constant in $Q_0 \setminus \overline{\Omega_0}$, that is exactly the form domain of $\tilde{A}_0^{(N)}$.
$\square$

Now we can state the following result on the convergence of the spectrum of A_η.

Theorem 4.9.1 *The spectrum of A^{p}_α converges to $\cup_{k\in\mathbb{N}^*}[\epsilon^{-1}\nu_k, \epsilon^{-1}\delta_k]$ as $\alpha \to 1$, in the sense that if $[\lambda^-_{\eta,k}, \lambda^+_{\eta,k}]$ is the k^{th} band of the spectrum of A^{p}_α, then*

$$\lambda^-_{\eta,k} \to \epsilon^{-1}\nu_k\ , \quad \lambda^+_{\eta,k} \to \epsilon^{-1}\delta_k\ , \quad \eta \to 0\ . \tag{4.9.65}$$

The convergence of the spectrum of A^{p}_α is uniform on any compact of $\mathbb{R}^+$, i.e., *for any compact I of $\mathbb{R}^+$ and any $C > 0$, there exists $0 < \alpha_0 < 1$ such that if $\alpha_0 < \alpha < 1$,*

$$dist_{\mathrm{H}}(\Sigma_\alpha \cap I, \bigcup_{k\in\mathbb{N}^*}[\epsilon^{-1}\nu_k, \epsilon^{-1}\delta_k] \cap I) < C\ . \tag{4.9.66}$$

Here $\mathrm{dist}_{\mathrm{H}}(E,F)$ denotes the Hausdorff distance between the subsets E and F.

Now we can see clearly the emergence of gaps in Σ_α as α goes to 1.

Corollary 4.9.3 *Suppose that for some $k \in \mathbb{N}^*$, $\delta_k < \nu_{k+1}$, then for any compact $I \subset\subset (\epsilon^{-1}\delta_k, \epsilon^{-1}\nu_{k+1})$, there exists $\alpha_0 > 0$ such that for any $\alpha_0 < \alpha < 1$,*

$$\Sigma_\alpha \cap I = \emptyset\ . \tag{4.9.67}$$

4.9.4 Existence of gaps in the limiting spectrum

The existence of gaps in Σ_α for α close enough to 1 is an obvious consequence of the existence of $k \in \mathbb{N}^*$ such that $\delta_k < \nu_{k+1}$. In a first step, let us prove that the eigenvalues ν_k and δ_k are enlaced.

Proposition 4.9.3 *The eigenvalues ν_k and δ_k of the operators respective $\tilde{A}_0^{(N)}$ and $\tilde{A}_0^{(D)}$ enlace,* i.e.,

$$0 = \nu_1 < \delta_1 \le \nu_2 \le \delta_2 \le \cdots \le \nu_k \le \delta_k \le \nu_{k+1} \le \delta_{k+1} \le \cdots\ . \tag{4.9.68}$$

Proof. Recalling the inclusion of the form domains $D(\mathfrak{a}_0^{(D)}) \subset D(\mathfrak{a}_0^{(N)})$, we deduce immediately that for any $k \in \mathbb{N}^*$,

$$\nu_k \leq \delta_k \ . \tag{4.9.69}$$

Let us denote $u_k^{(N)}$ the eigenvector of $\tilde{A}_0^{(N)}$ related to the eigenvalue ν_k. We recall that $\nu_1 = 0$ and $u_1^{(N)} = \mathbf{1}_{Q_0}$. Let $D_k^{(N)} = \mathrm{Vect}(u_l^{(N)})_{1\leq l\leq k}$. From the definition of $D(\mathfrak{a}_0^{(N)})$ there exist constants $c_l \in \mathbb{R}$ for $l \geq 2$ such that $u_l^{(N)} = c_l u_1^{(N)} + \tilde{u}_l^{(D)}$, where $\tilde{u}_l^{(D)} \in H_0^1(\Omega_0)$. It is also obvious that the dimension of $\tilde{D}_k^{(D)} = \mathrm{Vect}(\tilde{u}_l^{(D)})_{2\leq l\leq k+1}$ is k and that $\tilde{D}_k^{(D)} \subset D_{k+1}^{(N)}$

Finally, since

$$\mathfrak{a}_0^{(D)}[\tilde{u}] = \mathfrak{a}_0^{(N)}[\tilde{u}] \leq \nu_{k+1} \|\tilde{u}\|^2_{L^2(\Omega_0)} \ , \qquad \forall \tilde{u} \in \tilde{D}_k^{(D)} \ , \tag{4.9.70}$$

we deduce that

$$\delta_k \leq \nu_{k+1} \ , \tag{4.9.71}$$

which ends the proof. □

Now we give a condition for the existence of gaps in $\tilde{\Sigma}_\eta$ when η is sufficiently small.

Proposition 4.9.4 *Let $(\delta_k)_{k\geq 0}$ be the eigenvalues of $\tilde{A}_0^{(D)}$ ordered by the* $\min - \max$ *principle where formally $\delta_0 = -\infty$. Suppose that for some $k, m \geq 0$,*

$$\delta_{k-1} < \delta_k = \cdots = \delta_{k+m} < \delta_{k+m+1} \ . \tag{4.9.72}$$

(i) If there exists an eigenvector $u_0 \in H_0^1(\Omega_0)$ corresponding to the eigenvalue δ_k and satisfying

$$\int_{\Omega_0} u_0 \, dx \neq 0 \ , \tag{4.9.73}$$

then

$$\nu_k < \delta_k \ , \qquad \delta_{k+m} < \nu_{k+m+1} \ . \tag{4.9.74}$$

(ii) If all functions $u \in \ker(\tilde{A}_0^{(D)} - \delta_k)$ have zero mean value, then

$$\nu_k = \delta_k \ , \qquad \text{or} \qquad \delta_{k+m} = \nu_{k+m+1} \ . \tag{4.9.75}$$

To prove this proposition we need the following lemma.

Lemma 4.9.2 *We have $D(\tilde{A}_0^{(N)}) = \mathrm{Vect}\{\mathbf{1}_{Q_0}, D(\tilde{A}_0^{(D)})\}$ and*

$$\tilde{A}_0^{(N)} = P^* \tilde{A}_0^{(D)} P \ , \tag{4.9.76}$$

where P is the projection on $H_0^1(Q_0)$ along $\mathrm{Vect}\{\mathbf{1}_{Q_0}\}$ and P^*, the adjoint of P, is the projection on $\mathrm{Vect}\{\mathbf{1}_{Q_0}\}^\perp = \{u \in D(\mathfrak{a}_0^{(N)}) \ , \ \int_{Q_0} u(x)\, dx = 0\}$ along $H_0^1(Q_0)^\perp$.

This means that if $u \in D(\tilde{A}_0^{(N)})$ then $Pu \in D(\tilde{A}_0^{(D)})$ and

$$\tilde{A}_0^{(N)} u = P^* \tilde{A}_0^{(D)} P u = \tilde{A}_0^{(D)} u \ ;$$

conversely, if $u \in \mathrm{Vect}\{\mathbf{1}_{Q_0}, H_0^1(\Omega_0)\}$ *is such that* $Pu \in D(\tilde{A}_0^{(D)})$, *then necessarily* $u \in D(\tilde{A}_0^{(N)})$ *and* $\tilde{A}_0^{(N)}u = P^*\tilde{A}_0^{(D)}Pu$. *In particular, for any* $u \in D(\tilde{A}_0^{(D)})$ *we have*

$$\tilde{A}_0^{(N)}u = \tilde{A}_0^{(D)}u \quad \Longleftrightarrow \quad \int \tilde{A}_0^{(D)}u\, dx = 0\ . \tag{4.9.77}$$

Proof. Let $u \in D(\tilde{A}_0^{(N)})$, and let c_u be the real constant such that $Pu = u - c_u\mathbf{1}_{Q_0} \in H_0^1(\Omega_0)$. It is clear that $Pu \in D(\tilde{A}_0^{(N)})$, moreover, for any $v \in D(\mathfrak{a}_0^{(N)})$ we have $(\tilde{A}_0^{(N)}u, v) = \mathfrak{a}_0^{(N)}[u, v] = \mathfrak{a}_0^{(N)}[Pu, v]$. Recalling that $D(\mathfrak{a}_0^{(D)}) \subset D(\mathfrak{a}_0^{(N)})$, we deduce $(\tilde{A}_0^{(N)}u, w) = \mathfrak{a}_0^{(D)}[Pu, w]$ for any $w \in D(\mathfrak{a}_0^{(N)})$. This means that $Pu \in D(\tilde{A}_0^{(N)})$ and that $\tilde{A}_0^{(N)}u = \tilde{A}_0^{(D)}Pu$.

Finally, from $(\tilde{A}_0^{(N)}u, \mathbf{1}_{Q_0}) = \mathfrak{a}_0^{(N)}[u, \mathbf{1}_{Q_0}] = 0$ we deduce that

$$\int_{Q_0} \tilde{A}_0^{(N)}u\, dx = 0\ ,$$

and so $\tilde{A}_0^{(N)}u = P^*\tilde{A}_0^{(N)}u = P^*\tilde{A}_0^{(D)}Pu$.

Conversely, suppose that $u \in D(\tilde{A}_0^{(D)})$. For any $w = w_0 + c\mathbf{1}_{Q_0} \in D(\mathfrak{a}_0^{(N)})$, where $w_0 \in H_0^1(\Omega_0)$ and $c \in \mathbb{R}$, we have

$$\begin{aligned}\mathfrak{a}_0^{(N)}[u, w] &= \mathfrak{a}_0^{(N)}[u, w_0] = \mathfrak{a}_0^{(D)}[u, w_0] = (\tilde{A}_0^{(D)}u, w_0)\\ &= (P^*\tilde{A}_0^{(D)}u, w_0) + ((1 - P^*)\tilde{A}_0^{(D)}u, w_0) = (P^*\tilde{A}_0^{(D)}u, w)\ ,\end{aligned}$$

because $(1 - P^*)\tilde{A}_0^{(D)}u \in H_0^1(\Omega_0)^\perp$ and $P^*\tilde{A}_0^{(D)}u \in \mathbf{1}_{Q_0}^\perp$.

It follows that $u \in D(\tilde{A}_0^{(N)})$ and $\tilde{A}_0^{(N)}u = P^*\tilde{A}_0^{(D)}u$. □

Proof of Proposition 4.9.4:
(i) We define $K_{\delta_k}^{(D)}$ and $K_{\delta_k}^{(N)}$ as $\ker(\tilde{A}_0^{(D)} - \delta_k)$ and $\ker(\tilde{A}_0^{(N)} - \delta_k)$ respectively. We also define $\tilde{K}_{\delta_k}^{(D)} = \{u \in K_{\delta_k}^{(D)}\ ;\ \int_{\Omega_0} u\, dx = 0\}$. We first prove that $\tilde{K}_{\delta_k}^{(D)} = K_{\delta_k}^{(N)}$.

From Lemma 4.9.2 we have immediately

$$\tilde{K}_{\delta_k}^{(D)} \subset K_{\delta_k}^{(N)}\ .$$

Let us consider now $u \in K_{\delta_k}^{(N)}$. Then there exists $v \in D(\tilde{A}_0^{(D)})$ and $c \in \mathbb{R}$ such that $u = v + c\mathbf{1}_{Q_0}$. We have $v = Pu$. Since $\delta_k u = \tilde{A}_0^{(N)}u = P^*\tilde{A}_0^{(D)}Pu$, it is clear that $\int_{Q_0} u\, dx = 0$. Moreover,

$$(\tilde{A}_0^{(D)} - \delta_k)v = (\tilde{A}_0^{(N)} - \delta_k)(u - c\mathbf{1}_{Q_0}) = c\delta_k\mathbf{1}_{Q_0}\ . \tag{4.9.78}$$

Recalling the function u_0 of the hypothesis, we get

$$0 = ((\tilde{A}_0^{(D)} - \delta_k)u_0, v) = (u_0, (\tilde{A}_0^{(D)} - \delta_k)v) = c\delta_k \int_{\Omega_0} u_0\, dx\ . \tag{4.9.79}$$

Since $\int_{\Omega_0} u_0\, dx \neq 0$ we have $c = 0$ and so $u = v \in K_{\delta_k}^{(D)}$. As $\int_{Q_0} u\, dx = 0$, we deduce that $u \in \tilde{K}_{\delta_k}^{(D)}$. This proves

$$K_{\delta_k}^{(N)} \subset \tilde{K}_{\delta_k}^{(D)}\ .$$

Now suppose that $\nu_k = \delta_k$ or $\delta_{k+m} = \nu_{k+m+1}$, then the dimension of $K_{\delta_k}^{(N)}$ is at least $m+1$ while the dimension of $\tilde{K}_{\delta_k}^{(D)}$ is m which is impossible since $K_{\delta_k}^{(N)} = \tilde{K}_{\delta_k}^{(D)}$.

(ii) Suppose now that all functions in $K_{\delta_k}^{(D)}$ have 0 mean. Then $K_{\delta_k}^{(D)} = \tilde{K}_{\delta_k}^{(D)} \subset K_{\delta_k}^{(N)}$ and so the dimension of $K_{\delta_k}^{(N)}$ is at least $m+1$. Consequently, the inequalities in (4.9.74) can not be both strict.

4.10 Gaps opening in Σ_α: TM polarization

In the TM polarization we have exactly the same results replacing the Hilbert space $L^2(\mathbb{R}^2, dx)$ by the weighted Hilbert space $L^2(\mathbb{R}^2, \varepsilon_{\rm p}(x)\, dx)$.

Theorem 4.10.1 *The spectrum of $B_\alpha^{\rm p}$ converges to $\cup_{k\in\mathbb{N}}[\epsilon^{-1}\nu_k, \epsilon^{-1}\delta_k]$ as $\alpha \to 1$, in the sense that if $[\lambda_{\eta,k}^-, \lambda_{\eta,k}^+]$ is the $k^{\rm th}$ band of the spectrum of $A_\alpha^{\rm p}$, then*

$$\lambda_{\eta,k}^- \to \epsilon^{-1}\nu_k \ , \quad \lambda_{\eta,k}^+ \to \epsilon^{-1}\delta_k \ , \quad \eta \to 0 \ . \tag{4.10.80}$$

The convergence of the spectrum of $B_\alpha^{\rm p}$ is uniform on any compact of $\mathbb{R}^+$, i.e., for any compact I of $\mathbb{R}^+$, there exists a positive constant C independent of η such that

$$dist_{\rm H}(\Sigma_\alpha \cap I, \bigcup_{k\in\mathbb{N}} [\epsilon^{-1}\nu_k, \epsilon^{-1}\delta_k] \cap I) < C \ . \tag{4.10.81}$$

The eigenvalues (δ_k) and (ν_k) are exactly the same as those defined in the previous section. This is because $\varepsilon_{\rm p}(x) = \epsilon + 1$ in Ω and so the modification of the Hilbert space does not change the limiting operators.

4.11 Numerical experiments

In this section, we consider only the TE polarization. The periodic structures considered here are conformal to those in the previous section. The dielectric permittivity takes the value 5 in the domain Ω_0 and 1 otherwise. We give numerical results for different shapes of the domain Ω_0. The numerical tool used here is the *MIT Photonic-Bands* (MPB) package [42].

We compute the continuous spectrum of $A_\alpha^{\rm p}$ for different values of $\alpha \in [0,1]$. The 16 first bands are represented. The results are shown with the corresponding periodic medium in the figures below. The dark regions correspond to a dielectric permittivity 5.

All the structures shown here have no gaps for planar propagation, i.e. $\alpha = 0$. Figure 4.9 shows the bands of the structure with discs of radius 0.3 in the planar propagation. These bands are computed on the boundary of the irreductible Brillouin zone.

We notice clearly the appearance of one or more gaps in the spectra of each structure when α^2 approaches 1 ($\alpha^2 \geq 0.9$). The bottom of the first gap goes to the first eigenvalue of the Dirichlet-Laplacian in the domain Ω_0 when $\alpha^2 \to 1$. Actually, if f_0 is the limit of the bottom of the first gap and d_0^2 is the first eigenvalue of the Dirichlet-Laplacian in Ω_0, then

$$2\pi f_0 = \frac{1}{\sqrt{\epsilon}} d_0 \ , \tag{4.11.82}$$

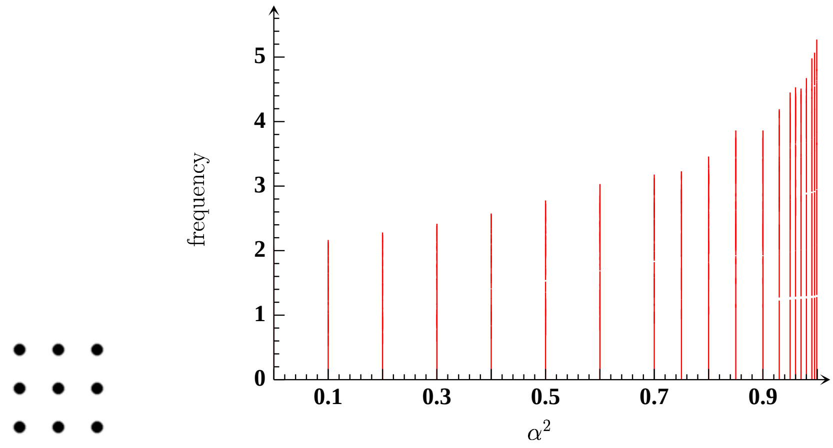


Figure 4.2: Spectrum of the structure with discs of radius 0.15.

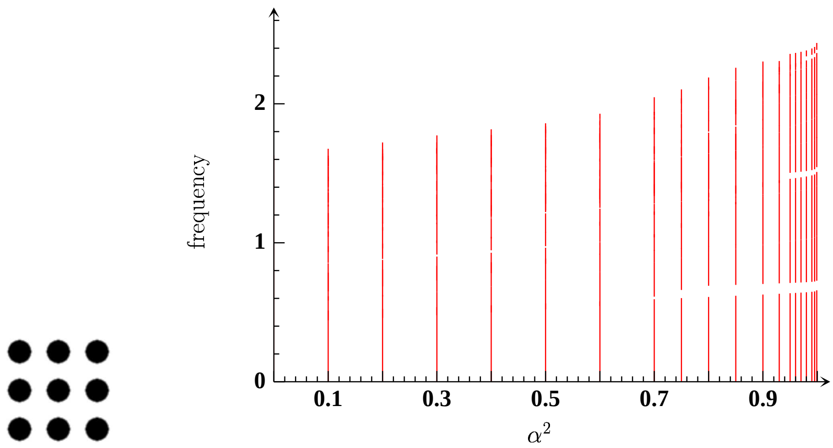


Figure 4.3: Spectrum of the structure with discs of radius 0.3.

where ϵ is defined in the previous section and is equal to 4 in our case.

When the size of Ω_0 increases, the midgap defect decreases and the width of the gap which corresponds to the interval (δ_1, ν_2) (defined in the previous section) increases.

When the gap is wider, the exponential decay of the electromagnetic energy in the periodic structure is higher which allows the use of very few periods in the cladding of the photonic fiber.

Next, we introduce a defect to the structure shown in Figure 4.3 and we compute the spectrum for different values of α^2. Two defects are investigated, the first one called "negative" consists in removing one rod from the structure, the second one called "positive" consists in increasing the radius of one rod in the structure. The way we call the defect comes from the sign of $(\delta\varepsilon)$. The method used for determining the spectrum is the "supercell" method. The size of the supercell is 5 or 7.

The parameter α^2 takes values in $[0.75, 0.90]$ for the negative defect and in

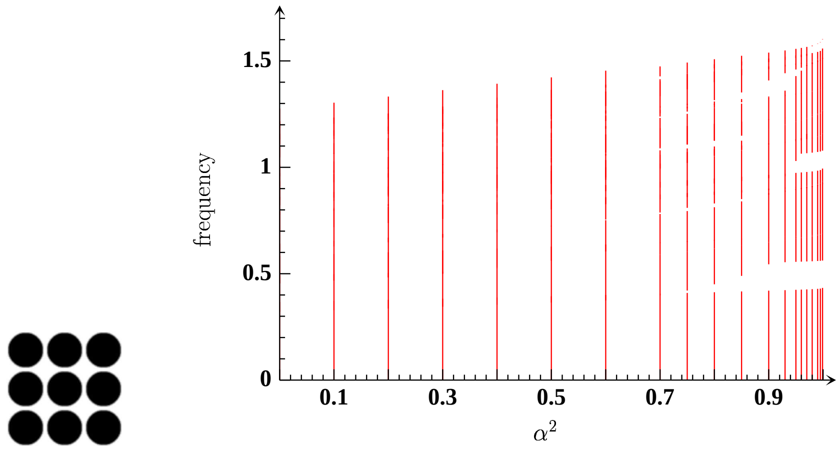


Figure 4.4: Spectrum of the structure with discs of radius 0.45.

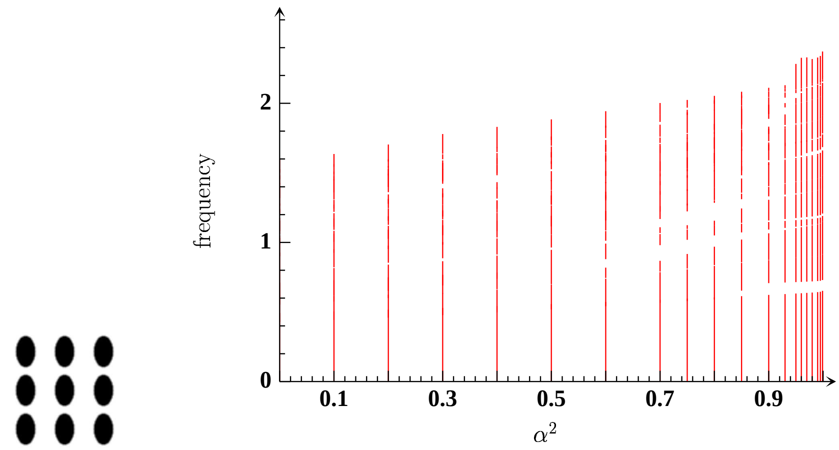


Figure 4.5: Spectrum of the structure with ellipses of axes 0.50 and 0.80.

$[0.80, 0.93]$ in the positive defect. When α^2 is too close to 1, the contrast between the coefficients is too high (more than 50) which, added to the complexity of the supercell, makes it impossible to get convergence to reliable results. For such limits we need dedicated preconditioners. We find one defect state for each case. The corresponding spectra are shown in Figures 4.10 and 4.11.

We notice that the defect frequency goes from the top to the bottom of the gap when $\alpha^2 \to 1$ in the positive defect and from the bottom to the top of the gap in the negative defect. When it is too close to the edge, the decay of the electromagnetic energy away from the defect is very weak.

Figures 4.12-4.19 represent the energy distribution of the defect modes in the supercell. The horizontal graduations represent the limits of unit cells.

Finally, we give in Tables 4.1-4.2 the percentage of the electromagnetic energy located in the defect region and the four closest dielectric rods.

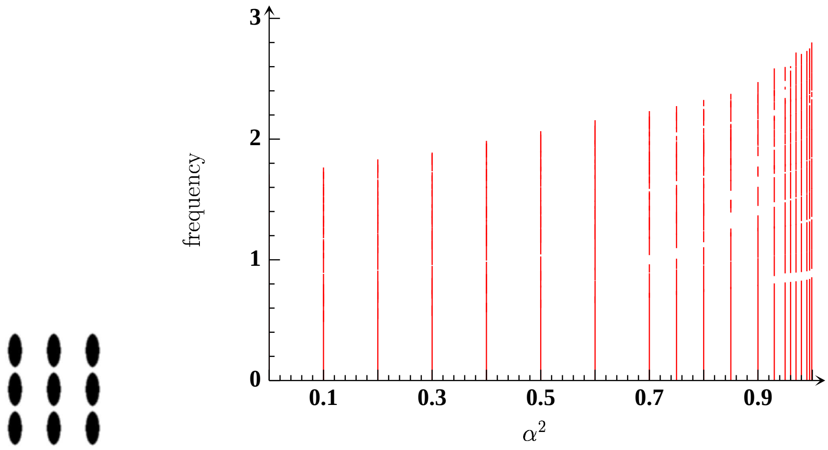


Figure 4.6: Spectrum of the structure with ellipses of axes 0.85 and 0.35.

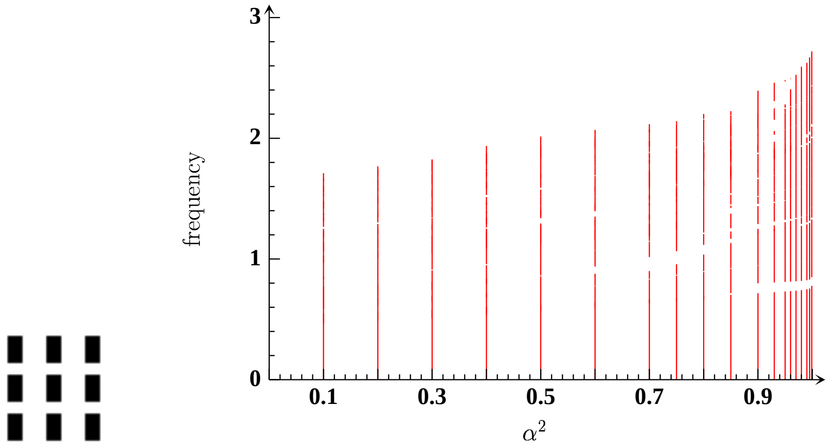


Figure 4.7: Spectrum of the structure with ellipses of axes 0.70 and 0.40.

4.12 Conclusion

We gave a rigorous proof for the origin of polarized guided modes in a photonic fiber. For a parameter α and a defect frequency $\omega_{\rm d}$, the corresponding guided mode will have the propagation constant $\beta = \alpha\omega_{\rm d}$.

It is also important to notice that we can get gaps and guide electromagnetic waves without any need to high dielectric contrast nor thin structures which is hard to achieve. The dielectric perturbation in the core of the fiber can be either positive or negative while the case of the classical fiber we can guide waves only with positive defects.

The integral formulation of guided modes could be used to achieve numerical tools for determining the defect frequencies in the fiber. This represents an alternative to the supercell method that could have some advantages. Actually, the supercell method does not distinguish defect eigenvalues from regular eigenvalues and computes all. But the degeneracy of the regular eigenvalues

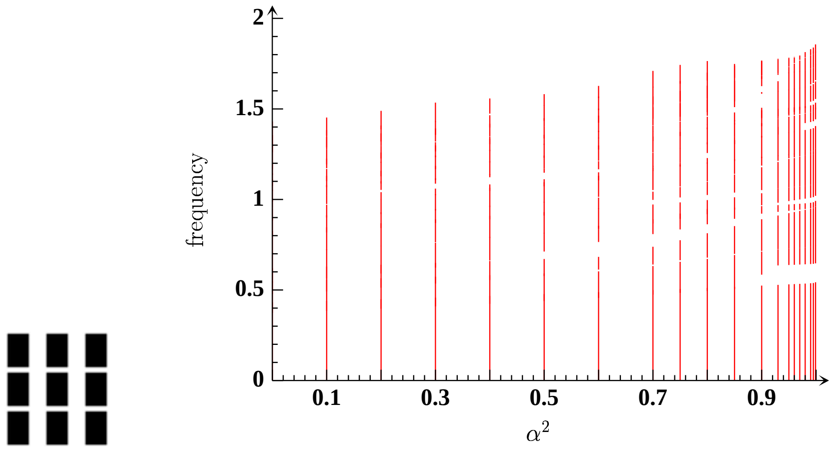


Figure 4.8: Spectrum of the structure with ellipses of axes 0.85 and 0.55.

α^2	defect frequency	% of energy around the defect
0.80	0.650	72.9
0.85	0.659	70.6
0.90	0.660	70.9
0.93	0.662	74.8

Table 4.1: Energy of positive defect modes located around the defect area.

grows as the square of the supercell size. This fact added to the growth of the computational domain makes the method slow. In the integral formulation, however, we have to compute an approximation of the Green's function once for every α value and then with this function we can determine the defect modes for different defects.

α^2	defect frequency	% of energy around the defect
0.75	0.617	87.7
0.80	0.639	92.9
0.85	0.656	95.1
0.90	0.685	64.0

Table 4.2: Energy of negative defect modes located around the defect area.

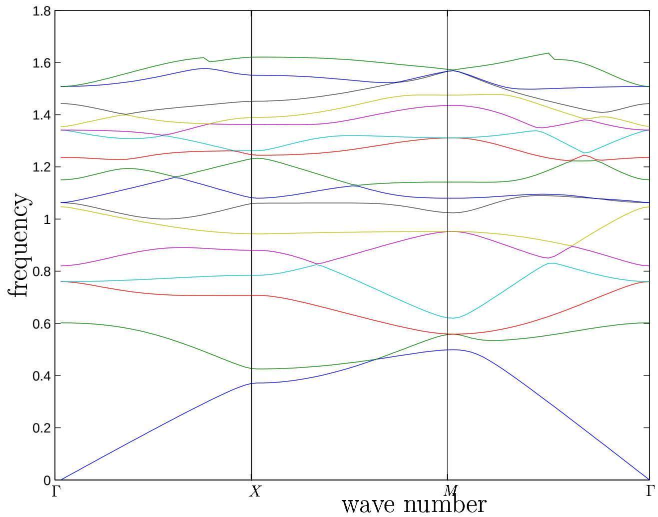


Figure 4.9: Band spectrum of the structure with discs of radius 0.3 in the planar propagation.

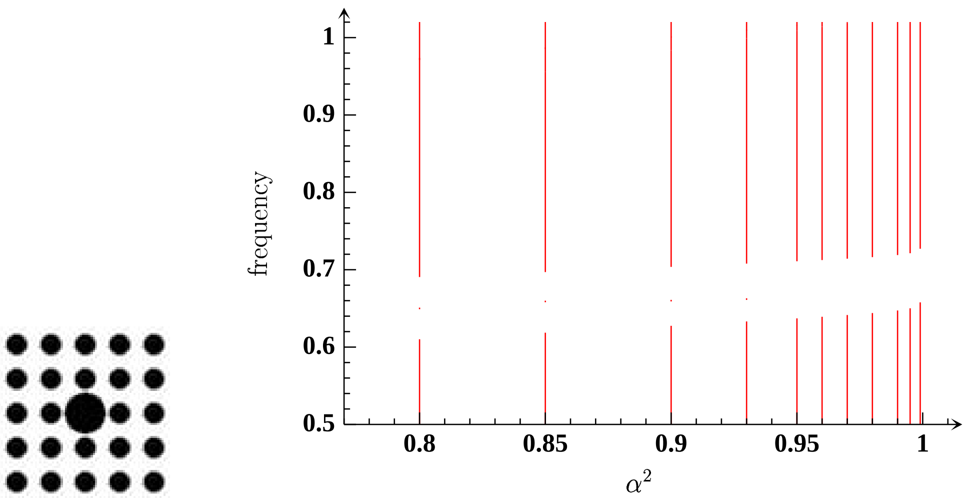


Figure 4.10: Spectrum of the structure with positive defect ($R_{\text{def}} = 0.6$).

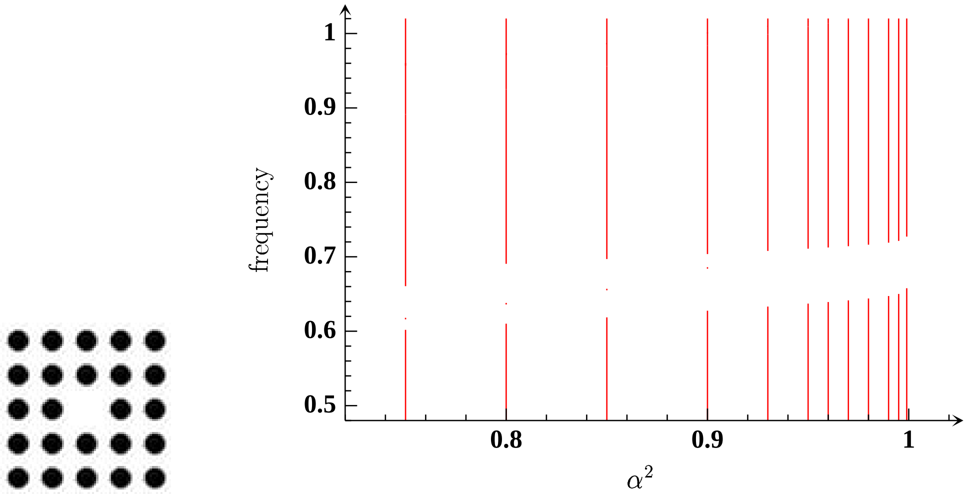


Figure 4.11: Spectrum of the structure with negative defect.

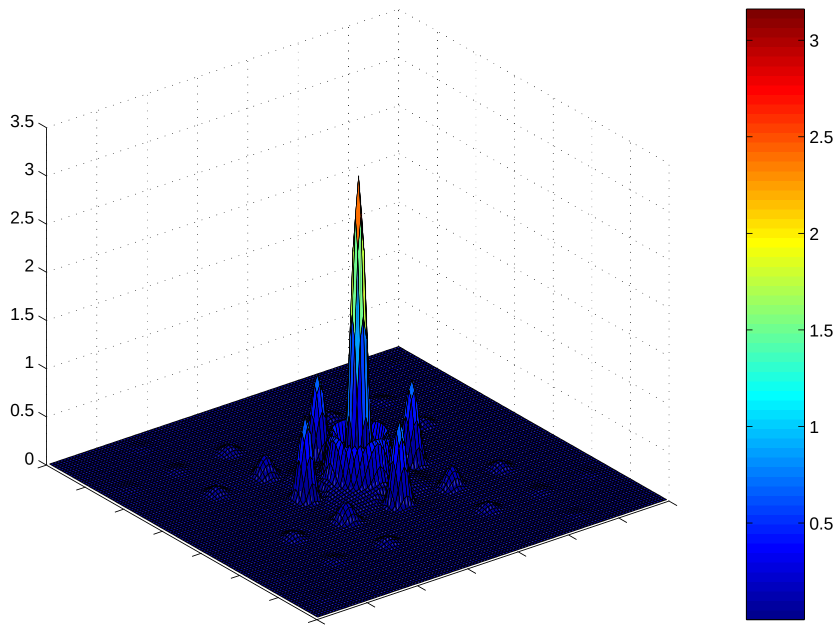


Figure 4.12: Energy density of the positive defect mode ($\alpha^2 = 0,80$).

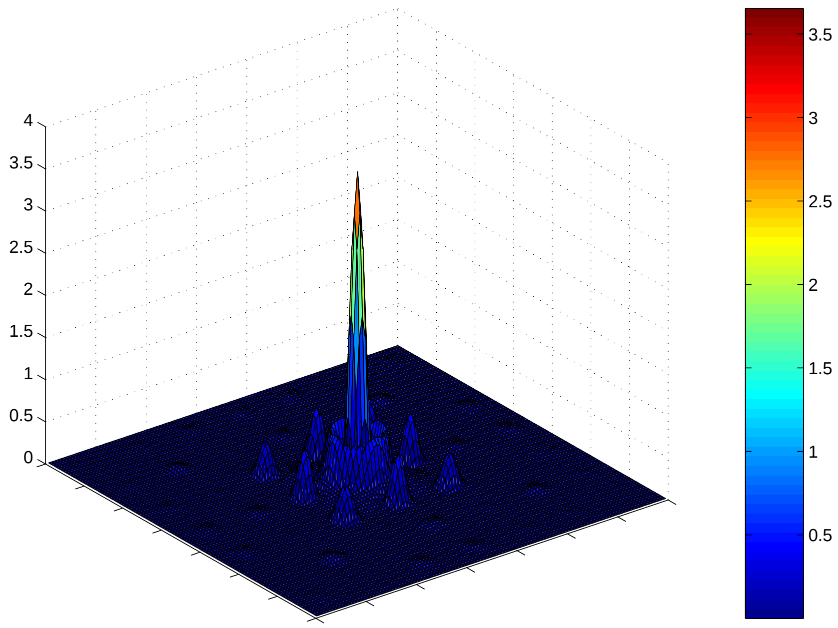


Figure 4.13: Energy density of the positive defect mode ($\alpha^2 = 0,85$).

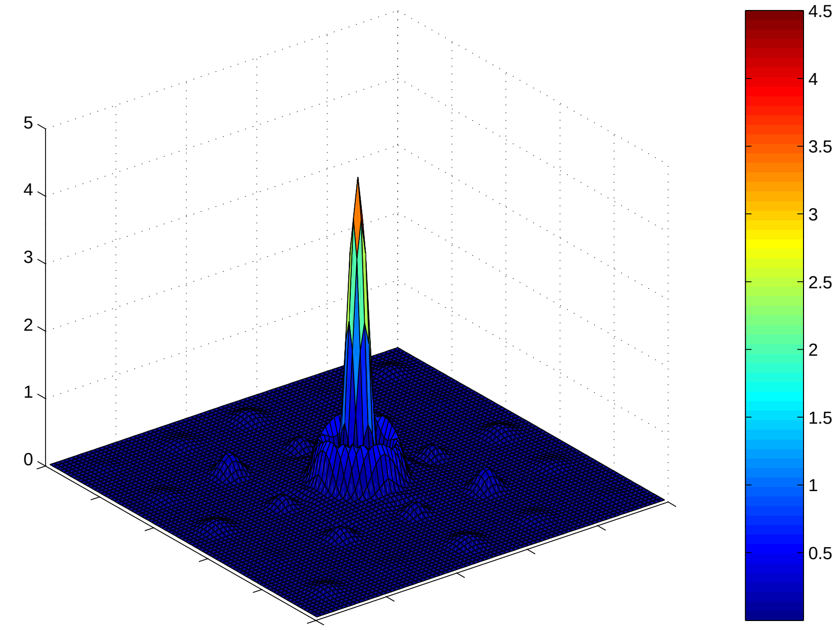


Figure 4.14: Energy density of the positive defect mode ($\alpha^2 = 0,90$).

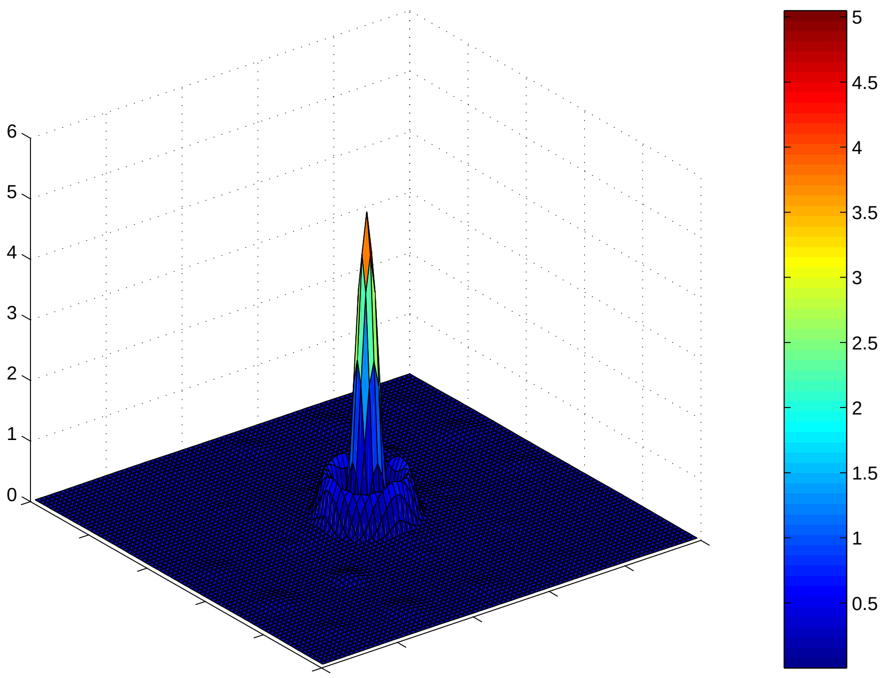


Figure 4.15: Energy density of the positive defect mode ($\alpha^2 = 0,93$).

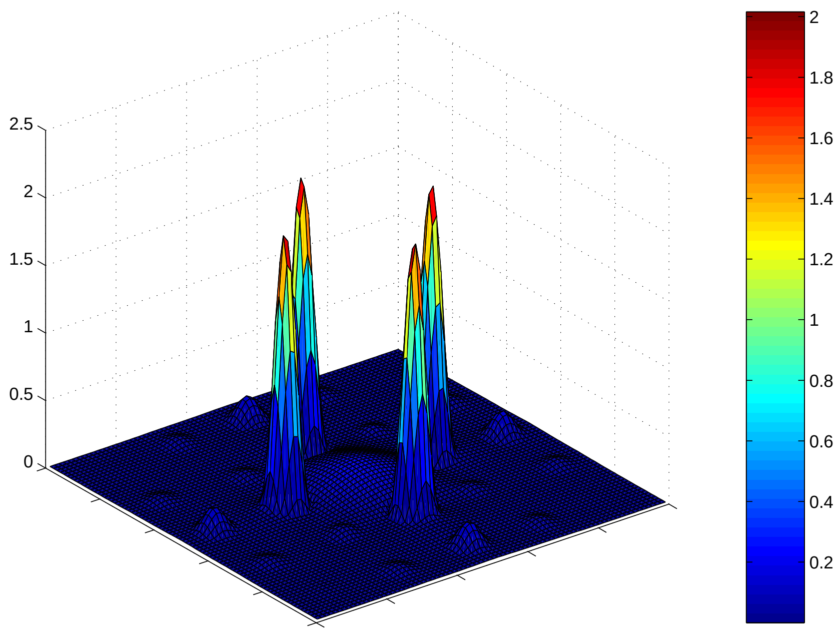


Figure 4.16: Energy density of the negative defect mode ($\alpha^2 = 0,75$).

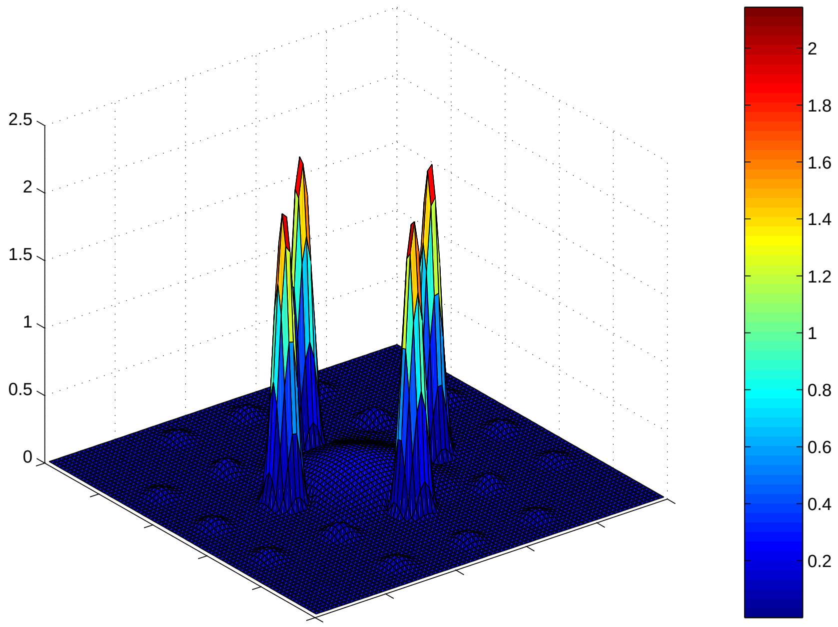


Figure 4.17: Energy density of the negative defect mode ($\alpha^2 = 0,80$).

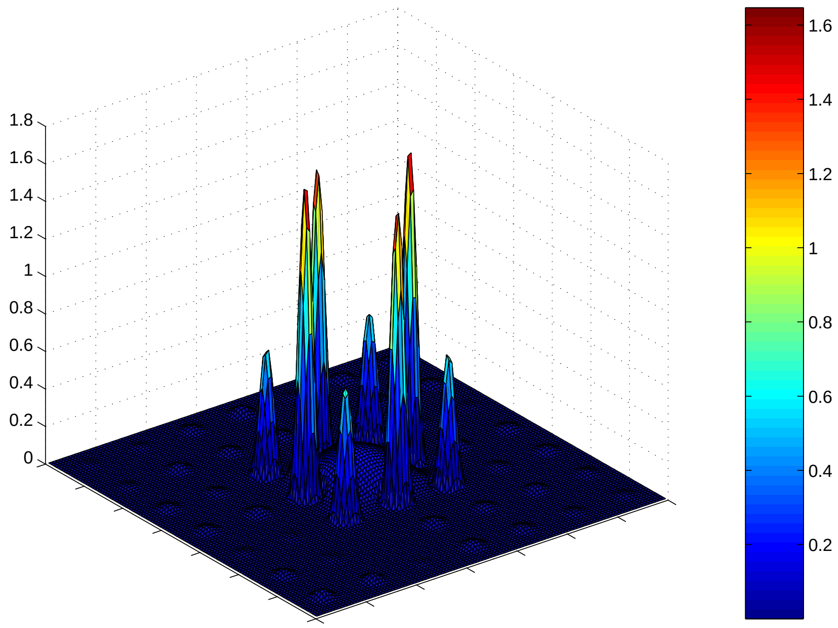


Figure 4.18: Energy density of the negative defect mode ($\alpha^2 = 0,85$).

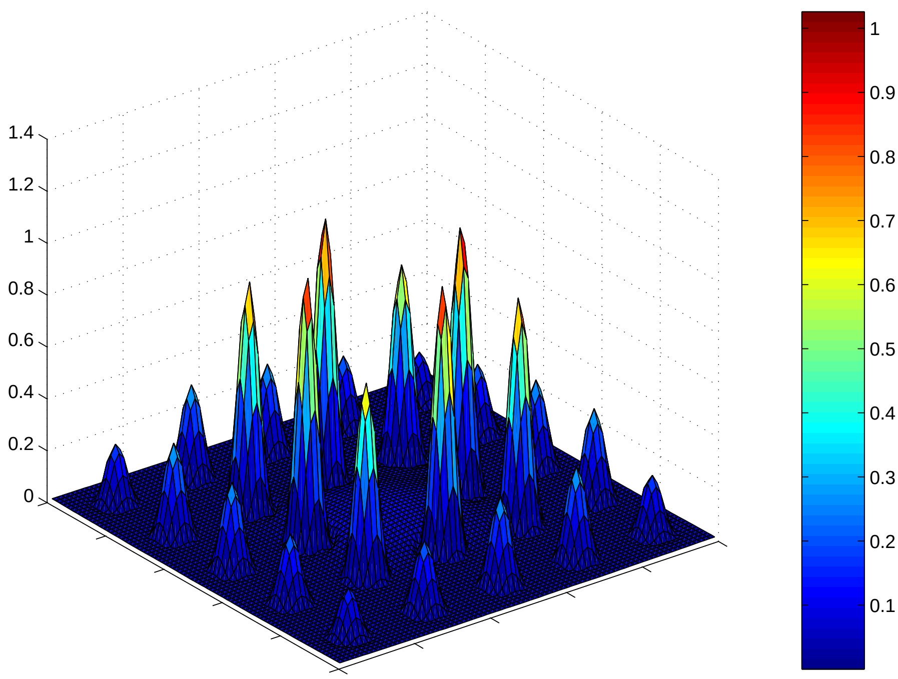


Figure 4.19: Energy density of the negative defect mode ($\alpha^2 = 0,90$).

Chapter 5

Appendices

A.1 Uniqueness results

We recall the following important result from the theory of the Helmholtz equation.

Lemma A.A.1.1 *Let $R_0 > 0$, $B_R = \{x : |x| < R\}$, and $S_R = \{x : |x| = R\}$. Let u satisfy the Helmholtz equation $\Delta u + k_0^2 = 0$ for $|x| > R_0$. Assume, furthermore that*

$$\lim_{R \to +\infty} \int_{S_R} |u(x)|^2 \, ds(x) = 0 \, .$$

Then, $u \equiv 0$ for $|x| > R_0$.

Let $W^{1,2}_{\mathrm{loc}}(\mathbb{R}^2 \setminus \overline{\Omega})$ denote the space of functions $f \in L^2_{\mathrm{loc}}(\mathbb{R}^2 \setminus \overline{\Omega})$ such that

$$hf \in W^{1,2}(\mathbb{R}^2 \setminus \overline{\Omega}), \forall \, h \in \mathcal{C}_0^\infty(\mathbb{R}^2 \setminus \overline{\Omega}) \, .$$

The following uniqueness result holds.

Lemma A.A.1.2 *Let Ω be a bounded Lipschitz domain in $\mathbb{R}^2$. Let $u \in W^{1,2}_{\mathrm{loc}}(\mathbb{R}^2 \setminus \overline{\Omega})$ satisfy*

$$\begin{cases} \Delta u + k_0^2 u = 0 \quad \text{in } \mathbb{R}^2 \setminus \overline{\Omega} \, , \\ \left| \dfrac{\partial u}{\partial |x|} - i k_0 u \right| = O\Big(|x|^{-3/2} \Big) \quad \text{as } |x| \to +\infty \quad \text{uniformly in } \dfrac{x}{|x|} \, , \\ \Im \displaystyle\int_{\partial \Omega} \overline{u} \frac{\partial u}{\partial \nu} \, ds = 0 \, . \end{cases}$$

Then, $u \equiv 0$ in $\mathbb{R}^2 \setminus \overline{\Omega}$.

Proof. Let $R > 0$ be large enough to have $\Omega \subset B_R$. Multiplying $\Delta u + k_0^2 u = 0$ by $\overline{u}$ and integrating by parts over $B_R \setminus \overline{\Omega}$, we get

$$\Im \int_{S_R} \overline{u} \frac{\partial u}{\partial \nu} \, ds = 0 \, ,$$

since $\Im \displaystyle\int_{\partial\Omega} \overline{u}\frac{\partial u}{\partial \nu}\,ds = 0$. Applying the Cauchy-Schwartz inequality to

$$\Im \int_{S_R} \overline{u}\left(\frac{\partial u}{\partial \nu} - ik_0 u\right) ds = -k_0 \int_{S_R} |u|^2\, ds \,,$$

we obtain

$$\left| \Im \int_{S_R} \overline{u}\left(\frac{\partial u}{\partial \nu} - ik_0 u\right) ds \right| \le \left(\int_{S_R} |u|^2 \right)^{1/2} \left(\int_{S_R} \left| \frac{\partial u}{\partial \nu} - ik_0 u \right|^2 \right)^{1/2} .$$

Then using the radiation condition yields

$$\Im \int_{S_R} \overline{u}\left(\frac{\partial u}{\partial \nu} - ik_0 u\right) ds \le \frac{C}{R}\left(\int_{S_R} |u|^2 \right)^{1/2} , \tag{A.1.1}$$

for some positive constant C independent of R. Finally, we obtain that

$$\left(\int_{S_R} |u|^2 \right)^{1/2} \le \frac{C}{R} ,$$

which gives by the Rellich's Lemma that $u \equiv 0$ in $\mathbb{R}^2 \setminus \overline{B}_R$. Hence, by the unique continuation property for $\Delta + k_0^2$, we can conclude that $u \equiv 0$ up to the boundary $\partial\Omega$. This finishes the proof. □

A.2 Proof of Lemma 2.3.1

Let $f \in H^{1/2}(S_R)$ and (f^n) its Fourier series with respect to the angular variable. Then

$$(C_R f)^n = k_0 \frac{H_n^{(1)\prime}(k_0 R)}{H_n^{(1)}(k_0 R)} f^n \,.$$

Using the following identity from [1]

$$n z^{n-2} H_n^{(1)}(z) + z^n H_n^{(1)\prime}(z) = z^{n-1} H_{n-1}^{(1)\prime}(z),$$

we get

$$0 \le -\frac{H_n^{(1)\prime}(k_0 R)}{H_n^{(1)}(k_0 R)} = +\frac{n}{(k_0 R)^2} - \frac{H_{n-1}^{(1)\prime}(k_0 R)}{k_0 R H_n^{(1)}(k_0 R)} \le C(1+n^2)^{1/2} \,.$$

It then follows that

$$(1+n^2)^{-1/2} |(C_R f)^n|^2 \le C(1+n^2)^{1/2} |f^n|^2$$

which proves that C_R is a bounded operator from $H^{1/2}(S_R)$ into $H^{-1/2}(S_R)$.

Next, let $f \in H^{1/2}(S_R)$ and let u be the unique solution to the Helmholtz equation $\Delta u + k_0^2 u = 0$ in $\mathbb{R}^2 \setminus \overline{B}_R$ satisfying $u|_{S_R} = f$ together with the radiation condition

$$\lim_{|x|\to\infty} \sqrt{|x|} \left| \frac{\partial u}{\partial |x|} - ik_0 u \right| = 0, \qquad \text{uniformly in } \frac{x}{|x|}.$$

For any $R' > R$, we have:

$$\begin{aligned} 0 &= \int_{B_{R'} \setminus \overline{B}_R} (\Delta u + k_0^2 u)\overline{u} \\ &= -\int_{B_{R'} \setminus \overline{B}_R} |\nabla u|^2 + \int_{B_{R'} \setminus \overline{B}_R} |u|^2 - \int_{S_R} \frac{\partial u}{\partial \nu}\overline{u} + \int_{S_{R'}} \frac{\partial u}{\partial \nu}\overline{u} \, . \end{aligned}$$

Recalling that $u|_{S_R} = f$ and $\dfrac{\partial u}{\partial \nu}|_{S_R} = C_R(f)$ and taking the imaginary part of the above identity, we get

$$\Im \int_{S_R} C_R(f)\overline{f} = \Im \int_{S_{R'}} \frac{\partial u}{\partial \nu}\overline{u} \, .$$

From the radiation condition, we obtain by using (A.1.1) that when R' goes to infinity,

$$\Im \int_{S_R} C_R(f)\overline{f} \sim k_0 \int_{S_{R'}} |u|^2 > 0 \, .$$

The second inequality (2.3.14) is a direct consequence of the explicit form of the operator C_R and can be found, for example, in [56].

A.3 Proof of Lemma 2.4.3

In view of Lemma 2.4.1 it suffices to prove Lemma 2.4.3 for $k = 0$. We have

$$\begin{aligned} &2\pi S^0_{\delta,\delta}\varphi(x) = \int_{\partial\Omega} \log|x - y + \delta(\nu(x) - \nu(y))|^2 (1 + \delta\rho(y))\varphi(y)\, ds(y) \\ &= \int_{\partial\Omega} \log(|x-y|^2 + \delta^2|\nu(x) - \nu(y)|^2 + 2\delta < \nu(x) - \nu(y), x - y >) \\ &\qquad\qquad\qquad\qquad\qquad\qquad (1 + \delta\rho(y))\varphi(y)\, ds(y) \\ &= 2\pi S^0_{0,0}\varphi(x) + 2\pi\delta S^0_{0,0}(\rho\varphi)(x) \\ &+ \int_{\partial\Omega} \log\left(1 + 2\delta\frac{< \nu(x) - \nu(y), x - y >}{|x-y|^2} + \delta^2\frac{|\nu(x) - \nu(y)|^2}{|x-y|^2}\right) \\ &\qquad\qquad\qquad\qquad\qquad\qquad (1 + \delta\rho(y))\varphi(y)\, ds(y) \, . \end{aligned}$$

Since $\partial\Omega$ is of class $\mathcal{C}^2$, $\dfrac{< \nu(x) - \nu(y), x - y >}{|x-y|^2}$ and $\dfrac{|\nu(x) - \nu(y)|^2}{|x-y|^2}$ are bounded. Therefore,

$$\begin{aligned} S^0_{\delta,\delta}\varphi(x) &= S^0_{0,0}\varphi(x) + \delta S^0_{0,0}(\rho\varphi)(x) + \frac{\delta}{\pi}\int_{\partial\Omega} \frac{< \nu(x) - \nu(y), x - y >}{|x-y|^2}\varphi(y)\, ds(y) \\ &\quad + O(\delta^2) \\ &= S^0_{0,0}\varphi(x) + \delta S^0_{0,0}(\rho\varphi)(x) + \delta(K^0_0)^*\varphi(x) + \delta K^0_0\varphi(x) + O(\delta^2) \, . \end{aligned}$$

On the other hand,

$$\pi(K_\delta^0)^*\varphi(x) = \int_{\partial\Omega} \frac{< \nu(x), x-y+\delta(\nu(x)-\nu(y)) >}{|x-y+\delta(\nu(x)-\nu(y))|^2}(1+\delta\rho)\varphi(y)\ ds(y)$$
$$= \int_{\partial\Omega} \frac{< \nu(x), x-y > +\delta < \nu(x), \nu(x)-\nu(y) >}{|x-y|^2}$$
$$\left(1 - 2\delta \frac{< \nu(x)-\nu(y), x-y >}{|x-y|^2}\right)(1+\delta\rho)\varphi(y)\ ds(y) + O(\delta^2),$$

or equivalently,

$$(K_\delta^0)^*\varphi(x) = (K_0^0)^*\varphi(x) + \delta(K_0^0)^*(\rho\varphi)(x) - 2\frac{\delta}{\pi}\int_{\partial\Omega} \frac{< \nu(x), x-y >^2}{|x-y|^4}\varphi(y)\ ds(y)$$
$$+2\frac{\delta}{\pi}\int_{\partial\Omega} \frac{< \nu(x), x-y >< \nu(y), x-y >}{|x-y|^4}\varphi(y)\ ds(y)$$
$$+\frac{\delta}{\pi}\int_{\partial\Omega} \frac{< \nu(x), \nu(x)-\nu(y) >}{|x-y|^2}\varphi(y)\ ds(y) + O(\delta^2)$$
$$= (K_0^0)^*\varphi(x) + \delta(K_0^0)^*(\rho\varphi)(x) + \delta M_0^0\varphi(x) + O(\delta^2)\ .$$

A.4 Proof of Lemma 2.4.4

We start by proving the inequalities for $s = 0$. Since the normal derivative of $\dfrac{\partial(S_{0,0}^k\varphi)_+}{\partial\nu}$ exists and is bounded from $L^2(\partial\Omega)$ into $L^2(\partial\Omega)$, we have

$$\|S_{0,\delta}^k\varphi - S_{0,0}^k\varphi\|_{L^2(\partial\Omega)} \le C\delta\|\varphi\|_{L^2(\partial\Omega)}\ ,$$

for some $C > 0$. It remains then to show that $\left\|\dfrac{\partial S_{0,\delta}^k\varphi}{\partial\tau} - \dfrac{\partial S_{0,0}^k\varphi}{\partial\tau}\right\|_{L^2(\partial\Omega)}$ goes uniformly to 0 as $\delta \to 0$. Once again, in view of Lemma 2.4.1 it suffices to prove this result for $k = 0$. Denoting by $\oint$ the Cauchy principal value, we compute

$$\frac{\partial S_{0,\delta}^0\varphi}{\partial\tau}(x) - \frac{\partial S_{0,0}^0\varphi}{\partial\tau}(x) = \int_{\partial\Omega} \frac{< \tau(x), x-y >}{|x-y|^2+\delta^2+2\delta < \nu(x), x-y >}$$
$$(1-\delta\rho(x))\varphi(y)\ ds(y) - \oint_{\partial\Omega} \frac{< \tau(x), x-y >}{|x-y|^2}\varphi(y)\ ds(y)$$
$$= \oint_{\partial\Omega} \frac{< \tau(x), x-y >}{|x-y|^2+\delta^2}\left(-2\delta\frac{< \nu(x), x-y >}{|x-y|^2+\delta^2}(1-\delta\rho(x)) - \frac{\delta^2}{|x-y|^2} + O(\delta^2)\right)$$
$$\varphi(y)\ ds(y)$$
$$= -2\delta\oint_{\partial\Omega} \frac{< \tau(x), x-y >}{|x-y|^2}\frac{|x-y|^2}{|x-y|^2+\delta^2}\frac{< \nu(x), x-y >}{|x-y|^2+\delta^2}(1-\delta\rho(x))\varphi(y)\ ds(y)$$
$$-\oint_{\partial\Omega} \frac{< \tau(x), x-y >}{|x-y|^2}\frac{\delta^2}{|x-y|^2+\delta^2}\varphi(y)\ ds(y) + \delta^2\oint_{\partial\Omega} \frac{< \tau(x), x-y >}{|x-y|^2}O(1)$$
$$\varphi(y)\ ds(y).$$

The two first integrals can be bounded by $\delta||\varphi||_{L^2(\partial\Omega)}$ while the last one is bounded by $\varepsilon_\delta||\varphi(x)||_{L^2(\partial\Omega)}$ for $\delta \leq \delta_0$. This ends the proof of the first inequality.

Let us now prove the third inequality. We write

$$
\begin{aligned}
&\frac{\partial S^k_{0,\delta}\varphi}{\partial\nu} - \frac{\partial(S^k_{0,0}\varphi)_+}{\partial\nu} = \int_{\partial\Omega} \frac{< \nu(x), x-y+\delta\nu(x) >}{|x-y|^2+\delta^2+2\delta < \nu(x), x-y >}\varphi(y)\ ds(y) \\
&- \int_{\partial\Omega} \frac{< \nu(x), x-y >}{|x-y|^2}\varphi(y)\ ds(y) - \frac{1}{2}\varphi(x) \\
&= \int_{\partial\Omega} \frac{< \nu(x), x-y > +\delta}{|x-y|^2+\delta^2}\left(1 - 2\delta\frac{< \nu(x), x-y >}{|x-y|^2+\delta^2} + O(\delta^2)\right)\varphi(y)\ ds(y) \\
&- \int_{\partial\Omega} \frac{< \nu(x), x-y >}{|x-y|^2}\varphi(y)\ ds(y) - \frac{1}{2}\varphi(x) \\
&= -\delta\int_{\partial\Omega} \frac{\delta}{|x-y|^2+\delta^2}\frac{< \nu(x), x-y >}{|x-y|^2}\varphi(y)\ ds(y) \\
&+\delta\int_{\partial\Omega} \frac{< \nu(x), x-y > +\delta}{|x-y|^2+\delta^2}\left(-2\frac{< \nu(x), x-y >}{|x-y|^2+\delta^2} + O(\delta)\right)\varphi(y)\ ds(y) \\
&+ \int_{\partial\Omega} \frac{\delta}{|x-y|^2+\delta^2}\varphi(y)\ ds(y) - \frac{1}{2}\varphi(x)\ .
\end{aligned}
$$

Since the Poisson kernel [44]

$$
\int_{\partial\Omega} \frac{\delta}{|x-y|^2+\delta^2}\varphi(y)\ ds(y)
$$

converges uniformly in $L^2(\partial\Omega)$ as $\delta \to 0$, the first integral is bounded by $|C\delta\varphi(x)|$, the second integral is bounded by $|C\delta(||\varphi||_{L^2(\partial\Omega)} + \varphi(x))|$, and the last one is uniformly bounded by $|\varepsilon_\delta\varphi(x)|$. Here C is a positive constant independent of x and $\varepsilon_\delta \to 0$ as $\delta \to 0$.

The second and the last inequalities can be proved in a very similar way. For the reader's convenience we give here the proof for the second one, that is,

$$
S^k_{\delta,\delta}\varphi - S^k_{\delta,0}\varphi = \big(S^k_{\delta,\delta} - S^k_{0,0}\big)\varphi + \big(S^k_{0,\delta} - S^k_{\delta,0}\big)\varphi - \big(S^k_{0,\delta} - S^k_{0,0}\big)\varphi\ .
$$

Using Lemma 2.4.3, the first and the third terms can be bounded uniformly in $H^1(\partial\Omega)$ by $\varepsilon_\delta||\varphi||_{L^2(\partial\Omega)}$. Then, in view of Lemma 2.4.1, we only need to investigate the second term for $k=0$. We compute

$$
\begin{aligned}
&2\big(S^0_{0,\delta}-S^0_{\delta,0}\big)\varphi(x)=\int_{\partial\Omega}\log\big(|x-y|^2-2\delta<\nu(y),x-y>+\delta^2\big)\\
&(1+\delta\rho)\varphi(y)\ ds(y)-\int_{\partial\Omega}\log\big(|x-y|^2+2\delta<\nu(x),x-y>+\delta^2\big)\varphi(y)\ ds(y)\\
&=\delta\int_{\partial\Omega}\log\big(|x-y|^2-2\delta<\nu(y),x-y>+\delta^2\big)\rho\varphi(y)\ ds(y)\\
&+\int_{\partial\Omega}\log\left(1+2\delta\frac{<\nu(x),x-y>}{|x-y|^2+\delta^2}\right)\varphi(y)\ ds(y)\\
&-\int_{\partial\Omega}\log\left(1-2\delta\frac{<\nu(y),x-y>}{|x-y|^2+\delta^2}\right)\varphi(y)\ ds(y)\\
&=\delta\int_{\partial\Omega}\log\big(|x-y|^2+\delta^2\big)\rho\varphi(y)\ ds(y)\\
&+2\delta\int_{\partial\Omega}\frac{<\nu(x)+\nu(y),x-y>}{|x-y|^2+\delta^2}\varphi(y)\ ds(y)+O(\delta^2)\\
&=\delta\int_{\partial\Omega}\log\big(|x-y|^2+\delta^2\big)\rho\varphi(y)\ ds(y)-2\delta K^0_0\varphi(x)+2\delta(K^0_0)^*\varphi(x)\\
&-2\delta^2\int_{\partial\Omega}\frac{\delta}{|x-y|^2+\delta^2}\frac{<\nu(x)+\nu(y),x-y>}{|x-y|^2}\varphi(y)\ ds(y)+O(\delta^2)\ .
\end{aligned}
$$

The first integral converges uniformly to $S^0_{0,0}(\rho\varphi)$ in $H^1(\partial\Omega)$ and the last integral converges uniformly to $\dfrac{\rho\varphi}{2}$ in $H^1(\partial\Omega)$. The proof is then complete.

For $s=1$, we need to suppose that $\partial\Omega$ is $\mathcal{C}^3$ or equivalently that ρ is $\mathcal{C}^1$. For the first inequality, we need then to proof that

$$
\left\|\frac{\partial^2 S^k_{0,\delta}\varphi}{\partial\tau^2}-\frac{\partial^2 S^k_{0,0}\varphi}{\partial\tau^2}\right\|_{L^2(\partial\Omega)}\le\varepsilon_\delta\left\|\frac{\partial\varphi}{\partial\tau}\right\|_{L^2(\partial\Omega)}.
$$

Let us then study the term $\dfrac{\partial^2 S^k_{0,\delta}\varphi}{\partial\tau^2}$. We rewrite this term as

$$
\begin{aligned}
&2\frac{\partial^2 S^0_{0,\delta}\varphi}{\partial\tau^2}(x)=\\
&\frac{\partial}{\partial\tau(x)}\int_{\partial\Omega}\left(\frac{\partial}{\partial\tau(x)}+\frac{\partial}{\partial\tau(y)}\right)\log(|x-y|^2+\delta^2+2\delta<\nu(x),x-y>)\varphi(y)\ ds(y)\\
&+\frac{\partial}{\partial\tau(x)}\int_{\partial\Omega}\log(|x-y|^2+\delta^2+2\delta<\nu(x),x-y>)\frac{\partial\varphi(y)}{\partial\tau(y)}\ ds(y)\ .
\end{aligned}
$$

The second term in the above identity converges uniformly to $\dfrac{\partial S^0_{0,0}(\partial_\tau\varphi)}{\partial\tau}$ for $\partial_\tau\varphi$ bounded in $L^2(\partial\Omega)$. It remains then to find the limit of the first term that we denote by $2I_\delta$. Direct computations give

$$\begin{aligned} I_\delta &= \int_{\partial\Omega}\left(\frac{\partial}{\partial\tau(x)}+\frac{\partial}{\partial\tau(y)}\right)(1-\delta\rho(x)) \\ &\qquad\qquad \frac{<\tau(x),x-y>}{|x-y|^2+\delta^2+2\delta<\nu(x),x-y>}\varphi(y)\ ds(y) \\ &= -\delta\partial_{\tau(x)}\rho(x)\int_{\partial\Omega}\frac{<\tau(x),x-y>}{|x-y|^2+\delta^2+2\delta<\nu(x),x-y>}\varphi(y)\,ds(y) \\ &\quad +(1-\delta\rho(x))\int_{\partial\Omega}\left(\frac{\partial}{\partial\tau(x)}+\frac{\partial}{\partial\tau(y)}\right) \\ &\qquad\qquad \frac{<\tau(x),x-y>}{|x-y|^2+\delta^2+2\delta<\nu(x),x-y>}\varphi(y)\ ds(y). \end{aligned}$$

In a similar way as done for $s=0$, we show that the first term in the expression of I_δ is uniformly bounded in $L^2(\partial\Omega)$, for φ in the unit ball of $L^2(\partial\Omega)$, by

$$\delta\partial_{\tau(x)}\rho(x)\oint_{\partial\Omega}\frac{<\tau(x),x-y>}{|x-y|^2}\varphi(y)\ ds(y)\ .$$

We look now into the integral in the second term of I_δ which we denote by J_δ. We have

$$\begin{aligned} J_\delta &= \int_{\partial\Omega}\frac{\rho(x)<\nu(x),x-y>}{|x-y|^2+\delta^2+2\delta<\nu(x),x-y>}\varphi(y)\ ds(y) \\ &+\int_{\partial\Omega}\frac{<\tau(x),\tau(x)-\tau(y)>}{|x-y|^2+\delta^2+2\delta<\nu(x),x-y>}\varphi(y)\ ds(y) \\ &-2\int_{\partial\Omega}\frac{<\tau(x),x-y><\tau(x)-\tau(y),x-y>}{(|x-y|^2+\delta^2+2\delta<\nu(x),x-y>)^2}\varphi(y)\ ds(y) \\ &+2\delta\int_{\partial\Omega}\frac{<\tau(x),x-y>(\rho(x)<\tau(x),x-y>+<\tau(x),\nu(x)-\nu(y)>)}{(|x-y|^2+\delta^2+2\delta<\nu(x),x-y>)^2} \\ &\qquad\qquad\varphi(y)\ ds(y). \end{aligned}$$

The last term is uniformly bounded in $L^2(\partial\Omega)$, for φ in the unit ball of $L^2(\partial\Omega)$, by

$$\delta\oint_{\partial\Omega}\frac{<\tau(x),x-y>}{|x-y|^2}\frac{\rho(x)<\tau(x),x-y>+<\tau(x),\nu(x)-\nu(y)>}{|x-y|^2}\varphi(y)\ ds(y)\ .$$

We prove then in a similar way as done for $s=0$ that J_δ converges uniformly in $L^2(\partial\Omega)$, for φ in the unit ball of $L^2(\partial\Omega)$ to J_0, given by

$$\begin{aligned} J_0 &= \int_{\partial\Omega}\frac{\rho(x)<\nu(x),x-y>}{|x-y|^2}\varphi(y)\ ds(y)+\oint_{\partial\Omega}\frac{<\tau(x),\tau(x)-\tau(y)>}{|x-y|^2} \\ &\quad \varphi(y)\ ds(y)-2\oint_{\partial\Omega}\frac{<\tau(x),x-y>}{|x-y|^2}\frac{<\tau(x)-\tau(y),x-y>}{|x-y|^2}\varphi(y)\ ds(y). \end{aligned}$$

Therefore, it follows that $\dfrac{\partial^2 S^0_{0,\delta}\varphi}{\partial\tau^2}$ converges uniformly to $\dfrac{\partial^2 S^0_{0,0}\varphi}{\partial\tau^2}$ in $L^2(\partial\Omega)$, for φ in the unit ball of $L^2(\partial\Omega)$, since it can be easily checked that

$$\begin{aligned}\frac{\partial^2 S^0_{0,0}\varphi}{\partial\tau^2}(x) &= \frac{\partial S^0_{0,0}(\partial_\tau\varphi)}{\partial\tau}(x) + \int_{\partial\Omega} \frac{\rho(x) < \nu(x), x-y >}{|x-y|^2}\varphi(y)\ ds(y)\\ &+ \oint_{\partial\Omega} \frac{< \tau(x), \tau(x)-\tau(y) >}{|x-y|^2}\varphi(y)\ ds(y)\\ &-2\oint_{\partial\Omega} \frac{< \tau(x), x-y >}{|x-y|^2}\frac{< \tau(x)-\tau(y), x-y >}{|x-y|^2}\varphi(y)\ ds(y).\end{aligned}$$

The proofs for the other inequalities essentially follow the same arguments.

Bibliography

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