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

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Abstract

We present a rigorous study of the convergence of the *supercell* method used for determing defect modes in photonic crystals with compactly supported perturbations. Transverse electric and transverse magnetic polarized waves are investigated in 2-D structures. We prove an exponential convergence of the defect frequencies with the *supercell* size and give a justification of the quasi independence of the corresponding eigenfunctions on the wave vector. We also give a characterization of the *supercell* eigenvalues corresponding to the background photonic crystal.

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 [18, 19, 28, 23] 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 [16, 17]. Other band gap structures have been found through computational and physical experiments. See [9, 8, 10, 2, 12].

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 [14, 15, 13]. See also Ammari and Santosa [1] and Kuchment and Ong [24] for the issue of existence of exponentially confined modes guided by line defects in photonic crystals.

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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 paper 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 paper 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 the supercell method and investigate its mathematical foundations in the TM case. Section 4 is devoted to the TE case. Finally in Section 5 the results of numerical experiments are presented to illustrate our main findings.

2 Notation and preliminary results

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

We assume that the crystal is periodic with period $[0,1]^2$, *i.e.*, that $\epsilon_{\rm p}(x + n) = \varepsilon(x)$ 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 one scalar partial differential equation and the other scalar functions follow immediately from that solution.

These equations are the Helmholtz equation:

$$\Delta u + \omega^2 \epsilon_{\rm p} u = 0 \ , \tag{2.1}$$

for the TM polarization, and the acoustic equation:

$$\nabla \cdot \frac{1}{\epsilon_{\rm p}} \nabla u + \omega^2 u = 0 \ , \tag{2.2}$$

for the TE polarization.

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

We first briefly present the Floquet-Bloch theory applied to the TM and TE operators in periodic media.

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 $\mathbb{Z}^2$, that is the transform assigning to a sufficiently decaying function $h(n)$ on $\mathbb{Z}^2$, 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 that is the appropriate transform in this case.

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

$$\mathcal{F}v(x, \xi) = \sum_{j \in \mathbb{Z}^2} v(x - j) e^{i\xi \cdot j} = \widehat{v(x - \cdot)} . \tag{2.3}$$

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:

$$(\mathcal{F}^{-1}v)(x) = \frac{1}{|\mathcal{B}|} \int_B v(x, \xi) d\xi , \tag{2.4}$$

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:

$$\begin{cases} \Phi v(x+n,\xi) = \Phi v(x,\xi) \ , & n\in\mathbb{Z}^2 \ , \\ \Phi v(x,\xi+\zeta) = e^{-i\zeta\cdot x}\Phi v(x,\xi) \ , & \zeta\in 2\pi\mathbb{Z}^2 \ . \end{cases} \tag{2.5}$$

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:

$$\Sigma = \cup_{\xi\in\mathcal{B}}\Sigma^\xi \ . \tag{2.6}$$

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:

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

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

$$-(\nabla_x - i\xi)\cdot\frac{1}{\epsilon_{\mathrm{p}}}(\nabla_x - i\xi)v(x,\xi) = \omega^2 v(x,\xi) \ , \quad v(\cdot,\xi)\in L^2(\mathbb{R}^2/\mathbb{Z}^2) \ . \tag{2.7}$$

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 $\Sigma_{\rm TE}$ and no propagation is possible for TE waves at the corresponding frequencies. This makes all the interest of photonic crystals.

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 $\Sigma_{TE} \neq \mathbb{R}^2$ and let ω be a frequency lying in a band gap. Let $G_{\rm p}$ be the Green's function of the TE operator defined by

$$\nabla \cdot \frac{1}{\epsilon_{\rm p}} \nabla G_{\rm p}(\omega; x, y) + \omega^2 G_{\rm p}(\omega; x, y) = \delta(x-y) \ , \quad x \in \mathbb{R}^2 \ . \tag{2.8}$$

It has been established in [7, 3] that the Floquet transform of $G_{\rm p}$ is analytic with respect to ω in a complex neighborhood of the real axis. In view of Paley-Wiener-type theorems, the analyticity of $\mathcal{F}G_{\rm p}$ is the key ingredient of the proof of the following result [14, 15, 13].

Lemma 2.1 *There exist two positive constants C_1 and C_2 depending only on $\omega_0^2 > 0$ such that for any $\omega^2 \notin \Sigma_{\rm TE}$,*

$$|G_{\rm p}(\omega; x, y)| \leq C_1 e^{-C_2 \, dist(\omega^2, \Sigma_{\rm TE})|x-y|} \ , \quad \textit{for } |x-y| \to +\infty \ . \tag{2.9}$$

Remark 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 $G_{\rm p}$ and thus inherit the exponential decay property.*

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

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

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

$$-\frac{1}{\epsilon_{\rm p}} (\nabla_x - i\xi) \cdot (\nabla_x - i\xi) v(x, \xi) = \omega^2 v(x, \xi) \ , \quad v(\cdot, \xi) \in L^2(\mathbb{R}^2/\mathbb{Z}^2) \ . \tag{2.10}$$

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

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

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

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 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 $\epsilon_{\rm p}$.

First, we introduce some simplified notations.

Definition 2.1 *We define the operator* A_{p} *by*

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

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*

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

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:

$$\varepsilon(x) = \epsilon_{\mathrm{p}}(x) - (\delta\varepsilon)\chi_{\Omega}(x) \ , \tag{2.11}$$

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

$$A = -\frac{1}{\varepsilon}\Delta \ , \tag{2.12}$$

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 [14]. 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 [14] is of importance to us.

Theorem 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 exists two constants* C_1 *and* C_2*, depending only on the distance of* ω^2 *to the spectrum* Σ_{p}*, such that*

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

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

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

$$\Delta u + \omega^2 \varepsilon(x) u = 0 \ . \tag{2.13}$$

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

$$u(x) = (\delta\varepsilon)\omega^2 \int_{\Omega} G_{\mathrm{p}}(\omega; x, y) u(y)\, dy \ . \tag{2.14}$$

The proof of the theorem is then a direct consequence of the exponential decay of the Green's function in Lemma 2.1. □

Remark 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 The supercell method

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

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:

$$\begin{cases} \varepsilon_N(x) = \varepsilon(x) \ , \quad \forall x \in]-N, N[^2 \ , \\ \varepsilon_N(x + 2Nj) = \varepsilon_N(x) \ , \quad \forall x \in \mathbb{R}^2 \ , \forall j \in \mathbb{N}^2 \ . \end{cases} \tag{3.15}$$

Definition 3.1 *We define the operator A_N on $L^2(\mathbb{R}^2)$ by:*

$$A_N = -\frac{1}{\varepsilon_N}\Delta \ , \tag{3.16}$$

and let Σ_N be its spectrum.

For $\xi \in \mathcal{B}_N = [-\frac{\pi}{2N}, \frac{\pi}{2N}[$, 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 3.2 *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*

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

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 [27], that will be useful for the convergence results.

Proposition 3.1 *Let A be a self-adjoint operator with a domain $\mathcal{D}(A)$ and a spectrum $\sigma(A)$, then, for $\mu \in \mathbb{R}$:*

$$dist(\mu, \sigma(A)) = \min_{\phi \in \mathcal{D}(A)} \frac{\|(A - \mu I)\phi\|}{\|\phi\|} \tag{3.17}$$

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 3.1 *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*

$$\max_{\omega^2 \in \cup_{k \in [-N+1, N-1[^2 \cap \mathbb{N}^2} \Sigma_{\mathrm{p}}^{\xi + k\pi/N} \cap [0, \omega_0^2]} dist(\omega^2, \Sigma_N^{\xi}) \leq \frac{C}{N^2} , \tag{3.18}$$

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

$$\left(\nabla - i\big(\xi + \frac{k\pi}{N}\big)\right) \cdot \left(\nabla - i\big(\xi + \frac{k\pi}{N}\big)\right)\phi + \omega^2 \epsilon_{\mathrm{p}} \phi = 0 \; . \tag{3.19}$$

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

$$\tilde{\phi}(x) = \phi(x) e^{-i\frac{\pi}{N} k \cdot x} \; . \tag{3.20}$$

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

$$(\nabla - i\xi) \cdot (\nabla - i\xi)\tilde{\phi} + \omega^2 \epsilon_{\mathrm{p}} \tilde{\phi} = 0 \; , \tag{3.21}$$

which can be rewritten as follows

$$(\nabla - i\xi) \cdot (\nabla - i\xi)\tilde{\phi} + \omega^2 \varepsilon \tilde{\phi} = -\chi_\Omega(\delta\varepsilon)\omega^2 \tilde{\phi} \; . \tag{3.22}$$

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:

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

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 3.1, 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

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

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

It follows from Proposition 3.1 that there exists an eigenvalue ω_ξ^2 belonging to the spectrum Σ_N^ξ of the operator A_N^ξ such that

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

which ends the proof. □

Remark 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. Larger is the size of the supercell, better is the approximation of the defect eigenvalues. But this will take much more time and need much more 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 $\Sigma_N = \cup_{\xi\in\mathcal{B}_N}\Sigma_N^\xi$ *is absolutely continuous, we deduce that each connected component of* $(\mathbb{R}^2 \setminus \Sigma_N) \cap \Sigma_{\rm p} \cap [0,\omega_0]$ *has a width smaller than* $\frac{2C}{N^2}$*.*

In practice, because of the growth of degeneracy of the eigenvalues located in $\Sigma_{\rm p}$ *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* $\Sigma_{\rm p}$ *is due to the presence of a defect eigenvalue in* Σ *close to the band or not.*

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

We also define $\Sigma_{\rm d}$ *as the set of the defect eigenvalues of the perturbed photonic crystal:*

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

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

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

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

The following proposition holds.

Proposition 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 $\xi_N \in \mathcal{B}_N$ and $\phi_N \in L^2(\mathbb{R}^2/2N\mathbb{Z}^2)$ with unit norm such that

$$(\nabla - i\xi_N)\cdot(\nabla - i\xi_N)\phi_N + \omega_N^2 \varepsilon_N \phi_N = 0 \quad \text{in } L^2(\mathbb{R}^2/2N\mathbb{Z}^2) \, . \tag{3.23}$$

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

$$\tilde{\phi}_N(x) = \int_\Omega G(\omega_N^2; x, y) e^{-i\xi_N\cdot y} \phi_N(y) \, dy \, . \tag{3.24}$$

The following lemma is needed.

Lemma 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:

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

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 [1]:

$$\sum_{j\in\mathbb{Z}^2, j\neq 0} \left|G(\omega^2; x, y+Nj)\right| \leq C_1 e^{-C_2 N}\ , \qquad \forall x \in]-N,N[^2\ ,\ \forall y \in \Omega\ . \quad (3.25)$$

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

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

We then deduce that:

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

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:

$$\|\tilde{\phi}_N\|_{L^2(\mathbb{R}^2)} \geq \|\tilde{\phi}_N\|_{L^2(]-N,N[^2)} \geq \frac{1}{2}\ . \quad (3.26)$$

Lemma 3.1 is then proved. $\square$

We now turn to the proof of Proposition 3.2. We have

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

Using estimate (3.25), 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

$$\Big|\sum_{j\in\mathbb{Z}^2, j\neq 0} G(\omega_N^2; x, y + Nj)e^{-i\xi_N\cdot(y+Nj)}\Big| \leq C_1 e^{-C_2 N}\,, \tag{3.27}$$

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:

$$\|\Delta\tilde{\phi}_N + \omega_N^2\varepsilon\tilde{\phi}_N\|_{L^2(\mathbb{R}^2)} \leq |(\delta\varepsilon)|\omega_N^2|\Omega| C_1 e^{-C_2 N}\,. \tag{3.28}$$

Lemma 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 3.2 *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 $\xi \in \mathcal{B}_{\mathcal{N}}$:

$$dist_{\mathcal{H}}\left(\Sigma_{\mathrm{d},N}^{\xi,\eta} \cap [0,\omega_0^2], \Sigma_{\mathrm{d}}^{\eta} \cap [0,\omega_0^2]\right) \leq C_1 e^{-C_2 N}. \tag{3.29}$$

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

$$\Delta u + \omega_{\mathrm{d}}^2 \varepsilon u = 0 \quad \text{in } \mathbb{R}^2 \,. \tag{3.30}$$

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 $x \in \mathbb{R}^2$,

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

Therefore

$$\Big((\nabla - i\xi)\cdot(\nabla - i\xi) + \omega_{\rm d}^2\varepsilon_N\Big)u^\xi(x)$$

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

From (3.25), it follows that there exist two positive constants C_1 and C_2, depending only on $\omega_{\rm d}^2$, such that

$$\begin{aligned}\left|\int_\Omega\Big(\sum_{j\in\mathbb{Z}^2, j\neq 0} G(\omega_{\rm d}^2; x+Nj, y)e^{i\xi\cdot(x+Nj)}\Big)u(y)\,dy\right| &\leq C_1 e^{-C_2N}\int_\Omega |u(y)|\,dy \\ &\leq C_1e^{-C_2N}|\Omega|^{\frac{1}{2}}\|u\|_{L^2(\Omega)} \\ &\leq |\Omega|^{\frac{1}{2}}C_1e^{-C_2N}\,.\end{aligned}$$

Therefore

$$\left\|(\nabla - i\xi)\cdot(\nabla - i\xi)u^\xi(x) + \omega_{\rm d}^2\varepsilon_N u^\xi(x)\right\|_{L^2(]-N,N[^2)} \leq (\delta\varepsilon)^2\omega_{\rm d}^4|\Omega|C_1e^{-C_2N}\,. \quad (3.31)$$

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

$$\|\sum_{j\in\mathbb{Z}^2, j\neq 0} u(x+Nj)e^{i\xi\cdot(x+Nj)}\|_{L^2(]-N,N[^2)} \leq |\Omega|^{\frac{1}{2}}NC_1e^{-C_2N}\ ,$$

we deduce that for N large enough,

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

Thus, we conclude that

$$\mathrm{dist}(\omega_{\rm d}^2, \Sigma_N^\xi) \leq C_1e^{-C_2N}\ ,$$

for two positive constants C_1 and C_2, depending only on $\omega_{\rm d}^2$.

It is clear that we can choose these constants such that

$$\max_{\omega_{\rm d}\in\Sigma_{\rm d}^\eta\cap[0,\omega_0^2]}\mathrm{dist}(\omega_{\rm d}^2, \Sigma_N^\xi) \leq C_1e^{-C_2N}\ , \quad (3.32)$$

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

Let $\eta > 0$ be small enough to get $\Sigma_{\rm d}^\eta \neq \emptyset$. Applying Proposition 3.2, we may see that there exists $N_0\in\mathbb{N}$ depending only on ω_0^2 and η such that $\Sigma_{{\rm d},N}^{\xi,\eta}\cap[0,\omega_0^2]$ has at least as many connected components as $\mathrm{card}(\Sigma_{\rm d}^\eta\cap[0,\omega_0^2])$ for $N\geq N_0$. To prove this, we take a neighborhood of $\Sigma_{\rm d}^{\eta} \cap [0, \omega_0^2]$ formed by disjoint intervals and that are away from $\Sigma_{\rm p}$, each one of them containing exactly one defect eigenvalue. Then from Proposition 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 $\Sigma_{{\rm d},N}^{\xi,\eta}$ is not empty if we take η small enough and then let N be large enough. By the same way, (3.32) can be written as

$$\max_{\omega_{\rm d} \in \Sigma_{\rm d}^{\eta} \cap [0,\omega_0^2]} \mathrm{dist}(\omega_{\rm d}^2, \Sigma_{{\rm d},N}^{\xi,\eta}) \le C_1 e^{-C_2 N} \,, \tag{3.33}$$

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

Now, let $\xi \in \mathcal{B}_N$ and let $\omega^2 \in \Sigma_{{\rm d},N}^{\xi,\eta}$. 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

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

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

$$\Big| \sum_{j\in\mathbb{Z}^2, j\neq 0} \Big(G(\omega^2; x, y+Nj) e^{-i\xi\cdot(y+Nj)}\Big)\Big| \le C_1 e^{-C_2 N} \,, \ \forall x \in]-N, N[^2 \,, \forall y \in \Omega \,, \tag{3.34}$$

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

$$\Big\| \int_{\Omega} \sum_{j\in\mathbb{Z}^2, j\neq 0} \Big(G(\omega^2; x, y + Nj) e^{-i\xi\cdot(y+Nj)}\Big)\phi(y)\, dy \Big\|_{L^2(]-N,N[^2)} \le N C_1 e^{-C_2 N} \,, \tag{3.35}$$

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

$$\|\phi\|_{L^2(\mathbb{R}^2)} \ge \|\phi\|_{L^2(]-N,N[^2)} \ge \frac{1}{2} \,. \tag{3.36}$$

On the other hand,

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

Therefore, it follows from (3.34) that

$$
\left|\Delta u(x) + \omega^2 \varepsilon u(x)\right| \leq |(\delta\varepsilon)| \omega_0^2 |\Omega|^{\frac{1}{2}} C_1 e^{-C_2 N}\, ,
$$

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

$$
\|\Delta u + \omega^2 \varepsilon u\|_{L^2(\mathbb{R}^2)} \leq |(\delta\varepsilon)| \omega_0^2 |\Omega| C_1 e^{-C_2 N}\, . \tag{3.37}
$$

From (3.36), we readily get

$$
\mathrm{dist}(\omega^2, \Sigma) \leq C_1 e^{-C_2 N}\, ,
$$

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

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

$$
\mathrm{dist}(\omega^2, \Sigma_{\rm d}^\eta) \leq C_1 e^{-C_2 N}\, ,
$$

which ends the proof of the theorem. □

An immediate consequence of this theorem is the following.

Corollary 3.1 *Suppose that the perturbation has created defect eigenvalues. Then, there exists $\eta_0 > 0$ and $N_0 \in \mathbb{N}$ such that $\Sigma_{{\rm d},N}^\eta \neq \emptyset$ 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 $\Sigma_{{\rm d},N}^\eta \cap [0, \omega_0^2]$ is at least equal to card $\left(\Sigma_{\rm d}^\eta \cap [0, \omega_0^2]\right)$ 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

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

$\square$

Remark 3.2 *These results are very important and practical 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.

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 $-\nabla.\frac{1}{\epsilon_{\mathrm{p}}}\nabla$ 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.

4.1 Definition and preliminary results

First we introduce some analogous notations to those in Definition 2.1.

Definition 4.1 *Let A_{p} be the operator defined by*

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

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

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

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

We perturb the background periodic medium on a bounded domain as done in (2.11).

It has been proved that the spectrum of A_{p} is absolutely continuous and that the perturbation is relatively compact and so does not affect the essential spectrum of A_{p}. The perturbation will then 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 3.1. 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 4.2 *Let B_{p} be the operator defined on $L^2(\mathbb{R}^2)^2$ by*

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

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

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

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

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

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 [23]). 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 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

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

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

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

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

We conclude that all the eigenvalues of $A_{\rm p}^{\xi}$ except for the eigenvalue 0 of $A_{\rm p}^{0}$ are eigenvalues of $B_{\rm p}^{\xi}$. We will see that 0 is an infinite multiplicity eigenvalue of $A_{\rm p}^{0}$.

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

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

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 $B_{\rm p}^{\xi}$ 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,

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

which means that ω^2 is an eigenvalue of $A_{\rm p}^{\xi}$. We can also show that if ψ_1 and ψ_2 are two linearly independent eigenvectors of $B_{\rm p}^{\xi}$ 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 A_N^{ξ} and B_N^{ξ} 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_N^{ξ} and A_N by studying those of B_N^{ξ} 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 2.1 for the operator $B_{\rm p}$.

Lemma 4.1 *For any $z \notin \Sigma_{\rm p}$ and $l > 0$ we have*

$$\|\chi_{x,l}R(z)\chi_{y,l}\| \leq \left(\frac{9}{\eta}\right) e^{(\sqrt{2}l/4)} e^{-m_z|x-y|} \quad \textit{for all } x, y \in \mathbb{R}^2 \ , \tag{4.38}$$

with

$$m_z = \frac{\eta}{4(2\varepsilon_-^{-1} + |z| + \eta)} \ , \tag{4.39}$$

where $\eta = dist(z, \Sigma_{\rm p})$, $\varepsilon_- = \min_{x\in\mathbb{R}^2} \epsilon_{\rm p}(x)$, *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 Combe-Thomas argument and can be found in [14, 15, 13].

Let B_a denote the operators formally given by

$$B_a = e^{a\cdot x} B_p e^{-a\cdot x} \ , \quad a \in \mathbb{R}^2 \ , \tag{4.40}$$

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

$$\mathcal{B}_a[\psi] = \langle \nabla\cdot(e^{a\cdot x}\psi), \frac{1}{\epsilon_{\rm p}(x)} \nabla\cdot(e^{-a\cdot x}\psi)\rangle = \langle(\nabla + a)\cdot\psi, \frac{1}{\epsilon_{\rm p}(x)}(\nabla - a)\cdot\psi\rangle \ . \tag{4.41}$$

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

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

Since

$$\left| \langle a\cdot\psi, \frac{1}{\epsilon_{\rm p}(x)}\nabla\cdot\psi\rangle \right| \le \frac{1}{2}|a| \left(\langle\psi, \frac{1}{\epsilon_{\rm p}(x)}\psi\rangle + \langle\nabla\cdot\psi, \frac{1}{\epsilon_{\rm p}(x)}\nabla\cdot\psi\rangle \right) \ , \tag{4.42}$$

we have

$$|\mathcal{Q}_a[\psi]| \le |a|\mathcal{B}_0[\psi] + |a|(1+|a|)\varepsilon_-^{-1}\|\psi\|^2 \quad \text{for all } \psi \in C_0^1(\mathbb{R}^2) \ . \tag{4.43}$$

Then we require $|a| < 1$ and use Theorem VI.3.9 in [21] 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

$$\Lambda \equiv 2\left\|(|a|(1+|a|)\varepsilon_-^{-1} + |a|B_{\rm p})(B_{\rm p} - zI)^{-1}\right\| < 1 \ , \tag{4.44}$$

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

$$\|R_a(z) - R_0(z)\| \le \frac{4\Lambda}{(1-\Lambda)^2}\|R_0(z)\| \ , \tag{4.45}$$

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

Since

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

it is sufficient to take

$$|a| < \frac{\eta}{2(2\varepsilon_-^{-1} + |z| + \eta)} \ , \tag{4.46}$$

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

$$|a| < m_z = \frac{\eta}{4(2\varepsilon_-^{-1} + |z| + \eta)} \ , \tag{4.47}$$

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

$$\|R_a(z)\| \leq \left(1 + \frac{4\Lambda}{(1-\Lambda)^2}\right) \|R_0(z)\| \leq \frac{9}{\eta} \ . \tag{4.48}$$

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

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

We also notice that

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

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

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

$$\nabla\nabla \cdot K(\omega^2; x, y) + \omega^2 \epsilon_{\rm p} K(\omega^2; x, y) = \delta(x - y) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \ . \tag{4.49}$$

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

$$|K(\omega^2; x, y)| \leq C_1 e^{-C_2\, dist(\omega^2, \Sigma_{\rm p})|x-y|} \ , \quad \textit{for } |x - y| \to +\infty \ . \tag{4.50}$$

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

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 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*

$$\max_{\omega^2 \in \cup_{k \in [-N+1, N-1[^2 \cap \mathbb{N}^2} \Sigma_\mathrm{p}^{\xi + k\pi/N} \cap [0,\omega_0^2]} dist(\omega^2, \Sigma_N^\xi) \leq \frac{C}{N^2} , \tag{4.51}$$

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 $\Sigma_\mathrm{p}^{\xi+k\pi/N} \cap [0, \omega_0^2]$. 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 $\omega^2 \neq 0$. From Theorem 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

$$\left(\nabla - i(\xi + \frac{k\pi}{N})\right)\left(\nabla - i(\xi + \frac{k\pi}{N})\right) \cdot \phi + \omega^2 \epsilon_\mathrm{p} \phi = 0 . \tag{4.52}$$

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

$$\tilde{\phi}(x) = \phi(x) e^{-i\frac{\pi}{N} k \cdot x} . \tag{4.53}$$

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

$$(\nabla - i\xi)(\nabla - i\xi) \cdot \tilde{\phi} + \omega^2 \epsilon_\mathrm{p} \tilde{\phi} = 0 , \tag{4.54}$$

which can be written as

$$(\nabla - i\xi)(\nabla - i\xi) \cdot \tilde{\phi} + \omega^2 \varepsilon \tilde{\phi} = -\chi_\Omega(\delta\varepsilon)\omega^2 \tilde{\phi} . \tag{4.55}$$

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

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

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

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

The theorem is then proved. □

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. The following proposition holds.

Proposition 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

$$(\nabla-i\xi_N)(\nabla-i\xi_N)\cdot\phi_N+\omega_N^2\varepsilon_N\phi_N=0\,,\quad\text{in } L^2(\mathbb{R}^2/2N\mathbb{Z}^2)^2\,. \tag{4.56}$$

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

$$\tilde{\phi}_N(x)=\int_\Omega K(\omega_N^2;x,y)e^{-i\xi_N\cdot y}\phi_N(y)\,dy\,. \tag{4.57}$$

Using $\tilde{\phi}_N$, we prove in a similar way as for Proposition 3.2 that

$$\frac{\|\nabla\nabla\cdot\tilde{\phi}_N+\omega_N^2\varepsilon\tilde{\phi}_N\|_{L^2(\mathbb{R}^2)^2}}{\|\tilde{\phi}_N\|_{L^2(\mathbb{R}^2)^2}}\leq C_1e^{-C_2N}\,, \tag{4.58}$$

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

$$\text{dist}(\omega_N^2,\Sigma)\leq C_1e^{-C_2N}\,, \tag{4.59}$$

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 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* $N\geq N_0$,

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

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* $\xi\in\mathcal{B}_\mathcal{N}$:

$$dist_\mathcal{H}\left(\Sigma_{{\rm d},N}^{\xi,\eta}\cap[0,\omega_0^2],\Sigma_{\rm d}^\eta\cap[0,\omega_0^2]\right)\leq C_1e^{-C_2N}\,. \tag{4.60}$$

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 3.2. □

Note that the Corollary 3.2 holds for the TE polarization.

5 Numerical experiments

The numerical simulations presented in this section are computed with the *MIT Photonic-Bands* (MPB) package [20]. 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 1 where the dark area corresponds to dielectric permittivity 12.

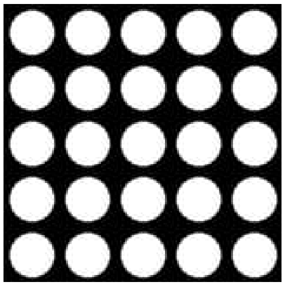


Figure 1: The periodic structure.

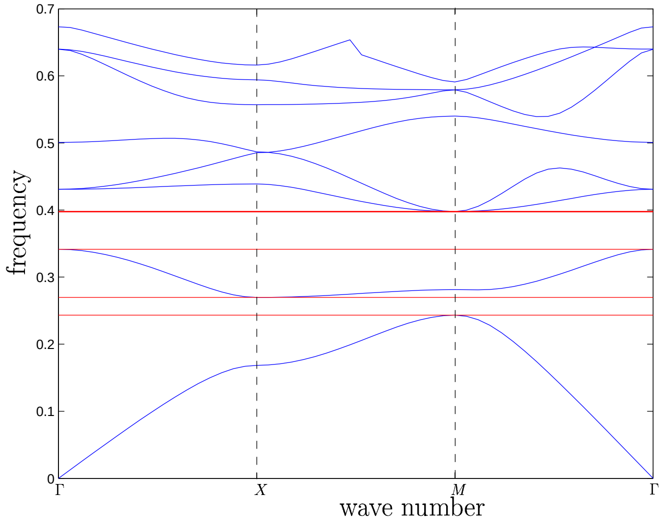


Figure 2: TE-spectrum of the periodic structure.

We investigate only the TE polarization. We compute the TE-spectrum of this structure for the first 8 bands. This is shown in Figure 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. 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 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 1.

The convergence of the continuous spectrum is in $1/N$ 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.

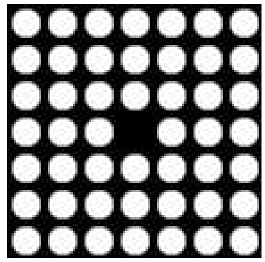


Figure 3: The 7x7 supercell.

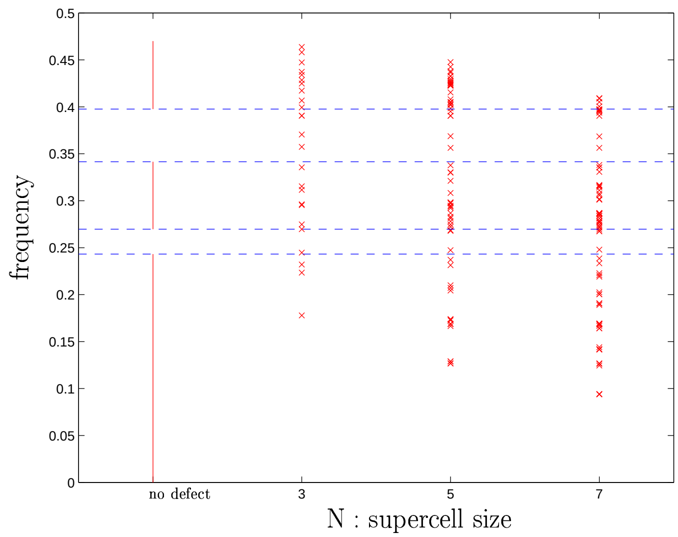


Figure 4: TE-spectrum of the supercell.

In Figure 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.

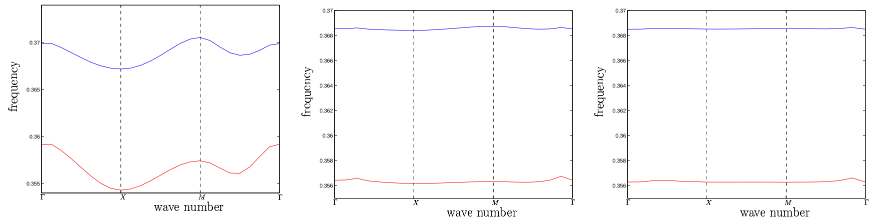
Finally, in Figures 6-9 we represent the energy distribution and the magnetic field for the defect modes in the case of the 7x7 supercell.

6 Conclusion

We presented in this paper 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	0.3706 0.6%	0.3687 0.05%	0.3685
Defect frequency 2	0.3574 0.3%	0.3563 $\leq$00.3%	0.3563

Table 1: Defect frequencies and relative difference with the 7x7 supercell.



(a) 3x3 (b) 5x5 (c) 7x7

Figure 5: Dependence of the defect frequencies on the wave number.

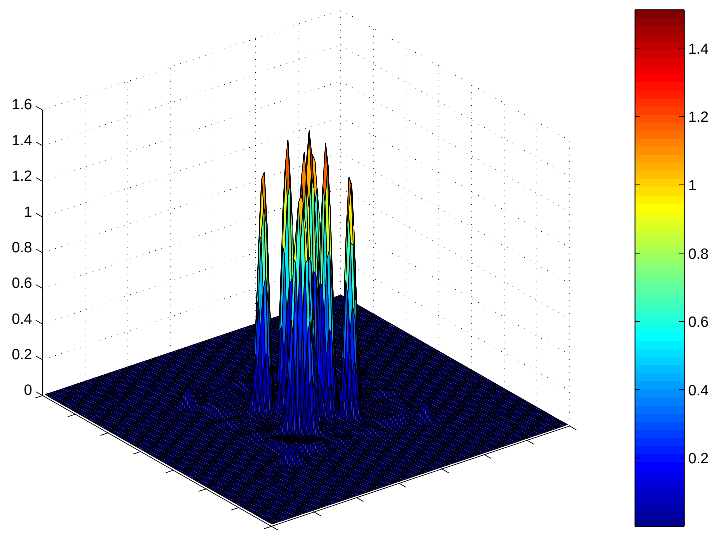


Figure 6: Energy distribution in the first defect mode.

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

$$O(\exp(-C\sqrt{|\omega^2 - \omega_a^2||\omega^2 - \omega_b^2|}\ |x|)). \tag{6.61}$$

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.

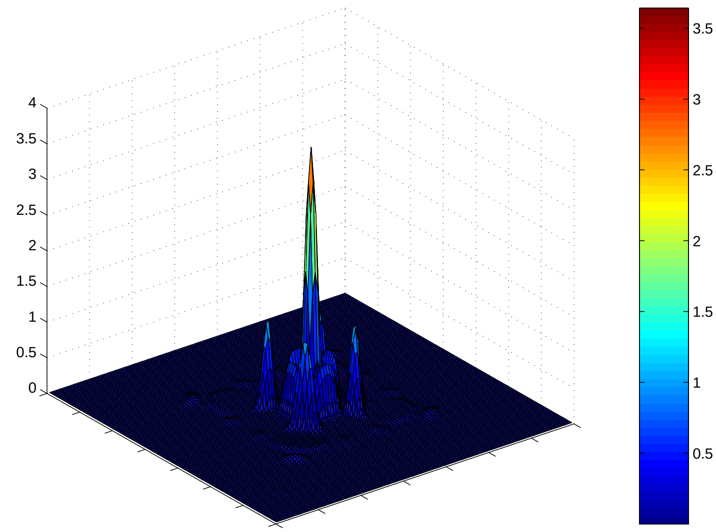


Figure 7: Energy distribution in the second defect mode.

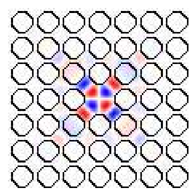


Figure 8: Magnetic field distribution in the first defect mode.

We believe that it should be possible to determine such eigenvalues in a faster way with integral operator methods.

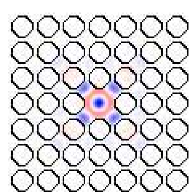


Figure 9: Magnetic field distribution in the second defect mode.

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