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SPECTRAL ANALYSIS OF THE DISCRETE MAXWELL OPERATOR: THE LIMITING ABSORPTION PRINCIPLE

OLIVIER POISSON
Aix Marseille Université, France

ABSTRACT. We make the beginning of the spectral analysis of the inhomogeneous discrete Maxwell operator \hat{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 \hat{H}^D at any not-zero real value. In particular, we analyse the case of thresholds of \hat{H}^D .

1. Introduction. We are interested in the limiting absorption principle (LAP) for the inhomogeneous discrete Maxwell operator \hat{H}^D defined on the square lattice \mathbf{Z}^3 , i.e. the limit in some usual or more abstract Besov spaces of the resolvents $\hat{R}(z) = (\hat{H}^D - z)^{-1}$ when $z \in \mathbb{C} \setminus \mathbb{R}$ tends to a spectral value λ of \hat{H}^D . It is equivalent and more convenient to deal with the Fourier series H^D of \hat{H}^D instead of \hat{H}^D since H^D is a multiplication operator on the three-dimensional real torus $\mathbb{T}^3 \approx (\mathbb{R}/(2\pi\mathbf{Z}))^3$. The operator H^D is so represented by the analytically fibered self-adjoint operator $\mathbb{T}^3 \ni x \mapsto H^D(x)$ on an Hilbert space \mathcal{H}^D where $H^D(x)$ is a 6×6 real matrix. We prove the LAP using the conjugate operator technique, as developed in the greatest generality by Gerard and Nier in a first version [3]. Actually, denoting $\Sigma = \{(\lambda, x) \mid \lambda \in \sigma(H^D(x))\}$ the energy-momentum set, where $\sigma(H^D(x))$ denotes the spectrum of an $H^D(x)$, we have the stratification $\Sigma = \cup_{j=1}^6 \Sigma_j$ where Σ_i is the semi-analytical set of elements (λ, x) for which λ is an eigenvalue of multiplicity i of $H^D(x)$ so we can introduce the (finite) set \mathcal{T} of thresholds. At this point we could simply apply [3, Theorem 3.1] and claim that for any interval $I \subset \subset \mathbb{R} \setminus \mathcal{T}$, there exists an operator A_I with domain $\mathcal{C}^\infty(\mathbb{T}^3; \mathbb{C}^6)$, essentially self-adjoint on \mathcal{H}^D , conjugated to H^D , and satisfying Points (i)-(iii) of [3, Theorem 3.1]. See Points (i)-(iv) of Theorem 3.1. However we go beyond this result. Moreover, the construction of the conjugate operator in [3] contains an error since, in fact, the analytically fibered self-adjoint operator for which the LAP is proved is not of class $\mathcal{C}^2(A_I)$. The authors of [3] have recently corrected it in the new version [4] at the cost of losing the (strict) globality of Mourre's inequality (3) which has to be replaced by a local one as (4). Nevertheless, following the ideas of the old version [3] and the new version [4] we construct an explicit conjugate operator A_ϕ to H^D with the same properties than the operator A_I of [3, Theorem 3.1]. Here we prefer to use as parameter for the conjugate a numerical smooth function ϕ instead of an interval I so A_ϕ is conjugated to H^D at each point of $\phi^{-1}(\mathbb{R}^*)$.

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We prove the LAP at any nonzero threshold. This result is optimal in the sense that there is no conjugate operator to H^D at 0 which is the obvious eigenvalue of H^D , and it shows also that H^D has no other eigenvalue. Denoting by \mathcal{X}^* the finite set of points $x \in \mathbb{T}^3$ such that $\sigma(H^D(x)) \cap \mathcal{T}$ is not reduced to the eigenvalue 0, we construct A_ϕ as a first order symmetric differential operator with smooth coefficients outside \mathcal{X}^* and with rational singularities at points $x \in \mathcal{X}^*$ such that $\sigma(H^D(x)) \cap \mathcal{T} \cap \phi^{-1}(\mathbb{R}^*)$ is not void. Then, the set of thresholds admits the partition $\mathcal{T} = \mathcal{T}_{sa} \cup \mathcal{T}_{sm}$: let $x^* \in \mathcal{X}^*$ and $\lambda \in \mathcal{T} \cap \sigma(H^D(x^*))$, if $\lambda \in \mathcal{T}_{sa}$ then the local part A_{x^*} of A_ϕ near x^* is essentially self-adjoint, and if $\lambda \in \mathcal{T}_{sm}$ then A_ϕ near x^* admits a maximal monotone extension. Thus, we obtain the LAP on $\mathbb{R}^* \setminus \mathcal{T}_{sm}$ in the same terms as [3, Theorem 3.3].

If $\lambda \in \phi^{-1}(\mathbb{R}^*) \cap \mathcal{T}_{sm}$ then A_ϕ may not have a maximal monotone extension since its singularities may come from several points of \mathcal{X}^* and since the sum of two maximal monotone operators, even with disjoint supports, is not necessarily maximal monotone. Nevertheless we prove the LAP on \mathcal{T}_{sm} by a slight extension of [2, Theorem 3.3].

In Part 2 we describe the operator H^D and the Hilbert space \mathcal{H}^D on which it is self-adjoint. In Part 3 we state the main results of our work, notably, the existence of a conjugate operator A_ϕ for H^D at Theorem 3.1, then several LAP in terms of abstract or usual Besov spaces at Corollaries 1-5. In Part 4 we describe the spectrum of $H^D(x)$, the stratification of the energy-momentum set Σ ; we define the thresholds and describe \mathcal{T} . It appears that \mathcal{T} depends mainly on the parameter $\beta = \varepsilon \times \mu$ where ε and μ denote respectively the permittivity and the permeability. In fact outside the first quite basic case $\beta = 0$ we have to deal with many special cases for which the set \mathcal{T} is no more obvious. In Part 5 we construct the conjugate operator A_ϕ according to the parameter β . We prove also the main properties of A_ϕ . In Part 6 we prove the main results (see Part 3).

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

$$\begin{aligned} y &= \sin x := (y_1 = \sin x_1, y_2 = \sin x_2, y_3 = \sin x_3) \in \mathbb{R}^3, \\ z &= y^2 := (z_1 = y_1^2, z_2 = y_2^2, z_3 = y_3^2) \in \mathbb{R}^3. \end{aligned}$$

(Although the letter z will be also used as a complex energy, there is no possible confusion with the notation above.) The other notations are standard. If $E \subset \mathcal{E} \in \{\mathbb{T}^3, \mathbb{R}^3\}$ and $\mathcal{F} \in \{\mathbb{R}^n, \mathbb{C}^n\}$, we denote by $\mathcal{C}_c^\infty(E, \mathcal{F})$ the real space of \mathcal{C}^∞ functions with values in \mathcal{F} , defined on E and with compact support in E .

Let T a self-adjoint operator, then $\sigma(T)$ is its spectrum; if $E \subset \mathbb{R}$ then $1_E(T)$ operator $\chi_{[a,b]}(T)$ where χ_J is the characteristic function of a set $J \subset \mathbb{R}$. If X and Y are two metrics spaces $B(X, Y)$ is the space of bounded operators from X into Y and $B(X) := B(X, X)$.

For $n \geq 1$ the space \mathbb{R}^n (respect., \mathbb{C}^n) is equipped with the scalar product $\langle \cdot, \cdot \rangle_{\mathbb{R}^n}$ (respect., with the hermitian product

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

Full notations are at the end of the text, Part 8.4.

2. The discrete Maxwell Operator.

2.1. The homogeneous discrete Maxwell Operator. Let $\mathbf{Z}^3 = \{n = (n_1, n_2, n_3); n_j \in \mathbf{Z}\}$ the square lattice, $\mathbb{T}^3 \approx (\mathbb{R}/(2\pi\mathbf{Z}))^3$ the 3-dimensional real torus, U the unitary transform between $L^2(\mathbb{T}^3)$ and $l^2(\mathbf{Z}^3)$:

$$(Uf)(n) := \hat{f}(n) \equiv (2\pi)^{-\frac{3}{2}} \int_{\mathbb{T}^3} e^{inx} f(x) dx, \quad n \in \mathbf{Z}^3,$$

so that any $f \in L^2(\mathbb{T}^3)$ can be written

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

The homogeneous discrete Maxwell operator is the bounded operator H_0 on $\mathcal{H} = (L^2(\mathbb{T}^3))^6$ defined by

$$\hat{H}_0 = UH_0U^*,$$

with $H_0(x)$ the real anti-symmetrical 6×6 matrix:

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

where $y = \sin x$ and $M(y)$ is the real anti-symmetrical 3×3 matrix:

$$M(y) = \begin{pmatrix} 0 & -y_3 & y_2 \\ y_3 & 0 & -y_1 \\ -y_2 & y_1 & 0 \end{pmatrix}, \quad y \in \mathbb{R}^3. \quad (1)$$

The space $\mathcal{H} = L^2(\mathbb{T}^3, dx; \mathbb{R}^6)$ can be written as the hilbertian sum

$$\mathcal{H} = \int_{\mathbb{T}^3}^{\oplus} \mathbb{R}^6 dx,$$

with the scalar product

$$(u, v) := \int_{\mathbb{T}^3} \langle u(x), v(x) \rangle_{\mathbb{R}^6} dx.$$

We then have

$$H_0 = \int_{\mathbb{T}^3}^{\oplus} H_0(x) dx$$

which shows that H_0 is a bounded self-adjoint operator on \mathcal{H} .

All along the article we consider that the vectorial functions u and v may be complex-valued so we denote by the same symbol \mathcal{H} the hilbertian space $\int_{\mathbb{T}^3}^{\oplus} \mathbb{C}^6 dx$ equipped with the hilbertian product

$$(u, v) := \int_{\mathbb{T}^3} \langle u(x), v(x) \rangle_{\mathbb{C}^6} dx = \int_{\mathbb{T}^3} \sum_{j=1}^6 u_j(x) \overline{v_j(x)} dx$$

and with norm $\|u\| := (u, u)^{\frac{1}{2}}$.

2.2. The discrete Maxwell Operator. Let ε and μ be 3×3 constant diagonal matrices with diagonal elements, respectively, $\varepsilon_1, \varepsilon_2, \varepsilon_3 \in (0, \infty)$ for ε , and $\mu_1, \mu_2, \mu_3 \in (0, \infty)$ for μ . The inhomogeneous discrete-Maxwell operator is defined by

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

where we set

$$\hat{D} = \begin{pmatrix} \varepsilon & 0_{3 \times 3} \\ 0_{3 \times 3} & \mu \end{pmatrix}.$$

The (unperturbed) discrete Maxwell operator is $H^D = U^* \hat{H}^D U$ so we have, since \hat{D} is constant,

$$H^D = U^*(\hat{D}\hat{H}_0)U = \hat{D}U^*\hat{H}_0U = \hat{D}H_0.$$

The relation

$$(\hat{D}^{-1}H^D u, v) = (H_0 u, v)$$

shows that the operator H^D is bounded and self-adjoint on the space $\mathcal{H}^D = \mathcal{H}$ equipped with the hilbertian product

$$(u, v)_{\mathcal{H}^D} := (\hat{D}^{-1}u, v) = \int_{\mathbb{T}^3} \langle \hat{D}^{-1}u(x), v(x) \rangle_{\mathbb{C}^6} dx$$

and with norm $\|u\|_{\mathcal{H}^D} := (u, u)_{\mathcal{H}^D}^{\frac{1}{2}}$. (Since the norms $\|\cdot\|$ and $\|\cdot\|_{\mathcal{H}^D}$ are equivalent, we can omit the index " \mathcal{H}^D ".) It appears that H^D is a multiplication operator and we write

$$H^D = \int_{\mathbb{T}^3}^{\oplus} H^D(x) dx,$$

where $H^D(x)$ is self-adjoint on \mathbb{C}^6 equipped with the hermitian product:

$$\langle u(x), v(x) \rangle_{\mathbb{C}^6, D} := \langle \hat{D}^{-1}u(x), v(x) \rangle_{\mathbb{C}^6}.$$

Since $H^D(x)$ depends only on $y = \sin(x)$ we write it $H^D(x) = h^D(y)$. It is known (see [11]) that

$$\sigma(H^D) = \overline{\cup_{x \in \mathbb{T}^3} \sigma(H^D(x))}, \quad (2)$$

which is a compact set of \mathbb{R} .

3. Results.

3.1. Main Theorem. We introduce the following settings:

$$\begin{aligned} \mathcal{X}_0 &:= \{x \in \mathbb{T}^3; z = 0\}, & \mathbb{T}_0^3 &= \mathbb{T}^3 \setminus \mathcal{X}_0, \\ \mathcal{X}^* &:= \{x \in \mathbb{T}^3; \sigma(H^D(x)) \cap \mathcal{T} \neq \{0\}\} \subset \mathbb{T}_0^3. \end{aligned}$$

We denote $\mathcal{D}_0 := \mathcal{C}_c^\infty(\mathbb{T}^3 \setminus \mathcal{X}^*)$ and $R(z) := (H^D - z)^{-1}$ the resolvent of H^D .

Theorem 3.1. Let $\mathcal{T}' \subset \mathcal{T}$ with $0 \in \mathcal{T}'$, and $\phi \in \mathcal{C}_c^\infty(\mathbb{R} \setminus \mathcal{T}')$. Then there exists a symmetric operator A_ϕ defined on $\mathcal{C}^\infty(\mathbb{T}^3)$ if $\mathcal{T}' = \mathcal{T}$ and on \mathcal{D}_0 if $\mathcal{T}' \neq \mathcal{T}$, and satisfying the following properties:

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

$$\phi(H^D)[H^D, iA_\phi]\phi(H^D) \geq \delta\phi^2(H^D). \quad (3)$$

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

(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 $\mathcal{T}' \neq \mathcal{T}$, and there exists $\tilde{\phi} \in \mathcal{C}_c^\infty(\mathbb{R} \setminus \mathcal{T}')$ so that $A_\phi = \tilde{\phi}(H^D)A_\phi = A_\phi\tilde{\phi}(H^D)$.

- (iv) If $\mathcal{T}_{sm} \subset \mathcal{T}'$ 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, $\text{supp } A_1 \cap \text{supp } A_2 = \emptyset$.

Remark 1. • Since the coefficients of A_ϕ are smooth in $\mathbb{T}^3 \setminus \mathcal{X}^*$ and, since \mathcal{D}_0 is dense in \mathcal{H}^D , then, for $u \in \mathcal{H}^D$, the distribution $A_\phi u$ belongs to the topological dual space of \mathcal{D}_0 so, since A_ϕ is symmetric,

$$A_\phi u \in \mathcal{H}^D \iff |(u, A_\phi v)_{\mathcal{H}^D}| \leq C \|v\| \quad \forall v \in \mathcal{D}_0.$$

Setting

$$\|u\|_{D(A_\phi)} := \|u\| + \|A_\phi u\| \quad \forall u \in \mathcal{D}_0,$$

the closure \bar{A}_ϕ of A_ϕ has domain

$$D(\bar{A}_\phi) := \overline{\mathcal{D}_0}^{\|\cdot\|_{D(A_\phi)}}.$$

The adjoint of \bar{A}_ϕ or of A_ϕ is the operator A_ϕ^* with domain $D(A_\phi^*) = \{v \in \mathcal{H}^D; |(A_\phi u, v)_{\mathcal{H}^D}| \leq C \|u\|, u \in D(A_\phi)\}$. If $\text{supp } \phi \cap \mathcal{T} = \emptyset$ then A_ϕ is essentially self-adjoint and its self-adjoint extension has domain $\overline{\mathcal{C}^\infty(\mathbb{T}^3)}^{\|\cdot\|_{D(A_\phi)}} \supset H^1(\mathbb{T}^3)$ (with dense inclusion).

- Our set \mathcal{T} of thresholds may defer to the set of thresholds in [3]. Anyway, \mathcal{T} is a discrete (and finite) set. The sets \mathcal{T} , \mathcal{T}_{sa} and \mathcal{T}_{sm} are precisely described in Part 5.7.3.
- In the case $\mathcal{T}' = \mathcal{T}$, the result of [3] 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 at Point B of Corollary 1). The new version [4] of [3] 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 explicite formula for A_ϕ which is easier to read than the general formula in [4] (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 [3] revised in [4].

The second consequence is that we can state the LAP outside $\mathcal{T}_{sm} \cup \{0\}$ in the same terms as those of Gérard and Nier in the old version [3] of their work. See also [9, 10]. Let us consider a compact interval $I \subset \mathbb{R}^* \setminus \mathcal{T}_{sm}$, and fix $\phi \in \mathcal{C}_c^\infty(\mathbb{R}^* \setminus \mathcal{T}_{sm})$ such that $\phi = 1$ on a neighborhood of I . We denote by $A_\phi^{sa} \subset A_\phi^*$ a self-adjoint extension of A_ϕ . We define the abstract Besov space \mathcal{B}_A by

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

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

$$\|u\|_{\mathcal{B}_A^*} = \sup_{j \geq 0} r_j^{1/2} \|1_{r_{j-1} \leq |A_\phi^{sa}| < r_j} u\|.$$

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

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

We can claim

Corollary 1. (LAP on $\mathbb{R}^* \setminus \mathcal{T}_{sm}$ in abstract Besov spaces.) We have

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

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

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

exist in $B(\mathcal{H}^D)$ and are bounded, with uniform convergence according to $\lambda \in I$. The mapping $\mathbb{R} \setminus \mathcal{T} \ni \lambda \mapsto R(\lambda \pm i0)$ is norm continuous in $B(D((1 + |A_\phi^{sa}|)^s), D((1 + |A_\phi^{sa}|)^{-s}))$ 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 [12] with the restriction to spectral values outside the thresholds. Thus, we consider the case $\text{supp } \phi \subset \mathbb{R} \setminus \mathcal{T}$ 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. Let $D'(\mathbb{T}^3, \mathbb{C}) = (\mathcal{C}^\infty(\mathbb{T}^3, \mathbb{C}))'$ the space of distribution on \mathbb{T}^3 and consider $D'(\mathbb{T}^3, \mathbb{C}^6) \approx (D'(\mathbb{T}^3, \mathbb{C}))^6 \approx (D'(\mathbb{T}^3, \mathbb{R}))^{12}$. We introduce the normed spaces

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

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 $s \geq 0$ and $u \in \mathcal{C}^\infty(\mathbb{T}^3, \mathbb{C}^6)$ we have $\|(1 + |A_\phi^{sa}|)^s u\| \leq C \|u\|_s$ where C does not depend on u . Thus, the following inclusion relations hold :

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

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

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

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

$$\|u\|_{\mathcal{B}^*} = \sup_{j \geq 0} r_j^{1/2} \|1_{r_{j-1} \leq |N| < r_j} u\|.$$

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, Lemma 2.8 of [5] says that there is a constant $C > 0$ such that

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

that is, $\mathcal{B} \subset \mathcal{B}_A$, and so, $\mathcal{B}_A^* \subset \mathcal{B}^*$. Hence, Corollary 1 can be extended as

Corollary 2. (LAP on $\mathbb{R} \setminus \mathcal{T}$ in usual Besov spaces.) We have

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

for all compact set $I \subset \mathbb{R} \setminus \mathcal{T}$. 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 $\mathbb{R} \setminus \mathcal{T} \ni \lambda \mapsto R(\lambda \pm i0)$ 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 [2, Theorem 3.3].

Corollary 3. (LAP on \mathbb{R}^* .) Let $I \subset \mathbb{R}^*$ a compact interval. There exists a constant C_I such that

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

for all $z = \lambda + i\mu$ with $\lambda \in I$, $\mu \neq 0$ real. Moreover if $z_1 = \lambda_1 + i\mu_1$, $z_2 = \lambda_2 + i\mu_2$ are two such numbers, and if μ_1 and μ_2 have the same sign, then

$$|(u, (R(z_1) - R(z_2))u)_{\mathcal{H}^D}| \leq C_I |z_1 - z_2|^{1/2} \|u\|_{D(\bar{A}_\phi)}^2 \quad \forall u \in D(\bar{A}_\phi).$$

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

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

An immediate consequence of Corollary 3 is

Corollary 4. 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 $H_V^D = H^D + V$, as done in [3]. We will simply recall some well known results in the Mourre theory (see [9, 10]) and refer the reader to the book [1] for a complete exposition of the Mourre method. In particular a sharper version of Corollary 5 is given in [1, Prop. 7.5.6].

Corollary 5. Let a compact interval $I \subset \mathbb{R}^* \setminus \mathcal{T}_{sm}$, and fix $\phi \in \mathcal{C}_c^\infty(\mathbb{R}^* \setminus \mathcal{T}_{sm})$ 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. $V \in C^{1,1}(A_\phi)$, i.e.,

$$\int \left\| R(i) \left(e^{itA_\phi} [V, iA_\phi] e^{-itA_\phi} - [V, iA_\phi] \right) R(i) \right\| \frac{dt}{t} < \infty.$$

Then, setting $H_V^D := H^D + V$, the following results hold:

1. There exists a constant $\delta > 0$ and a compact operator K so that,

$$\phi(H_V^D) [H_V^D, iA_\phi] \phi(H_V^D) \geq \delta \phi^2(H_V^D) + K.$$

Consequently point spectrum $\sigma_p(H_V^D)$ is of finite multiplicity in $\mathbb{R}^* \setminus \mathcal{T}_{sm}$ and has no accumulation point in $\mathbb{R}^* \setminus \mathcal{T}_{sm}$.

2. For each $\lambda \in I \setminus \sigma_p(H_V^D)$ there exist $\varepsilon > 0$ and $c > 0$ so that,

$$1_{[\lambda-\varepsilon, \lambda+\varepsilon]}(H_V^D) [H_V^D, iA_\phi] 1_{[\lambda-\varepsilon, \lambda+\varepsilon]} \geq c 1_{[\lambda-\varepsilon, \lambda+\varepsilon]}(H_V^D). \quad (4)$$

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

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

exist and are bounded for all $s > 1/2$.

Consequently the singular continuous spectrum of H_V^D is empty.

4. If the operator $(1 + |A_\phi|)^{-s} V (1 + |A_\phi|)^{-s}$ is bounded for some $s > 1/2$, then the wave operators

$$s - \lim_{t \rightarrow \pm\infty} e^{itH_V^D} e^{itH^D} 1_I(H^D) =: \Omega_I^\pm$$

exist and are asymptotically complete:

$$1_I^c(H_V^D) \mathcal{H}^D = \Omega_I^\pm \mathcal{H}^D.$$

4. First Spectral Properties.

4.1. **Spectrum of $h^D(y)$.** We introduce the new parameters:

$$\boldsymbol{\beta} = \boldsymbol{\varepsilon} \times \boldsymbol{\mu} = (\beta_1, \beta_2, \beta_3) \tag{5}$$

$$\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3), \quad \alpha_1 := (\varepsilon_2 \mu_3 + \varepsilon_3 \mu_2)/2 \quad \text{and, c.p.,}$$

$$\gamma_1 = \varepsilon_2 \varepsilon_3 \mu_2 \mu_3 \quad \text{and c.p. :} \tag{6}$$

$$\gamma_2 = \varepsilon_1 \varepsilon_3 \mu_1 \mu_3,$$

$$\gamma_3 = \varepsilon_1 \varepsilon_2 \mu_1 \mu_2.$$

(The abbreviation "c.p." means "circular permutation" so we have the other values by circular permutation, ex., $\beta_1 = \varepsilon_2 \mu_3 - \varepsilon_3 \mu_2$).

Let us describe the spectrum of $h^D(y)$.

Lemma 4.1. We have

$$\det(h^D(y) - k) = \det(\boldsymbol{\varepsilon} M(y) \boldsymbol{\mu} M(y) + k^2)$$

and the factorization

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

with

$$\tau^\pm = \Psi_0 \pm \sqrt{K_0}, \tag{7}$$

where

$$K_0(z) = \frac{1}{4} (\beta_1^2 z_1^2 - 2\beta_1 \beta_2 z_1 z_2) + c.p., \tag{8}$$

$$\Psi_0(z) = \boldsymbol{\alpha} \cdot \boldsymbol{z} := \alpha_1 z_1 + \alpha_2 z_2 + \alpha_3 z_3. \tag{9}$$

Proof in Appendix A. Since the characteristic polynomial $\det(H^D(x) - \lambda)$ depends on x via the new variable $z = (z_1, z_2, z_3) = \sin^2 x \in [0, 1]^3$ we set

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

Remark 2. If $z \neq 0$ then

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

Moreover there exists $C > 0$ such that

$$\tau^-(z) \geq C|z|, \quad z \in [0, 1]^3.$$

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

$$(A0): \beta_1 \geq \beta_2 > 0 > \beta_3 \text{ or } \beta_1 > \beta_2 = 0 > \beta_3.$$

The functions Ψ_0 and K_0 are homogeneous polynomials. The relation $K_0 \equiv 0$ is equivalent to $\beta = 0$ which is the special case where ε and μ are proportional. If one of the β_i 's vanishes, so, under Assumption (A0), $\beta_2 = 0$, then $\sqrt{K_0(z)}$ is polynomial. Thus, the functions $\mathbb{R}^3 \ni z \mapsto \tau^\pm(z)$ are homogeneous analytical complex functions with branch at $z = 0$ and at points z for which $K_0(z) = 0$ if $\beta_2 \neq 0$ for all i , and with branch point at $z = 0$ only if $\beta_2 \neq 0$.

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 4.2. (Spectrum of $h^D(y)$.) Let $z \in [0, +\infty)^3 \setminus \{0_{\mathbb{R}^3}\}$. 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 $\beta = 0$. 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 $\beta \neq 0$ (so (A0) holds). 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 $K_0(z) = 0$.

Assume $\beta \neq 0$ (so (A0) holds) with $\beta_2 = 0$. Then, τ^+ and τ^- are linear according to z :

$$\tau^+(z) = \varepsilon_2 \mu_3 z_1 + \varepsilon_3 \mu_1 z_2 + \varepsilon_2 \mu_1 z_3, \quad (10)$$

$$\tau^-(z) = \varepsilon_3 \mu_2 z_1 + \varepsilon_3 \mu_1 z_2 + \varepsilon_1 \mu_2 z_3. \quad (11)$$

(Hence we observe that:

If $(z_1, z_3) \neq 0_{\mathbb{R}^2}$, then the nonzero eigenvalues of $h^D(y)$ are $\pm \sqrt{\tau^+(z)}$, simple. If $(z_1, z_3) = 0_{\mathbb{R}^2}$ and $z_2 \neq 0$, then the nonzero eigenvalues of $h^D(y)$ are

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

double.)

The Proof of Theorem 4.2 follows from (8) and (9).

Lemma 4.3. Let us assume $\beta \neq 0$ (so (A0) holds). We have

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

The Proof is let to the reader.

We set

$$\lambda^* = \max\{\sqrt{\tau^+(z)}; z \in [0, 1]^3\} \in (0, +\infty).$$

The following result is a consequence of Theorem 4.2 and of relation (2):

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

$$\sigma(H^D) = [-\lambda^*, \lambda^*].$$

Proof in Appendix A.

4.2. Stratification and thresholds. Following [3] the set of energy-momentum is

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

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

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

It is clear that $P_{\mathbb{R}}|_{\Sigma}$ 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 set of energy-momentum Σ admits the partition

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

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

$$\mathcal{X}_j = P_M(\Sigma_j), \quad j \geq 1.$$

We see that $\Sigma_j = \emptyset$ for $j = 3, 4, 5$, $\Sigma_6 = \{0\} \times \mathcal{X}_0$ so $\mathcal{X}_6 = \mathcal{X}_0$, $\mathcal{X}_j = \emptyset$ for $j = 3, 4, 5$. Moreover,

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

If $\beta = 0$ then $\Sigma_1 = \emptyset$ and $(\lambda, x) \in \Sigma_2$ iff $z \neq 0$ and $\lambda^2 = \Psi_0(z)$.

If $\beta \neq 0$ 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 general definition of \mathcal{T} (which may defer from ours), see [3]. We set

$$\begin{aligned} \Sigma_1^* &:= \Sigma_1^{*+} \cup \Sigma_1^{*-}, \\ \Sigma_1^{*\pm} &:= \{(\lambda, x) \in \Sigma_1; \lambda^2 = \tau^{\pm}(x), \nabla_x \tau^{\pm}(z) = 0\}, \\ \Sigma_2^* &:= \{(\lambda, x) \in \Sigma_2; \lambda^2 = \sqrt{\Psi_0(z)}, \text{ and } \nabla_x \Psi_0(z) \text{ is normal to } \mathcal{X}_2 \text{ at } x\}, \end{aligned}$$

then,

$$\begin{aligned} \mathcal{T}_j &:= P_{\mathbb{R}}(\Sigma_j^*), \\ \mathcal{X}_j^* &:= P_M(\Sigma_j^*), \\ \mathcal{Z}_j^* &:= \sin^2(\mathcal{X}_j^*), \quad j = 1, 2. \end{aligned}$$

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

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

Let us describe \mathcal{T} . Setting

$$\mathcal{X}^* = \mathcal{X}_1^* \cup \mathcal{X}_2^*,$$

we see that λ is a threshold iff there exists $z^* \in \sin^2(\mathcal{X}^*)$ such that $p(z^*; \lambda) = 0$.

Setting

$$\begin{aligned} \mathcal{T}_1^{\pm} &:= P_{\mathbb{R}}(\Sigma_1^{*\pm}), \\ \mathcal{X}_1^{**\pm} &:= P_M(\Sigma_1^{*\pm}), \\ \mathcal{Z}_1^{**\pm} &:= \sin^2(\mathcal{X}_1^{*\pm}), \end{aligned}$$

we have

$$\begin{aligned}\mathcal{T}_1 &= \mathcal{T}_1^+ \cup \mathcal{T}_1^-, \\ \mathcal{X}_1^* &= \mathcal{X}_1^{*+} \cup \mathcal{X}_1^{*-}, \\ \sin^2(\mathcal{X}_1^*) &= \mathcal{Z}_1^{*+} \cup \mathcal{Z}_1^{*-},\end{aligned}$$

so

$$\mathcal{T} = \mathcal{T}_1^+ \cup \mathcal{T}_1^- \cup \mathcal{T}_2 \cup \{0\}. \quad (12)$$

Obviously \mathcal{T} is symmetric to 0 so we shall analyse H^D at the positive thresholds only.

Lemma 4.4. A) Assume $\beta = 0$. Then we have $\partial_{z_i} \tau^\pm(z) = \partial_{z_i} \Psi_0(z) > 0$ for all i .

B) Assume $\beta \neq 0$ (so (A0) holds.) We set

$$\nu := \frac{2\alpha_3 \sqrt{\beta_1 \beta_2} - \sqrt{\gamma_3}(\beta_1 + \beta_2)}{|\beta_3| \sqrt{\gamma_3}}. \quad (13)$$

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 3. Let $\tilde{\nu} \in \mathbb{R}$ there exist ε and μ such that $\nu = \tilde{\nu}$. Proof in Appendix A.

Lemma 4.4 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. Setting

$$\begin{aligned}Z_{\{0,1\}} &= \{0, 1\}^3, \quad Z_{\{0,1\}}^* = Z_{\{0,1\}} \setminus \{0_{\mathbb{R}^3}\}, \\ X_{\{0,1\}} &= \{x \in \mathbb{T}^3; z \in Z_{\{0,1\}}\}, \quad X_{\{0,1\}}^* = \{x \in \mathbb{T}^3; z \in Z_{\{0,1\}}^*\},\end{aligned}$$

we obtain the following (remember also (12))

Lemma 4.5. 1) Case $\beta = 0$. We have $K_0 \equiv 0$, $\mathcal{X}_1 = \emptyset$, $\Sigma_1 = \emptyset$, $\mathcal{X}_2 = \mathbb{T}_0^3$. Then $\sin^2(\mathcal{X}_2^*) = Z_{\{0,1\}}^*$, $\mathcal{T}_1 = \emptyset$, $\mathcal{T} = \{0\} \cup \mathcal{T}_2$ and

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

2) Case $\beta \neq 0$ (so (A0) holds). We set $\mathcal{Z}_\nu^* = \{(1, 1, \nu)\} \cap [0, 1]^3$. Then the sets \mathcal{X}_j , $j = 1, 2$, are not trivial (remember Lemma 4.3). We have $\mathcal{Z}_1^{*+} = Z_{\{0,1\}}^* \setminus \{(\frac{\beta_2}{\beta_1}, 1, 0)\}$, $\mathcal{Z}_1^{*-} = Z_{\{0,1\}}^* \cup \mathcal{Z}_\nu^* \setminus \{(\frac{\beta_2}{\beta_1}, 1, 0)\}$ and $\sin^2(\mathcal{X}_2^*) = \{(\frac{\beta_2}{\beta_1}, 1, 0)\}$,

so

$$\begin{aligned}\mathcal{T}_1^+ \cap \mathbb{R}^+ &= \{\sqrt{\tau^+(z)}, z \in Z_{\{0,1\}}^*, z \neq (\frac{\beta_2}{\beta_1}, 1, 0)\}, \\ \mathcal{T}_1^- \cap \mathbb{R}^+ &= \{\sqrt{\tau^-(z)}, z \in Z_{\{0,1\}}^* \cup \mathcal{Z}_\nu^*, z \neq (\frac{\beta_2}{\beta_1}, 1, 0)\}, \\ \mathcal{T}_2 \cap \mathbb{R}^+ &= \{\sqrt{\Psi_0(\frac{\beta_2}{\beta_1}, 1, 0)}\}.\end{aligned}$$

Proof in Appendix A.

Remark 4. We have $\mathcal{X}_1^{*+} \subset \mathcal{X}_1^{*-}$ and the inclusion is an equality if and only if $\nu \notin (0, 1)$.

Remark 5. Let us consider the case $\beta_2 = 0$. By definition of \mathcal{T}_2 we have

$$\mathcal{T}_2 \cap \mathbb{R}^+ = \{\sqrt{\Psi_0(z)}; z \neq 0, \nabla_x \sqrt{\Psi_0(z)} = 0\}.$$

Then, the eigenvalues $\sqrt{\tau^\pm}$ are analytic in $[0, +\infty)^3 \setminus \{0_{\mathbb{R}^3}\}$, since the functions τ^\pm are linear and positive in $[0, +\infty)^3 \setminus \{0_{\mathbb{R}^3}\}$. Hence it would be an alternative to replace \mathcal{T}_2 by \mathcal{T}'_2 where we set

$$\begin{aligned}\mathcal{T}'_2 &:= \mathcal{T}'_2^+ \cup \mathcal{T}'_2^-, \quad \mathcal{T}'_2^- := -\mathcal{T}'_2^+, \\ \mathcal{T}'_2^+ &:= \{\sqrt{\tau^\pm(z)}; z \neq 0, \nabla_x \sqrt{\tau^\pm(z)} = 0\} = \mathcal{T}'_2 \cap \mathbb{R}^+.\end{aligned}$$

But, thanks to Points B) 1) and 2) a) of Lemma 4.4 we obtain

$$\mathcal{T}'_2^+ = \{\sqrt{\tau^\pm(z)}; z \in \{0, 1\}^3, z \neq 0_{\mathbb{R}^3}\} = \mathcal{T}_2 \cap \mathbb{R}^+,$$

so the sets \mathcal{T}'_2 and \mathcal{T}_2 coincide.

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

5.1. Eigenprojectors. If $\beta = 0$ then $\Sigma_1 = \emptyset$ and the function $\sqrt{\Psi_0(y^2)}$ is analytic in $\mathbb{R}^3 \setminus \{0_{\mathbb{R}^3}\}$. The associated orthogonal eigenprojection

$$\pi_2(y) := \frac{1}{2i\pi} \int_{\mathcal{C}} (h^D(y) - \zeta)^{-1} d\zeta \quad \forall y \neq 0, \quad (14)$$

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

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

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

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 (14) 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

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

Each $\pi_1^\pm(y)$ has range one and $\pi_2(y)$ has range two. Each π_1^\pm is analytic at $y \in \sin(\mathcal{X}_1)$ (as subset of \mathbb{R}^3), π_2 is analytic on $\sin(\mathbb{R}^3) \setminus \{0_{\mathbb{R}^3}\} (\subset \mathbb{R}^3)$, and

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

5.2. Global tangent field to \mathcal{X}_2 . If $\beta_2 = 0$ then the τ^\pm 's and π_1^\pm 's extend analytically into $\mathbb{R}^3 \setminus \{0_{\mathbb{R}^3}\}$ with the relation

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

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 an nonzero eigenvalue of $H^D(x)$ (respect., of $h^D(y)$) is not simple then the stratification method explained in [3] involves a tangential vector field to the set \mathcal{X}_2 (respect., to $\sin(\mathcal{X}_2)$): $w(x) := (\sin(x_1) \cos(x_2), \cos(x_1) \sin(x_2), 0)$, (respect., $\tilde{w}(y) := (y_1, y_2, 0)$). 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 $f: \mathbb{T}^3$ or $\mathbb{R}^3 \rightarrow \mathbb{C}^n$ and a vector field $v(x) = (v_j(x))_{1 \leq j \leq n} \in \mathbb{C}^n$, 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

$$\begin{aligned} f_w &:= w \cdot \nabla_x f, \\ \tilde{f}_{\tilde{w}} &:= \tilde{w} \cdot \nabla_y f. \end{aligned}$$

We thus have

$$f_w(x) = \cos(x_1) \cos(x_2) \tilde{f}_{\tilde{w}}(y). \quad (15)$$

5.3. First cut-off functions. We consider the following metric on $\mathbb{T}^3 \approx (\mathbb{R}/(2\pi\mathbf{Z}))^3$:

$$d_0(x, x^*) = |e^{ix} - e^{ix^*}| \quad x^*, x \in \mathbb{T}^3.$$

We denote $d_0(x, E) = \inf\{d_0(x, x^*) \mid x^* \in E\}$ when $E \subset \mathbb{T}^3$. We consider a cut-off function $\varphi_1 \in \mathcal{C}^\infty(\mathbb{R}; [0, 1])$ such that $\text{supp } \varphi_1 \subset \{s \in \mathbb{R}; |s| < 1\}$ 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 \mathbb{R}^+ , and, equivalently, \mathcal{X}_0 from \mathbb{T}^3 , with the cut-off function $\chi_0(x) := \varphi_1(|z|/b_0)$. Since $\text{supp } \phi \subset (0, \infty)$, we can fix b_0 sufficiently small such that:

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

In addition we set

$$\begin{aligned} \chi_{x^*}(x) &:= \varphi_1(d_0(x, x^*)/b) \quad x^*, x \in \mathbb{T}^3, \\ \chi^{*+}(x) &:= (1 - \chi_0(x)) \prod_{x^* \in \mathcal{X}_1^{*+}} (1 - \chi_{x^*}), \\ \chi^{*-}(x) &:= (1 - \chi_0(x)) \prod_{x^* \in \mathcal{X}_1^{*-}} (1 - \chi_{x^*}), \\ \chi^*(x) &:= (1 - \chi_0(x)) \prod_{x^* \in \mathcal{X}^*} (1 - \chi_{x^*}), \end{aligned}$$

so χ^* vanishes in $\{x \in \mathbb{T}^3; d_0(x, \mathcal{X}^*) < b/2\}$ and in $\{x \in \mathbb{T}^3; |z| < b_0/2\}$; we have also $\chi^*(x) = 1$ if $d_0(x, \mathcal{X}^*) > b$ 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,

$$1 - \chi^*(x) = \chi_0(x) + \sum_{x^* \in \mathcal{X}^*} \chi_{x^*}(x),$$

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

5.4. The conjugated operator outside thresholds. Case $\beta = 0$. Remember that we have $\pi_1^+ = \pi_1^- = \pi_2$ which is analytic in $\mathbb{R}^3 \setminus \{0_{\mathbb{R}^3}\}$. We set, for $u \in \mathcal{C}^\infty(\mathbb{T}^3)$, $x \in \mathbb{T}^3$,

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

Case $\beta \neq 0$ and $\beta_2 = 0$ (with Assumption (A0)). Remember that the functions $\tau^\pm(\cdot)$ are analytic in \mathbb{R}^3 (see (10) and (11)) and are positive in $[0, +\infty)^3 \setminus \{0_{\mathbb{R}^3}\}$. Thus, the eigenvalues $\sqrt{\tau^\pm(\cdot)}$ are analytic in $[0, +\infty)^3 \setminus \{0_{\mathbb{R}^3}\}$. We set, for $u \in \mathcal{C}^\infty(\mathbb{T}^3)$, $x \in \mathbb{T}^3$,

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

Case $\beta_2 \neq 0$ (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 4.5) then the value $\sqrt{\tau^-(1, 1, \nu)}$ is a threshold be 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 $H^D \in \mathcal{C}^\infty(A_{out})$, we need to separate $\mathcal{X}_2 \subset \partial\mathcal{X}_1$ from \mathcal{X}_1 , as explained in [4]. 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 $\text{supp } \chi_2 \subset \{x; d_0(x, \mathcal{X}_2) \leq 2b\}$, $\chi_2(x) = 1$ if $d_0(x, \mathcal{X}_2) \leq b$, $\chi_1(x) = 1$ if $d_0(x, \mathcal{X}_2) \geq 3b$, and $\text{supp } \chi_1 \subset \{x; d_0(x, \mathcal{X}_2) \geq 2b\}$. Thus $\text{supp } \chi_1 \cap \text{supp } \chi_2 = \emptyset$ and $\chi_2 = 1$ on $\overline{\mathcal{X}_2}$. We then set $\chi_3 := 1 - \chi_1 - \chi_2$ so $\text{supp } \chi_3 \subset \{x; b \leq d_0(x, \mathcal{X}_2) \leq 3b\}$, and

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

See Figure 1. We have in addition (b being sufficiently small)

$$\text{supp } \chi_{x^*} \subset \text{supp } \chi_1 \setminus \text{supp } \chi_3 \quad \forall x^* \in \mathcal{X}_1^*, \quad (16)$$

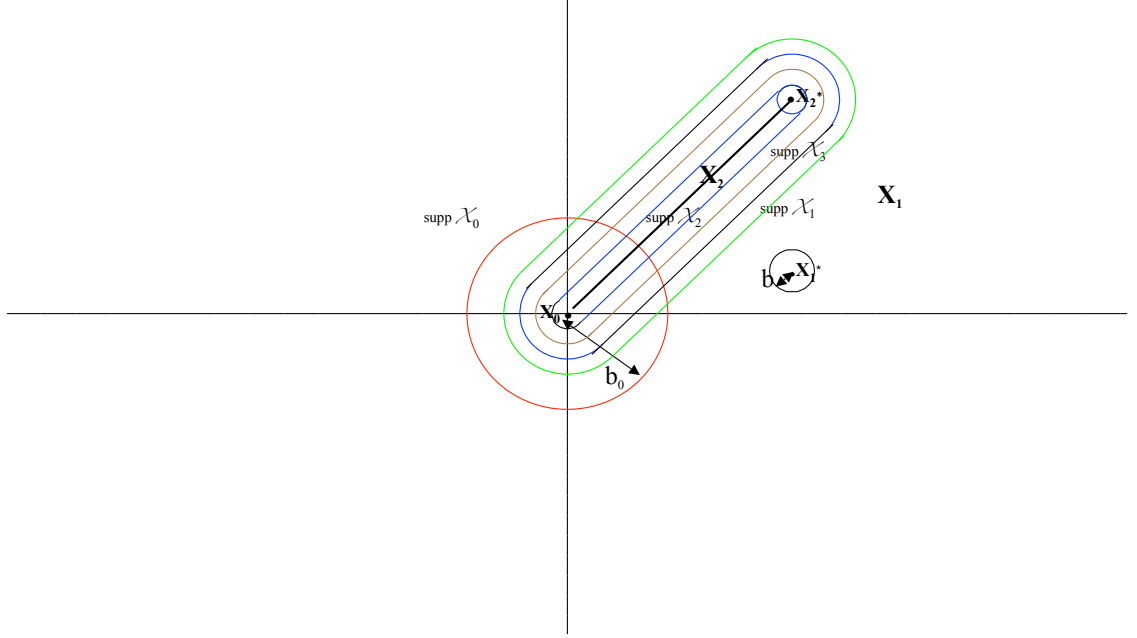
$$\text{supp } \chi_{x^*} \subset \text{supp } \chi_2 \setminus \text{supp } \chi_3 \quad \forall x^* \in \mathcal{X}_2^*. \quad (17)$$

$$\chi_j^*(x) := \chi^*(x)\chi_j(x) \quad j = 2, 3$$

$$\chi_1^{*\pm}(x) := \chi^{*\pm}(x)\chi_1(x).$$

(In fact, Relations (16) and (17) 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 $\mathcal{X}_1 \setminus \mathcal{X}_1^{*\pm}$.

FIGURE 1. Cut-off



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

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

Remark 6. The function $\sqrt{\Psi_0(z)}_w$ may vanish at points of \mathcal{X}^* but not of $\mathcal{X}_2 \setminus \mathcal{X}^*$ so $\chi_2^*(x) (\sqrt{\Psi_0(z)}_w)^{-1}$ is well-defined (for b sufficiently small). For more details, see the proof of (19) below. Similarly, the function $x \mapsto |\nabla_x \sqrt{\tau^\pm(z)}|$ is positive in $\text{supp } \chi_1^{*\pm}$.

In each case we symmetrize \mathcal{A}_{out} by setting

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

with domain $\mathcal{C}^\infty(\mathbb{T}^3)$. Here \mathcal{A}_{out}^* is the hermitian conjugate of \mathcal{A}_{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 [3, Lemma 3.10]). Since $D(H^D) = \mathcal{H}^D$, some possible problematic points of the Mourre Theory then become trivial (see [2]).

5.5. "Punctual" Mourre's estimate outside thresholds. We set

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

Similarly to proof of the Mourre's estimate in [3] we show that if the positive parameter b is sufficiently small then A_{out} is strictly conjugated to H on I .

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

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

By using

$$(\pi_1^\pm(y))^2 = \pi_1^\pm(y), \quad \pi_1^\pm(y) h^D(y) = h^D(y) \pi_1^\pm(y), \quad \pi_2(y) h^D(y) = h^D(y) \pi_2(y),$$

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

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

In \mathcal{X}_1 we have

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

so,

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

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

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

Thus,

$$\begin{aligned} \frac{1}{2} H_{1,out}(x) &= \sum_{\pm} (\chi_1^{*\pm}(x))^2 \pi_1^\pm(y) + ((\chi_2^*(x))^2 + (\chi_3^*(x))^2) \pi_2(y) \\ &\quad + (\chi_2^*(x))^2 \pi_2(y) (\sqrt{\Psi_0(z)})^{-1} \xi_w(x) \pi_2(y). \end{aligned} \quad (18)$$

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

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

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

$$\sqrt{\tilde{\Psi}_0(z)_{\tilde{w}}} = (\Psi_0(z))^{-1/2} (\alpha_1 z_1 + \alpha_2 z_2) > 0. \quad (19)$$

In addition, since the relation

$$(\sqrt{\Psi_0(z)_w})^{-1} \xi_w(x) = (\sqrt{\tilde{\Psi}_0(z)_{\tilde{w}}})^{-1} \tilde{\xi}_{\tilde{w}}(y)$$

holds true for $x \notin \mathcal{X}^*$ and $\sqrt{\tilde{\Psi}_0(z)}_{\tilde{w}} \neq 0$, then the function $(\sqrt{\Psi_0(z)}_w)^{-1} \xi_w$ is defined and is smooth in the compact set $\text{supp}(1 - \chi_0)\chi_2 \subset \text{supp}\chi_2 \subset \{x \in \mathbb{T}^3; d_0(x, \mathcal{X}_2) \leq 2b\}$, and vanishes on \mathcal{X}_2 . Hence, for b sufficiently small, we have

$$\|(\sqrt{\Psi_0(z)}_w)^{-1} \xi_w(x)\|_\infty < \frac{1}{2} \quad \forall x \in \text{supp}(1 - \chi_0)\chi_2, \quad (20)$$

where $\|\cdot\|_\infty$ denotes here the usual infinite norm on matrices. From (18), (20), we then obtain

$$H_{1,out}(x) \geq \sum_{\pm} (\chi_1^{*\pm}(x))^2 \pi_1^\pm(y) + ((\chi_2^*(x))^2 + (\chi_3^*(x))^2) \pi_2(y). \quad (21)$$

Remark 7. In the two other cases where $\beta_2 = 0$ we obtain

$$\frac{1}{2} H_{1,out}(x) = (\chi^*(x))^2 \pi_2(y), \quad (22)$$

so the punctual Mourre's estimate becomes simply

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

5.6. Smoothness. Relations (22) and (18) show that the symmetric form $H_{1,out}$ defined on $C^\infty(\mathbb{T}^3)$ is a multiplication operator on \mathcal{H}^D by smooth coefficients, so is bounded and closeable. Thus, $[H_{1,out}, iA_{out}]$ is a differential operator of order one at most. But when computing it's first order term we have to check only that $H_{1,out}$ is commuting with each coefficient of the first order terms of $-iA_{out}(x)$. In fact, the possible problematic bracket arising from the calculation of $[H_{1,out}, iA_{out}]$ is, in the case $\beta_2 \neq 0$,

$$\begin{aligned} & [(\chi_2^*(x))^2 (\sqrt{\Psi_0(z)}_w)^{-1} \pi_2(y) \xi_w(x) \pi_2(y) \quad , (\chi^{*\pm}(x))^2 \frac{\nabla_x \sqrt{\tau^\pm(z)}}{|\nabla_x \sqrt{\tau^\pm(z)}|^2} \cdot \\ & \quad \cdot \pi_1^\pm(y) \nabla_x (h^D(y) \pi_1^\pm(y)) \pi_1^\pm(y)]. \end{aligned}$$

But since $\chi_1 \chi_2 = 0$ then this bracket vanishes. Hence, $[H_{1,out}, iA_{out}]$ is a multiplication operator, is bounded in \mathcal{H} , and we have $H^D \in C^2(A_{out})$. By induction we see that $H^D \in C^\infty(A_{out})$. (See also [4].)

5.7. The conjugated operator near thresholds.

5.7.1. 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 β and of x^* , we enumerate the different cases as follows.

Case 1 $\beta = 0$ and $x^* \in \mathcal{X}_2^*$.

Case 2 $\beta \neq 0$ (so (A0) holds) and $x^* \in \mathcal{X}_1^*$.

Subcase 2-1 $\beta_2 = 0$.

Subcase 2-2 $\beta_2 > 0$.

Subcase 2-2-a $x^* \in \mathcal{X}_1^{*-}$ and $z_1^* = z_2^* = 1$ and $z_3^* = \nu \in (0, 1)$.

Subcase 2-2-b $x^* \in \mathcal{X}_1^{*-}$ and $z_1^* = z_2^* = 1$ and $z_3^* \neq \nu$.

Subcase 2-2-c $x^* \in \mathcal{X}_1^{*-}$ and $z_1^* = z_2^* = 1$ and $z_3^* = \nu \in \{0, 1\}$.

Subcase 2-2-d $x^* \in \mathcal{X}_1^{*-}$ and $(z_1^* = 0$ or $z_2^* = 0)$.

Subcase 2-2-e $x^* \in \mathcal{X}_1^{*+}$.

Case 3 $\beta \neq 0$ and $x^* \in \mathcal{X}_2^*$.

Subcase 3-1) $\beta_2 = 0$.

SubCase 3-2 $\beta_2 = \beta_1$.

SubCase 3-3 $\beta_2 \in (0, \beta_1)$.

Remark 8. In Case 2-2-c, if $\beta_1 = \beta_2$ then $(1, 1, 0) \in \sin^2 \mathcal{X}_2^*$ so $\nu = 1$.

5.7.2. *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 and 2-2-d and 2-2-e, and 3-1 we set $s_3 := s_3^*$;

- in Case 2-2-a we set $s_3 := 1$;

- in Case 2-2-b we set $s_3 := \text{sgn}(z_3^* - \nu)s_3^*$.

Lemma 5.1. In Cases 1 and 2-1 and 2-2-a and 2-2-b and 2-2-d and 2-2-e and 3-1 we have

$$dV(x) = \left(\sum_{j=1}^3 C_j s_j (x_j - x_j^*) dx_j \right) (1 + O(d_0(x, x^*))), \quad (23)$$

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

In Case 2-2-c we have

$$dV(x) = \left(- \sum_{j=1}^2 C_j (x_j - x_j^*) dx_j + C_3 (x_3 - x_3^*)^3 dx_3 \right) (1 + O(d_0(x, x^*))), \quad (24)$$

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

Proof in Appendix B.

Lemma 5.2. 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,

$$(\sqrt{\Psi_0(z)}_w) = C(x_1 - x_1^*)(x_2 - x_2^*)(1 + O(d_0(x, x^*))), \quad (25)$$

and, in Case 3-3,

$$(\sqrt{\Psi_0(z)}_w) = C(x_2 - x_2^*)(1 + O(d_0(x, x^*))), \quad (26)$$

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

Proof in Appendix B.

5.7.3. *Partition of the set of thresholds.* With the notations (the s_j 's notably) of Part 5.7.2 we set

$$\begin{aligned} \mathcal{T}_{sa} &:= \mathcal{T} \setminus (\mathcal{T}_{sm} \cup \{0\}), \\ \mathcal{T}_{sm} &:= \mathcal{T}_{sm}^+ \cup -\mathcal{T}_{sm}^+, \\ \mathcal{T}_{sm}^+ &:= \mathcal{T}_{ms,1}^+ \cup \mathcal{T}_{ms,2}^+, \end{aligned}$$

with, in Case $\beta = 0$:

$$\begin{aligned} \mathcal{T}_{ms,1}^+ &:= \emptyset, \\ \mathcal{T}_{ms,2}^+ &:= \{\sqrt{\Psi_0(z^*)}; x^* \in \mathcal{X}_2^* (= X_{\{0,1\}}^*), s_1 = s_2 = s_3 = \pm 1\}, \end{aligned}$$

in Case $\beta \neq 0$:

$$\begin{aligned} \mathcal{T}_{ms,1}^+ &:= \{\sqrt{\tau^+(z^*)}, \sqrt{\tau^-(z^*)}; x^* \in \mathcal{X}_1^*, s_1 = s_2 = s_3 = \pm 1\} \cup \mathcal{T}_\nu, \\ \mathcal{T}_{ms,2}^+ &:= \left\{ \sqrt{\Psi_0\left(\frac{\beta_2}{\beta_1}, 1, 0\right)} \right\}, \end{aligned}$$

with

$$\begin{aligned}\mathcal{T}_\nu &:= \{\sqrt{\tau^-(z^*)}; x^* \in \mathcal{X}_1^*, s_1 = s_2 = 1(=: s_3)\} \quad \nu \in (0, 1), \\ \mathcal{T}_\nu &:= \emptyset \quad \nu \notin (0, 1).\end{aligned}$$

5.7.4. *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 Part 5.7.2) 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 and 3-3.

With the notations of Lemma 5.1, in Cases 1, 2-1, 2-2-a, 2-2-b, 2-2-d, 2-2-e 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 2-2-c, 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 (23) and (24) of Lemma 5.1 can be written

$$dV(x) = (1 + O(d_0(x, x^*))) dp_1(x; x^*), \quad x \rightarrow x^*.$$

5.7.5. *The conjugated 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 ($\beta = 0, x^* \in \mathcal{X}_2^*$):

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

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

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

and $\mathcal{A}_{x^*} := \mathcal{A}_{x^*}^+ + \mathcal{A}_{x^*}^-$,

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

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

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

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

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

We set

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

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

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

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 ,

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

By a straight calculation as in Part 5.5 we obtain

Lemma 5.3. 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,

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

Lemma 5.3 shows that the quadratic forms H_{1,x^*} and $H_{1,in}$ 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 $H_{1,in}$. 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 $\text{supp } \chi_x \cap \text{supp } \chi_{x'} = \emptyset$ then $H^D \in \mathcal{C}^\infty(A_{in})$.

We set

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

The argumentation to prove the property $H^D \in \mathcal{C}^\infty(A_{out})$ at Part 5.6 still holds with A_{out} replaced by A_ϕ , so we obtain

Lemma 5.4. 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, $H^D \in \mathcal{C}^\infty(A_\phi)$.

5.8. **"Punctual" Mourre's estimate.** Let us prove that

$$\phi(H^D)(x)H_{1,\phi}(x)\phi(H^D)(x) \geq C\phi^2(H^D)(x), \quad (27)$$

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 Part 5.5 (see (18)) the calculation of $H_{1,\phi}$ yields

$$\begin{aligned} \frac{1}{2}H_{1,\phi}(x) &= \sum_{\pm} (\chi_1^{*\pm}(x))^2 \pi_1^\pm(y) + ((\chi_2^*(x))^2 + (\chi_3^*(x))^2) \pi_2(y) \\ &\quad + (\chi_2^*(x))^2 \pi_2(y) T_w(x)^{-1} \xi_w(x) \pi_2(y) \\ &\quad + \sum_{\pm} \sum_{x^* \in \mathcal{X}_{1,in}^{*\pm} \cup \mathcal{X}_{1,in}^{*-}} (\chi_{x^*}(x))^2 \pi_1^\pm(y) + \sum_{x^* \in \mathcal{X}_{2,in}^*} (\chi_{x^*}(x))^2 \pi_2(y) \\ &\quad + \sum_{x^* \in \mathcal{X}_{2,in}^*} (\chi_{x^*}(x))^2 \pi_2(y) (\sqrt{\Psi_0(z)}_w)^{-1} \xi_w(x) \pi_2(y) \quad x \notin \mathcal{X}^* \cup \mathcal{X}_0. \end{aligned}$$

Thus, as for Inequality (21), we get,

$$\begin{aligned} H_{1,\phi}(x) &\geq \sum_{\pm} (\chi_1^{*\pm}(x))^2 \pi_1^\pm(y) + ((\chi_2^*(x))^2 + (\chi_3^*(x))^2) \pi_2(y) \\ &\quad + \sum_{\pm} \sum_{x^* \in \mathcal{X}_{1,in}^{*\pm} \cup \mathcal{X}_{1,in}^{*-}} (\chi_{x^*}(x))^2 \pi_1^\pm(y) + \sum_{x^* \in \mathcal{X}_{2,in}^*} (\chi_{x^*}(x))^2 \pi_2(y). \end{aligned} \quad (28)$$

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

1. Case $d_0(x, \mathcal{X}^*) \geq b$. Then, $x \notin \text{supp } \chi_{x^*}$ for any $x^* \in \mathcal{X}^*$, and $\chi^*(x) = \chi^{*\pm}(x) = 1$. Hence (28) becomes

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

where $\delta_0 := \min_{\mathbb{T}^3} \sum_{j=1}^3 \chi_j^2 > 0$. Since $\phi(H^D(x)) \pi_2(x) = \phi(H^D(x))$, then (27) holds.

2. Case $d_0(x, \mathcal{X}^*) < b$. Then there exists exactly one $x^* \in \mathcal{X}^*$ such that $x \in \text{supp } \chi_{x^*}$ and $x \notin \text{supp } \chi_{x'}$ if $x' \in \mathcal{X}^* \setminus \{x^*\}$. We set

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

If $x^* \notin \mathcal{X}_{2,in}^* \cup \mathcal{X}_{1,in}^{*+} \cup \mathcal{X}_{1,in}^{*-}$ then $x \notin \text{supp } \phi(H^D(x))$ so (27) is trivial. We thus assume $x^* \in \mathcal{X}_{2,in}^* \cup \mathcal{X}_{1,in}^{*+} \cup \mathcal{X}_{1,in}^{*-}$.

- (a) Case $x^* \in \mathcal{X}_{2,in}^*$. Thus $x \notin \text{supp } \chi_1 \cup \text{supp } \chi_3$ and

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

Hence (28) becomes

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

Thus (27) holds.

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

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

Hence (28) becomes

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

Thus (27) holds.

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

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

Hence (28) becomes

$$\begin{aligned} H_{1,\phi}(x) &\geq \sum_{\pm} ((1 - \chi_{x^*}(x))^2 + (\chi_{x^*}(x))^2) \pi_1^{\pm}(y) \\ &\geq \delta(x^*) \pi_1^-(y). \end{aligned}$$

But we have also

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

Thus (27) holds.

As conclusion, (27) is proved with $C = \min(\delta_0, \min_{\mathcal{X}^*} \delta(x^*))$. \square

5.9. Self-adjointness and maximal monotonicity of parts of the conjugated operator. The conjugate operator A_ϕ with domain \mathcal{D}_0 is a symmetric first order differential operator in x whose coefficients belong to $\mathcal{C}^\infty(\mathbb{T}^3 \setminus \mathcal{X}^*; \mathcal{L}(\mathbb{C}^6))$. As we already saw, $\overline{A_{out}}$ with domain $\mathcal{C}^\infty(\mathbb{T}^3)$ is essentially self-adjoint and a self-adjoint extension is $\overline{A_{out}} = A_{out}$ with domain $D(\overline{A_{out}}) = \{u \in \mathcal{H}^D; A_{out}u \in \mathcal{H}^D\}$. (We may observe that $D(\overline{A_{out}})$ is also the closure of $\mathcal{C}^\infty(\mathbb{T}^3)$ under the norm $\|u\| + \|A_{out}u\|$.) Let us check that for all $x^* \in \mathcal{X}^*$ the operator A_{x^*} (with the same domain \mathcal{D}_0) is essentially self-adjoint or, at least, admits a maximal symmetric extension.

Lemma 5.5. Remembering the notations of Section 5.7.2 we then claim:

- A) Cases 1 and 2-1 and 2-2-a and 2-2-b 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 2-2-c. The operator A_{x^*} is essentially self-adjoint on \mathcal{H}^D .
- C) Cases 3-2 and 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 9. When A_{x^*} is essentially self-adjoint then the set \mathcal{D}_0 is not dense in the domain of the self-adjoint extension $\overline{A_{x^*}}$ of A_{x^*} . (The simple reason is that $\mathcal{C}_c^\infty(\mathbb{R}^*)$ is not dense in $H^1(\mathbb{R})$.)

We set

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

and

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

Corollary 6. 1) The operator A_{sa} is essentially self-adjoint on \mathcal{H}^D .
2) If $\mathcal{T}_{sm} \subset \mathcal{T}'$ then the operator A_ϕ defined on \mathcal{D}_0 is essentially self-adjoint on \mathcal{H}^D .

Proof. 1) 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 $\mathcal{T}' = \mathcal{T}_{sm}$ and we consider the case $\beta_2 \neq 0$ only. The operator $\bar{A} := A_\phi$ with domain $D(\bar{A}) := \{u \in \mathcal{H}^D; A_\phi u \in \mathcal{H}^D\}$ is a symmetric extension of A_ϕ . Let us prove that it is self-adjoint. Let $v \in D(\bar{A}^*)$ so

$$|(\bar{A}u, v)_{\mathcal{H}^D}| \leq C\|u\| \quad \forall u \in D(\bar{A}).$$

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

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

In addition, we have $B = \varphi_1 A_{sa} \varphi_1$ since \bar{A} coincides with A_{sa} in $\text{supp } \varphi_1$, 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

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

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 $v = \sum_{j=1}^2 \varphi_j^2 v \in D(\bar{A})$. \square

6. Proofs of the main results.

6.1. Proof of Theorem 3.1. Clearly, it is not restrictive to consider that $\text{supp } \phi \subset (0, +\infty)$ 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 5.4, the operator A_ϕ satisfies Point (ii). Point (i) is a straight consequence of (27).

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

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

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

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

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

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

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

Point (iv) is Point 2) of Corollary 6.

Point (v) is the consequence of Corollary 6.

6.2. Adaptation of the theory of Georgescu and alii. 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

$$\begin{aligned} \mathcal{X}_{sm1}^* &:= \{x^* \in \mathcal{X}_{sm}^*; A_{x^*} \text{ has default index } (N^+, N^- = 0)\}, \\ \mathcal{X}_{sm2}^* &:= \{x^* \in \mathcal{X}_{sm}^*; A_{x^*} \text{ has default index } (N^+ = 0, N^-)\}. \end{aligned}$$

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: $A_0 = A_{out}$, $A_1 = \sum_{x^* \in \mathcal{X}_{sm1}^* \cup \mathcal{X}_{sa}^*} A_{x^*}$, $A_2 = \sum_{x^* \in \mathcal{X}_{sm2}^*} A_{x^*}$. The proof of Corollary 6 shows that the operator A_0 is essentially self-adjoint.

Remark 10. We could have set more naturally $A_0 = A_{sa} + A_{out}$, $A_1 = \sum_{x^* \in \mathcal{X}_{sm1}^*}$ and A_2 unchanged. In such a choice some coefficients of A_0 have a rational singularity on \mathcal{X}_{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 $D(A_j^{sm})$ 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 [2, Theorem 3.3] and extend the statement of [2, Theorem 3.3] to our situation. We consider variables $z \in \rho(H^D)$ and ε real with $0 < |\varepsilon| < \varepsilon_0$ and $\Im m(z)\varepsilon \geq 0$. We set $H_\varepsilon := H^D - i\varepsilon H'$. (Thus $H_\varepsilon^* = H_{-\varepsilon}$.) Then, the resolvent $R_\varepsilon(z) := (H_\varepsilon - z)^{-1}$ is

well-defined if ε_0 is sufficiently small, see [2, Proposition 3.11]. Actually we make the following observations:

- The domain \mathcal{D}_0 of A_ϕ is dense in \mathcal{H}^D .
- Assumption [2, (M3)] becomes:
(M3*): [$\pm A_0^{sm}$ (respect., $(-1)^j A_j^{sm}$) is the generator of a C_0 -group $(W_t^{(0)})_{t \in \mathbb{R}}$ (respect., semigroup $(W_t^{(j)})_{t \geq 0}$) in \mathcal{H}^D .]
Clearly, Condition (M3*) is satisfied.
- Setting $\langle H \rangle := (1 + H^2)^{1/2}$, Assumption [2, (M2)] becomes:
(M2*): [a bounded open set $J \subset \mathbb{R}$ is given and there are numbers $a > 0$, $b \geq 0$, such that $H' \geq (a1_J(H^D) - b1_{\mathbb{R} \setminus J}) \langle H^D \rangle$ as forms on \mathcal{H}^D .]
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 (27).
- Assumption [2, (M4)] becomes:
(M4*): [There is $H'_j \in B(\mathcal{H}^D)$ such that the limits

$$\begin{aligned} \lim_{t \rightarrow 0^+} (-1)^j t^{-1} \{ (H^D u, W_t^{(j)} u)_{\mathcal{H}^D} - (u, W_t^{(j)} H^D u)_{\mathcal{H}^D} \} \quad (j \neq 0), \\ \lim_{t \rightarrow 0} t^{-1} \{ (H^D u, W_t^{(0)} u)_{\mathcal{H}^D} - (u, W_t^{(0)} H^D u)_{\mathcal{H}^D} \} \quad (j = 0) \end{aligned}$$

exist and are respectively equal to $(u, H'_j u)$ for all $u \in \mathcal{H}^D$.]

Clearly, Condition (M4*) is satisfied. We have $[H^D, iA_j]^\circ = H'_j$ and $[H^D, iA_\phi]^\circ = H' := \sum_{j=0}^2 H'_j \in B(\mathcal{H}^D)$, and we can write $H^D \in C^1(A_j^{sm})$, $H^D \in C^1(\bar{A}_\phi)$.

- The proofs of [2, Lemmas 3.13 and 3.14] with Conditions (M3*) and (M4*) satisfied imply the following relations:

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

In particular the map $\varepsilon \mapsto R_\varepsilon(z) \in B(\mathcal{H}^D)$ 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 [2, Remark 2.15]), then Assumption [2, (M1)] becomes:
(M1*): [for all j , $H^D \in C^1(H'_j)$.]
We see that (M1*) is obviously satisfied and $H^D \in C^1(H')$.
- Assumption [2, (M5)] becomes:
(M5*): [for all $j = 0, 1, 2$, there is $H''_j \in B(\mathcal{H}^D)$ such that the limits

$$\begin{aligned} \lim_{t \rightarrow 0^+} (-1)^j t^{-1} \{ (H' u, W_t^{(j)} u) - (u, W_t^{(j)} H' u) \} \quad j \neq 0, \\ \lim_{t \rightarrow 0} t^{-1} \{ (H' u, W_t^{(0)} u) - (u, W_t^{(0)} H' u) \} \quad (j = 0), \end{aligned}$$

exist and are respectively equal to $(u, H''_j u)$ for all $u \in \mathcal{H}^D$.]

Thanks to [2, Remark 3.1], Condition (M5*) is satisfied since it follows from the following facts: $H^D \in C^1(A_j^{sm})$ with $[H^D, iA_j^{sm}]^\circ = H'_j$, $H' \in C^1(A_j^{sm})$ with $[H', iA_j^{sm}]^\circ = H''_j$, so we can write $H^D \in C^2(\bar{A}_\phi)$.

Then the proof of [2, Theorem 3.3] implies the result of Corollary 3. \square

Conclusion. The results of this work, notably the LAP outside thresholds, is the first step to futur developments as:

- Extension of the result of Isozaki and Morioka [8] on Rellich type theorem for discrete Schrodinger operators to the case of discrete Maxwell operators.
- The LAP for perturbed discrete Maxwell operator of the form $\hat{H}^D = \hat{D}\hat{H}_0$ where \hat{D} is not constant but depends on $n \in \mathbf{Z}^3$.
- Conditions of radiation for perturbed discrete Maxwell operators. Actually, let \hat{f} in a suitable subspace of $L^2(\mathbf{Z}^3)$, particularly the space of sequences with compact support. We have to characterize $\hat{u}^\pm(n)$ for $|n|$ large where $\hat{u}^\pm := (\hat{H}^D - \lambda \pm i0)^{-1}\hat{f}$.
- Extension of the result of Isozaki and Jensen [6] on the continuum limit for lattice Schrödinger operators to the case of discrete Maxwell operators.
- Extension of the result of Isozaki and [7] on the inverse scattering for lattice Schrödinger operators to the case of discrete Maxwell operators.

7. Appendix A.

7.1. **Proof of Lemma 4.1.** We have

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

Thus,

$$\det(\hat{D}\hat{H}_0(x) - \lambda) = \det(\lambda^2 + \varepsilon M(y)\mu M(y)) =: p(z; \lambda).$$

We have

$$\begin{aligned} \varepsilon M \mu M &= \begin{pmatrix} 0 & -\varepsilon_1 y_3 & \varepsilon_1 y_2 \\ \varepsilon_2 y_3 & 0 & -\varepsilon_2 y_1 \\ -\varepsilon_3 y_2 & \varepsilon_3 y_1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -\mu_1 y_3 & \mu_1 y_2 \\ \mu_2 y_3 & 0 & -\mu_2 y_1 \\ -\mu_3 y_2 & \mu_3 y_1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} -\varepsilon_1 \mu_3 y_2^2 - \varepsilon_1 \mu_2 y_3^2 & \varepsilon_1 \mu_3 y_1 y_2 & \varepsilon_1 \mu_2 y_1 y_3 \\ \varepsilon_2 \mu_3 y_1 y_2 & -\varepsilon_2 \mu_3 y_1^2 - \varepsilon_2 \mu_1 y_3^2 & \varepsilon_2 \mu_1 y_2 y_3 \\ \varepsilon_3 \mu_2 y_1 y_3 & \varepsilon_3 \mu_1 y_2 y_3 & -\varepsilon_3 \mu_2 y_1^2 - \varepsilon_3 \mu_1 y_2^2 \end{pmatrix}. \end{aligned}$$

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

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

where $\Psi_0(z)$ is defined by (9)

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

We easily observe that the following relations hold (also, $+c.p.$):

$$\alpha_1^2 - \gamma_1 = \frac{1}{4} \beta_1^2, \quad (29)$$

$$\varepsilon_1 \mu_1 \alpha_1 - \alpha_2 \alpha_3 = \frac{1}{4} \beta_2 \beta_3, \quad (30)$$

$$\alpha_3 \beta_2 + \alpha_2 \beta_3 = -\varepsilon_1 \mu_1 \beta_1, \quad (31)$$

where γ is defined by (6) and β by (5). Thanks to (29), (30), (31), we compute:

$$\begin{aligned}\Psi_0^2 - \Phi_0 &= (\alpha_1 z_1 + \alpha_2 z_2 + \alpha_3 z_3)^2 / 4 - \{\gamma_1 z_1^2 + \gamma_2 z_2^2 \\ &\quad + \gamma_3 z_3^2 + 2\varepsilon_3 \mu_3 \alpha_3 z_1 z_2 + 2\varepsilon_1 \mu_1 \alpha_1 z_2 z_3 + 2\varepsilon_2 \mu_2 \alpha_2 z_1 z_3\} / 4 \\ &= K_0(z),\end{aligned}$$

where K_0 is defined by (8). Hence the eigenvalues of $\varepsilon M(y) \mu M(y)$ are 0 and

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

Then Relation (7) follows.

Remark 11. From (8) we obtain the relations

$$\begin{aligned}K_0(z) &= \frac{1}{4}(\beta_1 z_1 - \beta_2 z_2 - \beta_3 z_3)^2 - \beta_2 \beta_3 z_2 z_3, \\ K_0(z) &= \frac{1}{4}(\beta_3 z_3 - \beta_1 z_1 - \beta_2 z_2)^2 - \beta_1 \beta_2 z_1 z_2.\end{aligned}\tag{32}$$

7.2. Proof of Proposition 1. Similarly to (2) we have

$$\sigma(h^D) = \overline{\cup_{y \in [-1, 1]^3} \sigma(h^D(y))}.$$

In addition, since τ^+ and τ^- are continuous with $\tau^\pm(0) = 0$ and $\tau^+ \geq \tau^- \geq 0$ in $[0, 1]^3$, then

$$\cup_{y \in [-1, 1]^3} \sigma(h^D(y)) = \cup_{\pm} \{\pm \tau^+(z); z \in [0, 1]^3\} = [-\lambda^*, \lambda^*].$$

The conclusion follows.

7.3. Proof of Lemma 4.4. We set $z'_i = \beta_i z_i$ (so $z'_1, z'_2 \geq 0$ and $z'_3 \leq 0$). Remember that

$$(4\alpha_1^2 - \beta_1^2) = (2\alpha_1 - \beta_1)(2\alpha_1 + \beta_1) = 4\varepsilon_3 \mu_2 \varepsilon_2 \mu_3 = 4\gamma_1 > 0.$$

A) (Case $\beta = 0$). This point is obvious.

B) (Case $\beta \neq 0$.) Thanks to (32) we have

$$\begin{aligned}\frac{\partial}{\partial z_1} K_0 &= \frac{1}{2} \beta_1 (z'_1 - z'_2 - z'_3), \\ \frac{\partial}{\partial z_3} K_0 &= \frac{1}{2} \beta_3 (z'_3 - z'_1 - z'_2),\end{aligned}\tag{33}$$

and

$$\sqrt{K_0(z)} \geq \frac{1}{2} |z'_1 - z'_2 - z'_3|.\tag{34}$$

1) We have

$$\sqrt{K_0} \nabla_z \tau^\pm = \sqrt{K_0} \nabla_z \Psi_0 - \frac{1}{2} \nabla_z K_0,$$

so, by using (33), (34),

$$\begin{aligned}2\sqrt{K_0(z)} \partial_{z_1} \tau^\pm(z) &= 2\sqrt{K_0(z)} (\alpha_1 - \frac{1}{2} |\beta_1|) + |\beta_1| \sqrt{K_0(z)} \pm \frac{1}{2} \beta_1 |z'_1 - z'_2 - z'_3| \\ &\geq 2\sqrt{K_0(z)} (\alpha_1 - \frac{1}{2} |\beta_1|) > 0.\end{aligned}$$

Hence $\partial_{z_1} \tau^\pm(z) > 0$. Similarly, $\partial_{z_2} \tau^\pm(z) > 0$.

We have

$$2\sqrt{K_0} \partial_{z_3} \tau^\pm(z) = 2\sqrt{K_0} \alpha_3 \pm \frac{1}{2} \beta_3 (z'_3 - z'_1 - z'_2).$$

Since $\beta_3 < 0$ and $z'_3 - z'_1 - z'_2 \leq 0$ then $\partial_{z_3}\tau^+(z) \geq 0$. 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 (32), we have

$$2\sqrt{K_0}\partial_{z_3}\tau^-(z) = \alpha_3(z'_1 - z'_3) - \frac{1}{2}\beta_3(z'_3 - z'_1) = 2\sqrt{K_0}(\alpha_3 - \frac{1}{2}\beta_3) > 0.$$

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

(i) Assume $z_1 = 0$ or $z_2 = 0$. Then $\sqrt{K_0(z)} = \frac{1}{2}(z'_1 + z'_2 - z'_3)$ and

$$2\sqrt{K_0}\partial_{z_3}\tau^-(z) = (\alpha_3 - \frac{1}{2}|\beta_3|)(z'_1 + z'_2 - z'_3) > 0,$$

so, $\partial_{z_3}\tau^-(z) > 0$.

(ii) Assume $z_1 = z_2 = 1$. The functions $\xi := 4K_0(z)\partial_{z_3}\tau^-(z)\partial_{z_3}\tau^+(z)$ and $\partial_{z_3}\tau^-(z)$ 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

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

The conclusion follows.

7.4. Proof of Lemma 4.5. Lemma 4.5 is a straightforward consequence of Lemma 4.4 and of the following observations.

1) Case $\beta = 0$. We have $K_0 \equiv 0$ so $\mathcal{X}_1 = \emptyset$, $\mathcal{T}_1 = \emptyset$, $\mathcal{X}_2 = \mathbb{T}^3 \setminus \{0\}$. 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 iff $z \in \{0, 1\}^3$. Hence, noting that $\tau^\pm = \Psi_0$, we obtain $Z_2^* = Z_{\{0,1\}}^*$ and $\mathcal{T}_2 = \Psi_0(Z_{\{0,1\}}^*)$.

2) Case $\beta \neq 0$ (so (A0) holds). Thanks to Lemma 4.3 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 $(\beta_2 t / \beta_1, t, 0) \in \{0, 1\}^3 \setminus \{0_{\mathbb{R}^3}\}$ 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 (respect., to $\sin(\mathcal{X}_2)$) is then given by the vector field

$$w_0(x) := (\sin(x_1) \cos(x_2), \cos(x_1) \sin(x_2), 0), \quad (35)$$

(respect.,

$$\tilde{w}_0(y) := (y_1, y_2, 0)$$

).

Remark 12. In Case 3-1) (i.e, $\beta_2 = 0$) it is equivalent but more simple to set $w_0(x) = (0, 1, 0)$. However our choice in (35) 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 .

7.5. Proof of the statement of Remark 3. Step 1. We prove the following assertion. Let a real vector $\boldsymbol{\beta} \in \mathbb{R}^3$ and three positive real values $\varepsilon_1, \mu_1, \alpha_3$ such that $\beta_1 \geq \beta_2 > 0 > \beta_3$ and $\alpha_3 > |\beta_3|/2$. Then there exists positive values $\varepsilon_j, \mu_j, j = 2, 3$, such that $\boldsymbol{\beta} = \boldsymbol{\varepsilon} \times \boldsymbol{\mu}$ and $2\alpha_3 = \varepsilon_1\mu_2 + \varepsilon_2\mu_1$.

Proof. 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 $\varepsilon_1\mu_2 + \varepsilon_2\mu_1 = 2\alpha_3$. \square

Step 2. Let $\boldsymbol{\beta} \in \mathbb{R}^3$ such that $\beta_1 \geq \beta_2 > 0 > \beta_3$. Let us consider the function $(|\beta_3|/2, +\infty) \ni \alpha_3 \mapsto \nu(\alpha_3) = \nu$ defined by (13) and set

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

Then we have

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

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

8. Appendix B.

8.1. Proof of Lemma 5.1. Firstly we observe that if $z_j^* \in \{0, 1\}$ then

$$\begin{aligned} z_j - z_j^* &= \sin^2 x_j - \sin^2 x_j^* = \sin(2x_j^*)(x_j - x_j^*) + 2\cos(2x_j^*)(x_j - x_j^*)^2 \\ &\quad + O((x_j - x_j^*)^3) \\ &= 2s_j^*(x_j - x_j^*)^2 + O((x_j - x_j^*)^4), \end{aligned} \tag{36}$$

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

$$z_j - z_j^* = \sin(2x_j^*)(x_j - x_j^*) + O((x_j - x_j^*)^2), \tag{37}$$

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

Case 1. Assume $\beta = 0$ 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 (36),

$$\begin{aligned} \partial_{x_j} V(x) &= \partial_{z_j} V(x) \partial_{x_j} z_j = \partial_{z_j} V(x) \sin(2x_j) \\ &= (\partial_{z_j} V(x^*) + O(z - z^*)) (\sin(2x_j^*) + 2 \cos(2x_j^*) (x_j - x_j^*) \\ &\quad + O((x_j - x_j^*)^2)) \\ &= 2(\partial_{z_j} V(x^*) + O(z - z^*)) (s_j^* (x_j - x_j^*) + O((x_j - x_j^*)^2)) \\ &= C_j s_j^* (x_j - x_j^*) (1 + O(d_0(x, x^*))), \end{aligned}$$

where $C_j = 2\partial_{z_j} V(x^*) = \frac{\alpha_j}{\sqrt{\Psi_0(z^*)}} > 0$. Thus (23) 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 (10) and (11).)

Cases 2-1 and 2-2-a and 2-2-b are similar to Case 1, the sign of C_j being a consequence of Lemma 4.4.

Let us be more precise in Case 2-2-a. Since $z_3^* = \nu \in (0, 1)$ then $\sin(2x_3^*) \neq 0$ so, by using (37), (36), we have

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

Since $z_j - z_j^* = O((x_j - x_j^*)^2) = O(\partial_{x_j} \tau^-(z) d_0(x, x^*))$ for $j = 1, 2$, and $z_3 - z_3^* = \sin(2x_3^*) (x_3 - x_3^*) (1 + O(x_3 - x_3^*))$ then

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

where $C_3 = (2\sqrt{\tau^-(z^*)})^{-1} \partial_{z_3}^2 \tau^-(z^*) \sin^2(2x_3^*) > 0$. Thus (23) holds in Case 2-2-a too.

Case 2-2-c. 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 (36) we have

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

Hence

$$\partial_{x_3} V(x) = C_3 (x_3 - x_3^*)^3 + O(|\nabla_x V(x)| d_0(x, x^*)),$$

where $C_3 = 2(\sqrt{\tau^-(z^*)})^{-1} \partial_{z_3}^2 \tau^-(z^*) > 0$. Thus (24) holds too.

The lemma is proved.

8.2. Proof of Lemma 5.2. We remember that $y_1^* \neq 0$, $z_2^* \neq 0$ and $z_3^* = 0$, so,

$$\sqrt{\Psi_0(z)}_w = \cos(x_1) \cos(x_2) \sqrt{\tilde{\Psi}_0(z)}_{\tilde{w}}.$$

Thanks to (19) the function $x \mapsto \sqrt{\tilde{\Psi}_0(z)}_{\tilde{w}} = 2\alpha_1 z_1 + 2\alpha_2 z_2$ is smooth and positive in $\text{supp } \chi_2^*$.

In Case 3-3, we have $0 < z_1^* < z_2^* = 1$ then $\cos y_1^* \neq 0$ so $\cos(x_1) = \cos(x_1^*) + O(d_0(x, x^*))$ with $\cos(x_1^*) \neq 0$, and $\cos(x_2) = -y_2^* (x_2 - x_2^*) + O(x_2 - x_2^*)^3$. Hence (26) 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 (25) holds.

8.3. Proof of Lemma 5.5. We fix a representation of $x^* \in \mathbb{T}^3$ in \mathbb{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 $L_D^2(\mathbb{R}^3, \mathbb{C}^6) := L^2(\mathbb{R}^3, \mathbb{C}^6)$ equipped with the scalar product

$$(u, v)_{L_D^2(\mathbb{R}^3; \mathbb{C}^6)} := \int_{\mathbb{R}^3} \langle u(x), v(x) \rangle_{\mathbb{C}^6, D} dx = \int_{\mathbb{R}^3} \langle \hat{D}^{-1}u(x), v(x) \rangle_{\mathbb{C}^6} dx.$$

So, we can identify A_{x^*} with an unbounded symmetric operator on $L^2(\mathbb{R}^3; \mathbb{C}^6)$, 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 5.7.4, and in (23) or in (24) of Lemma 5.1. We set also $\rho' = \sqrt{x_1'^2 + x_2'^2}$, $r' = \sqrt{\rho'^2 + x_3'^2}$.

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

$$p_1(x) = \rho'^2 - x_3'^2,$$

and we set

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

The mapping $\mathbb{R}^2 \setminus \{(0, 0)\} \ni (x'_1, x'_2) \mapsto (\rho', p_3) \in \mathbb{R}^+ \times \mathbb{S}^1$ 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}^∞ -diffeomorphism from $(0, \infty) \times \mathbb{R}$ onto $\mathcal{O} := \mathbb{R}^2 \setminus (\mathbb{R}^- \times \{0\})$. Thus the mapping

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

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

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

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

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

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

$$u(x) = |J_\Phi(x')|^{1/2} \tilde{u}(p), \quad x' = \Phi^{-1}(p) \in \mathbb{R}^3, \quad (38)$$

so the transform

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

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

$$\sup_{x \in B(\mathbb{R}^3)} |\partial_{p_1}^j \tilde{\chi}(p(x))| = \sup_{\frac{r}{2} \leq d_0(x, x^*) \leq r} |\partial_{p_1}^j \tilde{\chi}(p(x))| \leq C.$$

The projector $\tilde{\pi}$ 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 $u, v \in \mathcal{C}_c^\infty((\mathbb{R}^2 \setminus \{x_1^*, x_2^*\}) \times \mathbb{R})$,

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

The projection $\tilde{\pi}$ has range two. Since $\beta = 0$, 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 $q(p)^T \in \ker(i\sqrt{\kappa}\varepsilon M(y) - \Psi_0(z)I_3)$, where $x = x(p)$, I_3 denotes the identity matrix of size 3, and $M(y)$ is the 3×3 matrix defined at (1). 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 $\langle \varepsilon^{-1}q(p), q(p) \rangle_{\mathbb{C}^3} = 1/2$, 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

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

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

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

where we set

$$\tilde{\xi}_j(\tilde{u})(p) := \langle \tilde{u}(p), \varphi_j(p) \rangle_{\mathbb{C}^6, D}. \quad (39)$$

We then have

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

Let us set

$$D(\tilde{A}_{x^*}) = \{\tilde{u} \in \tilde{H}; \tilde{\chi}^2 \partial_{p_1} \tilde{\xi}_j(\tilde{u}) \in L^2(\mathbb{R}^2 \times \mathbb{S}^1; \mathbb{C}; dp), j = 1, 2\}.$$

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

$$|(\tilde{A}_{x^*} \tilde{u}, \tilde{v})_{\tilde{H}}| \leq C \|\tilde{u}\|_{\tilde{H}}, \quad \forall \tilde{u} \in D(\tilde{A}_{x^*}), \quad (40)$$

that is,

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

We fix $j \in \{1, 2\}$ and choose $\tilde{u}(p) = f(p_1)g(p_2, p_3)\varphi_j(p)$ in the above estimate with arbitrary $f \in H^1(\mathbb{R}; \mathbb{C}; dp_1)$ and $g \in L^2(\mathbb{R} \times \mathbb{S}^1; \mathbb{C}; dp_2 dp_3)$. Then $\|\tilde{u}\|_{\tilde{H}} \leq C \|f\|_{H^1(\mathbb{R})} \|g\|_{L^2(\mathbb{R} \times \mathbb{S}^1)}$ so we have

$$\begin{aligned} \left| \int_{\mathbb{R}^2 \times \mathbb{S}^1} \frac{\partial f(p_1)}{\partial p_1} g(p_2, p_3) \tilde{\chi}^2(p) \overline{\tilde{\xi}_j(\tilde{v})} dp \right| &\leq C \|f\|_{H^1(\mathbb{R})} \|g\|_{L^2(\mathbb{R} \times \mathbb{S}^1)}, \\ &\forall f \in H^1(\mathbb{R}; dp_1), g \in L^2(\mathbb{R} \times \mathbb{S}^1, dp_2 dp_3). \end{aligned}$$

It shows that

$$K(p_1) := \int_{\mathbb{R} \times \mathbb{S}^1} \tilde{\chi}^2(p) \tilde{\xi}_j(\tilde{v}) g(p_2, p_3) dp_2 dp_3 \in H^1(\mathbb{R}; \mathbb{C}; dp_1)$$

with

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

But we have

$$\begin{aligned} \frac{\partial}{\partial p_1} K(p_1) &= \int_{\mathbb{R} \times \mathbb{S}^1} \tilde{\chi}^2(p) \frac{\partial}{\partial p_1} \tilde{\xi}_j(\tilde{v}) g(p_2, p_3) dp_2 dp_3 + L(p_1), \\ L(p_1) &:= \int_{\mathbb{R} \times \mathbb{S}^1} \tilde{\xi}_j(\tilde{v}) \left(\frac{\partial}{\partial p_1} \tilde{\chi}^2(p) \right) g(p_2, p_3) dp_2 dp_3, \end{aligned}$$

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

$$\tilde{\chi}^2 \frac{\partial}{\partial p_1} \tilde{\xi}_j(\tilde{v}) \in L^2(\mathbb{R}^2 \times \mathbb{S}^1, \mathbb{C}; dp).$$

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

Case 1 with the general situation $s_1 s_2 s_3 = -1$ is similar.

Cases 2-1 and 2-2-a and 2-2-b and 2-2-d and 2-2-d and 2-2-e, with $s_1 s_2 s_3 = -1$, are similar, except that the projection $\tilde{\pi}$ ($= \pi_1^+(y)$ 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

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

Thanks to Lemma 5.1 we have

$$k^\pm(x) = 1 + O(d_0(x, x^*)).$$

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 \tilde{H}^\pm replacing \tilde{H} so we have

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

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

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

and $\tilde{k}^\pm(p) := k^\pm(x)$, $\tilde{\pi}_1^\pm(p) := \pi_1^\pm(y)$, $\tilde{\chi}(p) := \chi_{x^*}(x)$. 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

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

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

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

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

Case 2-2-c. We have

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

and we set

$$\begin{aligned} p_2(x) &:= x_2' e^{-\frac{1}{2x_3'^2}}, \\ p_3(x) &:= x_1' e^{-\frac{1}{2x_3'^2}}, \end{aligned}$$

with $p_2|_{x_3'=0} = p_3|_{x_3'=0} = 0$, so $p_2, p_3 \in C^\infty(\mathbb{R}^3)$. Then,

$$\begin{aligned} \nabla p_1 &= 2(x_1', x_2', -x_3'^3), \\ \nabla p_2 &= e^{-\frac{1}{2x_3'^2}} (0, 1, x_2'/x_3'^3), \\ \nabla p_3 &= e^{-\frac{1}{2x_3'^2}} (1, 0, x_1'/x_3'^3), \end{aligned}$$

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

$$J_\Phi(x') = \frac{\rho'^2}{x_3'^3} e^{-\frac{1}{x_3'^2}}.$$

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

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

Let $p \in \mathbb{R} \times \mathbb{R}^{2*}$. We have $x_1' = p_3 e^{\frac{1}{2x_3'^2}}$, $x_2' = p_2 e^{\frac{1}{2x_3'^2}}$ so x_3' satisfies the equation $F(x_3'^2) = p_1$ where we set

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

Since $F' > 0$, $F(+\infty) = -\infty$ and $F(0^+) = +\infty$, then the equation is uniquely solvable by some $t_0 > 0$ so we obtain $x_3' = \pm\sqrt{t_0} \in \mathbb{R}^*$. Hence Φ^\pm is bijective. We let the lector to check that Φ^\pm is an homeomorphism from $\mathbb{R}^{2*} \times \mathbb{R}^{\pm*}$ into $\mathbb{R} \times \mathbb{R}^{2*}$. Hence, Φ^\pm is a C^∞ -diffeomorphism from $\mathbb{R}^{2*} \times \mathbb{R}^{\pm*}$ into $\mathbb{R} \times \mathbb{R}^{2*}$.

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

$$(\tilde{u}^\pm, \tilde{v}^\pm)_{\tilde{H}^\pm} := \int_{\mathbb{R}^{2*} \times \mathbb{R}^{\pm*}} \langle \tilde{u}^\pm(p), \tilde{v}^\pm(p) \rangle_{\mathbb{C}^6, D} dp,$$

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

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

so the transform

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

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

Setting again $\tilde{\chi}(p) = \chi_{x^*}(x)$, $\tilde{\pi}(p) = \pi_2(x)$, we have, for $u, v \in C_c^\infty(\mathbb{R}^2 \setminus \{(x_1^*, x_2^*)\} \times \mathbb{R} \setminus \{x_3^*\})$,

$$(A_{x^*} u, v)_{\mathcal{H}^D} = \int_{\mathbb{R}^3} i \left\langle \frac{\partial(\tilde{\chi}\tilde{\pi}\tilde{u})}{\partial p_1}, \tilde{\chi}\tilde{\pi}\tilde{v} \right\rangle_{\mathbb{C}^6, D} dp \equiv (\tilde{A}_{x^*} \tilde{u}, \tilde{v})_{\tilde{H}}.$$

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

A-2) Let us treat Case 1 with $s_1 = s_2 = -1$ (and $s_3 = -1$). We observe that

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

(where we set $x'_j = \sqrt{C_j/2}(x_j - x_j^*)$). We use the spherical coordinates: $x' = \rho\omega$ with $\rho = \sqrt{x_1'^2 + x_2'^2 + x_3'^2} > 0$, $\omega = \rho^{-1}x' \in \mathbb{S}^2$, 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 $\tilde{\xi}_j$ (defined by (39)) $j = 1, 2$. The mapping

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

is a \mathcal{C}^∞ -diffeomorphism from \mathbb{R}^{3*} onto $\mathbb{R}^{+*} \times \mathbb{S}^2$. 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 $\tilde{H} = L^2(\mathbb{R}^{+*} \times \mathbb{S}^2, \mathbb{C}^6; dp)$ equipped with the following scalar product:

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

For $\tilde{u} \in \tilde{H}$, $p \in \mathcal{U}$, we consider the transformation defined by (38) between u and \tilde{u} so it is a bijective isometry (up to a positive constant multiplicative factor) between $L^2(\mathbb{R}^3, \mathbb{C}^6)$ and \tilde{H} which we denote T again. Setting $\tilde{\pi}(p) = \pi_2(y)$, we have $\tilde{\chi} \in \mathcal{C}_c^\infty(\mathbb{R}^{+*} \times \mathbb{S}^2)$ and $\tilde{\chi} = 1$ near $p(x^*) = 0$. We thus have, for $u, v \in \mathcal{C}_c^\infty(\mathbb{R}^{+*} \times \mathbb{S}^2, \mathbb{C}^6)$,

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

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

$$D(\tilde{A}_{x^*}) = \mathcal{H}_{1,0} := \{\tilde{u} \in \tilde{H}; \tilde{\chi}^2 \partial_{p_1} \tilde{\xi}_j(\tilde{u}) \in L^2(\mathbb{R}^{+*} \times \mathbb{S}^2, \mathbb{C}; dp), \\ \tilde{\chi}^2 \partial_{p_1} \tilde{\xi}_j(\tilde{u})|_{p_1=0} = 0, j = 1, 2\}.$$

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

$$D((\tilde{A}_{x^*})^*) = \mathcal{H}_1 := \{\tilde{u} \in \tilde{H}; \tilde{\chi}^2 \partial_{p_1} \tilde{\xi}_j(\tilde{u}) \in L^2(\mathbb{R}^{+*} \times \mathbb{S}^2, \mathbb{C}; dp), j = 1, 2\}. \quad (41)$$

In fact an integration by parts shows that $D((\tilde{A}_{x^*})^*)$ contains \mathcal{H}_1 . Then, let $\tilde{v} \in D((\tilde{A}_{x^*})^*)$ so (40) holds. As in Case 1 with $\prod_{k=1}^3 s_k = -1$, let $j \in \{1, 2\}$ and choose $\tilde{u}(p) = f(p_1)g(p_2, p_3)\varphi_j(p)$ with arbitrary $f \in H^1(\mathbb{R}^{+*}; \mathbb{C}; dp_1)$ and $g \in L^2(\mathbb{S}^2; \mathbb{C}; dp_2 dp_3)$, so we have

$$\left| \int_{\mathbb{R}^{+*} \times \mathbb{S}^2} \frac{\partial f(p_1)}{\partial p_1} g(p_2, p_3) \tilde{\chi}^2(p) \overline{\tilde{\xi}_j(\tilde{v})} dp \right| \leq C \|f\|_{H^1(\mathbb{R}^{+*})} \|g\|_{L^2(\mathbb{S}^2)}, \\ \forall f \in H^1(\mathbb{R}; dp_1), g \in L^2(\mathbb{S}^2, dp_2 dp_3).$$

It implies $\frac{\partial}{\partial p_1}(\tilde{\chi}^2 \tilde{\xi}_j(\tilde{v})) \in L^2(\mathbb{R}^{+*} \times \mathbb{S}^2, \mathbb{C}; dp)$, then $\tilde{\chi}^2 \frac{\partial}{\partial p_1} \tilde{\xi}_j(\tilde{v}) \in L^2(\mathbb{R}^{+*} \times \mathbb{S}^2, \mathbb{C}; dp)$, so $\tilde{v} \in \mathcal{H}_1$. Therefore, (41) is proved. Now, let $\tilde{v} \in D((\tilde{A}_{x^*})^*)$ such that $(\tilde{A}_{x^*})^* \tilde{v} = i\tilde{v}$. Thus we have $(-i(\tilde{A}_{x^*})^* \tilde{v}, \tilde{v})_{\tilde{H}} = (\tilde{v}, \tilde{v})_{\tilde{H}}$. An integration by parts (according to the variable p_1) shows that $v = 0$. Consequently, A_{x^*} with domain $T^{-1}(D(\tilde{A}_{x^*}))$ is

a maximal symmetric operator with the default index $N^+ = 0$. (See also [2, 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 $\Phi: x \mapsto p = (p_1, p_2, p_3)$ is

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

We have $w \cdot \nabla_x u = u_w = -|\nabla p_1|^2 \partial_{p_1} u$ and, thanks to (15), $\sqrt{\Psi_0(z)}_w = p_1 \sqrt{\tilde{\Psi}_0(z)}_{\tilde{w}}$ where $\sqrt{\tilde{\Psi}_0(z)}_{\tilde{w}}$ is analytic and does not vanishes 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 \mathbb{R}^3 into a neighborhood of $0_{\mathbb{R}^3}$ in \mathbb{R}^3 . Hence, we have

$$(A_{x^*} u, v)_{\mathcal{H}^D} = -i \int_{\mathbb{R}^3} \frac{k(x)}{p_1} < \frac{\partial(\chi_2 \pi_2 u)}{\partial p_1}, \chi_2 \pi_2 v >_{\mathbb{C}^6, D} dp + \text{sym},$$

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 $j = 2, 3$, $\tilde{\chi}(q) = \chi_{x^*}(x)$, $\tilde{\pi}(q) = \pi_2(y)$, $\tilde{u}(q) = |k(x)|^{1/2} u(x)$. We then obtain

$$(A_{x^*} u, v)_{\mathcal{H}^D} = -i \int_{\mathbb{R}^3} \text{sgn}(q_1) < \frac{\partial(\tilde{\chi} \tilde{\pi} \tilde{u})}{\partial q_1}, \tilde{\chi}_2 \tilde{\pi}_2 \tilde{v} >_{\mathbb{C}^6, D} dq \equiv (\tilde{A}_{x^*} \tilde{u}, \tilde{v})_{\tilde{H}},$$

where $\tilde{H} = L^2(\mathbb{R}^3, (\mathbb{C}^6, <, >_{\mathbb{C}^6, D}); dq)$ is a usual Hilbert space. The projection $\tilde{\pi}$ has range two so Case 3-3 is similar to A-2) 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-1), i.e., there exists an Hilbert space \tilde{H} and an isometry $L^2(\mathbb{R}^3) \ni u \rightarrow \tilde{u} \in \tilde{H}$ such that

$$(A_{x^*} u, v)_{\mathcal{H}^D} = -i \int_{\mathbb{R}^2 \times \mathbb{S}^1} \text{sgn}(q_1) < \frac{\partial(\tilde{\chi} \tilde{\pi} \tilde{u})}{\partial q_1}, \tilde{\chi}_2 \tilde{\pi}_2 \tilde{v} >_{\mathbb{C}^6, D} dq,$$

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

8.4. Notations.

$$\begin{aligned}
y &= \sin x \quad (y_j = \sin x_j), \\
z &= y^2 \quad (z_j = y_j^2), \\
\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}}, \\
\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 + \text{c.p.}, \\
K_0 &= \frac{1}{4} (\beta_1^2 z_1^2 + \beta_2^2 z_2^2 + \beta_3^2 z_3^2 - 2\beta_1 \beta_2 z_1 z_2 - 2\beta_2 \beta_3 z_2 z_3 - 2\beta_1 \beta_3 z_1 z_3), \\
\Psi_0 &= \boldsymbol{\alpha} \cdot z = \alpha_1 z_1 + \alpha_2 z_2 + \alpha_3 z_3, \\
\tau^\pm &= \Psi_0 \pm \sqrt{K_0}, \\
\lambda^* &= \max\{\sqrt{\tau^+(z)} \mid z \in [0, 1]^3\}, \\
P_M &: \mathbb{R} \times \mathbb{T}^3 \ni (\lambda, x) \mapsto x \in \mathbb{T}^3, \\
P_{\mathbb{R}} &: \mathbb{R} \times \mathbb{T}^3 \ni (\lambda, x) \mapsto \lambda \in \mathbb{R}, \\
\Sigma &= \{(\lambda, x) \mid \lambda \in \sigma(H^D(x))\} = \cup_{j=1}^6 \Sigma_j, \\
\mathcal{X}_j &= P_M(\Sigma_j), \quad j = 1, 2, \\
\Sigma_1 &= \{(\lambda, x) \in \Sigma; K_0(z) \neq 0\}, \\
\Sigma_1^{\pm} &= \{(\lambda, x) \in \Sigma_1; \lambda^2 = \tau^\pm(z), \nabla_x \tau^\pm(z) = 0\}, \\
\Sigma_1^* &= \Sigma_1^{*+} \cup \Sigma_1^{*-}, \\
\Sigma_2 &= \{(\lambda, x) \in \Sigma; z \neq 0, K_0(z) = 0, \lambda^2 = \Psi_0(z)\}, \\
\Sigma_2^* &= \{(\lambda, x) \in \Sigma_2; \nabla_x \Psi_0(z) \text{ is normal to } \mathcal{X}_2 \text{ at } x\}, \\
\mathcal{X}_0 &= \{x \in \mathbb{T}^3; z = 0\}, \\
\mathbb{T}_0^3 &= \mathbb{T}^3 \setminus \mathcal{X}_0, \\
Z_{\{0,1\}} &= \{0, 1\}^3, \\
Z_{\{0,1\}}^* &= Z_{\{0,1\}} \setminus \{(0, 0, 0)\}, \\
X_{\{0,1\}} &= \{x \in \mathbb{T}^3; z \in Z_{\{0,1\}}\}, \\
X_{\{0,1\}}^* &= \{x \in \mathbb{T}^3; z \in Z_{\{0,1\}}^*\}, \\
\mathcal{T} &= \mathcal{T}_1 \cup \mathcal{T}_2 \cup \{0\}, \\
\mathcal{T}_j &= P_{\mathbb{R}}(\Sigma_j^*), \\
\mathcal{T}_1^\pm &= P_{\mathbb{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^*, \\
\mathcal{Z}_1^{\pm} &= \sin^2(\mathcal{X}_1^\pm), \\
\sin^2(\mathcal{X}^*) &= \sin^2(\mathcal{X}_1^*) \cup \sin^2(\mathcal{X}_2^*), \\
A_{out} &= \mathcal{A}_{out} + \mathcal{A}_{out}^*, \\
A_\phi &= A_{out} + A_{in} = A_0 + A_1 + A_2, \\
A_0 &= A_{out}.
\end{aligned}$$

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E-mail address: olivier.poisson@univ-amu.fr