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Spectral analysis of the discrete Maxwell operator: The limiting absorption principle [*]

Olivier Poisson [1]

Abstract. — We make the beginning of the spectral analysis of the anisotropic discrete Maxwell operator $\widehat{H}^D$ defined on the square lattice $\mathbf{Z}^3$: we prove that the limiting absorption principle holds. To this aim we construct a conjugate operator to the Fourier series of $\widehat{H}^D$ at any not-zero real value. In particular, we analyse the case of thresholds of $\widehat{H}^D$.

Résumé. — Nous commençons l'analyse spectrale de l'opérateur de Maxwell discret anisotrope $\widehat{H}^D$ défini sur le réseau carré $\mathbf{Z}^3$: nous prouvons que le principe d'absorption limite est valable. Pour ce faire nous construisons un opérateur conjugué à la série de Fourier de $\widehat{H}^D$, en toute valeur réelle non nulle. En particulier, le cas des seuils est résolu.

1. Introduction

In this article, we begin the investigation of the spectral properties of the anisotropic Maxwell operator $\widehat{H}^D$ on the square lattice $\mathbf{Z}^3$, which is a standard model for describing wave motions on periodic structures.

Let $\boldsymbol{\varepsilon}$ and $\boldsymbol{\mu}$ be, respectively, the permittivity and the permeability in the ambient space $\mathbf{Z}^3$. These are 3×3 constant diagonal matrices with diagonal elements, $\varepsilon_1, \varepsilon_2, \varepsilon_3 \in (0, \infty)$ for $\boldsymbol{\varepsilon}$, and $\mu_1, \mu_2, \mu_3 \in (0, \infty)$ for $\boldsymbol{\mu}$. Let $\widehat{H}_0$ be

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Article proposé par Jean-François Coulombel.

the isotropic discrete Maxwell operator with $\boldsymbol{\varepsilon} = \boldsymbol{\mu} = I_{3\times 3}$; the anisotropic Maxwell operator is defined by

$$\widehat{H}^D = \widehat{D}\widehat{H}_0,$$

where we put

$$\widehat{D} = \begin{pmatrix} \boldsymbol{\varepsilon} & 0_{3\times 3} \\ 0_{3\times 3} & \boldsymbol{\mu} \end{pmatrix} \tag{1.1}$$

The definition of $\widehat{H}_0$ is easier via the Fourier discrete transform between the square lattice $\mathbf{Z}^3$ and the flat torus $\mathbb{T}^3 \approx (\mathbf{R}/(2\pi\mathbf{Z}))^3$. The Fourier series of $\widehat{H}_0$ is the following symmetric real 6×6 matrix:

$$H_0(x) = \begin{pmatrix} 0_{3\times 3} & M(\sin x) \\ -M(\sin x) & 0_{3\times 3} \end{pmatrix} \in \mathbf{R}^6, \quad x \in \mathbb{T}^3, \tag{1.2}$$

where we write $\sin x := (\sin x_1, \sin x_2, \sin x_3)$, and where $M(y)$ is the real anti-symmetric 3×3 matrix:

$$M(y) = \begin{pmatrix} 0 & -y_3 & y_2 \\ y_3 & 0 & -y_1 \\ -y_2 & y_1 & 0 \end{pmatrix}, \quad y \in \mathbf{R}^3. \tag{1.3}$$

Then, the Fourier series $H^D(x)$ of the unperturbed anisotropic Maxwell operator $\widehat{H}^D$ defines a bounded analytically fibered self-adjoint operator $\mathbb{T}^3 \ni x \mapsto H^D(x) = \widehat{D}H_0(x)$ on the Hilbert space $\mathcal{H}^D = L^2(\mathbb{T}^3, \mathrm{d}x, \mathbb{C}^6)$, which is equipped with the hilbertian product

$$(u, v)_{\mathcal{H}^D} := \int_{\mathbf{R}^3} \left\langle \widehat{D}^{-1}u(x), v(x) \right\rangle_{\mathbb{C}^6} \mathrm{d}x, \tag{1.4}$$

where $\langle \cdot, \cdot \rangle_{\mathbb{C}^n}$ denotes the usual hermitian product on $\mathbb{C}^n$.

The complete spectral analysis of $\widehat{H}^D$ being too long for a single article, we devote ourselves to the limiting absorption principle (LAP) for the resolvent of $\widehat{H}^D + \widehat{V}$ where $\widehat{V}$ is a real perturbation of $\widehat{H}^D$. We also consider in this article a seemingly different form of perturbation of $\widehat{H}^D$, but one that has physical significance, the perturbed anisotropic Maxwell operator $\widehat{H}^{D_p} = \widehat{D}_p\widehat{H}_0$ where $\widehat{D}_p$ is a perturbation of $\widehat{D}$; see (3.4) later.

The LAP is the key step in clarifying the detailed spectral structure of $\widehat{H}^D + \widehat{V}$ (or of $\widehat{H}^{D_p}$). It analyses the existence of the limits of the resolvents $(\widehat{H}^D + \widehat{V} - \zeta)^{-1}$ when the complex variable ζ tends to a spectral value of $\widehat{H}^D$, $\lambda \in \mathbf{R}$, i.e.,

$$\left(\widehat{H}^D + \widehat{V} - \lambda \mp i0\right)^{-1} = \lim_{\varepsilon \to 0^+} \left(\widehat{H}^D + \widehat{V} - \lambda \mp i\varepsilon\right)^{-1}$$

where the limit $(\widehat{H}^D+\widehat{V}-\lambda\mp i0)^{-1}$ is a bounded operator from X into Y for suitable Banach spaces X, Y rigging $L^2(\mathbf{Z}^3)$, i.e. $X \subset L^2(\mathbf{Z}^3) \subset Y$ with dense inclusions. The LAP was considered by Agmon [1] to see the continuous spectrum of the Schrödinger operator $-\Delta+V$ on $\mathbf{R}^d$. To realize it Agmon derived a theorem of division in some weighted $L^2(\mathbf{R}^d)$-space. Agmon–Hörmander in [2, 11, 12] supplemented this approach by introducing Besov spaces B, B^*, which are optimal for the existence of the limit $(-\Delta+V-\lambda\mp i0)^{-1}$. Since all functions of the form $u^{\pm}=(-\Delta+V-\lambda\mp i0)^{-1}f \in B^*$ with $f \in B$ satisfy the equation $(-\Delta+V-\lambda)u^{\pm}=f$, it is relevant to distinguish them by an additional condition. Hence, Agmon–Hörmander introduced the radiation condition in terms of pseudo-differential operators to guarantee the uniqueness of the solution. However the question on a radiation condition for $\widehat{H}^D$ is outside the scope of this article and will be dealt with in future articles. The spectral properties of Schrödinger operators $-\widehat{\Delta}_{\text{disc}}+\widehat{V}$ on periodic lattices of dimension $d \geqslant 2$ have been analysed in depth by several authors since the 20^{st} century. In our notation, the Fourier series of $\widehat{\Delta}_{\text{disc}}$ defines the multiplication operator by the function $2\sum_{j=1}^{d}\cos(x_i)$ on $L^2(\mathbb{T}^d,\mathbb{C})$. Shaban–Vainberg [22] proved that the LAP holds for $-\widehat{\Delta}_{\text{disc}}+\widehat{V}$ outside eigenvalues and thresholds, and assert that it fails for the unperturbed operator $-\widehat{\Delta}_{\text{disc}}$ at the thresholds. In their case, the thresholds are the integers contained in the spectrum $[-2d,2d]$ of $-\widehat{\Delta}_{\text{disc}}$ of the form $\pm 4n$ when d is even and $\pm 2(2n+1)$ when d is odd. In fact, let λ be a threshold of $\widehat{\Delta}_{\text{disc}}$ and let $\widehat{G}_\zeta \in L^2(\mathbf{Z}^3,\mathbb{C})$ be the exponentially decaying at infinity fundamental solution of the operator $-\widehat{\Delta}_{\text{disc}}-\zeta$, $\Im\zeta \neq 0$. Shaban–Vainberg [22] proved that $\widehat{G}_\zeta(n)$ does not have a pointwise limit as $\zeta \to \lambda \pm i0$. However, the result of Shaban–Vainberg is not an impossibility for the LAP in our definition above. More recently, Isozaki et al. [4] have studied the spectral properties of Schrödinger operators on perturbed periodic lattices of dimension $d \geqslant 2$. In particular, they proved that outside an exceptional set, the LAP is valid in terms of Besov spaces.

An alternative way of performing the spectral analysis of Schrödinger operators is the commutator method invented by Eric Mourre in the famous paper [18]. The commutator method was then developed and applied in [6, 17, 19, 21]. An essentially optimal version of this method was developed in [3, 5]. Gérard–Nier [8] developed the Mourre theory for an abstract class of self-adjoint operators they call "analytically fibered operators". Then, they proved that the LAP and its main consequences are valid, such as the existence and asymptotic completeness of wave operators for perturbations of these operators.

In our article, we therefore adopt Mourre's method with the technical ideas of Gérard–Nier. Let's briefly recall part of it, denoting by H^D both our operator and the general analytically fibered operator of Gérard–Nier. Let $\lambda \in \sigma(H^D)$, $\sigma(H^D)$ being the spectrum of H^D, the commutator method consists in constructing a self-adjoint (unbounded with dense domain) operator A on $\mathcal{H}^D$, called the conjugate operator, which satisfies several conditions, the main ones being:

(i) The formal commutator $[H^D, iA] := H^D iA - iAH^D$ satisfies the strict Mourre's inequality which we write here for simplicity "$[H^D, iA] \geqslant \delta > 0$ near λ" and whose sense will be precised later.
(ii) the multi-commutators $\mathrm{ad}_A^k(H^D)$ are bounded on $\mathcal{H}^D$, $k \geqslant 1$. Here, formally $\mathrm{ad}_A^k(H^D) := [\mathrm{ad}_A^{k-1}(H^D), A]$ for $k \geqslant 1$, and $\mathrm{ad}_A^0(H^D) := H^D$.

(See [8, points (i)–(ii) of Theorem 3.1] or points (i)–(ii) of Theorem 3.1.) The construction of the conjugate operator is based on the stratification of the energy-momentum set. Let $\sigma(H^D(x))$ be the spectrum of $H^D(x)$, then the energy-momentum set $\Sigma = \{(\lambda, x) \mid \lambda \in \sigma(H^D(x))\}$ is stratified by $\Sigma = \bigcup_{j=1}^m \Sigma_j$, where Σ_i is the semi-analytical set of elements (λ, x) for which λ is an eigenvalue of multiplicity i of $H^D(x)$. In our case we have $m = 6$, $\Sigma_i = \emptyset$ for $i \in \{3, 4, 5\}$ and $\Sigma_6 = \{(0, x);\ \sin x = 0\}$. At this stage, we need to introduce our set $\mathcal{T}$ of thresholds, which may be different from and larger than the abstract set of thresholds introduced by Gérard–Nier. A full description of $\mathcal{T}$ is given in Section 2.4. For now, the reader can assume that $\mathcal{T}$ is a finite subset of $\sigma(H^D)$ defined from each stratum Σ_i, i.e., it has the form $\mathcal{T} = \bigcup_i \mathcal{T}_i$ (which is not a partition) with $\mathcal{T}_i \subset P_{\mathbf{R}}(\Sigma_i)$, where $P_{\mathbf{R}} : (\lambda, x) \mapsto \lambda$ is the first canonical projection from $\mathbf{R} \times \mathbb{T}^3$ into $\mathbf{R}$. It appears that the strata Σ_j and the set of thresholds depend mainly on the parameter $\boldsymbol{\beta} = \boldsymbol{\varepsilon} \times \boldsymbol{\mu} = (\beta_1, \beta_2, \beta_3)$ where $\boldsymbol{\varepsilon}$ and $\boldsymbol{\mu}$ denote permittivity and permeability respectively. In fact, apart from the first relatively simple case $\boldsymbol{\beta} = 0$, we have to deal with the following special cases: $\prod_{i=1}^3 \beta_i = 0$, $\prod_{i=1}^3 \beta_j \neq 0$ and two coordinates β_j, β_k with $k \neq j$ coincide (or not). Given any compact set $I \subset \mathbf{R} \backslash \mathcal{T}$, the authors of [8] construct a local conjugate operator A_{λ_i, x_0} to H^D near each point (λ_i, x_0) of a given stratum Σ_i such that $\lambda_i \in I$. By a compactness argument the conjugate operator A_I is defined as a finite sum of A_{λ_i, x_0}'s. The construction of A_I has very recently been revised by Gérard–Nier in [9] since it was pointed out to them by the author that their second commutator $\mathrm{ad}_{A_I}^2(H^D)$ is in fact not bounded. The problem appeared in the insufficient connection between several strata for A_I. Consequently, H^D would have been of class $\mathcal{C}^1(A_I)$ but not of class $\mathcal{C}^2(A_I)$. The property $H^D \in \mathcal{C}^1(A_I)$ is sufficient to obtain the structure of the spectrum of H^D but insufficient to garantee the completeness of the wave operators. In the new version [9] Gérard–Nier take into account the connection between the different strata by considering an additional term in A_I. The cost of correcting [8] in [9] is not high: the (strict) *globality* of Mourre's inequality (3.1) is lost but is replaced by a local inequality, as (3.3). This recent technical aspect is also exploited in our work. At this point we could simply apply [9, Theorem 1.1] and state that for any interval $I \subset\subset \mathbf{R} \setminus \mathcal{T}$ and for any $\lambda \in I$, there exists an operator A_I with domain $\mathcal{C}^\infty(\mathbb{T}^3, \mathbb{C}^6)$, essentially self-adjoint on $\mathcal{H}^D$, conjugate to H^D at λ, and satisfying [9, points (i)–(iii) of Theorem 1.1]. (Precisely, [9, points (i)–(ii) of Theorem 1.1] are respectively points (i)–(ii) above rigorously stated, and the additional [9, Theorem 1.1 (iii)] says that A_I is a first order differential operator with $\mathcal{C}^\infty$ coefficients satisfying Relation (3.2).) However we go beyond this result, notably because in the abstract framework of Gérard–Nier, the choice of the couples (λ_i, x_0) is not explicit, so their construction of A_I is not; because, too, their statement of the LAP avoids thresholds: the interval I does not touch $\mathcal{T}$ (their conjugate operator A_I vanishes in a neighborhood of $\mathcal{T}$). Following the ideas in the old version [8] and in the new version [9], we construct an explicit conjugate operator to H^D having, at least far from the thresholds, the same properties as the conjugate operator in [8, Theorem 3.1]. In fact, our (strict) Mourre's inequality (3.1) is still global. In addition, we complete the construction of the conjugate operator near the non-zero thresholds. Let's go into a little more detail. Let P_M be the second canonical projection from $\mathbf{R} \times \mathbb{T}^3$ into $\mathbb{T}^3$ and let $\mathcal{X}_j$ be the set $P_M(\Sigma_j)$. Since Σ_j is empty for $j = 3, 4, 5$ and $P_{\mathbf{R}}(\Sigma_6)$ is reduced to the eigenvalue 0, we then are concerned only with Σ_j and $\mathcal{X}_j$ for $j = 1, 2$, i.e., with the points $x \in \mathbb{T}^3$ for which $H^D(x)$ has positive or negative eigenvalues of order one or two. By ordering the eigenvalues $\lambda_1(x) \leqslant \cdots \leqslant \lambda_6(x)$ of $H^D(x)$, then, for $x^* \in \mathcal{X}_j$ $(j = 1, 2)$, the eigenvalue $\lambda_k(x^*)$ is a threshold in $\mathcal{T}_j$ iff it satisfies both:

- $\lambda_k(x^*)$ is of multiplicity j in $H^D(x^*)$, i.e., $(\lambda_k(x^*), x^*) \in \Sigma_j$;
- the variation of the restriction $\lambda_k(\cdot)|_{\mathcal{X}_j}$ of the function λ_k to the set $\mathcal{X}_j$ vanishes at x^*.

We denoted by $\mathcal{X}_j^*$ the set of such values x^* and we put $\mathcal{X}^* = \mathcal{X}_1^* \cup \mathcal{X}_2^*$ (which is a partition). It appears that $\mathcal{X}^*$ is finite and, for any $x^* \in \mathbb{T}^3$, we have $x^* \in \mathcal{X}^*$ if and only if $\sigma(H^D(x^*)) \cap (\mathcal{T} \setminus \{0\})$ is not void. We fix a smooth numerical function ϕ whose support is compact in $\mathbf{R}^*$ and has the same utility than the interval I in [8] and mentioned above. We construct A_ϕ as a symmetric first order differential operator with smooth coefficients outside $\mathcal{X}^*$ and with rational singularities at points $x^* \in \mathcal{X}^*$ for which $\sigma(H^D(x^*)) \cap \mathcal{T} \cap \phi^{-1}(\mathbf{R}^*)$ is not empty. Precisely, A_ϕ has the form $A_\phi = A_{\text{in}} + A_{\text{out}}$, A_{in} and A_{out} both beeing symmetric first order differential operators. The operator A_{out} is concerned with the part of $\operatorname{supp} \phi$ that does not touch $\mathcal{T}$; it is therefore very similar to the conjugate operator A_I in [9, 8]; in particular, it has smooth coefficients and is essentially self-adjoint. It is itself the sum of three terms in the most general case where $\mathcal{X}_1$ and $\mathcal{X}_2$ are not empty (in fact, when $\boldsymbol{\beta} \neq 0$; the case $\boldsymbol{\beta} = 0$ is simpler). The first two terms of this sum have support near $\mathcal{X}_1$ and $\mathcal{X}_2$ respectively. The third term is the connection between $\mathcal{X}_1$ and $\mathcal{X}_2$, and is based on the correction in [9]. The operator A_{in} is concerned with non-zero thresholds, so with the discrete set $\mathcal{X}^*$. It is the finite sum of firt order differential operators, A_{x^*}, where $x^* \in \mathcal{X}^*$. Each operator A_{x^*} has support in a small neighborhood of x^* and its coefficients have a rational singularity at x^*; it admits a maximal monotone extension which is possibly self-adjoint on $\mathcal{H}^D$. It then turns out that we can write $\mathcal{T}$ as a non trivial partition $\mathcal{T} = \{0\} \cup \mathcal{T}_{\text{sa}} \cup \mathcal{T}_{\text{sm}}$, where $\mathcal{T}_{\text{sm}}$ is the set of non zero extreme values of the functions $\lambda_k|_{\mathcal{X}_j}$ seen above, so if $\operatorname{supp}\phi$ doesn't touch $\mathcal{T}_{\text{sm}}$, then A_ϕ is essentially self-adjoint. We thus obtain the LAP on $\mathbf{R}^* \setminus \mathcal{T}_{\text{sm}}$ in the same terms as [8, Theorem 3.3] (see (i)–(iv) of Theorem 3.1). If $\operatorname{supp}\phi$ touchs $\mathcal{T}_{\text{sm}}$ we can't expect A_ϕ to be essentially self-adjoint. In fact, it may not have a maximal monotone extension, since its singularities may originate from several points of $\mathcal{X}^*$ and it is known that the sum of two maximal monotone operators, even with disjoint supports, is not necessarily maximal monotone. Nevertheless, we can prove that the LAP holds on $\mathcal{T}_{\text{sm}}$ by a slight extension of [7, Theorem 3.3] (see (i)–(iii) and (v) of Theorem 3.1).

Plan of the paper

In Section 2 we describe the analytically fibered self-adjoint operator H^D. Precisely, we compute in Section 2.3 the spectrum of $H^D(x)$ and we describe in Section 2.4 the stratification of the energy-momentum set Σ and the set of thresholds $\mathcal{T}$. In Section 3 we state the main results of our work, including the existence of a conjugate operator A_ϕ for H^D in Theorem 3.1; then we establish several LAPs in terms of abstract or usual Besov spaces in Corollaries 3.3–3.7. We then give three (abstract) examples to complete Corollary 3.7. In Section 4 we construct the conjugate operator A_ϕ according to the parameter $\boldsymbol{\beta}$. We prove also the main properties of A_ϕ. In Section 5 we prove the main results of Section 3 and slightly extend some of the results in [7]. In Section 6 we give a conclusion to our work and discuss possible future prospects.

Notations

All along the text we use the following notations. Let $\mathcal{E} \in \{\mathbb{T}^3, \mathbf{R}^3\}$ where $\mathbb{T}^3 \approx (\mathbf{R}/(2\pi\mathbf{Z}))^3$ is the 3-dimensional real torus. If f is a numerical function (from $\mathbf{R}$ into $\mathbf{R}$) we then denote by f again the mapping $\mathcal{E} \ni x \mapsto (f(x_1), f(x_2), f(x_3)) \in \mathbf{R}^3$, so if $E \subset \mathcal{E}$ then $f(E) = \{f(x);\ x \in E\} \subset \mathbf{R}^3$ and if $E \subset \mathbf{R}^3$ then $f^{-1}(E) = \{x \in \mathcal{E};\ f(x) \in E\}$. In particular we set, for $x \in \mathcal{E}$,

$$\begin{aligned} y = \sin x \ &:= (y_1 = \sin x_1, y_2 = \sin x_2, y_3 = \sin x_3) \in \mathbf{R}^3, \\ z = \sin^2 x &:= \big(\sin^2 x_1, \sin^2 x_2, \sin^2 x_3\big) \in \mathbf{R}^3. \end{aligned}$$

More generally, for $y \in \mathbf{R}^3$ we set $z = (z_1, z_2, z_3) = (y_1^2, y_2^2, y_3^2) \in [0, +\infty)^3$. The other notations are standard.

If $E \subset \mathcal{E} \in \{\mathbb{T}^3, \mathbf{R}^3\}$ and $\mathcal{F} \in \{\mathbf{R}^n, \mathbb{C}^n\}$, we denote by $\mathcal{C}_c^\infty(E, \mathcal{F})$ the real space of $\mathcal{C}^\infty$ functions with values in $\mathcal{F}$, defined on $\mathcal{E}$ and with compact support in E.

Let $J \subset \mathbf{R}$, we denote by $\chi_J \colon \mathbf{R} \to \mathbf{R}$ the characteristic function of J. Let $J, J' \subset \mathbf{R}$, we write $J \subset\subset J'$ when $\overline{J} \subset J'$. Let T be a self-adjoint operator, we denote by $\sigma(T)$ the spectrum of T, by $1_J(T)$ the spectral projection on J for T, and by $1_J^c(T)$ the spectral projection on the continuous spectral subspace of T in J.

If X and Y are two metrics spaces $B(X, Y)$ is the space of bounded operators from X into Y and $B(X) := B(X, X)$.

We denote by $\mathcal{L}(\mathbb{C}^m)$ the set of linear operators from $\mathbb{C}^m$ into itself. Thus, $\mathcal{L}(\mathbb{C}^m)$ is identified with the set of square complex matrices of size $m \times m$. Let $m \in \mathbf{N}^*$, the space $\mathbb{C}^m$ is equipped with the usual hermitian product

$$\langle f, g \rangle_{\mathbb{C}^m} = \sum_{j=1}^m f_j \overline{g_j}, \quad f = (f_j)_{1 \leqslant j \leqslant n},\ g = (g_j)_{1 \leqslant j \leqslant m},$$

which is associated with the norm $|f| := \langle f, f \rangle_{\mathbb{C}^m}^{1/2}$. Full notations are given at the end of the paper.

2. The discrete Maxwell Operator

2.1. Preliminaries

Let $\mathbf{Z}^3 = \{n = (n_1, n_2, n_3);\ n_j \in \mathbf{Z}\}$ be the square lattice and $\mathbb{T}^3 \approx (\mathbf{R}/(2\pi\mathbf{Z}))^3$ be the 3-dimensional real torus. Let $m \in \mathbf{N}^*$, the space $\mathcal{S}(\mathbf{Z}^3, \mathbb{C}^m)$ of rapidly decreasing sequences on $\mathbf{Z}^3$ with values in $\mathbb{C}^m$ is characterized by

$$\widehat{u} = (\widehat{u}_n)_{n \in \mathbf{Z}^3} \in \mathcal{S}(\mathbf{Z}^3, \mathbb{C}^m) \iff |\widehat{u}_n| \leqslant C_k (1 + |n|)^{-k}, \quad \forall\, n \in \mathbf{Z}^3,\ \forall\, k \geqslant 0.$$

The space $\mathcal{H} := L^2(\mathbb{T}^3, \mathrm{d}x, \mathbb{C}^m)$ can be written as the hilbertian sum

$$\mathcal{H} = \int_{\mathbb{T}^3}^{\oplus} \mathbb{C}^m \mathrm{d}x,$$

with the scalar product

$$(u, v) := \int_{\mathbb{T}^3} \langle u(x), v(x)\rangle_{\mathbb{C}^m} \mathrm{d}x.$$

All along the article we are mainly concerned by the case $m = 6$ and we make the identification between $\mathcal{H}$ and its dual space $\mathcal{H}'$. The dual space $\mathcal{S}'(\mathbf{Z}^3, \mathbb{C}^m)$ of $\mathcal{S}(\mathbf{Z}^3, \mathbb{C}^m)$ is therefore identified with the space of sequences $\widehat{u} = (\widehat{u}_n)_{n\in\mathbf{Z}^3}$ which satisfy the following condition:

there exist $k \geqslant 0$ and $C > 0$ such that $|\widehat{u}_n| \leqslant C(1 + |n|)^k, \quad \forall\, n \in \mathbf{Z}^3$.

The sets $\mathcal{S}(\mathbb{T}^3, \mathbb{C}^m) \supset \mathcal{D}(\mathbb{T}^3, \mathbb{C}^m) = \mathcal{C}^\infty(\mathbb{T}^3, \mathbb{C}^m)$ and their respective duals, $\mathcal{S}'(\mathbb{T}^3, \mathbb{C}^m) \subset \mathcal{D}'(\mathbb{T}^3, \mathbb{C}^m)$, are also standard: see [4].

For $f \in \mathcal{S}(\mathbb{T}^3, \mathbb{C}^m)$ we put its Fourier series:

$$\widehat{f}(n) := (2\pi)^{-\frac{3}{2}} \int_{\mathbb{T}^3} e^{\mathrm{inx}} f(x)\mathrm{d}x, \quad n \in \mathbf{Z}^3.$$

We then have the discrete Fourier transform U between $\mathcal{S}(\mathbf{Z}^3, \mathbb{C}^m)$ and $\mathcal{S}(\mathbb{T}^3, \mathbb{C}^m)$ by putting $(Uf)(n) := \widehat{f}(n)$, $n \in \mathbf{Z}^3$. Then, U realizes a unitary transform (denoted U again) between $l^2(\mathbf{Z}^3, \mathbb{C}^m)$ and $\mathcal{H}$, so that any $f \in \mathcal{H}$ can be written

$$f(x) = \big(U^*\widehat{f}\,\big)(x) \equiv (2\pi)^{-\frac{3}{2}} \sum_{n\in\mathbf{Z}^3} e^{-\mathrm{inx}} \widehat{f}(n), \quad \text{(a.e.) } x \in \mathbb{T}^3.$$

In addition, U extends continuously to an isomorphism (denoted U again) between $\mathcal{S}'(\mathbf{Z}^3, \mathbb{C}^m)$ and $\mathcal{S}'(\mathbb{T}^3, \mathbb{C}^m)$.

2.2. The discrete Maxwell Operator

The anisotropic unperturbed discrete-Maxwell operator is defined by

$$\widehat{H}^D = \widehat{D}\widehat{H}_0,$$

where $\widehat{D}$ is the diagonal 6×6 matrix in (1.1) and the Fourier series of $\widehat{H}_0$ is the matrice $H_0(x)$ defined by (1.2). Since $\widehat{D}$ is constant it turns that

$$H^D = \widehat{D}U^*\widehat{H}_0U = U^*\big(\widehat{D}\widehat{H}_0\big)U = U^*\widehat{H}^DU = \int_{\mathbb{T}^3}^{\oplus} H^D(x)\mathrm{d}x,$$

is an operator of multiplication, where $H^D(x)$ is self-adjoint on $\mathbb{C}^6$ equipped with the following hermitian product

$$\langle a,b\rangle_{\mathbb{C}^6,D} := \left\langle \widehat{D}^{-1}a, b\right\rangle_{\mathbb{C}^6}, \quad a,b\in\mathbb{C}^6.$$

Since $H^D(x)$ depends only on $y=\sin(x)$ we write it $H^D(x)=h^D(y)$. The relation $(\widehat{D}^{-1}H^D u,v)=(H_0u,v)$ shows that the operator H^D is bounded self-adjoint on the hilbertian space $\mathcal{H}^D = L^2(\mathbb{T}^3,\mathrm{d}x,\mathbb{C}^6)$ equipped with the hilbertian product (1.4). We denote by $\|u\|_{\mathcal{H}^D} := (u,u)^{\frac12}_{\mathcal{H}^D}$ the norm on $\mathcal{H}^D$. Since the norms $\|\cdot\|$ and $\|\cdot\|_{\mathcal{H}^D}$ are equivalent, we can omit the index "$\mathcal{H}^D$" in the above norm. Actually, the identification $\mathcal{H}'=\mathcal{H}$ is equivalent to the identification $(\mathcal{H}^D)'=\mathcal{H}^D$.

2.3. Spectrum of H^D

2.3.1. Spectrum of $h^D(y)$

Let us describe the spectrum of $h^D(y)$. We introduce the new parameters $\boldsymbol{\beta}=(\beta_j)_{j=1,2,3}, \boldsymbol{\alpha}=(\alpha_j)_{j=1,2,3}, \boldsymbol{\gamma}=(\gamma_j)_{j=1,2,3}\in\mathbf{R}^3$ by

$$\begin{aligned} &\boldsymbol{\beta} := \boldsymbol{\varepsilon}\times\boldsymbol{\mu}, && \\ &\alpha_1 := (\varepsilon_2\mu_3+\varepsilon_3\mu_2)/2 && \text{and c.p.}, \\ &\gamma_1 := \varepsilon_2\varepsilon_3\mu_2\mu_3 && \text{and c.p..} \end{aligned} \tag{2.1}$$

The abreviation "c.p." means "circular permutation" so we have the other values by circular permutation, ex., $\alpha_2 := (\varepsilon_3\mu_1+\varepsilon_1\mu_3)/2$.

Since $\boldsymbol{\beta}\cdot\boldsymbol{\varepsilon}=0$ and $\varepsilon_i>0$ for all $i\in[\![1,3]\!]$ there thus exists $j\in[\![1,3]\!]$ such that $\beta_j\beta_i\leqslant 0$ and $\beta_k\beta_i\geqslant 0$ for $i,k\neq j$. If two of the β_j's vanish then $\boldsymbol{\beta}$ vanishes. Moreover $\boldsymbol{\beta}$ is replaced by $-\boldsymbol{\beta}$ if $\boldsymbol{\varepsilon}$ and $\boldsymbol{\mu}$ are exchanged, which involves the same analysis. Hence, if $\boldsymbol{\beta}\neq 0$ we then can assume without any restriction:

$$\beta_1\geqslant\beta_2>0>\beta_3 \quad \text{or} \quad \beta_1>\beta_2=0>\beta_3. \tag{A0}$$

Note that, if $\boldsymbol{\beta}\neq 0$, the condition $\prod_{j=1}^3\beta_j=0$ is then equivalent, under assumption (A0), to $\beta_2=0$.

Lemma 2.1. — *We have*

$$\det\bigl(h^D(y)-k\bigr) = \det\bigl(\boldsymbol{\varepsilon}M(y)\boldsymbol{\mu}M(y)+k^2\bigr), \quad k\in\mathbb{C},$$

and the factorization

$$\det\bigl(h^D(y)-k\bigr) = k^2\bigl(\tau^+(z)-k^2\bigr)\bigl(\tau^-(z)-k^2\bigr),$$

with

$$\tau^{\pm} = \Psi_0 \pm \sqrt{K_0}, \tag{2.2}$$

where

$$K_0(z) = \frac{1}{4}\big(\beta_1^2 z_1^2 - 2\beta_1\beta_2 z_1 z_2\big) + c.p., \tag{2.3}$$

$$\Psi_0(z) = \boldsymbol{\alpha}\cdot z \;:=\; \alpha_1 z_1 + \alpha_2 z_2 + \alpha_3 z_3. \tag{2.4}$$

Proof in Appendix A.

Remark 2.2. — It is clear that $K_0 \geqslant 0$ on $[0,+\infty)^3$ since $z_j = y_j^2$, $j \in [\![1,3]\!]$, and since the matrix $h^D(y)$ is real symmetric for $y \in \mathbf{R}^3$. But we directly see that $K_0 \geqslant 0$ on $[0,+\infty)^3$ thanks to (2.3) which implies:

$$K_0(z) = \frac{1}{4}(\beta_1 z_1 - \beta_2 z_2 - \beta_3 z_3)^2 - \beta_2\beta_3 z_2 z_3. \tag{2.5}$$

(Observe that under assumption (A0) we have $\beta_2\beta_3 \leqslant 0$.)

Since the characteristic polynomial $\det(h^D(y) - \lambda)$ depends on $y \in \mathbf{R}^3$ via the new variable $z = (z_1, z_2, z_3) = (y_1^2, y_2^2, y_3^2) \in [0,+\infty)^3$ we put

$$p(z;\lambda) = \det\big(h^D(y) - \lambda\big) = \det\big(\boldsymbol{\varepsilon} M(y)\boldsymbol{\mu} M(y) + \lambda^2\big).$$

Remark 2.3. — If $z \in [0,+\infty)^3$, $z \neq 0$, then

$$\tau^+(z) = \Psi_0(z) + \sqrt{K_0(z)} \geqslant \tau^-(z) = \Psi_0(z) - \sqrt{K_0(z)} > 0.$$

Moreover there exists $C > 0$ such that

$$\tau^-(z) \geqslant C|z|, \quad z \in [0,+\infty)^3.$$

The functions Ψ_0 and K_0 are homogeneous polynomials. The relation $K_0 \equiv 0$ is equivalent to $\boldsymbol{\beta} = 0$ which is the special case where ε and μ are proportional. If one of the β_i's vanishes, then, under assumption (A0) with $\beta_2 = 0$, the function $\sqrt{K_0(\cdot)}$ is polynomial. So, the functions $\mathbf{R}^3 \ni z \mapsto \tau^{\pm}(z)$ are homogeneous analytical complex functions with branch points at $K_0^{-1}(0)$ (which contains 0) if $\beta_2 \neq 0$, and with branch point at $z = 0$ only if $\beta_2 = 0$.

If $z = 0$ then $h^D(y) = 0_{6\times 6}$ and all the eigenvalues vanish. Let us consider the case $z \neq 0$.

Theorem 2.4 (Spectrum of $h^D(y)$). — *Let $y \in \mathbf{R}^3 \setminus \{0_{\mathbf{R}^3}\}$. Then 0 is a double eigenvalue with eigenvectors $(y_1, y_2, y_3, 0, 0, 0) \equiv y \otimes 0_{\mathbb{C}^3}$ and $(0, 0, 0, y_1, y_2, y_3) \equiv 0_{\mathbb{C}^3} \otimes y$.*

Assume $\boldsymbol{\beta} = 0$. Then $K_0 \equiv 0$ and all the eigenvalues have multiplicity two. Moreover, the nonzero eigenvalues of $h^D(y)$ are

$$\pm\sqrt{\tau^+(z)} = \pm\sqrt{\tau^-(z)} = \pm\sqrt{\varepsilon_2\mu_3 z_1 + \varepsilon_3\mu_1 z_2 + \varepsilon_1\mu_2 z_3}.$$

Assume $\boldsymbol{\beta} \neq 0$. Then the nonzero eigenvalues of $h^D(y)$ are

- $\pm\sqrt{\tau^+(z)}$, *simple iff* $K_0(z) \neq 0$,
- $\pm\sqrt{\tau^-(z)}$, *simple iff* $K_0(z) \neq 0$.
- $\pm\sqrt{\tau^+(z)} = \pm\sqrt{\tau^-(z)}$, *double iff* $K_0(z) = 0$.

In addition, let us assume $\boldsymbol{\beta} \neq 0$ and $\prod_{j=1}^{3} \beta_j = 0$. Then, τ^+ and τ^- are linear according to z. Under (A0) *we have $\beta_2 = 0$, so*

$$\tau^+(z) = \varepsilon_2\mu_3 z_1 + \varepsilon_3\mu_1 z_2 + \varepsilon_2\mu_1 z_3, \tag{2.6}$$

$$\tau^-(z) = \varepsilon_3\mu_2 z_1 + \varepsilon_3\mu_1 z_2 + \varepsilon_1\mu_2 z_3. \tag{2.7}$$

(Hence we observe that:

- *if $(z_1, z_3) \neq 0_{\mathbf{R}^2}$, then the positive eigenvalues of $h^D(y)$ are $\sqrt{\tau^\pm(z)}$, simple;*
- *if $(z_1, z_3) = 0_{\mathbf{R}^2}$ and $z_2 \neq 0$, then the positive eigenvalues of $h^D(y)$ are*

$$\sqrt{\tau^+(z)} = \sqrt{\tau^-(z)} = \sqrt{\alpha_2}|y_2| = \sqrt{\varepsilon_3\mu_1}|y_2|,$$

  double.)

The proof of Theorem 2.4 follows from (2.3) and (2.4).

Lemma 2.5. — *Let us assume $\boldsymbol{\beta} \neq 0$ (so* (A0) *holds). We have*

$$K_0^{-1}(\{0\}) := \{z \in [0,1]^3\,;\, K_0(z) = 0\} = \left\{t(\beta_2, \beta_1, 0)\,;\, 0 \leqslant t \leqslant \frac{1}{\beta_1}\right\}.$$

The proof is left to the reader.

2.3.2. Spectrum of H^D

We put

$$\lambda_\pm := \max\left\{\sqrt{\tau^\pm(z)} \,\middle|\, z \in [0,1]^3\right\} \in (0, +\infty).$$

It is known (see [20, p. 90], [10]) that the spectrum of H^D is characterized by the formula:

$$\sigma(H^D) = \overline{\bigcup_{x \in \mathbb{T}^3} \sigma(H^D(x))}, \tag{2.8}$$

which is a compact set of $\mathbf{R}$. Thanks to Theorem 2.4 and to (2.8) we then obtain

Proposition 2.6.

(1) *The operator* H^D *admits* 0 *as eigenvalue of infinite order.*
(2) *The spectrum of* H^D *is*

$$\sigma\big(H^D\big) = [-\lambda_+, \lambda_+].$$

(The complete proof of this proposition is put in Appendix A.)

2.4. Stratification and thresholds

Following [8] the energy-momentum set is

$$\Sigma = \big\{(\lambda, x) \,\big|\, \lambda \in \sigma\big(H^D(x)\big)\big\} \subset \sigma\big(H^D\big) \times \mathbb{T}^3.$$

We have $(\lambda, x) \in \Sigma \iff p(z;\lambda) = 0$. We consider the canonical projections:

$$P_M : \mathbf{R} \times \mathbb{T}^3 \ni (\lambda, x) \mapsto x \in \mathbb{T}^3,$$
$$P_{\mathbf{R}} : \mathbf{R} \times \mathbb{T}^3 \ni (\lambda, x) \mapsto \lambda \in \mathbf{R}.$$

It is clear that $P_{\mathbf{R}}|_\Sigma$ is a proper map. The spectrum $\sigma(H^D(x))$ of $H^D(x)$ is discrete and depends continuously on x. The operators $H^D(x)$ are the fibers and the space $\mathbb{T}^3$ is the momentum space. The energy-momentum set Σ admits the partition

$$\Sigma = \bigcup_{i=1}^{6} \Sigma_i,$$

where Σ_i is the semi-analytical set of elements (λ, x) for which λ is an eigenvalue of multiplicity i of $H^D(x)$. We set

$$\mathcal{X}_j = P_M(\Sigma_j), \quad j \geqslant 1, \quad \mathcal{X}_0 = \big\{x \in \mathbb{T}^3;\ z = 0\big\}.$$

We see that $\Sigma_j = \emptyset$ for $j = 3, 4, 5$, $\Sigma_6 = \{0\} \times \mathcal{X}_0$; hence, $\mathcal{X}_6 = \mathcal{X}_0$, $\mathcal{X}_j = \emptyset$ for $j = 3, 4, 5$. Moroever, we can write

$$\Sigma_1 = \Sigma_1^+ \cup \Sigma_1^-,$$
$$\Sigma_1^\pm := \big\{(\lambda, x);\ 0 \neq \lambda^2 = \tau^\pm(z) \neq \tau^\mp(z)\big\},$$
$$\Sigma_2 = \big\{(\lambda, x);\ 0 \neq \lambda^2 = \tau^+(z) = \tau^-(z)\big\}.$$

- If $\boldsymbol{\beta} = 0$ then $\Sigma_1 = \emptyset$ and $(\lambda, x) \in \Sigma_2$ iff $z \neq 0$ and $\lambda^2 = \Psi_0(z)$.
- If $\boldsymbol{\beta} \neq 0$ holds then $(\lambda, x) \in \Sigma_1$ iff $K_0(z) \neq 0$ and $\lambda^2 \in \{\tau^+(z), \tau^-(z)\}$.

Let us define the set of thresholds, $\mathcal{T}$. For a more abstract definition (which may be more restrictive to ours) of $\mathcal{T}$ in the general case of analytically fibered operators, see [8]. We put

$$\Sigma_1^* := \Sigma_1^{*+} \cup \Sigma_1^{*-},$$
$$\Sigma_1^{*\pm} := \Big\{(\lambda, x) \in \Sigma_1^{\pm};\ \nabla_x \sqrt{\tau^{\pm}(z)} = 0\Big\},$$
$$\Sigma_2^* := \Big\{(\lambda, x) \in \Sigma_2;\ \nabla_x \sqrt{\Psi_0(z)} \text{ is normal to } \mathcal{X}_2 \text{ at } x\Big\},$$

then,

$$\mathcal{T}_j := P_{\mathbf{R}}(\Sigma_j^*), \quad j = 1, 2.$$

Remark. — Concerning the definitions of $\mathcal{T}_2$ and Σ_2^*, let us notice that, given $(\lambda, x) \in \Sigma_2$ (so we have $\lambda^2 = \Psi_0(z)$), the condition "$\nabla_x \sqrt{\Psi_0(z)}$ is normal to $\mathcal{X}_2$ at x" is equivalent to "$\nabla_x \Psi_0(z)$ is normal to $\mathcal{X}_2$ at x" and means that the derivative along $\mathcal{X}_2$ of the restriction of the eigenvalue function $\sqrt{\Psi_0} \circ \sin^2$ (of multiplicity two) on $\mathcal{X}_2$ vanishes at x.

Observing that $P_{\mathbf{R}}(\Sigma_6) = \{0\}$, we define the set of thresholds, $\mathcal{T}$, as

$$\mathcal{T} := \{0\} \cup \mathcal{T}_1 \cup \mathcal{T}_2.$$

Let us describe the sets $\mathcal{X}^*$ and $\mathcal{T}$. We put

$$\mathbb{T}_0^3 := \mathbb{T}^3 \setminus \mathcal{X}_0 = \big\{x \in \mathbb{T}^3;\ z \neq 0\big\},$$
$$\mathcal{X}_j^* := P_M\big(\Sigma_j^*\big),$$
$$\mathcal{X}^* := \mathcal{X}_1^* \cup \mathcal{X}_2^* = \big\{x \in \mathbb{T}^3;\ \sigma\big(H^D(x)\big) \cap \mathcal{T} \neq \{0\}\big\} \subset \mathbb{T}_0^3.$$

Thus, λ is a non zero threshold if and only if there exists $z^* \in \sin^2(\mathcal{X}^*)$ such that $p(z^*; \lambda) = 0$. Putting

$$\mathcal{T}_1^{\pm} := P_{\mathbf{R}}\big(\Sigma_1^{*\pm}\big),$$
$$\mathcal{X}_1^{*\pm} := P_M\big(\Sigma_1^{*\pm}\big),$$

we have

$$\mathcal{T}_1 = \mathcal{T}_1^+ \cup \mathcal{T}_1^-,$$
$$\mathcal{X}_1^* = \mathcal{X}_1^{*+} \cup \mathcal{X}_1^{*-},$$
$$\sin^2(\mathcal{X}_1^*) = \sin^2\big(\mathcal{X}_1^{*+}\big) \cup \sin^2\big(\mathcal{X}_1^{*-}\big),$$

so

$$\mathcal{T} = \mathcal{T}_1^+ \cup \mathcal{T}_1^- \cup \mathcal{T}_2 \cup \{0\}. \tag{2.9}$$

Obviously $\mathcal{T}$ is symmetrical to 0 and we analyse the positive eigenvalues of H^D only. See the schematic drawing 2.1 where the momentum space is two-dimensional.

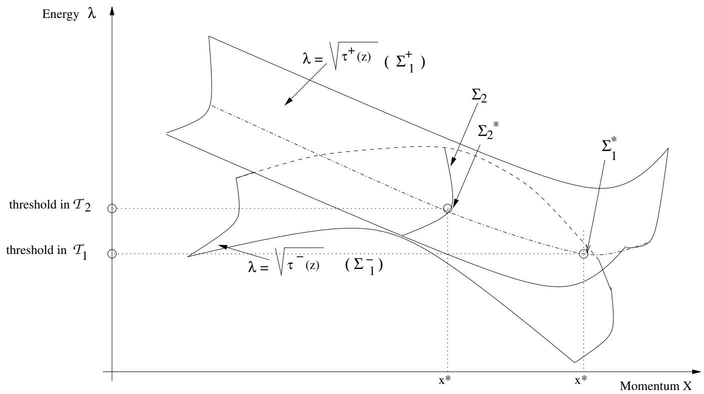

Figure 2.1.

Lemma 2.7.

(A) *Assume* $\boldsymbol{\beta} = 0$. *We then have*

$$\partial_{z_i}\tau^{\pm}(z) = \partial_{z_i}\Psi_0(z) > 0 \text{ for all } i.$$

(B) *Assume* $\boldsymbol{\beta} \neq 0$ *(so* (A0) *holds). We put*

$$\nu := \frac{2\alpha_3\sqrt{\beta_1\beta_2} - \sqrt{\gamma_3}(\beta_1+\beta_2)}{|\beta_3|\sqrt{\gamma_3}}. \tag{2.10}$$

Let $z \in [0,1]^3$ *such that* $K_0(z) \neq 0$.

(1) *We have* $\partial_{z_i}\tau^+(z) > 0$ *for* $i = 1,2,3$, *and* $\partial_{z_i}\tau^-(z) > 0$ *for* $i = 1,2$.

(2) (a) *Assume* $\beta_2 = 0$ *(so* $\nu < 0$*). Then* $\partial_{z_3}\tau^-(z) > 0$.

(b) *Assume* $\beta_2 > 0$.

(i) *If* $z_1 = 0$ *or* $z_2 = 0$ *then* $\partial_{z_3}\tau^-(z) > 0$.

(ii) *The derivative* $\partial_{z_3}\tau^-(1,1,z_3)$ *vanishes iff* $z_3 = \nu \in [0,1]$, *and if* $z_3 \neq \nu$ *then* $\partial_{z_3}\tau^-(1,1,z_3)$ *has the same sign than* $z_3 - \nu$.

Proof in Appendix A.

Remark 2.8. — Let $\widetilde{\nu} \in \mathbf{R}$, there exist then $\boldsymbol{\varepsilon}$ and $\boldsymbol{\mu}$ such that $\nu = \widetilde{\nu}$. Proof in Appendix A.

Lemma 2.7 implies that the thresholds of the analytically fibered family $(H^D(x), x \in \mathbb{T}^3)$ come from the values $x \in \mathbb{T}^3$ such that $\partial_{x_i} z_i(x) = 0$ at least for $i = 1,2$, so $z_1, z_2 \in \{0,1\}$, and, in addition, we have $z_3 \in \{0,\nu,1\}$.

We can determine now the set $\mathcal{T}$ of thresholds. Putting

$$Z_{\{0,1\}} = \{0,1\}^3, \qquad Z^*_{\{0,1\}} = Z_{\{0,1\}} \setminus \{0_{\mathbf{R}^3}\},$$
$$X_{\{0,1\}} = \big\{x \in \mathbb{T}^3;\ z \in Z_{\{0,1\}}\big\}, \qquad X^*_{\{0,1\}} = \Big\{x \in \mathbb{T}^3;\ z \in Z^*_{\{0,1\}}\Big\},$$

we obtain the following (remember also (2.9)).

Lemma 2.9.

(1) *Case $\boldsymbol{\beta} = 0$ (so, $K_0 \equiv 0$). We have $\mathcal{X}_1 = \emptyset$, $\Sigma_1 = \emptyset$, $\mathcal{X}_2 = \mathbb{T}^3_0$. Then, $\sin^2(\mathcal{X}^*_2) = Z^*_{\{0,1\}}$, $\mathcal{T}_1 = \emptyset$, $\mathcal{T} = \{0\} \cup \mathcal{T}_2$ and*

$$\mathcal{T}_2 \cap \mathbf{R}^+ = \Big\{\sqrt{\Psi_0(z)}; z \in Z^*_{\{0,1\}}\Big\}.$$

(2) *Case $\boldsymbol{\beta} \neq 0$ (so (A0) holds). The sets $\mathcal{X}_1$ and $\mathcal{X}_2$ are then not trivial (remember Lemma 2.5). We put $\mathcal{Z}^*_\nu = \{(1,1,\nu)\} \cap [0,1]^3$. We have*

$$\sin^2\big(\mathcal{X}^{*+}_1\big) = Z^*_{\{0,1\}} \setminus \left\{\left(\frac{\beta_2}{\beta_1}, 1, 0\right)\right\},$$
$$\sin^2\big(\mathcal{X}^{*-}_1\big) = Z^*_{\{0,1\}} \cup \mathcal{Z}^*_\nu \setminus \left\{\left(\frac{\beta_2}{\beta_1}, 1, 0\right)\right\}$$
$$\textit{and} \quad \sin^2(\mathcal{X}^*_2) = \left\{\left(\frac{\beta_2}{\beta_1}, 1, 0\right)\right\},$$

so

$$\mathcal{T}^+_1 \cap \mathbf{R}^+ = \left\{\sqrt{\tau^+(z)},\ z \in Z^*_{\{0,1\}},\ z \neq \left(\frac{\beta_2}{\beta_1}, 1, 0\right)\right\},$$
$$\mathcal{T}^-_1 \cap \mathbf{R}^+ = \left\{\sqrt{\tau^-(z)},\ z \in Z^*_{\{0,1\}} \cup \mathcal{Z}^*_\nu,\ z \neq \left(\frac{\beta_2}{\beta_1}, 1, 0\right)\right\},$$
$$\mathcal{T}_2 \cap \mathbf{R}^+ = \left\{\sqrt{\Psi_0\left(\frac{\beta_2}{\beta_1}, 1, 0\right)}\right\}.$$

Proof in Appendix A.

Remark 2.10. — Lemma 2.9 implies that $\mathcal{X}^*$ is finite.

Remark 2.11. — We have $\mathcal{X}^{*+}_1 \subset \mathcal{X}^{*-}_1$.

Remark 2.12. — Let us consider the case $\boldsymbol{\beta} \neq 0$ and $\beta_2 = 0$ (with Assumption (A0)). In one hand, we obtain that

$$\begin{aligned}\mathcal{T}_2 \cap \mathbf{R}^+ &= \Big\{\sqrt{\Psi_0(0,1,0)}\Big\} \\ &= \Big\{\sqrt{\Psi_0(z)};\ z \neq 0,\ K_0(z) = 0,\ \nabla_x \sqrt{\Psi_0(z)} = 0\Big\}.\end{aligned}$$

On the other hand, since the functions $\tau^{\pm}$ are linear and positive on $[0,+\infty)^3 \setminus \{0_{\mathbf{R}^3}\}$, the eigenvalues $\sqrt{\tau^{\pm}}$ are then analytic on $[0,+\infty)^3 \setminus \{0_{\mathbf{R}^3}\}$, so we can consider the following sets $\mathcal{T}_{2,\pm}$ instead of $\mathcal{T}_2 \cap \mathbf{R}^+$:

$$\mathcal{T}_{2,\pm} := \Big\{ \sqrt{\tau^{\pm}(z)};\ z \neq 0,\ K_0(z) = 0,\ \nabla_x \sqrt{\tau^{\pm}(z)} = 0 \Big\}.$$

Nevertheless, thanks to (1) and (a) of Lemma 2.7 we obtain

$$\mathcal{T}_{2,\pm} = \Big\{ \sqrt{\Psi_0(0,1,0)} \Big\} = \mathcal{T}_2 \cap \mathbf{R}^+,$$

so the sets $\mathcal{T}_{2,+}$, $\mathcal{T}_{2,-}$ and $\mathcal{T}_2 \cap \mathbf{R}^+$ coincide.

Similarly, if $\boldsymbol{\beta} = 0$ then the sets $\mathcal{T}_2 \cap \mathbf{R}^+$ and

$$\Big\{ \sqrt{\Psi_0(z)};\ z \neq 0,\ \nabla_x \sqrt{\Psi_0(z)} = 0 \Big\} \quad \text{coincide.}$$

So, when the eigenvalues of the fibers $H^D(x)$ are analytical, a simple and usual definition of the thresholds allows the stratification method to be bypassed.

Partition of the set of thresholds

We put

$$\lambda^* := \max_{\mathcal{X}_2} \sqrt{\Psi_0 \circ \sin^2}, \tag{2.11}$$

so $\lambda^* = \sqrt{\Psi_0\big(\frac{\beta_2}{\beta_1}, 1, 0\big)}$ if $\boldsymbol{\beta} \neq 0$ and (A0) hold, and $\lambda^* := \lambda_+ = \lambda_-$ if $\boldsymbol{\beta} = 0$ holds. We define the sets

$$\mathcal{T}_{\rm sm}^+ = \{\lambda_+, \lambda_-, \lambda^*\}, \tag{2.12}$$

$$\mathcal{T}_{\rm sm} := \mathcal{T}_{\rm sm}^+ \cup -\mathcal{T}_{\rm sm}^+ \tag{2.13}$$

$$\mathcal{T}_{\rm sa} := \mathcal{T} \setminus (\mathcal{T}_{\rm sm} \cup \{0\}). \tag{2.14}$$

In fact, remembering that

$$\lambda_+ = \max_{\mathbb{T}^3} \sqrt{\tau^+ \circ \sin^2} = \sqrt{\tau^+(1,1,1)},$$

$$\lambda_- = \max_{\mathbb{T}^3} \sqrt{\tau^- \circ \sin^2} = \max\Big(\sqrt{\tau^-(1,1,1)}, \sqrt{\tau^-(1,1,0)}, \sqrt{\tau^-(1,1,\nu)} \Big),$$

we observe that, if $\boldsymbol{\beta} \neq 0$ and (A0) hold,

(1) We then have $\lambda^* \leqslant \lambda_- < \lambda_+$. (Actually, thanks to Lemma 2.7, if $\sqrt{\tau^-(z)} = \lambda_-$ then $z_1 = z_2 = 1$ and $z_3 \in \{0,1\}$. If $z_3 = 1$ then $K_0(z) \neq 0$ so $\lambda_+ = \sqrt{\tau^+(z)} > \sqrt{\tau^-(z)} = \lambda_-$ and if $z_3 = 0$ then $\lambda_+ = \sqrt{\tau^+(1,1,1)} > \sqrt{\tau^+(1,1,0)} \geqslant \sqrt{\tau^-(z)} = \lambda_-$. Moreover, $\lambda^* = \sqrt{\tau^-(\frac{\beta_2}{\beta_1}, 1, 0)} \leqslant \lambda_-$.)

(2) If, in addition $\beta_1 > \beta_2$, then $\lambda^* < \lambda_-$, so $\mathcal{T}_{\rm sm}^+$ has exactly three elements.

3. Results

3.1. Main Theorem

We denote $\mathcal{D}_0 := \mathcal{C}_c^\infty(\mathbb{T}^3 \setminus \mathcal{X}^*, \mathbb{C}^6)$. Observe that it is dense in $\mathcal{H}^D$ since $\mathcal{X}^*$ is finite.

Our main result is

Theorem 3.1. — *Let $\mathcal{T}' \subset \mathcal{T}$ with $0 \in \mathcal{T}'$, and $\phi \in \mathcal{C}_c^\infty(\mathbf{R}\backslash\mathcal{T}', \mathbf{R})$. Then there exists a symmetric differential operator of order one, A_ϕ, defined on*

$$D(A_\phi) := \begin{cases} \mathcal{C}^\infty\big(\mathbb{T}^3, \mathbb{C}^6\big) & \text{if} \quad \mathcal{T}' = \mathcal{T} \\ \mathcal{D}_0 & \text{if} \quad \mathcal{T}' \neq \mathcal{T}, \end{cases}$$

satisfying the following properties:

(i) *There exists a constant $\delta = \delta(\phi) > 0$ so that we have*

$$\phi(H^D)\big[H^D, iA_\phi\big]\phi\big(H^D\big) \geqslant \delta\phi^2\big(H^D\big). \tag{3.1}$$

(ii) *The multi-commutators $ad^k_{A_\phi}(H^D)$ are bounded for all $k \in \mathbf{N}$.*

(iii) *The operator A_ϕ is a first order differential operator in x whose coefficients belong to $\mathcal{C}^\infty(\mathbb{T}^3, \mathcal{L}(\mathbb{C}^6))$ if $\mathcal{T}' = \mathcal{T}$ and to $\mathcal{C}^\infty(\mathbb{T}^3 \setminus \mathcal{X}^*, \mathcal{L}(\mathbb{C}^6))$ if $\mathcal{T}' \neq \mathcal{T}$. These coefficients vanish near any $x \in \mathbb{T}^3$ such that $z = 0$ or $s\sqrt{\tau^\pm(z)} \in \mathcal{T}' \cap \mathcal{T}_1^\pm$, or $s\sqrt{\Psi_0(z)} \in \mathcal{T}' \cap \mathcal{T}_2$, $s \in \{1, -1\}$, so, they vanish near $\mathcal{X}^*$ if $\mathcal{T}' = \mathcal{T}$. In addition, there exists $\widetilde{\phi} \in \mathcal{C}_c^\infty(\mathbf{R} \setminus \mathcal{T}')$ such that*

$$A_\phi = \widetilde{\phi}\big(H^D\big)A_\phi = A_\phi\widetilde{\phi}\big(H^D\big). \tag{3.2}$$

(iv) *If $\mathcal{T}_{\rm sm} \subset \mathcal{T}'$ then A_ϕ is essentially self-adjoint.*

(v) *If $\mathcal{T}' = \{0\}$ then A_ϕ has the form $\sum_{j=0}^3 A_j$ where A_0 has smooth coefficients and is essentially self-adjoint, A_1 and A_2 have coefficients with rational singularities at some points of $\mathcal{X}^*$ and, defined on the domain $\mathcal{D}_0$, admit a maximal symmetric extension; moreover,* $\operatorname{supp} A_1 \cap \operatorname{supp} A_2 = \emptyset$.

Remark 3.2.

- The property on H^D in the point (ii) can be written $H^D \in \mathcal{C}^\infty(A_\phi)$.

- The sets $\mathcal{C}^\infty(\mathbb{T}^3, \mathbb{C}^6)$ and $\mathcal{D}_0$ have well-known topologies. The differential operator A_ϕ is then a continuous mapping from $D(A_\phi)$ into itself. Letting $u \in \mathcal{H}^D$, since $D(A_\phi)$ is dense in $\mathcal{H}^D$, we then can define $A_\phi u$ as a distribution on $D(A_\phi)$, i.e., $A_\phi u \in D(A_\phi)'$ which is the topological dual space of $D(A_\phi)$. We then have the following characterization, since A_ϕ is symmetric,
$$A_\phi u \in \mathcal{H}^D \iff |(u, A_\phi v)_{\mathcal{H}^D}| \leqslant C\|v\| \quad \forall\, v \in D(A_\phi).$$
Putting the norm graph
$$\|u\|_{D(A_\phi)} := \|u\| + \|A_\phi u\| \quad \forall\, u \in D(A_\phi),$$
the closure $\bar{A}_\phi$ of A_ϕ has domain
$$D(\bar{A}_\phi) := \overline{D(A_\phi)}^{\|\cdot\|_{D(A_\phi)}}.$$
The adjoint of $\bar{A}_\phi$ or of A_ϕ is the operator $A_\phi{}^*$ with domain
$$D(A_\phi{}^*) = \left\{v \in \mathcal{H}^D;\ A_\phi v \in \mathcal{H}^D\right\} \supset D(\bar{A}_\phi).$$
- Let us consider the particular case $\operatorname{supp} \phi \cap \mathcal{T} = \emptyset$. Then, A_ϕ is a differential operator with smooth coefficients in $\mathcal{C}^\infty(\mathbb{T}^3, \mathbb{C}^6)$. Since, in addition, A_ϕ is symmetric and of order one, it is then essentially self-adjoint on $\mathcal{H}^D$ (see [8]). We let also the reader to prove the following assertions. The above extension $\bar{A}_\phi$ of A_ϕ is self-adjoint, and we have
$$H^1\big(\mathbb{T}^3, \mathbb{C}^6\big) \subset D(A_\phi{}^*) = D(\bar{A}_\phi)$$
where the above inclusion is dense.
- In the case $\mathcal{T}' = \mathcal{T}$, the result of [8] implies the existence of an essentially self-adjoint operator A_I with smooth coefficients such that points (i), (iii) and (iv) with A_ϕ replaced by A_I hold. But the first commutator $[H^D, A_I]$ is not a multiplication operator so point (ii) fails, and, in fact, $H^D \notin \mathcal{C}^{1,1}(A_I)$ (this set is defined in (2.2) of Corollary 3.7). The new version [9] of [8] provides an essentially self-adjoint operator A_{I,I_1} with smooth coefficients such that points (ii)–(iv) and a local (weaker) version of point (i) are maintained (with A_ϕ replaced by A_{I,I_1}).
- We give an explicit formula for A_ϕ which is easier to read than the general formula in [9] (which is only valid in the case $\mathcal{T}' = \mathcal{T}$).

3.2. Main consequences and extensions

The first obvious consequence of Theorem 3.1 is that the singular continuous spectrum of H^D is then empty. But it is actually a consequence of the general theorem in [8] revised in [9].

The second consequence is that we can state the LAP outside $\mathcal{T}_{\mathrm{sm}} \cup \{0\}$ in the same terms as those of Gérard and Nier in the old version [8] of their work. See also [18, 21]. Let us consider a compact interval $I \subset \mathbf{R}^* \setminus \mathcal{T}_{\mathrm{sm}}$, and fix $\phi \in \mathcal{C}_c^\infty(\mathbf{R}^* \setminus \mathcal{T}_{\mathrm{sm}})$ such that $\phi = 1$ on a neighborhood of I. We thus consider the conjugate operator A_ϕ which is evocated in Theorem 3.1 and Remark 3.2: it is an essentially self-adjoint unbounded operator on $\mathcal{H}^D$. We denote by $A_\phi^{\mathrm{sa}} \subset A_\phi{}^*$ a self-adjoint extension of A_ϕ and by $R(\zeta) := (H^D - \zeta)^{-1}$ the resolvent of H^D.

We define the abstract Besov space $\mathcal{B}_A$ by

$$\mathcal{B}_A = \left\{ f \in \mathcal{H};\ \|f\|_{\mathcal{B}_A} := \sum_{j=0}^{\infty} r_j^{1/2} \left\| 1_{r_{j-1} \leqslant |A_\phi^{\mathrm{sa}}| \leqslant r_j} f \right\| < \infty \right\}.$$

Its dual space $\mathcal{B}_A{}^*$ is the completion of $\mathcal{H}^D$ by the following norm

$$\|u\|_{\mathcal{B}_A{}^*} = \sup_{j \geqslant 0} r_j^{1/2} \left\| 1_{r_{j-1} \leqslant |A_\phi^{\mathrm{sa}}| < r_j} u \right\|.$$

For $s > 1/2$, the following inclusion relations hold:

$$\begin{aligned} D((1+|A_\phi^{\mathrm{sa}}|)^s) \subset \mathcal{B}_A \subset D\big((1+|A_\phi^{\mathrm{sa}}|)^{1/2}\big) \subset \mathcal{H}^D \\ \subset D\big((1+|A_\phi^{\mathrm{sa}}|)^{-1/2}\big) \subset \mathcal{B}_A{}^* \subset D\big(\big(1+|A_\phi^{\mathrm{sa}}|\big)^{-s}\big). \end{aligned}$$

We can claim

Corollary 3.3 (LAP on $\mathbf{R}^* \setminus \mathcal{T}_{\mathrm{sm}}$ in abstract Besov spaces.). — *Let a compact set $I \subset \mathbf{R}^* \setminus \mathcal{T}_{\mathrm{sm}}$. We have*

$$\sup_{\lambda \in I,\, \mu > 0} \|R(\lambda \pm i\mu) f\|_{\mathcal{B}_A{}^*} \leqslant C_I \|f\|_{\mathcal{B}_A} \quad \forall\, f \in \mathcal{B}_A.$$

Moreover letting $s > 1/2$ then the limits

$$\lim_{\varepsilon \to \pm 0} (1+|A_\phi^{\mathrm{sa}}|)^{-s} R(\lambda + i\varepsilon)(1+|A_\phi^{\mathrm{sa}}|)^{-s}$$

exist in $B(\mathcal{H}^D)$ and are bounded, with uniform convergence according to $\lambda \in I$. The mapping $\mathbf{R}^* \setminus \mathcal{T}^{\mathrm{sm}} \ni \lambda \mapsto R(\lambda \pm i0)$ is norm continuous in $B(D((1+|A_\phi^{\mathrm{sa}}|)^s, D((1+|A_\phi^{\mathrm{sa}}|)^{-s})$ and weakly continuous in $B(\mathcal{B}_A, \mathcal{B}_A{}^*)$.

For further developments we establish also the LAP in terms of the usual Besov spaces described by Isozaki and alii [4] with the restriction to spectral values outside the thresholds. Thus, we consider the case $\operatorname{supp}\phi \subset \mathbf{R} \setminus \mathcal{T}$ in Theorem 3.1. We set $N = (N_1, N_2, N_3)$, $N_j = i\partial/\partial x_j$ and the self-adjoint operators

$$|N| = \sqrt{N^2} = \sqrt{-\Delta}, \quad N^2 = \sum_{j=1}^{3} N_j^2 = -\Delta \quad \text{on } \mathbb{T}^3,$$

where Δ denotes the Laplacian on $\mathbb{T}^3 = [-\pi,\pi]^3$ with periodic boundary condition. We introduce the normed spaces:

$$\mathcal{H}^s = \{u \in D'(\mathbb{T}^3, \mathbb{C}^6),\ \|u\|_s < \infty\}, \quad \|u\|_s := \left\|\left(1+N^2\right)^{s/2} u\right\|, \quad s \in \mathbf{R},$$

so $\mathcal{H}^s$ is the completion of $D(|N|^s)$, the domain of $|N|^s$, with respect to the norm $\|u\|_s$ and we have $\mathcal{H}^D = \mathcal{H}^0 = L^2(\mathbb{T}^3, \mathbb{C}^6)$. For $s \geqslant 0$ and $u \in \mathcal{C}^\infty(\mathbb{T}^3, \mathbb{C}^6)$ we have $\|(1+|A_\phi^{\mathrm{sa}}|)^s u\| \leqslant C\|u\|_s$ where C does not depend on u. Thus, the following inclusion relations hold :

$$\mathcal{H}^s \subset D((1+|A_\phi^{\mathrm{sa}}|)^s) \subset \mathcal{H}^D \subset D((1+|A_\phi^{\mathrm{sa}}|)^{-s}) \subset \mathcal{H}^{-s} \quad \forall\, s \geqslant 0.$$

Using the sequence $(r_j)_{j\,\geqslant\,-1}$ where $r_{-1} = 0$, $r_j = 2^j$ for $j \geqslant 0$ we define the Besov space $\mathcal{B}$ by

$$\mathcal{B} := \left\{ f \in \mathcal{H}^D;\ \|f\|_{\mathcal{B}} := \sum_{j=0}^{\infty} r_j^{1/2} \left\|1_{r_{j-1}\,\leqslant\,|N|\,\leqslant\,r_j} f\right\| < \infty \right\}.$$

Its dual space $\mathcal{B}^*$ is the completion of $\mathcal{H}$ by the following norm

$$\|u\|_{\mathcal{B}^*} = \sup_{j\,\geqslant\,0} r_j^{1/2} \left\|1_{r_{j-1}\,\leqslant\,|N|\,<\,r_j} u\right\|.$$

For $s > 1/2$, the following inclusion relations hold :

$$\mathcal{H}^s \subset \mathcal{B} \subset \mathcal{H}^{1/2} \subset \mathcal{H}^D \subset \mathcal{H}^{-1/2} \subset \mathcal{B}^* \subset \mathcal{H}^{-s}.$$

Moreover, [14, Lemma 2.8] says that there is a constant $C > 0$ such that

$$\|f\|_{\mathcal{B}_A} \leqslant C\|f\|_{\mathcal{B}} \quad \forall\, f \in \mathcal{B},$$

i.e., $\mathcal{B} \subset \mathcal{B}_A$, and so, $\mathcal{B}_A^* \subset \mathcal{B}^*$. Hence, Corollary 3.3 can be extended as

Corollary 3.4. — *(LAP on $\mathbf{R} \setminus \mathcal{T}$ in usual Besov spaces.) Let a compact set $I \subset \mathbf{R} \setminus \mathcal{T}$. We have*

$$\sup_{\lambda\,\in\,I,\ \mu\,>\,0} \|R(\lambda \pm i\mu)\|_{B(\mathcal{B},\mathcal{B}^*)} < \infty.$$

Moreover letting $s > 1/2$ then the limits

$$R(\lambda \pm i0) := \lim_{\varepsilon \searrow 0} R(\lambda \pm i\varepsilon) \in B(\mathcal{H}^s, \mathcal{H}^{-s})$$

exist and are bounded, with uniform convergence according to $\lambda \in I$. The mapping $\mathbf{R} \setminus \mathcal{T} \ni \lambda \mapsto R(\lambda \pm i0)$ is norm continuous in $B(\mathcal{H}^s, \mathcal{H}^{-s})$ and weakly continuous in $B(\mathcal{B}, \mathcal{B}^*)$.

Another consequence of Theorem 3.1 is the following extension of the LAP to any nonzero spectral value, thanks to a slight adaptation of [7, Theorem 3.3].

Corollary 3.5 (LAP on $\mathbf{R}^*$). — *Let $I \subset \mathbf{R}^*$ a compact interval. There exists a constant C_I such that*

$$|(u, R(\zeta)u)_{\mathcal{H}^D}| \leqslant C_I \|u\|^2_{D(\bar{A}_\phi)} \quad \forall\, u \in D(\bar{A}_\phi),$$

for all $\zeta = \lambda + i\mu$ with $\lambda \in I$, $\mu \neq 0$ real. Moreover if $\zeta_1 = \lambda_1 + i\mu_1$, $\zeta_2 = \lambda_2 + i\mu_2$ are two such numbers, and if μ_1 and μ_2 have the same sign, then

$$\left|(u, (R(\zeta_1) - R(\zeta_2))u)_{\mathcal{H}^D}\right| \leqslant C_I |\zeta_1 - \zeta_2|^{1/2} \|u\|^2_{D(\bar{A}_\phi)} \quad \forall\, u \in D(\bar{A}_\phi).$$

In particular, if $u \in D(\bar{A}_\phi)$ then the limits

$$\lim_{\varepsilon \searrow 0^+} (u, R(\lambda \pm i\varepsilon)u)_{\mathcal{H}^D} =: (u, R(\lambda \pm i0)u)_{\mathcal{H}^D}$$

exist uniformly in $\lambda \in I$, and, for all $\lambda_1, \lambda_2 \in I$, we have

$$\big(u, (R(\lambda_1 \pm i0) - R(\lambda_2 \pm i0))u\big)_{\mathcal{H}^D} \leqslant C_I |\lambda_1 - \lambda_2|^{1/2} \|u\|^2_{D(\bar{A}_\phi)}.$$

An immediate consequence of Corollary 3.5 is

Corollary 3.6. — *The point spectrum $\sigma_p(H^D)$ of H^D is reduced to $\{0\}$.*

Before giving the proof of Theorem 3.1, we state the results for some natural class of perturbed Hamiltonians $H^D_V = H^D + V$, as done in [8]. We will simply recall some well known results in the Mourre theory (see [18, 21]) and refer the reader to the book [3] for a complete exposition of the Mourre method. In particular a sharper version of Corollary 3.7 is given in [3, Proposition 7.5.6].

Corollary 3.7. — *Let a compact interval $I \subset \mathbf{R}^* \setminus \mathcal{T}_{\mathrm{sm}}$, and fix $\phi \in \mathcal{C}^\infty_c(\mathbf{R}^* \setminus \mathcal{T}_{\mathrm{sm}})$ such that $\phi = 1$ on a neighborhood of I. Let V a symmetric operator on $\mathcal{H}^D$ so that*

(1) *$VR(i)$ and $R(i)[V, iA_\phi]R(i)$ are compact.*
(2) *$V \in \mathcal{C}^{1,1}(A_\phi)$, i.e.,*

$$\int \left\|R(i)\big(e^{\mathrm{it}\, A_\phi}[V, iA_\phi]e^{-\,\mathrm{it}\, A_\phi} - [V, iA_\phi]\big)R(i)\right\| \frac{\mathrm{d}t}{t} < \infty.$$

Then, putting $H^D_V := H^D + V$, the following results hold:

(3) *There exists a constant $\delta > 0$ and a compact operator K so that,*

$$\phi\big(H^D_V\big)\big[H^D_V, iA_\phi\big]\phi\big(H^D_V\big) \geqslant \delta\phi^2\big(H^D_V\big) + K.$$

Consequently the point spectrum $\sigma_p(H^D_V)$ is of finite multiplicity in $\mathbf{R}^* \setminus \mathcal{T}_{\mathrm{sm}}$ and has no accumulation point in $\mathbf{R}^* \setminus \mathcal{T}_{\mathrm{sm}}$.

(4) *For each $\lambda \in I \setminus \sigma_p(H^D_V)$ there exist $\varepsilon > 0$ and $c > 0$ so that,*

$$1_{[\lambda-\varepsilon,\lambda+\varepsilon]}\big(H^D_V\big)\big[H^D_V, iA_\phi\big]1_{[\lambda-\varepsilon,\lambda+\varepsilon]} \geqslant c1_{[\lambda-\varepsilon,\lambda+\varepsilon]}\big(H^D_V\big). \tag{3.3}$$

(5) *The LAP for H_V^D holds on $I \setminus \sigma_p(H_V^D)$: the limits*

$$\lim_{\varepsilon \to \pm 0} (1+|A_\phi|)^{-s} R(\lambda \pm i\varepsilon)(1+|A_\phi|)^{-s}$$

exist and are bounded for all $s > 1/2$. Consequently the singular continuous spectrum of H_V^D is empty.

(6) *If the operator $(1+|A_\phi|)^s V (1+|A_\phi|)^s$ is bounded for some $s > 1/2$, then for any open interval $J \subset I$, the wave operators*

$$s - \lim_{t \to \pm\infty} e^{\mathrm{it}\, H_V^D} e^{-\,\mathrm{it}\, H^D} 1_J\big(H^D\big) =: \Omega_J^{\pm}$$

exist and are asymptotically complete,

$$1_J^c\big(H_V^D\big)\mathcal{H}^D = \Omega_J^{\pm}\mathcal{H}^D,$$

where $1_J^c(H_V^D)$ is the spectral projection on the continuous spectral subspace of H_V^D in J.

Let us give three examples to complete Corollary 3.7.

First example. — Let $\widehat{V}$ an operator of multiplication on $L^2(\mathbf{Z}^3, \mathbb{C}^6)$ of the form $\widehat{V} = \widehat{D}\widehat{V}_0$ where $\widehat{V}_0$ has compact support and, for all $n \in \mathbf{Z}^3$, the matrix $\widehat{V}_0(n)$ is hermitian, i.e., $\widehat{V}_0(n)^* := \overline{\widehat{V}_0(n)}^{\,T} = \widehat{V}_0(n)$. Then, the operator V defined by the Fourier series $\widehat{V}(n)$ is compact and symmetric on $\mathcal{H}^D$. Let $I \subset \mathbf{R} \setminus \mathcal{T}$. Then, $\widehat{V}$ satisfies assumptions (1)–(2) of Corollary 3.7. In particular, the point spectrum $\sigma_p(H_V^D)$ is of finite multiplicity in $\mathbf{R} \setminus \mathcal{T}$ and has no accumulation point in $\mathbf{R} \setminus \mathcal{T}$.

Second example. — Let $\widehat{V}$ an operator on $L^2(\mathbf{Z}^3, \mathbb{C}^6)$ of the following form

$$\widehat{V} = \widehat{D}\widehat{W}_2\widehat{W}_1\widehat{W}_2$$

where $\widehat{W}_1$ is an operator of multiplication on $L^2(\mathbf{Z}^3, \mathbb{C}^6)$ by symmetric matrices $\widehat{W}_1(n)$ and has compact support, and the operator W_2 defined by the Fourier series of $\widehat{W}_2$ is a symmetric operator of multiplication on $L^2(\mathbb{T}^3, \mathbb{C}^6)$ (equipped with its hilbertian product) with sufficiently smooth coefficients and such that all its partial derivatives until a sufficient large order vanish on $\{x \in \mathcal{X}^*;\ \pm\sqrt{\tau^+(z)}, \pm\sqrt{\tau^-(z)} \in \mathcal{T}_{\mathrm{sm}}\}$. Let $I \subset \mathbf{R}^* \setminus \mathcal{T}_{\mathrm{sm}}$. Then, $\widehat{V}$ satisfies assumptions (1)–(2) of Corollary 3.7.

Although this example is purely academic, it shows that the case where $I \cap \mathcal{T} \neq \emptyset$ and H^D is perturbed by a non trivial potential is not void.

Third example. — This is the most interesting case, so we give the result as a corollary. Let $\widehat{D}_p$ be a perturbation of $\widehat{D}$ of the following form:

$$\widehat{D}_p = \begin{pmatrix} \widetilde{\boldsymbol{\varepsilon}} & 0_{3\times 3} \\ 0_{3\times 3} & \widetilde{\boldsymbol{\mu}} \end{pmatrix}, \tag{3.4}$$

under the assumptions that the 3×3 matrices $\widetilde{\boldsymbol{\varepsilon}}$ and $\widetilde{\boldsymbol{\mu}}$ are diagonal with positive but depending on n coefficients $\widetilde{\varepsilon}_j(n)>0$, $\widetilde{\mu}_j(n)>0$ for $1\leqslant j\leqslant 3$, $n\in\mathbf{Z}^3$, and $\widehat{D}_p-\widehat{D}$ has compact support. We denote by H^{D_p} the operator defined by the Fourier series of $\widehat{H}^{D_p}$.

Corollary 3.8. — *Let a compact interval $I\subset\mathbf{R}\setminus\mathcal{T}$, and fix $\phi\in\mathcal{C}_c^\infty(\mathbf{R}\setminus\mathcal{T})$ such that $\phi=1$ on a neighborhood of I. Then, the points* (1)–(3) *and the conclusion of* (4) *in Corollary 3.7 with H_V^D replaced by H^{D_p} hold.*

Proof in Section 5.2.

4. The conjugate operator

In this section we consider a set $\mathcal{T}'\subset\mathcal{T}$ and a function $\phi\in\mathcal{C}_c^\infty((0,+\infty)\setminus\mathcal{T}',\mathbf{R})$. We construct an adequate conjugate operator A_ϕ to H on $\operatorname{supp}\phi$.

4.1. Eigenprojectors

Assume $\boldsymbol{\beta}=0$. Then, $\Sigma_1=\emptyset$, and the function $y\mapsto\sqrt{\Psi_0(z)}$ is analytic in $\mathbf{R}^3\setminus\{0_{\mathbf{R}^3}\}$. The associated orthogonal eigenprojection

$$\pi_2(y):=\frac{1}{2i\pi}\int_{\mathcal{C}}\big(h^D(y)-\zeta\big)^{-1}\mathrm{d}\zeta\quad\forall\,y\neq 0,\tag{4.1}$$

where $\mathcal{C}\subset\mathbb{C}$ is a complex contour containing $\sqrt{\Psi_0(z)}$ but not 0, is then analytic in $\mathbf{R}^3\setminus\{0_{\mathbf{R}^3}\}$ and has rank two.

Let us assume $\boldsymbol{\beta}\neq 0$. Let us denote by $\pi_1^\pm(y)$ the orthogonal eigenprojection on $\ker(h^D(y)-\sqrt{\tau^\pm(z)})$, i.e.,

$$\pi_1^\pm(y):=\frac{1}{2i\pi}\int_{\mathcal{C}}\big(h^D(y)-\zeta\big)^{-1}\mathrm{d}\zeta\quad\forall\,y\in\sin(\mathcal{X}_1),$$

where $\mathcal{C}$ is a contour containing $\sqrt{\tau^\pm(z)}$ but no other eigenvalue of $h^D(y)$. Let again $\pi_2(y)$ defined by (4.1) where now $\mathcal{C}$ is a contour containing both $\sqrt{\tau^+(z)}$ and $\sqrt{\tau^-(z)}$ but no other eigenvalue. Thus $\pi_2(y)$ is the orthogonal eigenprojection on $\ker(h^D(y)-\sqrt{\tau^+(z)})+\ker(h^D(y)-\sqrt{\tau^-(z)})$, and

$$\pi_2(y)=\pi_1^+(y)\oplus\pi_1^-(y)\quad\forall\,y\in\sin(\mathcal{X}_1).$$

Each $\pi_1^\pm(y)$ has range one and $\pi_2(y)$ has range two. Each $\pi_1^\pm$ is analytic on $\sin(\mathcal{X}_1)\subset\mathbf{R}^3$, π_2 is analytic on $\sin(\mathbf{R}^3)\setminus\{0_{\mathbf{R}^3}\}$ ($\subset\mathbf{R}^3$), and

$$\begin{aligned}h^D(y)\pi_2(y)&=\sqrt{\tau^+(z)}\pi_1^+(y)+\sqrt{\tau^-(z)}\pi_1^-(y)&&\forall\,y\in\sin(\mathcal{X}_1),\\ h^D(y)\pi_2(y)&=\sqrt{\Psi_0(z)}\pi_2(y)&&\forall\,y\in\sin(\mathcal{X}_2).\end{aligned}$$

4.2. Global tangent field to $\mathcal{X}_2$

If $\beta_2 = 0$ then the $\tau^{\pm}$'s and $\pi_1^{\pm}$'s extend analytically into $\mathbf{R}^3 \setminus \{0_{\mathbf{R}^3}\}$ with the relation

$$\pi_2(y) = \pi_1^+(y) + \pi_1^-(y) \quad \forall\, y \neq 0_{\mathbf{R}^3}.$$

In addition, in case (A0) (with $\beta_2 = 0$), the sum $\pi_1^+(y) + \pi_1^-(y)$ is direct.

Let us assume $\beta_2 \neq 0$ (with assumption (A0)) and make a precise description of $\mathcal{X}_2$. A point $x \in \mathbb{T}^3$ belongs to $\mathcal{X}_2$ iff $z \neq 0$ and $z_3 = 0 = \beta_1 z_1 - \beta_2 z_2$. The last relation can be written

$$\beta_1 y_1^2 = \beta_2 y_2^2, \quad y_2 \in [-1,1] \setminus \{0\}.$$

When a nonzero eigenvalue of $H^D(x)$ (resp., of $h^D(y)$) is not simple then the stratification method explained in [8] involves a tangential vector field to the set $\mathcal{X}_2$ (resp., to $\sin(\mathcal{X}_2)$): $w(x) := (\sin(x_1)\cos(x_2), \cos(x_1)\sin(x_2), 0)$, (resp., $\widetilde{w}(y) := (y_1, y_2, 0)$). We observe that $|w(x)| \neq 0$ for all $x \in \mathcal{X}_2 \setminus \mathcal{X}^*$, and $|w(x)| \neq 0$ for all $x \in \mathcal{X}_2$ if $\beta_2 \in (0, \beta_1)$. If $\beta_2 = \beta_1$ then w vanishes at all $x^* \in \mathcal{X}_2^*$ since $z_1^* = z_2^* = 1$.

We introduce the following notations. Letting a function f from $\mathbb{T}^3$ or $\mathbf{R}^3$ into $\mathbb{C}^n$ and a vector field $v(x) = (v_j(x))_{1 \leqslant j \leqslant n} \in \mathbb{C}^n$, then $v \cdot \nabla_x f$ is the vectorial function $x \mapsto \sum_{j=1}^n v_j(x) \partial_{x_j} f(x) \in \mathbb{C}^n$. We set also

$$f_w := w \cdot \nabla_x f,$$
$$\widetilde{f}_{\widetilde{w}} := \widetilde{w} \cdot \nabla_y f.$$

We thus have

$$f_w(x) = \cos(x_1)\cos(x_2) \widetilde{f}_{\widetilde{w}}(y). \tag{4.2}$$

4.3. First cut–off functions

We consider the following metric on $\mathbb{T}^3 \approx (\mathbf{R}/(2\pi\mathbf{Z}))^3$:

$$\mathrm{d}_0(x, x^*) = \left| e^{ix} - e^{ix^*} \right| x^*, \quad x \in \mathbb{T}^3.$$

We denote $\mathrm{d}_0(x, E) = \inf\{\mathrm{d}_0(x, x^*) \mid x^* \in E\}$ when $E \subset \mathbb{T}^3$. We consider a cut–off function $\varphi_1 \in \mathcal{C}^\infty(\mathbf{R}; [0,1])$ such that $\operatorname{supp} \varphi_1 \subset \{s \in \mathbf{R};\, |s| < 1\}$ and $\varphi_1 = 1$ in $\{s;\, |s| < 1/2\}$. Let b, b_0 with $0 < b < b_0/2$ two small parameters which will be precised later. We separate the eigenvalue 0 from $\mathbf{R}^+$, and, equivalently, $\mathcal{X}_0$ from $\mathbb{T}^3$, with the cut–off function $\chi_0(x) := \varphi_1(|z|/b_0)$. Let ϕ with $\operatorname{supp} \phi \subset (0, \infty)$ be as in the statement of Theorem 3.1, we can fix b_0 sufficiently small such that:

$$\left\{ \sqrt{\tau^+(z)}, \sqrt{\tau^-(z)} \right\} \cap \operatorname{supp} \phi \neq \emptyset \Rightarrow \chi_0(x) = 1.$$

In addition we set

$$\begin{aligned}
\chi_{x^*}(x) &:= \varphi_1(\mathrm{d}_0(x,x^*)/b) \quad x^*,\, x \in \mathbb{T}^3, \\
\chi^{*+}(x) &:= (1-\chi_0(x)) \prod_{x^* \in \mathcal{X}_1^{*+}} (1-\chi_{x^*}), \\
\chi^{*-}(x) &:= (1-\chi_0(x)) \prod_{x^* \in \mathcal{X}_1^{*-}} (1-\chi_{x^*}), \\
\chi^{*}(x) &:= (1-\chi_0(x)) \prod_{x^* \in \mathcal{X}^{*}} (1-\chi_{x^*}),
\end{aligned}$$

so χ^* vanishes in $\{x \in \mathbb{T}^3; \mathrm{d}_0(x,\mathcal{X}^*) < b/2\}$ and in $\{x \in \mathbb{T}^3; |z| < b_0/2\}$; we have also $\chi^*(x) = 1$ if $\mathrm{d}_0(x,\mathcal{X}^*) > b$ and $|z| > b_0$. It means that χ^* is a smooth cut-off function localizing in the complement of $\mathcal{X}^* \cup \mathcal{X}_0$, and, since $\mathcal{X}^* \cup \mathcal{X}_0$ is a discrete set (and finite), we then have, for $b_0 > 0$ sufficiently small,

$$\begin{aligned}
1-\chi^*(x) &= \chi_0(x) + \sum_{x^* \in \mathcal{X}^*} \chi_{x^*}(x), \\
1-\chi^{*\pm}(x) &= \chi_0(x) + \sum_{x^* \in \mathcal{X}_1^{*\pm}} \chi_{x^*}(x).
\end{aligned}$$

4.4. The conjugate operator outside thresholds

Case 1: $\boldsymbol{\beta} = 0$. — Remember that we have $\pi_1^+ = \pi_1^- = \pi_2$ which is analytic in $\mathbf{R}^3 \setminus \{0_{\mathbf{R}^3}\}$. We set, for $u \in \mathcal{C}^\infty(\mathbb{T}^3)$, $x \in \mathbb{T}^3$,

$$\mathcal{A}_{\mathrm{out}} u\,(x) := i\chi^*(x)\pi_2(y) \frac{\nabla_x \sqrt{\Psi_0(z)}}{|\nabla_x \sqrt{\Psi_0(z)}|^2} \cdot \nabla_x \big(\chi^*(x)\pi_2(y)u(x)\big). \tag{4.3}$$

Let us give a brief explanation. For a simple scalar multiplication operator h on $L^2((0,1),\mathbb{C})$ which is the multiplication by a smooth function h with a positive (or negative) derivative h', the most usual conjugate operator is the hermitian conjugate $\frac{1}{2}(\mathcal{A}+\mathcal{A}^*)$ of the operator $u(x) \mapsto \mathcal{A}u(x) = iu'(x)/h'(x) = i\mathrm{d}u/\mathrm{d}h$. In fact, it is easy to see that, at least formally, the commutator satisfies the relation $[h, i\mathcal{A}] = \mathrm{id}$ which is the simplest form of Mourre's inequality (3.1). In our case the multiplication operator H^D is not scalar-valued, but, in place of it we can consider the multiplication operator $H^D(x)\pi_2(y)$ which is scalar-valued since it multiplies functions of x by the eigenvalue $\sqrt{\Psi_0(z)}$. In (4.3) the differential operator $|\nabla_x\sqrt{\Psi_0(z)}|^{-2}(\nabla_x\sqrt{\Psi_0(z)})\nabla_x\cdot$ is the operator of partial derivation according to the coordinate $x \mapsto \sqrt{\Psi_0(z)}$ and generalizes the above operator $\mathrm{d}\cdot/\mathrm{d}h$.

Case 2: $\boldsymbol{\beta} \neq 0$ and $\beta_2 = 0$ (with assumption (A0)*).* — Remember that the functions $\tau^{\pm}(\cdot)$ are analytic in $\mathbf{R}^3$ (see (2.6) and (2.7)) and are positive in $[0,+\infty)^3 \setminus \{0_{\mathbf{R}^3}\}$. Thus, the eigenvalues $\sqrt{\tau^{\pm}(\cdot)}$ are analytic in $[0,+\infty)^3 \setminus \{0_{\mathbf{R}^3}\}$. We set, for $u \in \mathcal{C}^\infty(\mathbb{T}^3)$, $x \in \mathbb{T}^3$,

$$\mathcal{A}_{\text{out}} u\,(x) := \sum_{\pm} i\chi^*(x)\pi_1^{\pm}(y)\frac{\nabla_x\sqrt{\tau^{\pm}(z)}}{\left|\nabla_x\sqrt{\tau^{\pm}(z)}\right|^2}\cdot\nabla_x\big(\chi^*(x)\pi_1^{\pm}(y)u(x)\big).$$

Case 3: $\beta_2 \neq 0$ (with assumption (A0)*).* — Firstly, we have $\mathcal{X}_1^{*+} \subset \mathcal{X}_1^{*-}$, but not necessarily the converse inclusion. Actually, if $\nu \in (0,1)$ (remember Lemma 2.9) then the value $\sqrt{\tau^-(1,1,\nu)}$ is a threshold but not necessarily $\sqrt{\tau^+(1,1,\nu)}$, so we may have $x_\nu^* \in \mathcal{X}_1^{*-} \setminus \mathcal{X}_1^{*+}$.

Secondly, in aim to have $H^D \in \mathcal{C}^\infty(\mathcal{A}_{\text{out}})$ we need to separate $\mathcal{X}_2 \subset \partial\mathcal{X}_1$ from $\mathcal{X}_1$, as explained in [9]. (Remember that a short definition of a class as $\mathcal{C}^\infty(\mathcal{A}_{\text{out}})$ is given in Remark 3.2). Since $\overline{\mathcal{X}_2} = \mathcal{X}_2 \cup \mathcal{X}_0 = \{x \in \mathbb{T}^3; K_0(z) = 0\}$ is compact then there exist two smooth cut-off functions, χ_1 and χ_2 in $\mathcal{C}^\infty(\mathbb{T}^3;[0,1])$, such that $\operatorname{supp}\chi_2 \subset \{x;\, \mathrm{d}_0(x,\mathcal{X}_2) \leqslant 2b\}$, $\chi_2(x) = 1$ if $\mathrm{d}_0(x,\mathcal{X}_2) \leqslant b$, $\chi_1(x) = 1$ if $\mathrm{d}_0(x,\mathcal{X}_2) \geqslant 3b$, and $\operatorname{supp}\chi_1 \subset \{x;\, \mathrm{d}_0(x,\mathcal{X}_2) \geqslant 2b\}$. Thus $\operatorname{supp}\chi_1 \cap \operatorname{supp}\chi_2 = \emptyset$ and $\chi_2 = 1$ on $\overline{\mathcal{X}_2}$. We then set $\chi_3 := 1 - \chi_1 - \chi_2$ so $\operatorname{supp}\chi_3 \subset \{x;\, b \leqslant \mathrm{d}_0(x,\mathcal{X}_2) \leqslant 3b\}$, and

$$\sum_{j=1}^{3}\chi_j^2(x) > 0 \quad \forall\, x \in \mathbb{T}^3.$$

We have in addition (b being sufficiently small)

$$\operatorname{supp}\chi_{x^*} \subset \operatorname{supp}\chi_1 \setminus \operatorname{supp}\chi_3 \quad \forall\, x^* \in \mathcal{X}_1^*, \tag{4.4}$$

$$\operatorname{supp}\chi_{x^*} \subset \operatorname{supp}\chi_2 \setminus \operatorname{supp}\chi_3 \quad \forall\, x^* \in \mathcal{X}_2^*. \tag{4.5}$$

We set

$$\begin{aligned}\chi_j^*(x) &:= \chi^*(x)\chi_j(x) \quad j = 2,3\\ \chi_1^{*\pm}(x) &:= \chi^{*\pm}(x)\chi_1(x).\end{aligned}$$

(In fact, Relations (4.4) and (4.5) imply $\chi_3^* = (1-\chi_0)\chi_3$.) The function χ_2^* is a smooth cut-off localizing in $\mathcal{X}_2 \setminus \mathcal{X}^*$ while $\chi_1^{*\pm}$ is a smooth cut-off localizing in $\mathcal{X}_1 \setminus \mathcal{X}_1^{*\pm}$.

For $u \in \mathcal{C}^\infty(\mathbb{T}^3)$, $x \in \mathbb{T}^3$, we set,

$$\begin{aligned}\mathcal{A}_{\mathrm{out}} u\,(x) := &\sum_{\pm} i\chi_1^{*\pm}(x)\pi_1^{\pm}(y)\frac{\nabla_x\sqrt{\tau^{\pm}(z)}}{\left|\nabla_x\sqrt{\tau^{\pm}(z)}\right|^2}\cdot\nabla_x\big(\chi_1^{*\pm}(x)\pi_1^{\pm}(y)u(x)\big)\\ &+ i\chi_2^*(x)\Big(\sqrt{\Psi_0(z)}_w\Big)^{-1}\pi_2(y)\ \big(\chi_2^*(x)\pi_2(y)u(x)\big)_w\\ &+\sum_{\pm} i\chi_3^*(x)\Big(\sqrt{\Psi_0(z)}_w\Big)^{-1}\pi_1^{\pm}(y)\ \big(\chi_3^*(x)\pi_1^{\pm}(y)u(x)\big)_w.\end{aligned}$$

Remark 4.1. — The function $\sqrt{\Psi_0(z)}_w$ may vanish at points of $\mathcal{X}^*$ but not of $\mathcal{X}_2\setminus\mathcal{X}^*$ so $\chi_2^*(x)(\sqrt{\Psi_0(z)}_w)$ is well-defined (for b sufficiently small). For more details, see the proof of (4.7) below. Similarly, the function $x\mapsto |\nabla_x\sqrt{\tau^{\pm}(z)}|$ is positive in $\operatorname{supp}\chi_1^{*\pm}$.

In each case we symmetrize $\mathcal{A}_{\mathrm{out}}$ by putting

$$A_{\mathrm{out}} := \mathcal{A}_{\mathrm{out}} + \mathcal{A}_{\mathrm{out}}^*,$$

with domain $\mathcal{C}^\infty(\mathbb{T}^3)$. Here $\mathcal{A}_{\mathrm{out}}^*$ is the hermitian conjugate of $\mathcal{A}_{\mathrm{out}}$. By observing that the mappings $x\mapsto\chi_j(x)\pi_1^{\pm}(y)$ for $j=1,3$, and $x\mapsto(1-\chi_0(x))\,\pi_2(y)$ are smooth, then A_{out} is a symmetric first order differential operator in x whose coefficients belong to $\mathcal{C}^\infty(\mathbb{T}^3,\mathcal{L}(\mathbb{C}^6))$. It is then essentially self-adjoint on $\mathcal{H}^D$ (see [8, Lemma 3.10]). Since $D(H^D)=\mathcal{H}^D$, some possible problematic points of the Mourre Theory then become trivial (see [7]).

4.5. "Punctual" Mourre's estimate outside thresholds

We set

$$H_{1,\mathrm{out}}(x) := \big[H^D, iA_{\mathrm{out}}\big](x).$$

Similarly to proof of the Mourre's estimate in [8] we show that if the positive parameter b is sufficiently small then A_{out} is strictly conjugated to H on I.

Case 1: $\beta_2\neq 0$ under assumption (A0). — Let $u\in\mathcal{C}^\infty(\mathbb{T}^3)$, we have

$$\begin{aligned}-\,i\mathcal{A}_{\mathrm{out}}\circ H^D u\,(x)\\ =&\sum_{\pm}\chi_1^{*\pm}(x)\pi_1^{\pm}(y)\frac{\nabla_x\sqrt{\tau^{\pm}(z)}}{\left|\nabla_x\sqrt{\tau^{\pm}(z)}\right|^2}\cdot\nabla_x\big(\chi_1^{*\pm}(x)\pi_1^{\pm}(y)h^D(y)u(x)\big)\\ &+\chi_2^*(x)\pi_2(y)\Big(\sqrt{\Psi_0(z)}_w\Big)^{-1}\ \big(\chi_2^*(x)\pi_2(y)h^D(y)u(x)\big)_w\\ &+\sum_{\pm}\chi_3^*(x)\pi_1^{\pm}(y)\Big(\sqrt{\Psi_0(z)}_w\Big)^{-1}\ \big(\chi_3^*(x)\pi_1^{\pm}(y)h^D(y)\big)_w.\end{aligned}$$

By using

$$\begin{aligned}\big(\pi_1^{\pm}(y)\big)^2 &= \pi_1^{\pm}(y),\\ \pi_1^{\pm}(y)h^D(y) &= h^D(y)\pi_1^{\pm}(y),\\ \pi_2(y)h^D(y) &= h^D(y)\pi_2(y),\end{aligned}$$

we obtain the expression of $[H^D, i\mathcal{A}_{\mathrm{out}}]$ as a multiplication operator:

$$\begin{aligned}\big[H^D, i\mathcal{A}_{\mathrm{out}}\big](x) &= \big(iH^D\circ\mathcal{A}_{\mathrm{out}} - i\mathcal{A}_{\mathrm{out}}\circ H^D\big)(x)\\ &= \sum_{\pm}\big(\chi_1^{*\pm}(x)\big)^2\frac{\nabla_x\sqrt{\tau^{\pm}(z)}}{\big|\nabla_x\sqrt{\tau^{\pm}(z)}\big|^2}\pi_1^{\pm}(y)\cdot\nabla_x\big(\pi_1^{\pm}(y)h^D(y)\big)\pi_1^{\pm}(y)\\ &\quad+(\chi_2^*(x))^2\Big(\sqrt{\Psi_0(z)}_w\Big)^{-1}\,\pi_2(y)\big(h^D(y)\pi_2(y)\big)_w\pi_2(y)\\ &\quad+\sum_{\pm}(\chi_3^*(x))^2\Big(\sqrt{\Psi_0(z)}_w\Big)^{-1}\,\pi_1^{\pm}(y)\big(h^D(y)\pi_1^{\pm}(y)\big)_w\pi_1^{\pm}(y).\end{aligned}$$

In $\mathcal{X}_1$ we have

$$\pi_1^{\pm}(y)\nabla_x\big(h^D(y)\pi_1^{\pm}(y)\big)\pi_1^{\pm}(y) = \nabla_x\sqrt{\tau^{\pm}(z)}\pi_1^{\pm}(y),$$

so,

$$\begin{aligned}\Big|\nabla_x\sqrt{\tau^{\pm}}(z)\Big|^{-2}\pi_1^{\pm}(y)\nabla_x\sqrt{\tau^{\pm}}(z)\cdot\nabla_x\big(h^D(y)\pi_1^{\pm}(y)\big)\pi_1^{\pm}(y) &= \pi_1^{\pm}(y),\\ \sum_{\pm}\pi_1^{\pm}(y)\Big(\sqrt{\tau^{\pm}}_w(x)\Big)^{-1}w\cdot\nabla_x\big(h^D(y)\pi_1^{\pm}(y)\big) = \sum_{\pm}\pi_1^{\pm}(y) &= \pi_2(y).\end{aligned}$$

Let us make the following computations near $\mathcal{X}_2$, precisely, in $\operatorname{supp}\chi_2^*\cup\operatorname{supp}\chi_3^*$. Putting $\xi(y) := h^D(y)\pi_2(y) - \sqrt{\Psi_0(z)}\pi_2(y)$, we have

$$\pi_2(y)\;w(x)\cdot\nabla_x\big(h^D(y)\pi_2(y)\big)\pi_2(y) = \sqrt{\Psi_0(z)}(x)\pi_2(y) + \pi_2(y)\;\xi_w(x)\pi_2(y).$$

Thus,

$$\begin{aligned}\frac{1}{2}H_{1,\mathrm{out}}(x) = \sum_{\pm}\big(\chi_1^{*\pm}(x)\big)^2\pi_1^{\pm}(y) + \big((\chi_2^*(x))^2 + (\chi_3^*(x))^2\big)\pi_2(y)\\ + (\chi_2^*(x))^2\pi_2(y)\Big(\sqrt{\Psi_0(z)}\Big)^{-1}\,\xi_w(x)\pi_2(y). \quad (4.6)\end{aligned}$$

For $x\in\mathcal{X}_2$ we have $\xi(y)=0$, so, since $\widetilde{w}$ is a tangent field to $\sin(\mathcal{X}_2)$,

$$\widetilde{\xi}_{\tilde{w}}(y) = 0, \quad \forall\, x\in\mathcal{X}_2.$$

For $x\in\mathcal{X}_2$ we have

$$\widetilde{\sqrt{\Psi_0(z)}}_{\tilde{w}} = (\Psi_0(z))^{-1/2}(\alpha_1 z_1 + \alpha_2 z_2) > 0. \quad (4.7)$$

In addition, since the relation

$$\left(\sqrt{\Psi_0(z)}_w\right)^{-1}\xi_w(x)=\left(\widetilde{\sqrt{\Psi_0(z)}_{\tilde w}}\right)^{-1}\widetilde{\xi}_{\tilde w}(y)$$

holds true for $x\notin\mathcal{X}^*$ and $\widetilde{\sqrt{\Psi_0(z)}_{\tilde w}}\neq 0$, then the function $(\sqrt{\Psi_0(z)}_w)^{-1}\xi_w$ is defined and is smooth in the compact set $\operatorname{supp}(1-\chi_0)\chi_2\subset\operatorname{supp}\chi_2\subset\{x\in\mathbb{T}^3;\ \mathrm{d}_0(x,\mathcal{X}_2)\leqslant 2b\}$, and vanishes on $\mathcal{X}_2$. Hence, for b sufficiently small, we have

$$\left\|(\sqrt{\Psi_0(z)}_w)^{-1}\xi_w(x)\right\|_\infty<\frac{1}{2}\quad\forall\, x\in\operatorname{supp}(1-\chi_0)\chi_2,\tag{4.8}$$

where $\|\cdot\|_\infty$ denotes here the usual infinite norm on matrices. From (4.6), (4.8), we then obtain

$$H_{1,\mathrm{out}}(x)\geqslant\sum_{\pm}\big(\chi_1^{*\pm}(x)\big)^2\pi_1^{\pm}(y)+\big((\chi_2^*(x))^2+(\chi_3^*(x))^2\big)\pi_2(y).\tag{4.9}$$

Remark 4.2. — In the two other cases where $\beta_2=0$ we obtain

$$\frac{1}{2}H_{1,\mathrm{out}}(x)=(\chi^*(x))^2\pi_2(y),\tag{4.10}$$

so the punctual Mourre's estimate becomes simply

$$H_{1,\mathrm{out}}(x)\geqslant 2(\chi^*(x))^2\pi_2(y).$$

4.6. Smoothness

Relations (4.6)–(4.10) show that the symmetric form $H_{1,\mathrm{out}}$ defined on $\mathcal{C}^\infty(\mathbb{T}^3)$ is a multiplication operator on $\mathcal{H}^D$ by smooth coefficients, so is bounded and closeable. Thus, $[H_{1,\mathrm{out}},iA_{\mathrm{out}}]$ is a differential operator of order one at most. But when computing its first order term we have to check only that $H_{1,\mathrm{out}}$ is commuting with each coefficient of the first order terms of $-i\mathcal{A}_{\mathrm{out}}(x)$. In fact, the possible problematic bracket arising from the calculation of $[H_{1,\mathrm{out}},i\mathcal{A}_{\mathrm{out}}]$ is, in the case $\beta_2\neq 0$,

$$\begin{bmatrix}(\chi_2^*(x))^2\left(\sqrt{\Psi_0(z)}_w\right)^{-1}\pi_2(y)\ \xi_w(x)\pi_2(y),\\ \big(\chi^{*\pm}(x)\big)^2\dfrac{\nabla_x\sqrt{\tau^{\pm}(z)}}{\left|\nabla_x\sqrt{\tau^{\pm}(z)}\right|^2}\pi_1^{\pm}(y)\nabla_x\big(h^D(y)\pi_1^{\pm}(y)\big)\pi_1^{\pm}(y)\end{bmatrix}.$$

But since $\chi_1\chi_2=0$ then this bracket vanishes. Hence, $[H_{1,\mathrm{out}},iA_{\mathrm{out}}]$ is a multiplication operator, is bounded in $\mathcal{H}$, and we have $H^D\in\mathcal{C}^2(A_{\mathrm{out}})$. By induction we see that $H^D\in\mathcal{C}^\infty(A_{\mathrm{out}})$. (See also [9].)

4.7. The conjugate operator near thresholds

4.7.1. Enumeration of the different cases

Since our proof of the LAP at each threshold related to some $x^* \in \mathcal{X}^*$ requires a special treatment which depends on the values of $\boldsymbol{\beta}$ and of x^*, we enumerate the different cases as follows.

(1) $\boldsymbol{\beta} = 0$ and $x^* \in \mathcal{X}_2^*$.
(2) $\boldsymbol{\beta} \neq 0$ (so (A0) holds) and $x^* \in \mathcal{X}_1^*$.
 (2-1) $\beta_2 = 0$.
 (2-2) $\beta_2 > 0$.
  (2-1a) $x^* \in \mathcal{X}_1^{*-}$ and $z_1^* = z_2^* = 1$ and $z_3^* = \nu \in (0,1)$.
  (2-1b) $x^* \in \mathcal{X}_1^{*-}$ and $z_1^* = z_2^* = 1$ and $z_3^* \neq \nu$.
  (2-1c) $x^* \in \mathcal{X}_1^{*-}$ and $z_1^* = z_2^* = 1$ and $z_3^* = \nu \in \{0,1\}$.
  (2-1d) $x^* \in \mathcal{X}_1^{*-}$ and ($z_1^* = 0$ or $z_2^* = 0$).
  (2-1e) $x^* \in \mathcal{X}_1^{*+}$.
(3) $\boldsymbol{\beta} \neq 0$ and $x^* \in \mathcal{X}_2^*$.
 (3-1) $\beta_2 = 0$.
 (3-2) $\beta_2 = \beta_1$.
 (3-3) $\beta_2 \in (0, \beta_1)$.

Remark 4.3. — In (2-1c), if $\beta_1 = \beta_2$ then $(1,1,0) \in \sin^2 \mathcal{X}_2^*$ so $\nu = 1$.

4.7.2. Behaviour of the eigenvalues of $H^D(x)$ at a threshold

We set $s_j^* = 1 - 2z_j^*$ if $z_j^* \in \{0,1\}$, $j \in [\![1,3]\!]$, so $s_j^* \in \{-1,1\}$. We set also $s_j = s_j^*$ for $j = 1,2$.

- In Case (1) we set $V = \sqrt{\ } \circ \Psi_0 \circ \sin^2$ and $s_3 := s_3^*$.
- In Case (2) with $x^* \in \mathcal{X}_1^{*\pm}$ and in Case (3-1) we set $V = \sqrt{\ } \circ \tau^{\pm} \circ \sin^2$ and
  - in Cases (2-1), (2-1d) and (2-1e), and (3-1) we set $s_3 := s_3^*$;
  - in Case (2-1a) we set $s_3 := 1$;
  - in Case (2-1b) we set $s_3 := \operatorname{sgn}(z_3^* - \nu) s_3^*$.

Lemma 4.4. — *In Cases* (1)*,* (2-1)*,* (2-1a)*,* (2-1b)*,*(2-1d)*,* (2-1e) *and* (3-1) *we have*

$$\mathrm{d}V(x) = \left(\sum_{j=1}^{3} C_j s_j (x_j - x_j^*) \mathrm{d}x_j \right) (1 + O(\mathrm{d}_0(x, x^*))), \qquad (4.11)$$

as $x \to x^*$*, where* $C_j > 0$*,* $j = 1, 2, 3$*. In Case* (2-1d) *we have*

$$\begin{aligned} &\mathrm{d}V(x) \\ &= \left(-\sum_{j=1}^{2} C_j (x_j - x_j^*) \mathrm{d}x_j + C_3 (x_3 - x_3^*)^3 \mathrm{d}x_3 \right) (1 + O(\mathrm{d}_0(x, x^*))), \quad (4.12) \end{aligned}$$

as $x \to x^*$*, where* $C_j > 0$*,* $j = 1, 2, 3$*.*

Proof in Appendix B.

Lemma 4.5. — *Consider Cases* (3-2) *or* (3-3) *(i.e., assumption* (A0) *with* $\beta_2 \neq 0$ *and* $x^* \in \mathcal{X}_2^*$*). We then have the following estimates.*

In Case (3-2)*,*

$$\left(\sqrt{\Psi_0(z)}_w\right) = C(x_1 - x_1^*)(x_2 - x_2^*)\big(1 + O(\mathrm{d}_0(x, x^*))\big), \qquad (4.13)$$

and, in Case (3-3)*,*

$$\left(\sqrt{\Psi_0(z)}_w\right) = C(x_2 - x_2^*)(1 + O\big(\mathrm{d}_0(x, x^*))\big), \qquad (4.14)$$

for some $C \neq 0$ *as* $x \to x^*$*.*

Proof in Appendix B.

4.7.3. New coordinate near an element of $\mathcal{X}^*$

We give an approximation of a vector proportional to $\nabla_x V(x)$ (where V is defined in Section 4.7.2) of the form $\nabla_x p_1$ near a point $x^* \in \mathcal{X}_j^*$. We then give an approximation of a vector proportional to $w(x)$ near a point $x^* \in \mathcal{X}_2^*$ in Cases (3-2)–(3-3).

With the notations of Lemma 4.4, in Cases (1), (2-1), (2-2), (2-1a), (2-1b), (2-1d), (2-1e) and (3-1), we set

$$p_1(x; x^*) = \frac{1}{2} \sum_{j=1}^{3} C_j s_j (x_j - x_j^*)^2;$$

in Case (2-1c), we set

$$p_1(x; x^*) = \frac{1}{2} \sum_{j=1}^{2} C_j (x_j - x_j^*)^2 - \frac{1}{4} C_3 (x_3 - x_3^*)^4.$$

Then, Relations (4.11)–(4.12) of Lemma 4.4 can be written

$$\mathrm{d}V(x) = (1 + O(\mathrm{d}_0(x, x^*)))\mathrm{d}p_1(x; x^*), \quad x \to x^*.$$

4.7.4. The conjugate operator near thresholds

Let $x^* \in \mathcal{X}^*$. For simplicity we then write $p_1(x;x^*) = p_1(x)$. For $u \in \mathcal{D}_0$ and $x \in \mathbb{T}^3 \setminus \{x^*\}$ we set,

- in Case (1) ($\boldsymbol{\beta} = 0$, $x^* \in \mathcal{X}_2^*$):

$$\mathcal{A}_{x^*} u\,(x) := i\chi_{x^*}(x)\pi_2(y) \frac{\nabla_x p_1(x)}{\nabla_x p_1(x) \cdot \nabla_x \sqrt{\Psi_0(z)}} \cdot \nabla_x(\chi_{x^*}(x)\pi_2(y)u(x)),$$

- in Case (2) ($\boldsymbol{\beta} \neq 0$, $x^* \in \mathcal{X}_1^{*\pm}$) and Case (3-1) ($\boldsymbol{\beta} \neq 0$, $\beta_2 = 0$, $x^* \in \mathcal{X}_2^*$):

$$\mathcal{A}_{x^*}^{\pm} u\,(x) := i\chi_{x^*}(x)\pi_1^{\pm}(y) \frac{\nabla_x p_1(x)}{\nabla_x p_1(x) \cdot \nabla_x \sqrt{\tau^{\pm}(z)}} \cdot \nabla_x\big(\chi_{x^*}(x)\pi_1^{\pm}(y)u(x)\big),$$

  and $\mathcal{A}_{x^*} := \mathcal{A}_{x^*}^{+} + \mathcal{A}_{x^*}^{-}$,
- in Cases (3-2)–(3-3) ($\beta_2 \neq 0$, $x^* \in \mathcal{X}_2^*$):

  $$\mathcal{A}_{x^*} u\,(x) := i\chi_{x^*}(x)\pi_2(y)\big(\sqrt{\Psi_0(z)}_w\big)^{-1}(\chi_{x^*}(x)\pi_2(y)u(x))_w.$$

  In each case we symmetrize $\mathcal{A}_{x^*}$ and $\mathcal{A}_{x^*}^{\pm}$ by putting

  $$A_{x^*} := \mathcal{A}_{x^*} + \mathcal{A}_{x^*}{}^*, \quad A_{x^*}^{\pm} := \mathcal{A}_{x^*}^{\pm} + (\mathcal{A}_{x^*}^{\pm})^*,$$

  where $\mathcal{A}_{x^*}{}^*$ (resp., $(\mathcal{A}_{x^*}^{\pm})^*$) denotes the formal adjoint to $\mathcal{A}_{x^*}$ (resp., to $\mathcal{A}_{x^*}^{\pm}$). It is defined on $\mathcal{D}_0$ too.

We set

$$\mathcal{T}_{\text{in}} := (\mathcal{T} \setminus \mathcal{T}') \cap (0, +\infty),$$
$$\mathcal{X}_{1,\text{in}}^{*\pm} := \Big\{x \in \mathcal{X}_1^{*\pm};\ \sqrt{\tau^{\pm}(z)} \in \mathcal{T}_{\text{in}}\Big\},$$
$$\mathcal{X}_{2,\text{in}}^{*} := \Big\{x \in \mathcal{X}_2^{*};\ \sqrt{\Psi_0(z)} \in \mathcal{T}_{\text{in}}\Big\}.$$

(We have, in Case (1), $\mathcal{X}_{1,in}^{*\pm} = \emptyset$.) We set

$$A_{\text{in}} := \sum_{x^* \in \mathcal{X}_{2,\text{in}}^*} A_{x^*} + \sum_{\pm} \sum_{x^* \in \mathcal{X}_{1,\text{in}}^{*\pm}} A_{x^*}^{\pm}.$$

Then the operator A_{in} with domain $\mathcal{D}_0$ is symmetric, closable and densely defined on $\mathcal{H}^D$.

We set, as quadratic forms defined on $\mathcal{D}_0$,

$$H_{1,x^*} := \big[H^D, iA_{x^*}\big], \quad H_{1,\text{in}} := \big[H^D, iA_{\text{in}}\big].$$

By a straight calculation as in Section 4.5 we obtain

Lemma 4.6. — *We have for $x \neq x^*$, in Cases* (1) *and* (2)*:*

$$\frac{1}{2} H_{1,x^*}(x) = (\chi_{x^*}(x))^2 \pi_2(y),$$

and, in Cases (3-2) *and* (3-3)*,*

$$\frac{1}{2} H_{1,x^*}(x) = (\chi_{x^*}(x))^2 \pi_2(y) + (\chi_{x^*}(x))^2 \pi_2(y) \left(\sqrt{\Psi_0(z)}_w\right)^{-1} \xi_w(x) \pi_2(y).$$

Lemma 4.6 shows that the quadratic forms H_{1,x^*} and $H_{1,\mathrm{in}}$ extend continuously as bounded quadratic forms on $\mathcal{H}^D$ which are associated with bounded self-adjoint operators, as multiplication operators by smooth real symmetric coefficients, denoted, respectively, H_{1,x^*} and $H_{1,\mathrm{in}}$. In addition, these coefficients (as functions of x) are commuting with $\pi_2(y)$. Then, an obvious iteration shows that $H^D \in \mathcal{C}^\infty(A_{x^*})$ for all $x^* \in \mathcal{X}^*$. Since $x \neq x'$ implies $\operatorname{supp} \chi_x \cap \operatorname{supp} \chi_{x'} = \emptyset$ then $H^D \in \mathcal{C}^\infty(A_{\mathrm{in}})$.

We set

$$A_\phi := A_{\mathrm{out}} + A_{\mathrm{in}}.$$

The argumentation to prove the property $H^D \in \mathcal{C}^\infty(A_{\mathrm{out}})$ at Section 4.6 still holds with A_{out} replaced by A_ϕ, so we obtain

Lemma 4.7. — *The quadratic form $H_{1,\phi} := [H^D, iA_\phi]$ defined on $\mathcal{D}_0$ defines a bounded self-adjoint multiplication operator on $\mathcal{H}^D$. In addition, $H^D \in \mathcal{C}^\infty(A_\phi)$.*

4.8. "Punctual" Mourre's estimate

Proof. — Let us prove that

$$\phi(H^D)(x) H_{1,\phi}(x) \phi(H^D)(x) \geqslant C \phi^2(H^D)(x), \tag{4.15}$$

for all $x \in \mathbb{T}^3$, where $C > 0$ does not depend on x but on ϕ only.

We consider the case $\beta_2 \neq 0$ (under assumption (A0)) only. The other case $\beta_2 = 0$ is more simple and omitted. As in Section 4.5 (see (4.6)) the calculation of $H_{1,\phi}$ yields

$$\begin{aligned} &\frac{1}{2} H_{1,\phi}(x) \\ &= \sum_{\pm} \left(\chi_1^{*\pm}(x)\right)^2 \pi_1^{\pm}(y) + \left((\chi_2^*(x))^2 + (\chi_3^*(x))^2\right) \pi_2(y) \\ &\quad + (\chi_2^*(x))^2 \pi_2(y) T_w(x)^{-1} \xi_w(x) \pi_2(y) \\ &\quad + \sum_{\pm} \sum_{x^* \in \mathcal{X}_{1,\mathrm{in}}^{*+} \cup \mathcal{X}_{1,\mathrm{in}}^{*-}} (\chi_{x^*}(x))^2 \pi_1^{\pm}(y) + \sum_{x^* \in \mathcal{X}_{2,\mathrm{in}}^*} (\chi_{x^*}(x))^2 \pi_2(y) \end{aligned}$$

$$+ \sum_{x^* \in \mathcal{X}^*_{2,\mathrm{in}}} (\chi_{x^*}(x))^2 \pi_2(y) \big(\sqrt{\Psi_0(z)}_w\big)^{-1} \xi_w(x)\pi_2(y), \quad x \notin \mathcal{X}^* \cup \mathcal{X}_0.$$

Thus, as for inequality (4.9), we get,

$$\begin{aligned} H_{1,\phi}(x) \geqslant & \sum_{\pm} (\chi_1^{*\pm}(x))^2 \pi_1^{\pm}(y) + \big((\chi_2^*(x))^2 + (\chi_3^*(x))^2\big)\pi_2(y) \\ & + \sum_{\pm} \sum_{x^* \in \mathcal{X}^{*\pm}_{1,\mathrm{in}} \cup \mathcal{X}^{*-}_{1,\mathrm{in}}} (\chi_{x^*}(x))^2 \pi_1^{\pm}(y) \;+ \sum_{x^* \in \mathcal{X}^*_{2,\mathrm{in}}} (\chi_{x^*}(x))^2 \pi_2(y). \quad (4.16) \end{aligned}$$

Let us fix $x \in \operatorname{supp} \phi(H^D(x))$. Thus $\chi_0(x) = 1$. We consider the following cases.

Case 1: $\mathrm{d}_0(x, \mathcal{X}^*) \geqslant b$. — Then, $x \notin \operatorname{supp} \chi_{x^*}$ for any $x^* \in \mathcal{X}^*$, and $\chi^*(x) = \chi^{*\pm}(x) = 1$. Hence (4.16) becomes

$$\begin{aligned} H_{1,\phi}(x) &\geqslant \sum_{\pm} \chi_1^2(x)\pi_1^{\pm}(y) + \big(\chi_2^2(x) + \chi_3^2(x)\big)\pi_2(y) = \sum_{j=1}^{3} \chi_j^2(x)\pi_2(y) \\ &\geqslant \delta_0 \pi_2(y), \end{aligned}$$

where $\delta_0 := \min_{\mathbb{T}^3} \sum_{j=1} \chi_j^2 > 0$. Since $\phi(H^D(x))\pi_2(x) = \phi(H^D(x))$, then (4.15) holds.

Case 2: $\mathrm{d}_0(x, \mathcal{X}^*) < b$. — Then there exists exactly one $x^* \in \mathcal{X}^*$ such that $x \in \operatorname{supp} \chi_{x^*}$ and $x \notin \operatorname{supp} \chi_{x'}$ if $x' \in \mathcal{X}^* \setminus \{x^*\}$. We set

$$\delta(x^*) := \min_{\{\chi_0 = 1\}} (1 - \chi_{x^*})^2 + (\chi_{x^*})^2 > 0.$$

If $x^* \notin \mathcal{X}^*_{2,\mathrm{in}} \cup \mathcal{X}^{*+}_{1,\mathrm{in}} \cup \mathcal{X}^{*-}_{1,\mathrm{in}}$ then $x \notin \sup \phi(H^D)(x)$ so (4.15) is trivial. We thus assume $x^* \in \mathcal{X}^*_{2,\mathrm{in}} \cup \mathcal{X}^{*+}_{1,\mathrm{in}} \cup \mathcal{X}^{*-}_{1,\mathrm{in}}$.

(a) *Case* $x^* \in \mathcal{X}^*_{2,\mathrm{in}}$: Thus $x \notin \operatorname{supp} \chi_1 \bigcup \operatorname{supp} \chi_3$ and

$$\chi_2^*(x) = (1 - \chi_{x^*}(x))\chi_2(x) = (1 - \chi_{x^*}(x)).$$

Hence (4.16) becomes

$$H_{1,\phi}(x) \geqslant (\chi_2^*(x))^2 \pi_2(y) + (\chi_{x^*}(x))^2 \pi_2(y) \geqslant \delta(x^*).$$

Thus (4.15) holds.

(b) *Case* $x^* \in \mathcal{X}^{*+}_{1,\mathrm{in}}$ (which is included in $\mathcal{X}^{*-}_{1,\mathrm{in}}$ and does not intersect $\mathcal{X}^*_{2,\mathrm{in}}$). Thus $x \notin \operatorname{supp} \chi_2 \cup \operatorname{supp} \chi_3$ and

$$\chi_1^{*\pm}(x) = (1 - \chi_{x^*}(x))\chi_1(x) = 1 - \chi_{x^*}(x).$$

Hence (4.16) becomes

$$H_{1,\phi}(x) \geqslant \sum_{\pm}((1-\chi_{x^*}(x))^2 + (\chi_{x^*}(x))^2)\pi_1^{\pm}(y)$$
$$= ((1-\chi_{x^*}(x))^2 + (\chi_{x^*}(x))^2)\pi_2(y) \geqslant \delta(x^*)\pi_2(y).$$

Thus (4.15) holds.

(c) *Case* $x^* \in \mathcal{X}_{1,\text{in}}^{*-} \setminus \mathcal{X}_{1,\text{in}}^{*+}$ (which does not intersect $\mathcal{X}_{2,\text{in}}^*$). Thus $x \notin \operatorname{supp}\chi_2 \cup \operatorname{supp}\chi_3$ and

$$\chi_1^{*-}(x) = (1-\chi_{x^*}(x))\chi_1(x) = 1-\chi_{x^*}(x), \quad \chi_1^{*+}(x) = 0$$

Hence (4.16) becomes

$$H_{1,\phi}(x) \geqslant \sum_{\pm}\big((1-\chi_{x^*}(x))^2 + (\chi_{x^*}(x))^2\big)\pi_1^-(y)$$
$$\geqslant \delta(x^*)\pi_1^-(y).$$

But we have also

$$\phi(H^D)(x) = \phi\big(\sqrt{\tau^-(x)}\big)\pi_1^-(y).$$

Thus (4.15) holds.

As conclusion, (4.15) is proved with $C = \min(\delta_0, \min_{\mathcal{X}^*}\delta(x^*))$. □

4.9. Self-adjointness and maximal monotonicity of parts of the conjugate operator

The conjugate operator A_ϕ with domain $\mathcal{D}_0$ is a symmetric first order differential operator in x whose coefficients belong to $\mathcal{C}^\infty(\mathbb{T}^3 \setminus \mathcal{X}^*, \mathcal{L}(\mathbb{C}^6))$. The symmetric first order differential operator A_{out} is acting from $\mathcal{C}^\infty(\mathbb{T}^3, \mathbb{C}^6)$ into itself, so, by duality from $\mathcal{C}^\infty(\mathbb{T}^3, \mathbb{C}^6)'$ into itself. Its restriction to $\mathcal{C}^\infty(\mathbb{T}^3, \mathbb{C}^6)$ which we denote A_{out} too is essentially self-adjoint and admits a self-adjoint extension to $\mathcal{H}^D$, $\overline{A_{\text{out}}}$, with domain $D(\overline{A_{\text{out}}}) = \{u \in \mathcal{H}^D;\ A_{\text{out}}u \in \mathcal{H}^D\}$. (We may observe that $D(\overline{A_{\text{out}}})$ is also the closure of $\mathcal{C}^\infty(\mathbb{T}^3, \mathbb{C}^6)$ under the graph norm $\|u\| + \|A_{\text{out}}u\|$.) Let us check that for all $x^* \in \mathcal{X}^*$ the operator A_{x^*} with domain $\mathcal{D}_0$ is essentially self-adjoint or, at least, admits a maximal symmetric extension.

Lemma 4.8. — *Remembering the notations of Section 4.7.2 we then claim:*

(A) *Cases* (1), (2-1), (2-1a), (2-1b) *and* (3-1)*: if* $\{s_1, s_2, s_3\} = \{-1, 1\}$, *then* A_{x^*} *is essentially self-adjoint on* $\mathcal{H}^D$*. Otherwise, i.e., if all the* s_j*'s have the same sign, then* A_{x^*} *admits a maximal symmetric extension on* $\mathcal{H}^D$*.*

(B) *Case* (2-1c)*: the operator* A_{x^*} *is essentially self-adjoint on* $\mathcal{H}^D$*.*
(C) *Cases* (3-2)–(3-3) *(so we have* (A0) *with* $\beta_2 \in (0, \beta_1]$*,* $x^* \in \mathcal{X}_2^*$*,* $|y_2^*| = 1$*): the operator* A_{x^*} *admits a maximal symmetric extension on* $\mathcal{H}^D$*.*

Proof in Appendix B.

Remark 4.9. — When A_{x^*} is essentially self-adjoint then the set $\mathcal{D}_0$ is not dense for the graph norm in the domain $D(\overline{A_{x^*}})$ of the self-adjoint extension $\overline{A_{x^*}}$ of A_{x^*} (the simple reason is that $\mathcal{C}_c^\infty(\mathbf{R}^*)$ is not dense in $H^1(\mathbf{R})$).

We set

$$\begin{aligned}\mathcal{X}_{\mathrm{sa}}^* &:= \{x^* \in \mathcal{X}^*;\ A_{x^*} \text{ is essentially self-adjoint}\},\\ \mathcal{X}_{\mathrm{sm}}^* &:= \mathcal{X}^* \setminus \mathcal{X}_{\mathrm{sa}}^*,\end{aligned}$$

and

$$A_{\mathrm{sa}} := \sum_{x^* \in \mathcal{X}_{\mathrm{sa}}^*} A_{x^*},\ D(A_{\mathrm{sa}}) := \mathcal{D}_0.$$

Corollary 4.10.

(1) *The operator* A_{sa} *is essentially self-adjoint on* $\mathcal{H}^D$*.*
(2) *If* $\mathcal{T}_{\mathrm{sm}} \subset \mathcal{T}'$ *then the operator* A_ϕ *defined on* $\mathcal{D}_0$ *is essentially self-adjoint on* $\mathcal{H}^D$*.*

Proof. — As a preliminary, we observe that, remembering the definitions of s_j at Section 4.7.2 and (2.11), (2.12), (2.13), (2.14), we have,

$$\mathcal{T}_{\mathrm{sm}}^+ = \begin{cases} \left\{\sqrt{\Psi_0(z^*)};\ x^* \in \mathcal{X}_2^*\left(= X_{\{0,1\}}^*\right),\ s_1 = s_2 = s_3 = \pm 1\right\} & \text{if } \boldsymbol{\beta} = 0,\\ \left\{\sqrt{\tau^+(z^*)}, \sqrt{\tau^-(z^*)};\ x^* \in \mathcal{X}_1^*,\ s_1 = s_2 = s_3 = \pm 1\right\} & \text{if } \boldsymbol{\beta} \neq 0.\end{cases}$$

(1). — Hence, the operator A_{sa} is the finite sum of essentially self-adjoint operators A_{x^*} defined on $\mathcal{D}_0$ and with disjoint supports so A_{sa} is essentially self-adjoint too. □

(2). — For simplicity we assume that $\mathcal{T}' = \mathcal{T}_{\mathrm{sm}}$ and we consider the case $\beta_2 \neq 0$ only. The operator $\overline{A} := A_\phi$ with domain $D(\overline{A}) := \{u \in \mathcal{H}^D;\ A_\phi u \in \mathcal{H}^D\}$ is a symmetric extension of A_ϕ. Let us prove that it is self-adjoint. Let $v \in D(\overline{A}^*)$ so

$$\left|(\overline{A}u, v)_{\mathcal{H}^D}\right| \leqslant C\|u\| \quad \forall\, u \in D(\overline{A}).$$

Let $u \in D(\overline{A})$. Let $\varphi_1 \in \mathcal{C}^\infty(\mathbb{T}^3 \setminus \mathcal{X}_{\mathrm{sm}}^*; [0,1])$ such that $\operatorname{supp} \varphi_1$ is a small neighbourhood of $\mathcal{X}_{\mathrm{sa}}^*$ and $\varphi_1 = 1$ near $\mathcal{X}_{\mathrm{sa}}^*$. Putting $B := \varphi_1 A_\phi \varphi_1$, since

$\nabla\varphi_1$ vanishes near $\mathcal{X}^*$ then $B - A_\phi\varphi_1^2$ is bounded on $\mathcal{H}^D$, $\varphi_1^2 u \in D(\bar{A})$ and we get

$$|(Bu, v)_{\mathcal{H}^D}| \leqslant |(\bar{A}(\varphi_1^2 u), v)_{\mathcal{H}^D}| + C'\|u\| \leqslant C''\|u\|.$$

In addition, we have $B = \varphi_1 A_{\mathrm{sa}}\varphi_1$ since $\bar{A}$ coincides with A_{sa} in $\operatorname{supp}\varphi_1$, so B is essentially self-adjoint (the proof is similar to those of A_{sa}). Hence, $Bv \in \mathcal{H}^D$ and then $\varphi_1^2 v \in D(\bar{A})$. Let $\varphi_2 \in \mathcal{C}_c^\infty(\mathbb{T}^3 \setminus \mathcal{X}^*; [0,1])$. Then, $\varphi_2 A_\phi \varphi_2 - A_\phi\varphi_2^2$ is bounded on $\mathcal{H}^D$, $\varphi_2^2 u \in D(\bar{A})$ and

$$|(\varphi_2\bar{A}(\varphi_2 u), v)_{\mathcal{H}^D}| \leqslant \left|(A(\varphi_2^2 u), v)_{\mathcal{H}^D}\right| + C'\|u\| \leqslant C''\|u\|.$$

Since $\varphi_2 A_\phi \varphi_2$ is a symmetric first order differential operator with smooth coefficients it is so essentially self-adjoint and we get $\varphi_2 A_\phi\varphi_2 v \in \mathcal{H}^D$, and $\varphi_2^2 v \in D(\bar{A})$. Letting φ_1 such that its derivatives at any order vanish on $\varphi_1^{-1}(\{1\})$ we can choose $\varphi_2 := \sqrt{1-\varphi_1^2}$. Then $v = \sum_{j=1}^2 \varphi_j^2 v \in D(\bar{A})$. □

5. Proofs of the main results

5.1. Proof of Theorem 3.1

Proof. — Clearly, it is not restrictive to consider that $\operatorname{supp}\phi \subset (0,+\infty)$ so $\phi \in \mathcal{C}_c^\infty((0,+\infty)\setminus\mathcal{T}')$. We then construct the operators A_{out}, A_{in}, A_ϕ as above. Thanks to Lemma 4.7, the operator A_ϕ satisfies point (ii). Point (i) is a straight consequence of (4.15).

Proof of point (iii). — We consider the cases $\operatorname{supp}\phi \subset (0,+\infty)$ and $\beta_2 \neq 0$ only. We have $\operatorname{supp} A_\phi \subset \mathcal{X}_A$ where we set

$$\mathcal{X}_A := \operatorname{supp}\chi_1^{*+} \cup \operatorname{supp}\chi_1^{*-} \cup \operatorname{supp}\chi_2^* \cup \operatorname{supp}\chi_3^* \cup \bigcup_{\substack{x^* \in \mathcal{X}_{1,\mathrm{in}}^{*+} \\ \cup \mathcal{X}_{1,\mathrm{in}}^{*-} \cup \mathcal{X}_{2,\mathrm{in}}^*}} \operatorname{supp}\chi_{x^*}.$$

The set $\mathcal{K} := \bigcup_\pm \sqrt{\tau^\pm(\sin^2(\mathcal{X}_A))}$ is then a compact subset of $(0,\infty)\setminus\mathcal{T}'$. Thus there exists $\widetilde{\phi} \in \mathbb{C}_c^\infty((0,\infty)\setminus\mathcal{T}')$ with $\widetilde{\phi} = 1$ in $\mathcal{K}$. Thus if $x \in \operatorname{supp} A_\phi \cap \mathcal{X}_1$ then

$$\widetilde{\phi}(H^D)(x) = \sum_\pm \widetilde{\phi}\big(\sqrt{\tau^\pm(z)}\big)\pi_1^\pm(y) = \pi_2(y),$$

and, if $x \in \operatorname{supp} A_\phi \cap \mathcal{X}_2$, then

$$\widetilde{\phi}(H^D)(x) = \widetilde{\phi}\big(\sqrt{\Psi_0(z)}\big)\pi_2(y) = \pi_2(y).$$

Hence, $\widetilde{\phi}(H^D)(x) = \pi_2(y)$ on $\operatorname{supp} A_\phi$. In addition, $A_\phi(x)$ is obviously commuting with $\pi_2(y)$ for all x. It shows that point (iii) holds. □

Point (iv) is Corollary 4.10 (2).

Point (v) is the consequence of Lemma 4.8 and Corollary 4.10. □

5.2. Proof of Corollary 3.8

Proof. — Let $\widehat{L}$ be the invertible operator on $l^2(\mathbf{Z}^3, \mathbb{C}^6)$ defined by

$$\widehat{L}(n) := \widehat{D}_p(n)^{1/2}\widehat{D}^{-1/2}, \quad n \in \mathbf{Z}^3.$$

We put $\widehat{Q}_1 := \widehat{L} - I$ and $\widehat{Q}_2 := \widehat{L}^{-1}\widehat{D}_p\widehat{D}^{-1} - I = \widehat{D}^{1/2}\widehat{D}_p^{1/2}\widehat{D}^{-1} - I$.

For $\zeta \in \mathbb{C} \setminus \mathbf{R}$ the equation

$$\big(\widehat{H}^{D_p} - \zeta\big)\widehat{u} = \widehat{f} \tag{5.1}$$

is then equivalent to

$$\big(\widehat{H}^{D} + \widehat{V} - \zeta\big)\widehat{v} = \widehat{g} \tag{5.2}$$

where $\widehat{v} := \widehat{L}^{-1}\widehat{u}$, $\widehat{g} := \widehat{L}^{-1}\widehat{f}$, $\widehat{V} := \widehat{Q}_2\widehat{H}^D + \widehat{H}^D\widehat{Q}_1 + \widehat{Q}_2\widehat{H}^D\widehat{Q}_1$. Since the $\widehat{Q}_j$'s have compact support and since $\widehat{H}^D(x)$ is a polynomial function of (e^{ix}, e^{-ix}) then $\widehat{V}$ has compact support. Thus, the Fourier series of $\widehat{V}$ defines a compact and smoothing operator V on $\mathcal{H}^D$. Hence, for all differential operators P_1, P_2 on $\mathcal{S}'(\mathbb{T}^3, \mathbb{C}^6)$ with smooth coefficients, the operator $P_1 V P_2$ is bounded (and also compact) on $\mathcal{H}^D$. Moreover, since $\operatorname{supp}\phi \cap \mathcal{T} = \emptyset$, the conjugate operator A_ϕ has smooth coefficients. We thus have $V \in \mathcal{C}^2(A_\phi) \subset \mathcal{C}^{1,1}(A_\phi)$. In addition, V is symmetric on $\mathcal{H}^D$ (but not on $\mathcal{H}$!), since we have $\widehat{V} = \widehat{D}^{1/2}\widehat{D}_p^{1/2}\widehat{H}^D\widehat{D}_p^{1/2}\widehat{D}^{-1/2} - \widehat{H}^D$. Thus, V satisfies (1)–(2) of Corollary 3.7. Hence, Corollary 3.7 applies. In addition, since $\widehat{L} - I$ and $\widehat{L}^{-1} - I$ are operators of multiplication in $\mathcal{S}'(\mathbf{Z}^3, \mathbb{C}^6)$ with compact support, then $\widehat{L}$ is an isomorphism both of $B(\mathcal{B}(\mathbf{Z}^3, \mathbb{C}^6)$, $B(\mathcal{B}^*(\mathbf{Z}^3, \mathbb{C}^6))$, $B(H^s(\mathbf{Z}^3, \mathbb{C}^6))$ and of $B(D((1 + |A_\phi|))^s)$ for all s. Actually, $Q_1 = L - I$ and $Q_3 := L^{-1} - I$ are continuous mappings from $\mathcal{S}'(\mathbb{T}^3, \mathbb{C}^6)$ into $\mathcal{S}(\mathbb{T}^3, \mathbb{C}^6)$, so $Q_j \in B(\mathcal{B}(\mathbf{Z}^3, \mathbb{C}^6) \cap B(\mathcal{B}^*(\mathbf{Z}^3, \mathbb{C}^6)) \cap B(H^s(\mathbf{Z}^3, \mathbb{C}^6)) \cap B(D((1 + |A_\phi|))^s)$, $j = 1, 3$. Consequently, (1), (2), (3) of Corollary 3.7 with H_V^D replaced by H^{D_p} hold. Corollary 3.8 is proved. □

5.3. Adaptation of the theory of Georgescu et al.

Notation. — If Q is a bounded quadratic form on $\mathcal{H}$ we denote by Q° the bounded operator associated with Q. Let us consider the case $\mathcal{T}' = \{0\}$

so A_{in} may not be essentially self-adjoint. We set

$$\mathcal{X}^*_{\mathrm{sm}\,1} := \big\{x^* \in \mathcal{X}^*_{\mathrm{sm}};\ A_{x^*} \text{ has default index } (N^+, N^- = 0)\big\},$$
$$\mathcal{X}^*_{\mathrm{sm}\,2} := \big\{x^* \in \mathcal{X}^*_{\mathrm{sm}};\ A_{x^*} \text{ has default index } (N^+ = 0, N^-)\big\}.$$

We write

$$A_\phi = A_0 + A_1 + A_2$$

where all the A_j are differential operators of first order defined at least on $\mathcal{D}_0$ by: $A_0 = A_{\mathrm{out}}$, $A_1 = \sum_{x^* \in \mathcal{X}^*_{\mathrm{sm}\,1} \bigcup \mathcal{X}^*_{\mathrm{sa}}} A_{x^*}$, $A_2 = \sum_{x^* \in \mathcal{X}^*_{\mathrm{sm}\,2}} A_{x^*}$. The proof of Corollary 4.10 shows that the operator A_0 is essentially self-adjoint.

Remark 5.1. — We could have set more naturally $A_0 = A_{\mathrm{sa}} + A_{\mathrm{out}}$, $A_1 = \sum_{x^* \in \mathcal{X}^*_{\mathrm{sm}\,1}}$ and A_2 unchanged. In such a choice some coefficients of A_0 have a rational singularity on $\mathcal{X}^*_{\mathrm{sa}}$.

Since the supports of the A_{x^*}, $x^* \in \mathcal{X}^*$, are two-by-two disjoint then the operators $\pm A_0$ and $(-1)^j A_j$, $j = 1, 2$, admit a maximal symmetric extension with deficiency index of the form $(N, 0)$. We denote by A_j^{sm} with domain $D(A_j^{\mathrm{sm}})$ the maximal symmetric extension of A_j (with domain $\mathcal{D}_0$).

Let us show that we can modify the main hypotheses (M1)–(M5) of [7, Theorem 3.3] and extend the statement of [7, Theorem 3.3] to our situation. We consider variables $\zeta \in \rho(H^D)$ and ε real with $0 < |\varepsilon| < \varepsilon_0$ and $\Im m(\zeta)\varepsilon \geqslant 0$. We set $H' := [H^D, iA_\phi]^\circ$ and $H_\varepsilon := H^D - i\varepsilon H'$. (Thus $H_\varepsilon^* = H_{-\varepsilon}$.) Then, the resolvent $R_\varepsilon(\zeta) := (H_\varepsilon - \zeta)^{-1}$ is well-defined if ε_0 is sufficiently small, see [7, Proposition 3.11]. Actually we make the following observations:

- The domain $\mathcal{D}_0$ of A_ϕ is dense in $\mathcal{H}^D$.
- Assumption [7, (M3)] becomes:

$$\begin{bmatrix} \pm A_0^{\mathrm{sm}} \big(\text{resp.}, (-1)^j A_j^{\mathrm{sm}}\big) \text{is the generator of a } C_0\text{-group} \\ \big(W_t^{(0)}\big)_{t \in \mathbf{R}} \Big(\text{resp., semigroup } \big(W_t^{(j)}\big)_{t \geqslant 0}\Big) \text{in } \mathcal{H}^D. \end{bmatrix} \tag{M3*}$$

  Clearly, Condition (M3*) is satisfied.
- Putting $\langle H \rangle := (1 + H^2)^{1/2}$, Assumption [7, (M2)] becomes:

$$\begin{bmatrix} \text{a bounded open set } J \subset \mathbf{R} \text{ is given and there are numbers} \\ a > 0, b \geqslant 0, \text{ such that } H' \geqslant \big(a 1_J\big(H^D\big) - b 1_{\mathbf{R}\setminus J}\big)\big\langle H^D\big\rangle \\ \text{as forms on } \mathcal{H}^D. \end{bmatrix} \tag{M2*}$$

  Thus, for all bounded open set $J \subset\subset (0, +\infty)$, Condition (M2*) is satisfied (by choosing ϕ such that $\phi = 1$ on J, and with $b = 0$), thanks to Mourre's inequality (4.15).

- Assumption [7, (M4)] becomes:

$$\left[\begin{array}{l} \text{There } H'_j \in B(\mathcal{H}^D) \text{ such that the limits} \\ \lim_{t\to 0^+} (-1)^j t^{-1}\Big\{\Big(H^D u, W_t^{(j)} u\Big)_{\mathcal{H}^D} - \Big(u, W_t^{(j)} H^D u\Big)_{\mathcal{H}^D}\Big\} \; (j \neq 0), \\ \qquad \lim_{t\to 0} t^{-1}\Big\{\Big(H^D u, W_t^{(0)} u\Big)_{\mathcal{H}^D} - \Big(u, W_t^{(0)} H^D u\Big)_{\mathcal{H}^D}\Big\} \; (j = 0) \\ \text{exist and are respectively equal to } \big(u, H'_j u\big) \text{ for all } u \in \mathcal{H}^D. \end{array}\right] \tag{M4*}$$

  Clearly, by choosing $H'_j := [H^D, iA_j]^\circ$, Condition (M4*) is satisfied. Since $[H^D, iA_\phi]^\circ = H' = \sum_{j=0}^{2} H'_j \in B(\mathcal{H}^D)$, we have $H^D \in C^1(A_j^{\mathrm{sm}})$ and $H^D \in C^1(\bar{A}_\phi)$.
- The proofs of [7, Lemmas 3.13 and 3.14] with conditions (M3*) and (M4*) satisfied imply the following relations:

$$\begin{aligned} [R_\varepsilon(\zeta), iA_j^{\mathrm{sm}}]^\circ &= R_\varepsilon(\zeta)(iH'_j + \varepsilon H''_j)R_\varepsilon(\zeta) \quad j = 0, 1, 2, \\ [R_\varepsilon(\zeta), iA_\phi]^\circ &= R_\varepsilon(\zeta)(iH' + \varepsilon H'')R_\varepsilon(\zeta), \\ \frac{\mathrm{d}R_\varepsilon(\zeta)}{\mathrm{d}\varepsilon} &= [R_\varepsilon(\zeta), iA_\phi]^\circ - \varepsilon R_\varepsilon(\zeta) H'' R_\varepsilon(\zeta). \end{aligned}$$

  In particular the map $\varepsilon \mapsto R_\varepsilon(\zeta) \in B(\mathcal{H}^D)$ is C^1 in norm on $]0, 1]$.
- Since H^D and the H'_j's are symmetric bounded self-adjoint operators on $\mathcal{H}^D$ (so H'_j is regular; see also [7, Remark 2.15]), then Assumption [7, (M1)] becomes:

$$\big[H^D \in C^1\big(H'_j\big) \text{ for all } j.\big] \tag{M1*}$$

  We see that (M1*) is obviously satisfied and $H^D \in C^1(H')$.
- Assumption [7, (M5)] becomes:

$$\left[\begin{array}{l} \text{For all } j = 0, 1, 2, \text{there is } H''_j \in B(\mathcal{H}^D) \text{ such that the limits} \\ \lim_{t\to 0^+} (-1)^j t^{-1}\Big\{\Big(H' u, W_t^{(j)} u\Big) - \Big(u, W_t^{(j)} H' u\Big)\Big\} \quad j \neq 0, \\ \qquad \lim_{t\to 0} t^{-1}\Big\{\Big(H' u, W_t^{(0)} u\Big) - \Big(u, W_t^{(0)} H' u\Big)\Big\} \quad (j = 0), \\ \text{exist and are respectively equal to } (u, H''_j u) \text{for all } u \in \mathcal{H}^D. \end{array}\right] \tag{M5*}$$

  Thanks to [7, Remark 3.1], by choosing $H''_j := [H', iA_j^{\mathrm{sm}}]^\circ$, Condition (M5*) is satisfied since it follows from the following facts:
  - $H^D \in C^1(A_j^{\mathrm{sm}})$ since $[H^D, iA_j^{\mathrm{sm}}]^\circ = H'_j \in B(\mathcal{H}^D)$,
  - $H' \in C^1(A_j^{\mathrm{sm}})$ since $H''_j \in B(\mathcal{H}^D)$.

  (We can write $H^D \in C^2(\bar{A}_\phi)$.)

Then the proof of [7, Theorem 3.3] implies the result of Corollary 3.5.

6. Conclusion

The results of this work, in particular the LAP outside thresholds, are the first step in the future development of the following points.

- A Rellich type theorem for discrete Maxwell operators. In the article we have proved that the point spectrum of the unperturbed operator $\widehat{H}^D$ is reduced to 0, but this property is unclear concerning the perturbed operator $\widehat{H}^{D_p}$. A property of Rellich type combined with a unique continuation property, as described by Isozaki–Morioka in [15] for discrete Schrödinger operators is a usefull tool to answer this question, and will be soon presented by the author in collaboration with H. Isozaki in the framework of the anisotropic discrete Maxwell operator.
- Conditions of radiation for perturbed discrete Maxwell operators. Actually, let $\widehat{f}$ in a suitable subspace of $L^2(\mathbf{Z}^3, \mathbb{C}^6)$, particularly the space of sequences with compact support. We have to characterize $\widehat{u}^{\pm}(n)$ for $|n|$ large where $\widehat{u}^{\pm} := (\widehat{H}^{D_p} - \lambda \pm i0)^{-1}\widehat{f}$.
- Extension of the result of Isozaki and Jensen [13] on the continuum limit for lattice Schrödinger operators to the case of discrete Maxwell operators.
- Extension of the result of Isozaki and [16] on the inverse scattering for lattice Schrödinger operators to the case of discrete Maxwell operators. (In addition, the Rellich property is an important tool for such the problems.)

Appendix A.

A.1. Proof of Lemma 2.1

We have

$$\widehat{D}\widehat{H}_0(x) - k = \begin{pmatrix} -k & \boldsymbol{\varepsilon} M \\ -\boldsymbol{\mu} M & -k \end{pmatrix}.$$

Thus,

$$\det\Big(\widehat{D}\widehat{H}_0(x) - k\Big) = \det\big(k^2 + \boldsymbol{\varepsilon} M(y)\boldsymbol{\mu} M(y)\big) =: p(z;k).$$

We have

$$\boldsymbol{\varepsilon} M \boldsymbol{\mu} M = \begin{pmatrix} 0 & -\varepsilon_1 y_3 & \varepsilon_1 y_2 \\ \varepsilon_2 y_3 & 0 & -\varepsilon_2 y_1 \\ -\varepsilon_3 y_2 & \varepsilon_3 y_1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -\mu_1 y_3 & \mu_1 y_2 \\ \mu_2 y_3 & 0 & -\mu_2 y_1 \\ -\mu_3 y_2 & \mu_3 y_1 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} -\varepsilon_1\mu_3 y_2^2 - \varepsilon_1\mu_2 y_3^2 & \varepsilon_1\mu_3 y_1 y_2 & \varepsilon_1\mu_2 y_1 y_3 \\ \varepsilon_2\mu_3 y_1 y_2 & -\varepsilon_2\mu_3 y_1^2 - \varepsilon_2\mu_1 y_3^2 & \varepsilon_2\mu_1 y_2 y_3 \\ \varepsilon_3\mu_2 y_1 y_3 & \varepsilon_3\mu_1 y_2 y_3 & -\varepsilon_3\mu_2 y_1^2 - \varepsilon_3\mu_1 y_2^2 \end{pmatrix}.$$

Then, for $t = k^2 \in \mathbb{C}$,

$$\begin{aligned} &\det(\boldsymbol{\varepsilon} M \boldsymbol{\mu} M + t) \\ &\quad = t^3 - t^2\big\{(\varepsilon_2\mu_3 + \varepsilon_3\mu_2)y_1^2 + (\varepsilon_1\mu_3 + \varepsilon_3\mu_1)y_2^2. + (\varepsilon_1\mu_2 + \varepsilon_2\mu_1)y_3^2\big\} \\ &\qquad + t\big\{\varepsilon_2\varepsilon_3\mu_2\mu_3 y_1^4 + \varepsilon_1\varepsilon_3\mu_1\mu_3 y_2^4 \\ &\qquad + \varepsilon_1\varepsilon_2\mu_1\mu_2 y_3^4 + (\varepsilon_2\varepsilon_3\mu_1\mu_3 + \varepsilon_1\varepsilon_3\mu_2\mu_3)y_1^2 y_2^2 \\ &\qquad + (\varepsilon_2\varepsilon_3\mu_1\mu_2 + \varepsilon_1\varepsilon_2\mu_2\mu_3)y_1^2 y_3^2 + (\varepsilon_1\varepsilon_3\mu_1\mu_2 + \varepsilon_1\varepsilon_2\mu_1\mu_3)y_2^2 y_3^2\big\} \\ &\quad \equiv t^3 - 2t^2\Psi_0 + t\Phi_0, \end{aligned}$$

where $\Psi_0(z)$ is defined by (2.4), and

$$\Phi_0 := \varepsilon_2\varepsilon_3\mu_2\mu_3 z_1^2 + (\varepsilon_2\varepsilon_3\mu_1\mu_3 + \varepsilon_1\varepsilon_3\mu_2\mu_3)z_1 z_2 + c.p..$$

We easily observe that the following relations hold with *c.p.*:

$$\alpha_1^2 - \gamma_1 = \frac{1}{4}\beta_1^2, \tag{A.1}$$

$$\varepsilon_1\mu_1\alpha_1 - \alpha_2\alpha_3 = \frac{1}{4}\beta_2\beta_3, \tag{A.2}$$

$$\alpha_3\beta_2 + \alpha_2\beta_3 = -\varepsilon_1\mu_1\beta_1, \tag{A.3}$$

where $\boldsymbol{\gamma}$ is defined by (2.1). Thanks to (A.1), (A.2), (A.3), we compute:

$$\begin{aligned} \Psi_0^2 - \Phi_0 = (\alpha_1 z_1 + \alpha_2 z_2 + \alpha_3 z_3)^2 - \big(\gamma_1 z_1^2 + \gamma_2 z_2^2 + \gamma_3 z_3^2 \\ + 2\varepsilon_3\mu_3\alpha_3 z_1 z_2 + 2\varepsilon_1\mu_1\alpha_1 z_2 z_3 + 2\varepsilon_2\mu_2\alpha_2 z_1 z_3\big) = K_0(z), \end{aligned}$$

where K_0 is defined by (2.3). Hence the eigenvalues of $\boldsymbol{\varepsilon} M(y)\boldsymbol{\mu} M(y)$ are 0 and

$$t = k^2 = \Psi_0(z) \pm \sqrt{K_0(z)}.$$

Relation (2.2) then follows.

A.2. Proof of Proposition 2.6

Proof. — Since τ^+ and τ^- are continuous with $\tau^\pm(0) = 0$ and $\tau^+ \geqslant \tau^- \geqslant 0$ in $[0,1]^3$, we then have

$$\bigcup_{y \in [-1,1]^3} \sigma\big(h^D(y)\big) = \bigcup_{\pm}\Big\{\pm\sqrt{\tau^+(z)};\ z \in [0,1]^3\Big\} = [-\lambda_+, \lambda_+].$$

Thanks to (2.8) the conclusion follows. □

A.3. Proof of Lemma 2.7

Proof. — We set $z'_i = \beta_i z_i$ (so $z'_1, z'_2 \geqslant 0$ and $z'_3 \leqslant 0$). Remember that
$$\left(4\alpha_1^2 - \beta_1^2\right) = (2\alpha_1 - \beta_1)(2\alpha_1 + \beta_1) = 4\varepsilon_3\mu_2\varepsilon_2\mu_3 = 4\gamma_1 > 0.$$

(A) (Case $\boldsymbol{\beta} = 0$.) This point is obvious.
(B) (Case $\boldsymbol{\beta} \neq 0$.) Thanks to (2.5) we have
$$\begin{aligned} \frac{\partial}{\partial z_1} K_0 &= \frac{1}{2}\beta_1(z'_1 - z'_2 - z'_3), \\ \frac{\partial}{\partial z_3} K_0 &= \frac{1}{2}\beta_3(z'_3 - z'_1 - z'_2), \end{aligned} \tag{A.4}$$
and
$$\sqrt{K_0(z)} \geqslant \frac{1}{2}|z'_1 - z'_2 - z'_3|. \tag{A.5}$$

(1) We have
$$\sqrt{K_0}\nabla_z \tau^{\pm} = \sqrt{K_0}\nabla_z \Psi_0 \pm \frac{1}{2}\nabla_z K_0,$$
so, by using (A.4), (A.5),
$$\begin{aligned} &2\sqrt{K_0(z)}\partial_{z_1}\tau^{\pm}(z) \\ &\quad = 2\sqrt{K_0(z)}\left(\alpha_1 - \frac{1}{2}\beta_1\right) + \beta_1\sqrt{K_0(z)} \pm \frac{1}{2}\beta_1(z'_1 - z'_2 - z'_3) \\ &\quad \geqslant 2\sqrt{K_0(z)}\left(\alpha_1 - \frac{1}{2}\beta_1\right) > 0. \end{aligned}$$
Thus, $\partial_{z_1}\tau^{\pm}(z) > 0$. Similarly, $\partial_{z_2}\tau^{\pm}(z) > 0$. We have
$$2\sqrt{K_0(z)}\partial_{z_3}\tau^{\pm}(z) = 2\sqrt{K_0(z)}\alpha_3 \pm \frac{1}{2}\beta_3(z'_3 - z'_1 - z'_2).$$
Since $\beta_3 < 0$ and $z'_3 - z'_1 - z'_2 \leqslant 0$ then $\partial_{z_3}\tau^{+}(z) \geqslant 0$. Moreover if $\partial_{z_3}\tau^{+}(z) = 0$ then $\sqrt{K_0(z)} = 0$ which is forbidden. Hence $\partial_{z_3}\tau^{+}(z) > 0$.

(2) (a) (Case $\beta_2 = 0$.) Thanks to (2.5), we have
$$2\sqrt{K_0(z)}\partial_{z_3}\tau^{-}(z) = \alpha_3(z'_1 - z'_3) - \frac{1}{2}\beta_3(z'_3 - z'_1) = 2\sqrt{K_0(z)}\left(\alpha_3 + \frac{1}{2}\beta_3\right) > 0.$$

(b) (Case $\beta_2 > 0$.)

(bi) Assume $z_1 = 0$ or $z_2 = 0$. Then $\sqrt{K_0(z)} = \frac{1}{2}(z'_1 + z'_2 - z'_3)$ and
$$2\sqrt{K_0(z)}\partial_{z_3}\tau^{-}(z) = \left(\alpha_3 + \frac{1}{2}\beta_3\right)(z'_1 + z'_2 - z'_3) > 0,$$
so, $\partial_{z_3}\tau^{-}(z) > 0$.

(bii) Assume $z_1 = z_2 = 1$. The functions

$$\xi := 4K_0(z)\partial_{z_3}\tau^-(z)\partial_{z_3}\tau^+(z) \quad \text{and} \quad \partial_{z_3}\tau^-(z)$$

have the same sign outside $K_0^{-1}(\{0\})$. We have

$$\begin{aligned}\xi &= 4\alpha_3^2 K_0(z) - (\partial_{z_3}K_0(z))^2\\ &= 4\alpha_3^2\left(\frac{1}{4}(\beta_1+\beta_2-z_3')^2-\beta_1\beta_2\right)-\frac{1}{4}\beta_3^2(\beta_1+\beta_2-z_3')^2\\ &= \gamma_3(\beta_1+\beta_2-z_3')^2-4\alpha_3^2\beta_1\beta_2.\end{aligned}$$

Thus, if $\gamma_3 = 0$ then $\xi < 0$ and if $\gamma_3 \neq 0$ then

$$\begin{aligned}\xi = 0 &\iff \sqrt{\gamma_3}(\beta_1+\beta_2-\beta_3 z_3) = 2\alpha_3\sqrt{\beta_1\beta_2}\\ &\iff z_3 = \nu.\end{aligned}$$

Moreover, we have

$$\partial_{z_3}\xi = -2\gamma_3\beta_3(\beta_1+\beta_2-\beta_3 z_3) > 0.$$

The conclusion follows. □

A.4. Proof of Lemma 2.9

Proof. — Lemma 2.9 is a straightforward consequence of Lemma 2.7 and of the following observations.

Case $\boldsymbol{\beta} = 0$. We have $K_0 \equiv 0$ so, obviously, $\mathcal{X}_1 = \emptyset$, $\mathcal{T}_1 = \emptyset$, $\mathcal{X}_2 = \mathbb{T}^3 \setminus \mathcal{X}_0$. In addition we have $\partial_{x_i}\Psi_0 = 2\alpha_i \sin x_i \cos x_i$. Hence $\nabla_x \Psi_0(z)$ vanishes if and only if $z \in \{0,1\}^3$. Hence, noting that $\tau^\pm = \Psi_0$, we obtain $\sin^2(\mathcal{X}_2^*) = Z^*_{\{0,1\}}$ and $\mathcal{T}_2 = \sqrt{\Psi_0}(Z^*_{\{0,1\}})$.

Case $\boldsymbol{\beta} \neq 0$ *(so* (A0) *holds).* — Thanks to Lemma 2.5 we have

$$\sin^2(\mathcal{X}_1^*) \subset [0,1]^3 \setminus \left\{\left(\frac{\beta_2}{\beta_1}t, t, 0\right), t \in [0,1]\right\}.$$

For $t \in [0,1]$ we have $(\beta_2 t/\beta_1, t, 0) \in \{0,1\}^3 \setminus \{0_{\mathbf{R}^3}\}$ iff $t = 1$ and $\beta_2 = \beta_1$, or $t = 1$ and $\beta_2 = 0$. The characterization of $\sin^2(\mathcal{X}_1^*)$ follows, then those of $\mathcal{X}_1^*$ and of $\mathcal{T}_1$. Let us determine $\mathcal{X}_2^*$. We look for a tangent vector field to $\mathcal{X}_2$. A point $x \in \mathbb{T}^3$ belongs to $\mathcal{X}_2$ iff $z \neq 0$ and $z_3 = 0 = \beta_1 z_1 - \beta_2 z_2 = 0$. The last relation can be written

$$\beta_1 y_1^2 = \beta_2 y_2^2,$$

and $y_2 \neq 0$. (If $y_2 = 0$ then $y_1 = 0$ so $z = 0$ which is forbidden.) Then a tangent field to $\mathcal{X}_2$ (resp., to $\sin(\mathcal{X}_2)$) is then given by the vector field

$$w_0(x) := \big(\sin(x_1)\cos(x_2), \cos(x_1)\sin(x_2), 0\big), \tag{A.6}$$

(resp., $\widetilde{w}_0(y) := (y_1, y_2, 0)$).

Remark A.1. — In Case (3-1), (i.e, $\beta_2 = 0$) it is equivalent but simpler to put $w_0(x) = (0, 1, 0)$. However our choice in (A.6) is general.

We then observe that $|w(x)| \neq 0$ for all $x \in \mathcal{X}_2 \setminus \mathcal{X}^*$, and $|w(x)| \neq 0$ for all $x \in \mathcal{X}_2$ if $\beta_2 \in [0, \beta_1)$. If $\beta_2 = \beta_1$ then $w(x)$ vanishes at all $x^* \in \mathcal{X}_2^*$ since $z_1^* = z_2^* = 1$. The determination of $\sin^2(\mathcal{X}_2^*)$ follows, then those of $\mathcal{X}_2^*$ and of $\mathcal{T}_2$. □

A.5. Proof of the statement of Remark 2.8

Proof.

Step 1. — We prove the following assertion. Let a real vector $\boldsymbol{\beta} \in \mathbf{R}^3$ and three positive real values ε_1, μ_1, α_3 such that $\beta_1 \geqslant \beta_2 > 0 > \beta_3$ and $\alpha_3 > |\beta_3|/2$. Then there exist positive values ε_j, μ_j, $j = 2, 3$, such that $\boldsymbol{\beta} = \boldsymbol{\varepsilon} \times \boldsymbol{\mu}$ and $2\alpha_3 = \varepsilon_1\mu_2 + \varepsilon_1\mu_2$.

We set successively

$$\begin{aligned} \delta^{\pm} &:= \alpha_3 \pm \frac{1}{2}\beta_3 > 0, \\ \varepsilon_2 &:= \frac{\delta^-}{\mu_1} > 0, \\ \mu_2 &:= \frac{\delta^+}{\varepsilon_1} > 0, \\ \varepsilon_3 &:= \frac{\varepsilon_1\beta_1 + \varepsilon_2\beta_2}{-\beta_3} > 0, \\ \mu_3 &:= \frac{\mu_1\beta_1 + \mu_2\beta_2}{-\beta_3} > 0. \end{aligned}$$

A direct calculation provides $\boldsymbol{\varepsilon} \times \boldsymbol{\mu} = \boldsymbol{\beta}$ and $\varepsilon_1\mu_2 + \varepsilon_2\mu_1 = 2\alpha_3$.

Step 2. — Let $\boldsymbol{\beta} \in \mathbf{R}^3$ such that $\beta_1 \geqslant \beta_2 > 0 > \beta_3$. Let us consider the function $(|\beta_3|/2, +\infty) \ni \alpha_3 \mapsto \nu(\alpha_3) = \nu$ defined by (2.10) and set

$$\begin{aligned} F(r) &:= \frac{2r}{\sqrt{r^2 - \frac{1}{4}\beta_3^2}} - 2 \quad \text{for } r > |\beta_3|/2, \\ \nu^*(\boldsymbol{\beta}) &:= -\frac{\left(\sqrt{\beta_1} - \sqrt{\beta_2}\right)^2}{|\beta_3|}. \end{aligned}$$

We then have

$$\nu(\alpha_3) = \widetilde{\nu} \Longleftrightarrow F(\alpha_3) = \frac{|\beta_3|}{\sqrt{\beta_1\beta_2}}(\widetilde{\nu} - \nu^*(\boldsymbol{\beta})).$$

Obviously, the function F realizes a decreasing bijection from $(|\beta_3|/2, +\infty)$ into $(0, +\infty)$. Thus if $\nu^*(\boldsymbol{\beta}) < \widetilde{\nu}$ then there exists a unique value $\alpha_3 > |\beta_3|/2$ such that $\nu(\alpha_3) = \widetilde{\nu}$. But the condition $\nu^*(\boldsymbol{\beta}) < \widetilde{\nu}$ is easily satisfied since $\nu^*(\boldsymbol{\beta}) \to -\infty$ as $\beta_3 \to 0^-$ if $\beta_1 > \beta_2$. The conclusion follows. □

Appendix B.

Proof of Lemma 4.4

Proof. — Firstly we observe that if $z_j^* \in \{0,1\}$ then

$$\begin{aligned} z_j - z_j^* &= \sin^2 x_j - \sin^2 x_j^* \\ &= \sin(2x_j^*)(x_j - x_j^*) + \cos(2x_j^*)(x_j - x_j^*)^2 \\ &\quad - \frac{2}{3}\sin(2x_j^*)(x_j - x_j^*)^3 + O\big((x_j - x_j^*)^4\big) \\ &= s_j^*(x_j - x_j^*)^2 + O\big((x_j - x_j^*)^4\big), \end{aligned} \tag{B.1}$$

and if $z_j \notin \{0,1\}$ then

$$z_j - z_j^* = \sin(2x_j^*)(x_j - x_j^*) + O\big((x_j - x_j^*)^2\big), \tag{B.2}$$

with $\sin(2x_j^*) \neq 0$.

Case (1). — Assume $\boldsymbol{\beta} = 0$ so $V(x) = \sqrt{\Psi_0(z)}$. We have

$$\partial_{z_j} V(x^*) = \frac{\alpha_j}{2\sqrt{\Psi_0(z^*)}} > 0$$

for $j = 1, 2, 3$. So, by using (B.1),

$$\begin{aligned} \partial_{x_j} V(x) &= \partial_{z_j} V(x) \partial_{x_j} z_j = \partial_{z_j} V(x) \sin(2x_j) \\ &= \big(\partial_{z_j} V(x^*) + O(z - z^*)\big) \\ &\quad \cdot \big(\sin(2x_j^*) + 2\cos(2x_j^*)(x_j - x_j^*) + O\big((x_j - x_j^*)^2\big)\big) \\ &= 2\big(\partial_{z_j} V(x^*) + O(z - z^*)\big)t\big(s_j^*(x_j - x_j^*) + O\big((x_j - x_j^*)^2\big)\big) \\ &= C_j s_j^*(x_j - x_j^*)\big(1 + O(\mathrm{d}_0(x, x^*))\big), \end{aligned}$$

where $C_j = 2\partial_{z_j} V(x^*) = \frac{\alpha_j}{\sqrt{\Psi_0(z^*)}} > 0$. Thus (4.11) is proved.

Case (3-1) is similar since the six partial derivatives $\partial_{z_j} \tau^{\pm}$ are all constant and positive, and $\tau^{\pm}(z^*) > 0$ (see (2.6) and (2.7).).

Cases (2-1), (2-1a)(2-1b) are similar to Case (1), the sign of C_j being a consequence of Lemma 2.7. Let us be more precise in Case (2-1a). Since $z_3^* = \nu \in (0,1)$ then $\sin(2x_3^*) \neq 0$ so, by using (B.2), (B.1), we have

$$\begin{aligned}\partial_{x_3} V^2(x) &= \partial_{z_3}\tau^-(z)\sin(2x_3)\\ &= \big(O(z_1 - z_1^*) + O(z_2 - z_2^*) + \partial_{z_3}^2\tau^-(z^*)\big)(z_3 - z_3^*)\\ &\quad \cdot (1 + O((z_3 - z_3^*)))(\sin(2x_3^*) + O(x_3 - x_3^*)).\end{aligned}$$

Since $z_j - z_j^* = O((x_j - x_j^*)^2) = O(\partial_{x_j}\tau^-(z)\mathrm{d}_0(x,x^*))$ for $j = 1,2$, and $z_3 - z_3^* = \sin(2x_3^*)(x_3 - x_3^*)(1 + O(x_3 - x_3^*))$ then

$$\begin{aligned}\partial_{x_3} V(x) = \frac{\partial_{x_3} V^2(x)}{2V(x)} &= C_3(x_3 - x_3^*) + O\big(d_0^2(x,x^*)\big)\\ &= C_3(x_3 - x_3^*) + |\nabla_x V(x)| O(\mathrm{d}_0(x,x^*)),\end{aligned}$$

where $C_3 = (2\sqrt{\tau^-(z^*)})^{-1}\partial_{z_3}^2\tau^-(z^*)\sin^2(2x_3^*) > 0$. Thus (4.11) holds in Case (2-1a) too. Case (2-1c). The computation of the derivatives $\partial_{x_j} V(x)$, $j = 1,2$, is similar to the other cases (with $s_j = s_j^* = -1$). By using (B.1) we have

$$\begin{aligned}\partial_{x_3} V^2(x) &= \partial_{z_3}\tau^-(z)\sin(2x_3)\\ &= \Big(\big(O(z_1 - z_1^*) + O(z_2 - z_2^*) + \partial_{z_3}^2\tau^-(z^*)\big)(z_3 - z_3^*)\\ &\quad + O(z_3 - z_3^*)^2\Big) \cdot \Big(2s_3^*(x_3 - x_3^*) + O\big((x_3 - x_3^*)^3\big)\Big).\end{aligned}$$

Hence

$$\partial_{x_3} V(x) = C_3(x_3 - x_3^*)^3 + O(|\nabla_x V(x)|\,\mathrm{d}_0(x,x^*)),$$

where $C_3 = 2(\sqrt{\tau^-(z^*)})^{-1}\partial_{z_3}^2\tau^-(z^*) > 0$. Thus (4.12) holds too.

The Lemma 4.4 is proved. □

Proof of Lemma 4.5

Proof. — We remember that $y_1^* \neq 0$, $z_2^* \neq 0$ and $z_3^* = 0$, so,

$$\sqrt{\Psi_0(z)}_w = \cos(x_1)\cos(x_2)\widetilde{\sqrt{\Psi_0(z)}}_{\tilde{w}}.$$

Thanks to (4.7) the function $x \mapsto \widetilde{\sqrt{\Psi_0(z)}}_{\tilde{w}} = 2\alpha_1 z_1 + 2\alpha_2 z_2$ is smooth and positive in $\operatorname{supp}\chi_2^*$.

In Case (3-3), we have $0 < z_1^* < z_2^* = 1$ then $\cos y_1^* \neq 0$ so $\cos(x_1) = \cos(x_1^*) + O(\mathrm{d}_0(x,x^*))$ with $\cos(x_1^*) \neq 0$, and $\cos(x_2) = -y_2^*(x_2 - x_2^*) + O(x_2 - x_2^*)^3$. Hence (4.14) holds. In Case (3-2), we have $z_1^* = z_2^*$, $\cos y_1^* = 0$ so $\cos(x_j) = -y_j^*(x_j - x_j^*) + O(x_j - x_j^*)^3$, $j = 1,2$. Hence (4.13) holds. □

Proof of Lemma 4.8

Proof. — We fix a representation of $x^* \in \mathbb{T}^3$ in $\mathbf{R}^3$ which we denote again x^*. Then, the multiplication by χ_{x^*} is an isometry (non surjective) from $\mathcal{H}^D$ into the Hilbert space $L^2_D(\mathbf{R}^3, \mathbb{C}^6) := L^2(\mathbf{R}^3, \mathbb{C}^6)$ equipped with the scalar product

$$(u, v)_{L^2_D(\mathbf{R}^3,\mathbb{C}^6)} := \int_{\mathbf{R}^3} \langle u(x), v(x)\rangle_{\mathbb{C}^6,D} \mathrm{d}x = \int_{\mathbf{R}^3} \left\langle \widehat{D}^{-1} u(x), v(x)\right\rangle_{\mathbb{C}^6} \mathrm{d}x.$$

So, we can identify A_{x^*} with an unbounded symmetric operator on $L^2(\mathbf{R}^3, \mathbb{C}^6)$, which we denote A_{x^*} again.

We set $x'_j = \sqrt{C_j/2}(x_j - x^*_j)$ where the C_j's are the positive constants of Section 4.7.3, and in (4.11) or in (4.12) of Lemma 4.4. We set also $\rho' = \sqrt{x'^2_1 + x'^2_2}$, $r' = \sqrt{\rho'^2 + x'^2_3}$.

(A). — Let us consider Case (1) with $s_1 = s_2 = 1$ and $s_3 = -1$. Since $\boldsymbol{\beta} = 0$ then we have $\boldsymbol{\mu} = \kappa\boldsymbol{\varepsilon}$, with the scalar $\kappa > 0$. We have

$$p_1(x) = \rho'^2 - x'^2_3,$$

and we set

$$p_2(x) := 2\rho' x'_3,$$
$$p_3(x) := \frac{(x'_1, x'_2)}{\rho'} \in \mathbb{S}^1 \approx \mathbf{R}/(2\pi\mathbf{Z}).$$

The mapping $\mathbf{R}^2 \backslash \{(0,0)\} \ni (x'_1, x'_2) \mapsto (\rho', p_3) \in \mathbf{R}^+ \times \mathbb{S}^1$ is the polar change of coordinates. Since $p_1 + ip_2 = (\rho' + ix'_3)^2$, then the mapping $(\rho', x'_3) \mapsto (p_1, p_2)$ is a $\mathcal{C}^\infty$-diffeomorphism from $(0,\infty) \times \mathbf{R}$ onto $\mathcal{O} := \mathbf{R}^2 \setminus (\mathbf{R}^- \times \{0\})$. Thus the mapping

$$\Phi : \; x' = (x'_1, x'_2, x'_3) \mapsto p = (p_1, p_2, p_3)$$

is a $\mathcal{C}^\infty$-diffeomorphism from $\mathbf{R}^{2*} \times \mathbf{R}$ onto $\mathcal{U} := \mathcal{O} \times \mathbb{S}^1$, with jacobian

$$J_\Phi(x') = -\frac{r'^2}{\rho'}.$$

We set $\widetilde{H} = L^2(\mathbf{R}^{2*} \times \mathbb{S}^1, \mathbb{C}^6; \mathrm{d}p)$ equipped with the following scalar product:

$$(\widetilde{u}, \widetilde{v})_{\widetilde{H}} := \int_{\mathbf{R}^2 \times \mathbb{S}^1} \langle \widetilde{u}(p), \widetilde{v}(p)\rangle_{\mathbb{C}^6,D} \mathrm{d}p.$$

For $\widetilde{u} \in \widetilde{H}$, $p \in \mathcal{U}$, we set

$$u(x) = |J_\Phi(x')|^{1/2} \widetilde{u}(p), \quad x' = \Phi^{-1}(p) \in \mathbf{R}^3, \tag{B.3}$$

so the transform

$$T : \; L^2\big(\mathbf{R}^3, \mathbb{C}^6\big) \ni u \mapsto \widetilde{u} \in \widetilde{H}$$

is a bijective isometry. Putting $\widetilde{\pi}(p) = \pi_2(x)$ and $\widetilde{\chi}(p) = \chi_{x^*}(x)$, the partial derivatives $\partial^j_{p_1}\widetilde{\chi}$, $j \geqslant 0$, are bounded in $\mathbf{R}^{2*} \times \mathbb{S}^1$ since $\widetilde{\chi} = 1$ near $p(x^*) = 0$ and the function $|\nabla_x p_1|$ on $\operatorname{supp} \nabla \chi_{x^*}$ is smooth and bounded by below by a positive constant. For example if $j = 1$, we have

$$\sup_{x \in B(\mathbf{R}^3)} \left|\partial^j_{p_1}\widetilde{\chi}(p(x))\right| = \sup_{\frac{r}{2} \leqslant \mathrm{d}_0(x,x^*) \leqslant r} \left|\partial^j_{p_1}\widetilde{\chi}(p(x))\right| \leqslant C.$$

The projector $\widetilde{\pi}$ is continuous but admits a singular of first order at $p = 0$. Observing that

$$\frac{\nabla p_1(x) \nabla u(x)}{|\nabla p_1|^2} = \frac{\partial u}{\partial p_1},$$

and denoting by "+ sym." the terms of symmetrization of $\mathcal{A}_{x^*}$, we have, for $u, v \in \mathcal{C}^\infty_c((\mathbf{R}^2 \setminus \{(x^*_1, x^*_2)\} \times \mathbf{R})$,

$$\begin{aligned}
&(A_{x^*}u, v)_{\mathcal{H}^D} \\
&= \int_{\mathbf{R}^3} i\chi_{x^*}(x)\left\langle \pi_2(y)\frac{\nabla p_1(x) \cdot \nabla(\chi_{x^*}(x)\pi_2(y)u(x))}{|\nabla p_1(x)|^2}, v(x)\right\rangle_{\mathbb{C}^6,D} \mathrm{d}x + \mathrm{sym.} \\
&= \int_{\mathbf{R}^2\times\mathbb{S}^1} i\left\langle \frac{\partial(\widetilde{\pi}\widetilde{u})}{\partial p_1}, \widetilde{\chi}^2(p)\widetilde{\pi}(p)\widetilde{v}(p)\right\rangle_{\mathbb{C}^6,D} \mathrm{d}p + \mathrm{sym.} \\
&= \int_{\mathbf{R}^2\times\mathbb{S}^1} i\left\langle \frac{\partial(\widetilde{\chi}\widetilde{\pi}\widetilde{u})}{\partial p_1}, \widetilde{\chi}\widetilde{\pi}\widetilde{v}\right\rangle_{\mathbb{C}^6,D} \mathrm{d}p \equiv \left(\widetilde{A}_{x^*}\widetilde{u}, \widetilde{v}\right)_{\tilde{H}}.
\end{aligned}$$

The projection $\widetilde{\pi}$ has range two. Since $\boldsymbol{\beta} = 0$, we have, for $z \neq 0$, a basis of the eigenspace $\ker(H^D(x) - \sqrt{\Psi_0(z)})$ of the form $(\varphi_1(p), \varphi_2(p) = \overline{\varphi_1(p)})^T$, with $\varphi_1 = (q, i\sqrt{\kappa}q)$ and $q(p)^T \in \ker(i\sqrt{\kappa}\boldsymbol{\varepsilon}M(y) - \Psi_0(z)I_3)$, where $x = x(p)$, I_3 denotes the identity matrix of size 3, and $M(y)$ is the 3×3 matrix defined at (1.3). Moreover we can choose $q(p)$ such that $x \mapsto q(p(x))$ is analytic in the support of χ_{x^*} at least, and with $\langle \boldsymbol{\varepsilon}^{-1}q(p), q(p)\rangle_{\mathbb{C}^3} = 1/2$, so $(\varphi_1(p), \varphi_2(p))$ is orthonormal in $\mathbb{C}^6$ equipped with $\langle , \rangle_{\mathbb{C}^6,D}$. We thus have $\langle \varphi_i(p), \varphi_j(p)\rangle_{\mathbb{C}^6,D} = \delta_{i,j}$, $i, j \in \{1, 2\}$, but also

$$\begin{aligned}
\langle \partial_p\varphi_1, \varphi_2\rangle_{\mathbb{C}^6,D} &= \left\langle \boldsymbol{\varepsilon}^{-1}\partial_p q, q\right\rangle_{\mathbb{C}^3} + \left\langle \boldsymbol{\mu}^{-1}\partial_p(i\sqrt{\kappa}q), -i\sqrt{\kappa}q\right\rangle_{\mathbb{C}^3} \\
&= \left\langle \boldsymbol{\varepsilon}^{-1}\partial_p q, q\right\rangle_{\mathbb{C}^3} + \left\langle i\boldsymbol{\varepsilon}^{-1}\partial_p q, -iq\right\rangle_{\mathbb{C}^3} \\
&= 0.
\end{aligned}$$

Similarly, $\langle \varphi_1, \partial_p\varphi_2\rangle_{\mathbb{C}^6,D} = 0$. Hence we have

$$\widetilde{\pi}(p)\widetilde{u}(p) = \widetilde{\xi}_1(\widetilde{u})(p)\varphi_1(p) + \widetilde{\xi}_2(\widetilde{u})(p)\varphi_2(p),$$

where we set

$$\widetilde{\xi}_j(\widetilde{u})(p) := \langle \widetilde{u}(p), \varphi_j(p)\rangle_{\mathbb{C}^6,D}. \tag{B.4}$$

We then have

$$\big(\widetilde{A}_{x^*}\widetilde{u},\widetilde{v}\big)_{\tilde{H}} = i\sum_{j=1}^{2}\int_{\mathbf{R}^2\times\mathbb{S}^1}\frac{\partial}{\partial p_1}\big(\widetilde{\chi}\widetilde{\xi}_j(\widetilde{u})\big)\overline{\widetilde{\chi}\widetilde{\xi}_j(\widetilde{v})}\mathrm{d}p.$$

Let us set

$$D\big(\widetilde{A}_{x^*}\big) = \Big\{\widetilde{u}\in\widetilde{H};\ \widetilde{\chi}^2\partial_{p_1}\widetilde{\xi}_j(\widetilde{u})\in L^2\big(\mathbf{R}^2\times\mathbb{S}^1,\mathbb{C};\mathrm{d}p\big),\ j=1,2\Big\}.$$

Let us show that $D(\widetilde{A}^*_{x^*}) = D(\widetilde{A}_{x^*})$. Let $\widetilde{v}\in D(\widetilde{A}^*_{x^*})$, so we have:

$$\Big|\big(\widetilde{A}_{x^*}\widetilde{u},\widetilde{v}\big)_{\tilde{H}}\Big| \leqslant C\|\widetilde{u}\|_{\tilde{H}},\quad \forall\,\widetilde{u}\in D\big(\widetilde{A}_{x^*}\big), \tag{B.5}$$

i.e.,

$$\left|\sum_{j=1}^{2}\int_{\mathbf{R}^2\times\mathbb{S}^1}\frac{\partial\widetilde{\xi}_j(\widetilde{u})}{\partial p_1}\widetilde{\chi}^2(p)\overline{\widetilde{\xi}_j(\widetilde{v})}\mathrm{d}p\right| \leqslant C\|\widetilde{u}\|_{\tilde{H}},\quad \forall\,\widetilde{u}\in D\big(\widetilde{A}_{x^*}\big).$$

We fix $j\in\{1,2\}$ and choose $\widetilde{u}(p) = f(p_1)g(p_2,p_3)\varphi_j(p)$ in the above estimate with arbitrary $f\in H^1(\mathbf{R},\mathbb{C};\mathrm{d}p_1)$ and $g\in L^2(\mathbf{R}\times\mathbb{S}^1,\mathbb{C};\mathrm{d}p_2\mathrm{d}p_3)$. Then $\|\widetilde{u}\|_{\tilde{H}}\leqslant C\|f\|_{H^1(\mathbb{C})}\|g\|_{L^2(\mathbf{R}\times\mathbb{S}^1)}$ so we have

$$\left|\int_{\mathbf{R}^2\times\mathbb{S}^1}\frac{\partial f(p_1)}{\partial p_1}g(p_2,p_3)\widetilde{\chi}^2(p)\overline{\widetilde{\xi}_j(\widetilde{v})}\mathrm{d}p\right| \leqslant C\|f\|_{H^1(\mathbf{R})}\|g\|_{L^2(\mathbf{R}\times\mathbb{S}^1)},$$
$$\forall\, f\in H^1(\mathbf{R},\mathbb{C};\mathrm{d}p_1), g\in L^2\big(\mathbf{R}\times\mathbb{S}^1,\mathbb{C};\mathrm{d}p_2\mathrm{d}p_3\big).$$

It shows that

$$K(p_1) := \int_{\mathbf{R}\times\mathbb{S}^1}\widetilde{\chi}^2(p)\widetilde{\xi}_j(\widetilde{v})g(p_2,p_3)\mathrm{d}p_2\mathrm{d}p_3 \in H^1(\mathbf{R},\mathbb{C};\mathrm{d}p_1)$$

with

$$\left\|\frac{\partial}{\partial p_1}K(p_1)\right\|_{L^2(\mathbf{R})} \leqslant C\|g\|_{L^2(\mathbf{R}\times\mathbb{S}^1)}.$$

But we have

$$\frac{\partial}{\partial p_1}K(p_1) = \int_{\mathbf{R}\times\mathbb{S}^1}\widetilde{\chi}^2(p)\frac{\partial}{\partial p_1}\widetilde{\xi}_j(\widetilde{v})g(p_2,p_3)\mathrm{d}p_2\mathrm{d}p_3 + L(p_1),$$
$$L(p_1) := \int_{\mathbf{R}\times\mathbb{S}^1}\widetilde{\xi}_j(\widetilde{v})\left(\frac{\partial}{\partial p_1}\widetilde{\chi}^2(p)\right)g(p_2,p_3)\mathrm{d}p_2\mathrm{d}p_3,$$

with $\|L_1\|_{L^2(\mathbf{R})}\leqslant C\|g\|_{L^2(\mathbf{R}\times\mathbb{S}^1)}$. Hence we have

$$\widetilde{\chi}^2\frac{\partial}{\partial p_1}\widetilde{\xi}_j(\widetilde{v}) \in L^2\big(\mathbf{R}^2\times\mathbb{S}^1,\mathbb{C};\mathrm{d}p\big).$$

Thus, $\widetilde{v}\in D(\widetilde{A}_{x^*})$ and so $\widetilde{A}_{x^*}$ is self-adjoint. Consequently, A_{x^*} with domain $T^{-1}(D(\widetilde{A}_{x^*}))$ is a self-adjoint operator.

Case (1) with the general situation $s_1s_2s_3 = -1$ is similar.

Cases (2-1), (2-1a), (2-1b), (2-1d) and (2-1e), with $s_1 s_2 s_3 = -1$, are similar, except that the projection $\widetilde{\pi}$ ($= \pi_1^+(y)$ or $= \pi_1^-(y)$) has range one, which simplifies the proof.

Case (3-1) with $s_1 s_2 s_3 = -1$. We set $\pi_1^\pm A_{x^*} \pi_1^\pm =: A^\pm$ so $A_{x^*} = \sum_\pm A^\pm$ with $D(A^\pm) = \mathcal{D}_0$. We prove that $A^\pm$ is essentially self-adjoint on $\mathcal{H}^D$. We set

$$k^\pm(x) := \frac{|\nabla_x p_1(x)|}{\left|\nabla_x p_1(x) \cdot \nabla_x \sqrt{\tau^\pm(z)}\right|^{1/2}}.$$

Thanks to Lemma 4.4 we have

$$k^\pm(x) = 1 + O(\mathrm{d}_0(x, x^*)).$$

Thus $k^\pm(x)$ is defined for $x \simeq x^*$ and $x \neq x^*$, extends as a positive lipschitzian function near x^*. We then consider the same transforms than in Case (1) with $\widetilde{H}^\pm$ replacing $\widetilde{H}$ so we have

$$\begin{aligned}\left(A^\pm u^\pm, v^\pm\right)_{\mathcal{H}^D} &= i \int_{\mathbf{R}^2 \times \mathbb{S}^1} \left\langle \frac{\partial}{\partial p_1} (\widetilde{\chi} \widetilde{u}^\pm), \widetilde{\chi} \widetilde{v}^\pm \right\rangle_{\mathbb{C}^6, D} \mathrm{d}p \\ &\equiv \left(\widetilde{A}^\pm \widetilde{u}^\pm, \widetilde{v}^\pm\right)_{\tilde{H}},\end{aligned}$$

where we set $\widetilde{A}^\pm := i \widetilde{\chi} \circ \frac{\partial}{\partial p_1} \circ \widetilde{\chi}$, and

$$\widetilde{u}^\pm(p) := |\nabla_x p_1(x)| \, |J_\Phi(x')|^{-1/2} \widetilde{k}^\pm(p) u(x) \quad x' = \Phi^{-1}(p) \in \mathbf{R}^3,$$

and $\widetilde{k}^\pm(p) := k^\pm(x)$, $\widetilde{\pi}_1^\pm(p) := \pi_1^\pm(y)$, $\widetilde{\chi}(p) := \chi_{x^*}(x)$. Thus, as in Case 2-1 with $\pi_j s_j = 1$, $A^\pm = \pi_1^\pm A^\pm \pi_1^\pm$ is essentially self-adjoint on $\mathcal{H}^D$. We denote by $D^\pm$ the domain of the self-adjoint extension of $A^\pm$, so $D^\pm = \{u \in \mathcal{H}^D;\ A^\pm u \in \mathcal{H}^D\}$. Then, A_{x^*} extends as a symmetric operator, $A'_{x^*} = A_{x^*}$ with domain $D(A'_{x^*}) := D^+ \cap D^-$. Now, let $v \in D((A'_{x^*})^*)$ so

$$|(A_{x^*} u, v)_{\mathcal{H}^D}| \leqslant C\|u\| \quad \forall\, u \in D(A'_{x^*}).$$

Let $u \in D^\pm$. Then $A_{x^*} \pi_1^\pm u = A^\pm u \in \mathcal{H}^D$, so $\pi_1^\pm u \in D(A'_{x^*})$. Thus

$$\left|\left(A^\pm u, v\right)_{\mathcal{H}^D}\right| = \left|\left(A_{x^*} \pi_1^\pm u, v\right)_{\mathcal{H}^D}\right| \leqslant C\left\|\pi_1^\pm u\right\| \leqslant C\|u\| \quad \forall\, u \in D^\pm.$$

Hence $v \in D^\pm$. Thus, $v \in D(A'_{x^*})$, so A'_{x^*} is self-adjoint.

Case (2-1c). — We have

$$p_1(x) = \rho'^2 - \frac{1}{2} x_3'^4,$$

and we set

$$p_2(x) := x_2' e^{-\frac{1}{2x_3'^2}},$$

$$p_3(x) := x_1' e^{-\frac{1}{2x_3'^2}},$$

with $p_2|_{x'_3=0} = p_3|_{x'_3} = 0$, so $p_2, p_3 \in \mathcal{C}^\infty(\mathbf{R}^3)$. Then,

$$\begin{aligned}\nabla p_1 &= 2\big(x'_1, x'_2, -x'^3_3\big),\\ \nabla p_2 &= e^{-\frac{1}{2x'^2_3}}\big(0, 1, x'_2/x'^3_3\big),\\ \nabla p_3 &= e^{-\frac{1}{2x'^2_3}}\big(1, 0, x'_1/x'^3_3\big),\end{aligned}$$

$\nabla p_1 \perp \nabla p_j$, $j = 2, 3$, and the Jacobian of the mapping Φ: $x' \mapsto p$ is

$$J_\Phi(x') = \frac{\rho'^2}{x'^3_3} e^{-\frac{1}{x'^2_3}}.$$

It does not vanish if $x'_3 \neq 0$ or $\rho' \neq 0$. Let us invert Φ. The sign of x'_3 is not determined by p so we consider

$$\Phi^\pm :\ \mathbf{R}^{2*} \times \mathbf{R}^{\pm *} \ni x' \mapsto p \in \mathbf{R} \times \mathbf{R}^{2*}.$$

Let $p \in \mathbf{R} \times \mathbf{R}^{2*}$. We have $x'_1 = p_3 e^{\frac{1}{2x'^2_3}}$, $x'_2 = p_2 e^{\frac{1}{2x'^2_3}}$ so x'_3 satisfies the equation $F(x'^2_3) = p_1$ where we set

$$F(t) := \big(p_2^2 + p_3^2\big)e^{1/t} - \frac{1}{2}t^2, \quad t > 0.$$

Since $F' > 0$, $F(+\infty) = -\infty$ and $F(0^+) = +\infty$, then the equation is uniquely solvable by some $t_0 > 0$ so we obtain $x'_3 = \pm\sqrt{t_0} \in \mathbf{R}^*$. Hence $\Phi^\pm$ is bijective. We let the lector to check that $\Phi^\pm$ is an homeomorphism from $\mathbf{R}^{2*} \times \mathbf{R}^{\pm *}$ into $\mathbf{R} \times \mathbf{R}^{2*}$. Hence, $\Phi^\pm$ is a $\mathcal{C}^\infty$-diffeomorphism from $\mathbf{R}^{2*} \times \mathbf{R}^{\pm *}$ into $\mathbf{R} \times \mathbf{R}^{2*}$.

We set the Hilbert spaces $\widetilde{H}^\pm = L^2(\mathbf{R}^{2*} \times \mathbf{R}^{\pm *}, \mathbb{C}^6; \mathrm{d}p)$ equipped with the scalar product

$$\big(\widetilde{u}^\pm, \widetilde{v}^\pm\big)_{\widetilde{H}^\pm} := \int_{\mathbf{R}^{2*} \times \mathbf{R}^{\pm *}} \big\langle \widetilde{u}^\pm(p), \widetilde{v}^\pm(p)\big\rangle_{\mathbb{C}^6, D} \mathrm{d}p,$$

then $\widetilde{H} := \widetilde{H}^+ \oplus \widetilde{H}^-$. For $\widetilde{u} = (\widetilde{u}^+, \widetilde{u}^-) \in \widetilde{H}$, $x' \in \mathbf{R}^{2*} \times \mathbf{R}^{\pm *}$, we set

$$u(x) = |J_\Phi(x')|^{1/2} \widetilde{u}^\pm\big(\Phi^\pm(x')\big),$$

so the transform

$$T :\ L^2(\mathbf{R}^3) \ni u \mapsto \widetilde{u} \in \widetilde{H}$$

is a bijective isometry (up to a nonzero constant multiplicative factor).

Putting again $\widetilde{\chi}(p) = \chi_{x*}(x)$, $\widetilde{\pi}(p) = \pi_2(x)$, we have, for $u, v \in \mathcal{C}_c^\infty(\mathbf{R}^2 \setminus \{(x_1^*, x_2^*)\} \times \mathbf{R} \setminus \{x_3^*\}, \mathbb{C})$,

$$(A_{x^*}u, v)_{\mathcal{H}^D} = \int_{\mathbf{R}^3} i\bigg\langle \frac{\partial(\widetilde{\chi}\widetilde{\pi}\widetilde{u})}{\partial p_1}, \widetilde{\chi}\widetilde{\pi}\widetilde{v}\bigg\rangle_{\mathbb{C}^6, D} \mathrm{d}p \equiv \big(\widetilde{A}_{x^*}\widetilde{u}, \widetilde{v}\big)_{\widetilde{H}}.$$

The projection $\widetilde{\pi}$ has range one so this case is similar to Case (2-1), so A_{x^*} is essentially self-adjoint. □

(B). — Let us treat Case (1) with $s_1 = s_2 = -1$ (and $s_3 = -1$). We observe that

$$p_1(x) = \sum_{j=1}^{3} (x'_j)^2 \geqslant 0.$$

(where we set $x'_j = \sqrt{C_j/2}(x_j - x^*_j)$). We use the spherical coordinates: $x' = \rho\omega$ with $\rho = \sqrt{x'^2_1 + x'^2_2 + x'^2_3} > 0$, $\omega = \rho^{-1}x' \in \mathbb{S}^2$, so we have $p_1 = \rho^2$ and choose two other coordinates, p_2, p_3, on the sphere $\mathbb{S}^2$.

We then follow the above method (Case (1) with $s_1 = s_2 = 1 = -s_3$) with similar notations, notably, with the same couple (φ_1, φ_2) and coordinates $\widetilde{\xi}_j$ (defined by (B.4)) $j = 1, 2$. The mapping

$$\Phi:\ x' = (x'_1, x'_2, x'_3) \mapsto p = (p_1, p_2, p_3)$$

is a $\mathcal{C}^\infty$-diffeomorphism from $\mathbf{R}^{3*}$ onto $\mathbf{R}^{+*} \times \mathbb{S}^2$. The jacobian of Φ has the form

$$J_\Phi(x') = j(p_2, p_3)\sqrt{p_1},$$

where j is a positive smooth function on $\mathbb{S}^2$. We set $\widetilde{H} = L^2(\mathbf{R}^{+*} \times \mathbb{S}^2, \mathbb{C}^6; \mathrm{d}p)$ equipped with the following scalar product:

$$(\widetilde{u}, \widetilde{v})_{\widetilde{H}} := \int_{\mathbf{R}^{+*}\times\mathbb{S}^2} \big\langle \widetilde{u}(p), \widetilde{v}(p)\big\rangle_{\mathbb{C}^6, D} \mathrm{d}p.$$

For $\widetilde{u} \in \widetilde{H}$, $p \in \mathcal{U}$, we consider the transformation defined by (B.3) between u and $\widetilde{u}$ so it is a bijective isometry (up to a positive constant multiplicative factor) between $L^2(\mathbf{R}^3, \mathbb{C}^6)$ and $\widetilde{H}$ which we denote T again. Setting $\widetilde{\pi}(p) = \pi_2(y)$, we have $\widetilde{\chi} \in \mathcal{C}^\infty_c(\mathbf{R}^{+*} \times \mathbb{S}^2)$ and $\widetilde{\chi} = 1$ near $p(x^*) = 0$. We thus have, for $u, v \in \mathcal{C}^\infty_c(\mathbf{R}^{+*} \times \mathbb{S}^2, \mathbb{C}^6)$,

$$(A_{x^*}u, v)_{\mathcal{H}^D} = \sum_{j=1}^{2} \int_{\mathbf{R}^{+*}\times\mathbb{S}^2} i\widetilde{\chi}\frac{\partial\big(\widetilde{\chi}\widetilde{\xi}_j(\widetilde{u})\big)}{\partial p_1}\overline{\widetilde{\xi}_j(\widetilde{v})}\mathrm{d}p \equiv (\widetilde{A}_{x^*}\widetilde{u}, \widetilde{v})_{\widetilde{H}}.$$

The above formula defines the symmetric operator $\widetilde{A}_{x^*}$ on $\widetilde{H}$ with domain $\mathcal{C}^\infty_c(\mathbf{R}^{+*} \times \mathbb{S}^2)$. Thus, $\widetilde{A}_{x^*}$ extends to the operator with the same formula defined on

$$D(\widetilde{A}_{x^*}) = \mathcal{H}_{1,0} := \left\{ \begin{matrix} \widetilde{u} \in \widetilde{H};\ \widetilde{\chi}^2\partial_{p_1}\widetilde{\xi}_j(\widetilde{u}) \in L^2\big(\mathbf{R}^{+*} \times \mathbb{S}^2, \mathbb{C}; \mathrm{d}p\big), \\ \widetilde{\chi}^2\partial_{p_1}\widetilde{\xi}_j(\widetilde{u})|_{p_1=0} = 0,\ j = 1, 2 \end{matrix} \right\}.$$

Let us prove that the default index N^+ of $\widetilde{A}_{x^*}$ vanishes. Firstly, observe that

$$\begin{aligned} D((\widetilde{A}_{x^*})^*) &= \mathcal{H}_1 \\ &:= \Big\{ \widetilde{u} \in \widetilde{H};\ \widetilde{\chi}^2\partial_{p_1}\widetilde{\xi}_j(\widetilde{u}) \in L^2\big(\mathbf{R}^{+*} \times \mathbb{S}^2, \mathbb{C}; \mathrm{d}p\big),\ j = 1, 2 \Big\}. \end{aligned} \tag{B.6}$$

In fact an integration by parts shows that $D((\widetilde{A}_{x^*})^*)$ contains $\mathcal{H}_1$. Then, let $\widetilde{v} \in D((\widetilde{A}_{x^*})^*)$ so (B.5) holds. As in Case (1) with $\prod_{k=1}^3 s_k = -1$, let $j \in \{1,2\}$ and choose $\widetilde{u}(p) = f(p_1)g(p_2,p_3)\varphi_j(p)$ with arbitrary $f \in H^1(\mathbf{R}^{+*}, \mathbb{C}; \mathrm{d}p_1)$ and $g \in L^2(\mathbb{S}^2, \mathbb{C}; \mathrm{d}p_2\mathrm{d}p_3)$, so we have

$$\left| \int_{\mathbf{R}^+ \times \mathbb{S}^2} \frac{\partial f(p_1)}{\partial p_1} g(p_2,p_3)\widetilde{\chi}^2(p)\overline{\widetilde{\xi}_j(\widetilde{v})}\mathrm{d}p \right| \leqslant C\|f\|_{H^1(\mathbf{R}^+,\mathbb{C})}\|g\|_{L^2(\mathbb{S}^2,\mathbb{C})},$$
$$\forall\, f \in H^1(\mathbf{R}, \mathbb{C}; \mathrm{d}p_1),\ g \in L^2\big(\mathbb{S}^2, \mathbb{C}; \mathrm{d}p_2\mathrm{d}p_3\big).$$

It implies $\frac{\partial}{\partial p_1}(\widetilde{\chi}^2\widetilde{\xi}_j(\widetilde{v})) \in L^2(\mathbf{R}^{+*} \times \mathbb{S}^2, \mathbb{C}; \mathrm{d}p)$, then $\widetilde{\chi}^2 \frac{\partial}{\partial p_1}\widetilde{\xi}(\widetilde{v}) \in L^2(\mathbf{R}^{+*} \times \mathbb{S}^2, \mathbb{C}; \mathrm{d}p)$, so $\widetilde{v} \in \mathcal{H}_1$. Therefore, (B.6) is proved. Now, let $\widetilde{v} \in D((\widetilde{A}_{x^*})^*)$ such that $(\widetilde{A}_{x^*})^*\widetilde{v} = i\widetilde{v}$. Thus we have $(-i(\widetilde{A}_{x^*})^*\widetilde{v},\widetilde{v})_{\tilde{H}} = (\widetilde{v},\widetilde{v})_{\tilde{H}}$. An integration by parts (according to the variable p_1) shows that $v = 0$. Consequently, A_{x^*} with domain $T^{-1}(D(\widetilde{A}_{x^*}))$ is a maximal symmetric operator with the default index $N^+ = 0$. (See also[7, Lemma 1.3] for results of the same kind). □

(C)*(Cases* (3-2) *and* (3-3)*).* — We set

$$p_1 = \cos(x_1)\cos(x_2),$$

so p_1 vanishes at $x = x^* \in \mathcal{X}_2^*$ (such that $z^* = (\frac{\beta_2}{\beta_1}, 1, 0)$). We have

$$\nabla_x p_1 = -w = (\sin x_1 \cos x_2, \sin x_2 \cos x_1, 0).$$

We set

$$p_2 = \frac{\sin x_1}{\sin x_2} - \frac{\sin x_1^*}{\sin x_2^*}, \quad p_3 = x_3,$$

so $\nabla_x p_i \cdot \nabla_x p_j = 0$ if $i \neq j$ and the jacobian of the map $\Phi\colon x \mapsto p = (p_1,p_2,p_3)$ is

$$J_\Phi(x) = \prod_{j=1}^3 \nabla_x p_j.$$

We have $\underset{\frown}{w \cdot \nabla_x u} = \underset{\frown}{u_w} = -|\nabla p_1|^2\partial_{p_1}u$ and, thanks to (4.2), $\sqrt{\Psi_0(z)}_w = p_1\sqrt{\Psi_0(z)}_{\tilde{w}}$ where $\sqrt{\Psi_0(z)}_{\tilde{w}}$ is analytic and does not vanish at x^*.

Case (3-3). — We have $\nabla_x p_1(x^*) \neq 0$ and $J_\Phi(x^*) \neq 0$, so Φ is a local diffeomorphism from a neighborhood of x^* in $\mathbf{R}^3$ into a neighborhood of $0_{\mathbf{R}^3}$ in $\mathbf{R}^3$. Hence, we have

$$(A_{x^*}u, v)_{\mathcal{H}^D} = -i\int_{\mathbf{R}^3} \frac{k(x)}{p_1}\left\langle \frac{\partial(\chi_2\pi_2 u)}{\partial p_1}, \chi_2\pi_2 v\right\rangle_{\mathbb{C}^6,D} \mathrm{d}p + \mathrm{sym},$$

where k is smooth with $k(x^*) > 0$. As in the above cases, we thus set $q = (q_1,q_2,q_3)$, $q_1 = p_1|p_1|$, $q_j = p_j$ for $j = 2,3$, $\widetilde{\chi}(q) = \chi_{x^*}(x)$, $\widetilde{\pi}(q) = \pi_2(y)$,

$\widetilde{u}(q) = |k(x)|^{1/2}u(x)$. We then obtain

$$(A_{x^*}u, v)_{\mathcal{H}^D} = -i\int_{\mathbf{R}^3} \operatorname{sgn}(q_1)\Big\langle \frac{\partial(\widetilde{\chi}\widetilde{\pi}\widetilde{u})}{\partial q_1}, \widetilde{\chi}\widetilde{\pi}\widetilde{v}\Big\rangle_{\mathbb{C}^6,D} \mathrm{d}q \equiv \big(\widetilde{A}_{x^*}\widetilde{u}, \widetilde{v}\big)_{\widetilde{H}},$$

where $\widetilde{H} = L^2(\mathbf{R}^3, (\mathbb{C}^6, \langle\,,\rangle_{\mathbb{C}^6,D}); \mathrm{d}q)$ is a usual Hilbert space. The projection $\widetilde{\pi}$ has range two so Case (3-3) is similar to (B)) with A_{x^*} replaced by $-A_{x^*}$. Hence, A_{x^*} has default index $N^- = 0$ and admits a maximal symmetric extension.

Case (3-2). — We have $\nabla_x p_1(x^*) = 0$ so $J_\Phi(x^*) = 0$. Let us "invert" $x \mapsto p$. For simplicity we assume $y_1^* = y_2^* = 1$. Set $x_j' = x_j - x_j^*$ for $j = 1, 2$. Since $\sin x_j \simeq 1 - (x_j')^2/2$ and $\cos(x_j) \simeq -x_j'$ for $j = 1, 2$ then $p_1 \simeq x_1'x_2'$ and $-2p_2 \simeq (x_1')^2 - (x_2')^2$. Thus $(x_1' + ix_2')^2 \simeq 2i(p_1 + ip_2)$.

It means that we have the same transform than in Case (A)), i.e., there exists an Hilbert space $\widetilde{H}$ and an isometry $L^2(\mathbf{R}^3) \ni u \to \widetilde{u} \in \widetilde{H}$ such that

$$(A_{x^*}u, v)_{\mathcal{H}^D} = -i\int_{\mathbf{R}^2\times\mathbb{S}^1} \operatorname{sgn}(q_1)\Big\langle \frac{\partial(\widetilde{\chi}\widetilde{\pi}\widetilde{u})}{\partial q_1}, \widetilde{\chi}\widetilde{\pi}\widetilde{v}\Big\rangle_{\mathbb{C}^6,D} \mathrm{d}q,$$

where $\widetilde{\chi}(q) := \chi_{x^*}(x)$, $\widetilde{\pi}(q) := \pi_2(y)$. Hence, as in Case (3-3), A_{x^*} has default index $N^- = 0$) and admits a maximal symmetric extension. $\square$

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Notations

$$\begin{aligned}
y &= \sin x \quad (y_j = \sin x_j),\\
z &= \sin^2 x \quad (z_j = \sin^2 x_j),\\
\boldsymbol{\beta} &= \boldsymbol{\varepsilon} \times \boldsymbol{\mu} = (\beta_1, \beta_2, \beta_3),\\
\boldsymbol{\alpha} &= (\alpha_1, \alpha_2, \alpha_3), \quad \alpha_1 := (\varepsilon_2\mu_3 + \varepsilon_3\mu_2)/2 \quad \text{and c.p.},\\
\gamma_1 &= \varepsilon_2\varepsilon_3\mu_2\mu_3 \quad \text{and c.p.},\\
\nu &= \frac{2\alpha_3\sqrt{\beta_1\beta_2} - \sqrt{\gamma_3}(\beta_1 + \beta_2)}{|\beta_3|\sqrt{\gamma_3}},
\end{aligned}$$

$$h^D(y) = H^D(x),$$

$$\begin{aligned}
\Phi_0(z) &= \varepsilon_2\varepsilon_3\mu_2\mu_3 z_1^2 + (\varepsilon_2\varepsilon_3\mu_1\mu_3 + \varepsilon_1\varepsilon_3\mu_2\mu_3)z_1z_2 + \text{c.p.},\\
K_0(z) &= \frac{1}{4}\big(\beta_1^2z_1^2 + \beta_2^2z_2^2 + \beta_3^2z_3^2 - 2\beta_1\beta_2z_1z_2 - 2\beta_2\beta_3z_2z_3 - 2\beta_1\beta_3z_1z_3\big),\\
\Psi_0(z) &= \boldsymbol{\alpha}\cdot z \;=\; \alpha_1z_1 + \alpha_2z_2 + \alpha_3z_3,\\
\tau^{\pm} &= \Psi_0 \pm \sqrt{K_0},\\
\lambda_{\pm} &= \max\Big\{\sqrt{\tau^{\pm}(z)}\;\Big|\; z\in[0,1]^3\Big\},\\
\lambda^* &= \max_{\mathcal{X}_2}\sqrt{\Psi_0\circ\sin^2},\\
\mathcal{X}_0 &= \big\{x\in\mathbb{T}^3;\; z=0\big\},\\
\mathbb{T}_0^3 &= \mathbb{T}^3\setminus\mathcal{X}_0,\\
P_M &: \mathbf{R}\times\mathbb{T}^3 \ni (\lambda,x)\mapsto x\in\mathbb{T}^3,\\
P_{\mathbf{R}} &: \mathbf{R}\times\mathbb{T}^3 \ni (\lambda,x)\mapsto \lambda\in\mathbf{R},\\
\Sigma &= \big\{(\lambda,x);\; \lambda\in\sigma(H^D(x))\big\} = \bigcup_{j=1}^{6}\Sigma_j,\\
\Sigma_1 &= \{(\lambda,x)\in\Sigma;\; K_0(z)\neq 0\;\},\\
\Sigma_2 &= \big\{(\lambda,x)\in\Sigma;\; z\neq 0,\; K_0(z)=0,\; \lambda^2=\Psi_0(z)\big\},\\
\mathcal{X}_j &= P_M(\Sigma_j),\quad j=1,2,\\
\Sigma_1^{*\pm} &= \big\{(\lambda,x)\in\Sigma_1;\; \lambda^2=\tau^{\pm}(z), \nabla_x\tau^{\pm}(z)=0\big\},\\
\Sigma_1^* &= \Sigma_1^{*+}\cup\Sigma_1^{*-},\\
\Sigma_2^* &= \{(\lambda,x)\in\Sigma_2;\; \nabla_x\Psi_0(z) \text{ is normal to } \mathcal{X}_2 \text{ at } x\},\\
Z_{\{0,1\}} &= \{0,1\}^3,\\
Z_{\{0,1\}}^* &= Z_{\{0,1\}}\setminus\{(0,0,0)\},\\
X_{\{0,1\}} &= \big\{x\in\mathbb{T}^3;\; z\in Z_{\{0,1\}}\big\},\\
X_{\{0,1\}}^* &= \Big\{x\in\mathbb{T}^3;\; z\in Z_{\{0,1\}}^*\Big\},\\
\mathcal{T} &= \mathcal{T}_1\cup\mathcal{T}_2\cup\{0\},\\
\mathcal{T}_j &= P_{\mathbf{R}}(\Sigma_j^*),\\
\mathcal{T}_1^{\pm} &= P_{\mathbf{R}}(\Sigma_1^{*\pm}),\\
\mathcal{X}_j^* &= P_M(\Sigma_j^*),\\
\mathcal{X}_1^{*\pm} &= P_M(\Sigma_1^{*\pm}),\\
\mathcal{X}^* &= \mathcal{X}_1^*\cup\mathcal{X}_2^*,\\
\sin^2(\mathcal{X}_j^*) &= \{\sin^2 x;\; x\in\mathcal{X}_j^*),
\end{aligned}$$

$$\begin{aligned}
\mathcal{T}_{\mathrm{sm}}^{+} &= \{\lambda_{+}, \lambda_{-}, \lambda^{*}\},\\
\mathcal{T}_{\mathrm{sm}} &:= \mathcal{T}_{\mathrm{sm}}^{+} \cup -\mathcal{T}_{\mathrm{sm}}^{+},\\
\mathcal{T}_{\mathrm{sa}} &:= \mathcal{T} \setminus (\mathcal{T}_{\mathrm{sm}} \cup \{0\});\\
A_{\mathrm{out}} &= \mathcal{A}_{\mathrm{out}} + \mathcal{A}_{\mathrm{out}}^{*},\\
A_{\phi} &= A_{\mathrm{out}} + A_{\mathrm{in}} = A_0 + A_1 + A_2,\\
A_0 &= A_{\mathrm{out}}.
\end{aligned}$$

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