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Opérateurs conjugués et invariance de translation en théorie de la diffusion

THÈSE

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Toute chose a une fin, sauf le saucisson qui en a deux.
Anonyme

Première partie

Introduction

1.1 Préambule

Une théorie générale, un choix contextuel délibéré et un outil technique spécifique. Voici les trois ingrédients génériques qui, souvent, structurent le travail scientifique. C'est en accord avec ce schéma que doit être interprété le titre de cette thèse : opérateurs conjugués (l'outil technique) et invariance de translation (le choix contextuel) en théorie de la diffusion (la théorie générale). Trois notions que nous allons nous efforcer de définir dans le reste de l'introduction.

Dans la section 1.2, nous décrivons succinctement certains aspects de la théorie spectrale et de la théorie de la diffusion en mécanique quantique. Dans la section 1.3, nous introduisons brièvement la méthode dite de l'opérateur conjugué. Et dans la section 1.4, nous expliquons pourquoi se restreindre à l'étude de systèmes physiques invariants sous translation (dans un sens à préciser) peut permettre d'obtenir des résultats additionnels.

Les parties II, III et IV de cette thèse sont quant à elles consacrées à la discussion de trois applications s'inscrivant dans ce canevas théorique. Elles s'articulent toutes autour du même principe : une première section consistant en la présentation résumée des résultats et une seconde contenant l'article publié (ou en voie de publication) correspondant.

1.2 Théorie de la diffusion

Considérons une particule élémentaire de spin s évoluant dans un espace de configurations $\Omega \subset \mathbb{R}^d$, $d \geq 1$, en présence d'un potentiel (ou d'un champ) externe V. A chaque temps t, l'ensemble des états possibles de la particule constitue le même espace (hilbertien) de fonctions $\mathcal{H} := \mathsf{L}^2(\Omega; \mathbb{C}^{2s+1})$. La dynamique de la particule est contrainte par le principe de conservation de l'énergie, lui-même formalisé par la donnée d'une équation différentielle appelée équation de Schrödinger :

$$i\,\frac{\partial \varphi_t}{\partial t} = H\varphi_t \qquad (\hbar = 1),$$

où φ_t est l'état de la particule au temps t et H est l'opérateur autoadjoint $-\Delta + V$ agissant dans $\mathcal{H}$. Par analogie à la situation classique, l'opérateur différentiel de Laplace-Beltrami Δ est usuellement associé à (moins) l'énergie cinétique de la particule alors que l'opérateur (matriciel) de multiplication V représente son énergie potentielle. L'opérateur H est donc naturellement interprété comme l'hamiltonien du système $\{$particule+potentiel externe$\}$ et le groupe unitaire $\{\mathrm{e}^{-itH}\}_{t\in\mathbb{R}}$ comme son groupe d'évolution temporelle. Deux approches complémentaires sont communément employées pour déterminer certaines propriétés du système : la théorie spectrale et la théorie de la diffusion.

La théorie spectrale a pour objet d'étude le sous-ensemble $\sigma(H)$ de $\mathbb{R}$, dit spectre de H, qui tient lieu de support au calcul fonctionnel[1] associé à l'opérateur H. L'analyse

[1] Dans sa version simple, le calcul fonctionnel associé à H consiste en le fait qu'il existe une mesure $E(\cdot)$ sur $\sigma(H)$ (la mesure spectrale de H) à valeurs dans les opérateurs bornés telle que

$$f(H) = \int_{\sigma(H)} \mathrm{d}E(\lambda)\, f(\lambda)$$

pour toute fonction $f : \sigma(H) \to \mathbb{C}$ continue. Pour chaque $\varphi \in \mathcal{H}$, l'application $\lambda \mapsto \|E(\lambda)\varphi\|^2$, où $\|\cdot\|$ est la norme de $\mathcal{H}$, définit une mesure μ^φ. Cette mesure admet une décomposition unique

$$\mu^\varphi = \mu^\varphi_{\mathrm{p}} + \mu^\varphi_{\mathrm{ac}} + \mu^\varphi_{\mathrm{sc}},$$

où μ^φ_{p}, $\mu^\varphi_{\mathrm{ac}}$ et $\mu^\varphi_{\mathrm{sc}}$ sont respectivement des mesures ponctuelle, absolument continue et singulièrement continue de cet ensemble permet entre autres de déterminer complètement (ou partiellement) la décomposition de l'espace de Hilbert $\mathcal{H}$ en deux composantes $\mathcal{H}_{\rm p}(H)$ et $\mathcal{H}_{\rm c}(H)$ ayant chacune une interprétation physique. $\mathcal{H}_{\rm p}(H)$ est le sous-espace (associé à la partie ponctuelle du spectre de H) engendré par l'ensemble des vecteurs propres de H tandis que $\mathcal{H}_{\rm c}(H)$ est le sous-espace (associé à la partie continue du spectre de H) de continuité par rapport à H. Les vecteurs propres de H sont considérés comme les états liés du système puisqu'ils demeurent invariants (à une phase près) sous le groupe d'évolution temporelle $\{{\rm e}^{-itH}\}_{t\in\mathbb{R}}$. Les vecteurs de $\mathcal{H}_{\rm c}(H)$ sont pour leur part interprétés comme les états de diffusion du système car ils quittent, au moins en moyenne temporelle, toute partie finie de l'espace de configurations lorsque $t \to +\infty$.

Dans la pratique, la théorie spectrale tire souvent profit du schéma perturbatif suivant : si le potentiel V est borné relativement au laplacien Δ avec borne $b < 1$, le système caractérisé par l'hamiltonien H peut être considéré comme une perturbation[2] du système sans interaction externe décrit par l'opérateur $-\Delta$.

Cette structure additionnelle, facultative en théorie spectrale, est en quelque sorte la donnée première de la théorie de la diffusion. En effet, cette dernière a pour objectif principal la description asymptotique du groupe d'évolution (total) $\{{\rm e}^{-itH}\}_{t\in\mathbb{R}}$ en termes d'un groupe d'évolution (libre) $\{{\rm e}^{-itH_0}\}_{t\in\mathbb{R}}$. Un des buts de la théorie de la diffusion est de déterminer un opérateur H_0 (plus simple que H) tel que pour chaque état de diffusion $\psi \in \mathcal{H}_{\rm ac}(H)$ au temps $t = 0$, il existe des états de diffusion $\varphi_\pm \in \mathcal{H}_{\rm ac}(H_0)$ tel que la différence

$${\rm e}^{-itH}\psi - {\rm e}^{-itH_0}\varphi_\pm$$

converge en norme vers 0 lorsque $t \to \pm\infty$. Pour l'essentiel, ce problème est équivalent à la question de l'existence et de la complétude[3] des opérateurs d'onde (généralisés)

$$W^\pm := \text{s-}\lim_{t\to\pm\infty} {\rm e}^{itH}{\rm e}^{-itH_0}P_{\rm ac}(H_0),$$

où $P_{\rm ac}(H_0)$ est le projecteur orthogonal sur $\mathcal{H}_{\rm ac}(H_0)$ et "s- lim" fait référence à la limite forte dans $\mathcal{H}$. L'interprétation usuelle des opérateurs $W^\pm$ est esquissée dans la figure 1.1.

La méthode de l'opérateur conjugué, technique apparue dans les années 60 [Put67] et continuellement développée depuis lors, permet d'obtenir une large part des résultats rencontrés en théorie spectrale et en théorie de la diffusion. Elle repose sur l'introduction d'un opérateur autoadjoint auxiliaire A ayant certaines propriétés de compatibilité (exprimées en termes de la résolvante de H et du groupe unitaire $\{{\rm e}^{-itA}\}_{t\in\mathbb{R}}$) vis-à-vis de l'hamiltonien H. Si ces conditions de régularité sont satisfaites, et si le commutateur $[iH, A]$ est un opérateur strictement positif lorsque localisé sur un sous-ensemble J du spectre de H, alors plusieurs informations relatives à H peuvent être déduites localement dans J.

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par rapport à la mesure de Lebesgue. En conséquence, l'espace de Hilbert $\mathcal{H}$ se décompose en la somme directe

$$\mathcal{H} = \mathcal{H}_{\rm p}(H) \oplus \mathcal{H}_{\rm ac}(H) \oplus \mathcal{H}_{\rm sc}(H),$$

où $\mathcal{H}_{\rm p}(H) := \{\varphi \in \mathcal{H} : \mu^\varphi = \mu^\varphi_{\rm p}\}$, $\mathcal{H}_{\rm ac}(H) := \{\varphi \in \mathcal{H} : \mu^\varphi = \mu^\varphi_{\rm ac}\}$ et $\mathcal{H}_{\rm sc}(H) := \{\varphi \in \mathcal{H} : \mu^\varphi = \mu^\varphi_{\rm sc}\}$.

[2]Ici, l'expression "l'opérateur $T + S$ est une perturbation de l'opérateur T" fait référence à la préservation des propriétés d'autoadjonction dans le sens du théorème de Rellich-Kato. C'est-à-dire, si T est un opérateur autoadjoint (essentiellement autoadjoint) dans un espace de Hilbert $\mathcal{H}$ et S est symétrique et borné relativement à T avec borne $b < 1$, alors l'opérateur $T + S$ est autoadjoint (essentiellement autoadjoint), $\overline{T + S} = \overline{T} + \overline{S}$ et le domaine de $\overline{T + S}$ est égal au domaine de $\overline{T}$.

[3]Les opérateurs d'onde $W^\pm$ sont dit complets si et seulement si leurs images $\mathrm{Ran}(W^\pm)$ dans $\mathcal{H}$ vérifient l'identité

$$\mathrm{Ran}(W^-) = \mathrm{Ran}(W^+) = \mathrm{Ran}\left[P_{\rm ac}(H_0)\right].$$

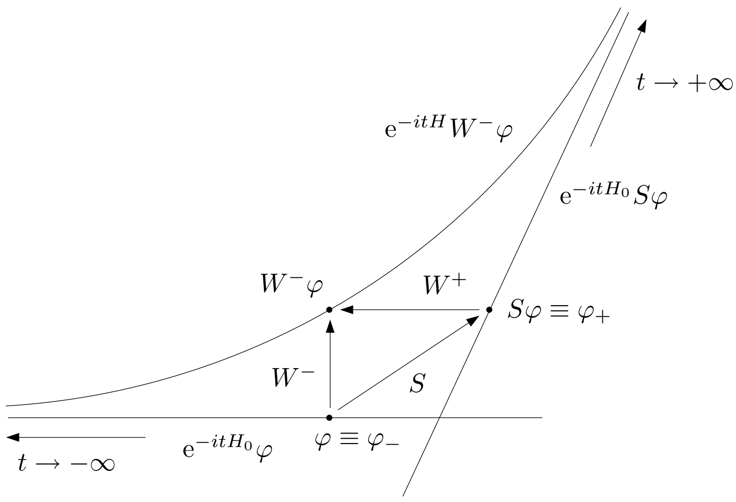


FIG. 1.1 – Opérateurs d'onde $W^\pm$ et opérateur S de diffusion

Comme la méthode de l'opérateur conjugué ne repose que sur la donnée d'un triplet abstrait $\{H, A, \mathcal{H}\}$ adéquat, son domaine d'application surpasse celui de beaucoup d'approches concurrentes. Les exemples qui suivent forment une liste révélatrice de contextes physiques où la méthode de l'opérateur conjugué a déjà permis d'obtenir des résultats subtils : opérateurs de Schrödinger (simples ou à N corps), milieux stratifiés, opérateurs de Dirac, théorie quantique des champs non relativiste, diffusion sur des graphes, mécanique statistique, effet Hall quantique, diffusion dans la métrique de Kerr, etc. De surcroît, comme cette technique est aussi un outil commun aux trois travaux présentés dans cette thèse, elle constitue le sujet de la section qui suit (nous renvoyons à [Ric04] pour une présentation alternative).

1.3 Opérateurs conjugués

1.3.1 Hypothèses générales

Considérons un opérateur autoadjoint H agissant dans un espace de Hilbert $\mathcal{H}$ de produit scalaire $\langle \cdot, \cdot \rangle$ et de norme $\| \cdot \|$. Désignons par $\mathcal{D}(H)$ le domaine de H équipé du produit scalaire graphe $\langle \cdot, \cdot \rangle_{\mathcal{D}(H)} := \langle \cdot, \cdot \rangle + \langle H \cdot, H \cdot \rangle$. Ainsi défini, $\mathcal{D}(H)$ constitue un nouvel espace de Hilbert plongé continûment et densément dans $\mathcal{H}$. En identifiant $\mathcal{H}$ avec son adjoint[4] via l'isomorphisme de Riesz, nous obtenons la suite usuelle de plongements continus et denses :

$$\mathcal{D}(H) \subset \mathcal{H} \subset \mathcal{D}(H)^*.$$

La première propriété de régularité de H requise dans la méthode de l'opérateur conjugué permet d'étendre cette suite dans le sens qui suit. Soit A un second operateur autoadjoint

[4]L'ajoint d'un espace de Banach F, not´e F^*, est l'espace vectoriel des fonctions continues anti-lin´eaires $\varphi : F \to \mathbb{C}$ muni de la norme duale

$$\|\varphi\|_{F^*} := \sup\{|\varphi(f)| : f \in F,\ \|f\| \le 1\}.$$

dans $\mathcal{H}$ dont le domaine $\mathcal{D}(A)$ est aussi équipé du produit scalaire graphe. Alors H est dit de classe $C^1(A)$ si l'application (de conjugaison)

$$\mathbb{R} \ni t \mapsto \mathrm{e}^{itA}(H-i)^{-1}\mathrm{e}^{-itA},$$

à valeurs dans l'ensemble $\mathscr{B}(\mathcal{H})$ des opérateurs bornés sur $\mathcal{H}$, est fortement differentiable. De façon équivalente, H est de classe $C^1(A)$ s'il existe une constante $\mathrm{c} > 0$ telle que

$$\left|\left\langle (H+i)^{-1}\varphi, A\varphi\right\rangle - \left\langle A\varphi, (H-i)^{-1}\varphi\right\rangle\right| \leq \mathrm{c}\,\|\varphi\|^2$$

pour tout $\varphi \in \mathcal{D}(A)$. Dans ce cas, si l'ensemble $\mathcal{D}(A) \cap \mathcal{D}(H)$ est muni de la topologie de l'intersection, tous les plongements dans la suite

$$\mathcal{D}(A) \cap \mathcal{D}(H) \subset \mathcal{D}(H) \subset \mathcal{H} \subset \mathcal{D}(H)^* \subset (\mathcal{D}(A) \cap \mathcal{D}(H))^*$$

sont continus et denses. De surcroît, pour $z \in \mathbb{C} \setminus \sigma(H)$, le commutateur $[(H-z)^{-1}, A]$, défini au sens des formes sur $\mathcal{D}(A)$, s'étend par continuité à un opérateur borné sur $\mathcal{H}$. Similairement, le commutateur $[H, A]$, défini au sens des formes sur $\mathcal{D}(A) \cap \mathcal{D}(H)$, s'étend par continuité à un opérateur borné de $\mathcal{D}(H)$ dans $\mathcal{D}(H)^*$. Les extensions de $[(H-z)^{-1}, A]$ et $[H, A]$ (chacune notée avec le même symbole) vérifient alors, au sens des formes sur $\mathcal{H}$, la relation fondamentale :

$$[(H-z)^{-1}, A] = -(H-z)^{-1}[H, A](H-z)^{-1}.$$

En plus du fait que H doive être de classe $C^1(A)$, la méthode de l'opérateur conjugué s'appuie de manière cruciale sur l'hypothèse suivante de positivité locale du commutateur $[iH, A]$.

Soit $E(\,\cdot\,)$ la mesure spectrale de H. Si H est de classe $C^1(A)$, alors l'opérateur $E(J)[iH, A]E(J)$ est bien défini et borné pour tout sous-ensemble $J \subset \mathbb{R}$ ouvert et borné. Aussi, il existe des nombres $a \in \mathbb{R}$ tels que

$$E(J)[iH, A]E(J) \geq aE(J). \tag{1.1}$$

Si cette inégalité est vérifiée pour un nombre $a > 0$, on dit que A est localement strictement conjugué à H sur J (d'où le qualificatif d'opérateur conjugué pour désigner A).

Dans le reste de cette section, nous expliquons quels résultats peuvent être déduits, tant en théorie spectrale qu'en théorie de la diffusion, des hypothèses faites ci-dessus.

1.3.2 Opérateurs conjugués et théorie spectrale

Si $\lambda \in \sigma(H)$ et $\mu > 0$, l'opérateur borné $(H - \lambda - i\mu)^{-1}$ n'admet pas de limite dans $\mathscr{B}(\mathcal{H})$ lorsque $\mu \searrow 0$. En revanche, la limite

$$\lim_{\mu \searrow 0} \left\langle \varphi, (H - \lambda - i\mu)^{-1}\varphi\right\rangle \tag{1.2}$$

peut tout de même exister pour certains $\varphi \in \mathcal{H}$. Si pour tout λ dans un sous-ensemble $J \subset \mathbb{R}$ ouvert et pour tout φ dans un sous-ensemble dense de $\mathcal{H}$ cette limite existe et si la convergence est uniforme en λ sur tout sous-ensemble compact de J, on dit qu'un principe d'absorption limite pour H est vérifié sur J. L'existence d'un tel principe a pour conséquence principale le fait que le spectre de H dans J est purement absolument continu (*cf.* [ABG96, Sec. 7.1.1 & 7.1.2]).

A la fin des années 70, E. Mourre [Mou81, Mou83] a remarqué que si l'inégalité (1.1) est vérifiée pour un nombre $a > 0$ et si certaines conditions supplémentaires sont aussi satisfaites alors un principe d'absorption limite existe. C'est pourquoi on parle d'estimation de Mourre stricte lorsque l'inégalité (1.1) est satisfaite pour un nombre $a > 0$. Les démonstrations de l'existence de la limite (1.2) à partir d'une estimation de Mourre stricte se fondent sur une méthode, dite des inégalités différentielles, relativement technique. Nous renvoyons le lecteur à [ABG96, Sec. 7.3 & 7.4] pour un traitement général du sujet et à [ABG96, p. 267–268] pour un exposé du cas particulier (fondateur) où $[iH, A] = H$.

Un principe d'absorption limite est démontré dans chacune des applications présentées dans cette thèse (voir les chapitres II.2, III.2 et IV.2). Bien qu'un cadre abstrait existe, la démonstration d'un tel principe requiert l'obtention d'un certain nombre de résultats intermédiaires non triviaux. Etant donné un hamiltonien H, le problème principal réside en la construction d'un opérateur adéquat A conjugué à H. Si l'opérateur H ne diffère pas trop du laplacien négatif $-\Delta$ dans $\mathbb{R}^d$, on fait usuellement appel au générateur du groupe des dilatations $A = D$ (*cf.* section 1.4) qui vérifie la règle de commutation

$$[i\Delta, D] = 2\Delta. \tag{1.3}$$

Si l'hamiltonien H diffère sensiblement de $-\Delta$ dans $\mathbb{R}^d$, alors le choix d'un opérateur conjugué constitue un problème ouvert ne faisant encore l'objet d'aucune théorie générale. Dans la section 1.4, nous expliquons comment une part de la construction associée à la règle de commutation (1.3) peut être sauvegardée dans le cas où la dynamique libre est invariante par translation le long d'une ligne de coordonnées.

Avant d'expliquer comment certains résultats de la théorie de la diffusion peuvent également être déduits du cadre introduit dans la sous-section 1.3.1, nous indiquons une variante moins forte de l'inégalité (1.1). On dit qu'une estimation de Mourre (non stricte) est vérifiée sur le sous-ensemble $J \subset \mathbb{R}$ ouvert et borné s'il existe un nombre $a > 0$ et un opérateur compact K dans $\mathcal{H}$ tels que l'inégalité

$$E(J)[iH, A]E(J) \geq aE(J) + K \tag{1.4}$$

est satisfaite. Les propriétés spectrales que l'on peut inférer d'une telle estimation sont légèrement moins fortes que celles déduites d'une estimation de Mourre stricte. Essentiellement, si l'inégalité (1.4) est vérifiée pour un nombre $a > 0$, alors le spectre de H dans J n'est pas absolument continu mais absolument continu en dehors de (possibles) valeurs propres de multiplicité finie. Ce type de résultats est obtenu dans les chapitres II.2, III.2 et IV.2.

1.3.3 Opérateurs conjugués et théorie de la diffusion

De nombreuses propriétés de propagation de l'état $\mathrm{e}^{-itH}\varphi$ sont obtenues via la méthode de l'opérateur conjugué. Nous expliquons ici comment une estimation de Mourre (locale) induit l'existence d'opérateurs (localement) H-lisses, laquelle permet à son tour d'inférer l'existence (locale) des opérateurs d'onde. Ce schéma est mis à profit dans les chapitres II.2 et IV.2.

Commençons par rappeler la relation entre opérateurs H-lisses et opérateurs d'onde. Un opérateur T fermé avec $\mathcal{D}(H) \subset \mathcal{D}(T)$ est dit localement H-lisse sur J si, pour tout intervalle $[b, c] \subset J$, il existe une constante $\mathrm{c} > 0$ telle que l'inégalité

$$\big\| T \operatorname{Im}(H - \lambda - i\mu)^{-1} T^* \big\| \leq \mathrm{c} \tag{1.5}$$

est vérifiée pour tout $\lambda \in [b,c]$, $\mu \in (0,1)$. En utilisant la relation

$$\mathsf{Im}(H-\lambda-i\mu)^{-1} = \tfrac{1}{2}\int_{\mathbb{R}} \mathrm{d}t\, \mathrm{e}^{i\lambda t}\mathrm{e}^{-itH-\mu|t|} \qquad (\mu > 0),$$

on peut montrer que T est localement H-lisse sur J si et seulement si, pour tout intervalle $[b,c] \subset J$, il existe une constante $\mathrm{C} > 0$ telle que

$$\int_{\mathbb{R}} \mathrm{d}t\, \big\|T\mathrm{e}^{-itH}E([b,c])\varphi\big\|^2 \le \mathrm{C}\|\varphi\|^2$$

pour tout $\varphi \in \mathcal{H}$. Ainsi, l'existence d'un opérateur T localement H-lisse sur J fournit des informations relatives à la propagation de l'état $\mathrm{e}^{-itH}E([b,c])\varphi$. En fait, en supposant que la différence entre les hamiltoniens libre et total puisse être exprimée en termes d'opérateurs localement H-lisses, on peut alors montrer des théorèmes d'existence des opérateurs d'onde du type suivant :

Théorème 1.3.1. *Soit H_1 et H_2 deux opérateurs autoadjoints dans $\mathcal{H}$, $E_j(\cdot)$ la mesure spectrale de H_j et J un sous-ensemble ouvert de $\mathbb{R}$. Supposons que pour tout $\varphi_j \in \mathcal{D}(H_j)$ l'égalité $\langle H_1\varphi_1, \varphi_2\rangle - \langle \varphi_1, H_2\varphi_2\rangle = \langle T_1\varphi_1, T_2\varphi_2\rangle$ soit vérifiée avec T_j un opérateur localement H_j-lisse sur J. Alors la limite*

$$W^{\pm}(H_1,H_2;J) := \mathsf{s}\text{-}\lim_{t\to\pm\infty} \mathrm{e}^{itH_1}\mathrm{e}^{-itH_2}E_2(J)$$

existe et est une isométrie partielle de $E_2(J)\mathcal{H}$ sur $E_1(J)\mathcal{H}$. De plus, les opérateurs d'onde $W^{\pm}(H_1,H_2;J)$ satisfont l'identité

$$W^{\pm}(H_1,H_2;J)^* = \mathsf{s}\text{-}\lim_{t\to\pm\infty} \mathrm{e}^{itH_2}\mathrm{e}^{-itH_1}E_1(J) \equiv W^{\pm}(H_2,H_1;J).$$

Supposons maintenant qu'un principe d'absorption limite pour H soit obtenu sur un sous-ensemble $J \subset \mathbb{R}$ ouvert à partir d'une estimation de Mourre. Alors, l'ensemble des vecteurs pour lesquels la limite (1.2) existe comprend le domaine $\mathcal{D}(A)$ (*cf.* [ABG96, Sec. 7.4]). De plus, si l'intervalle $[b,c]$ est inclus dans J, il existe une constante $\mathrm{C} > 0$ (dépendante de b et c) telle que

$$\big|\langle\varphi, (H-\lambda-i\mu)^{-1}\varphi\rangle\big| \le \mathrm{C}\left(\|\varphi\|^2 + \|A\varphi\|^2\right)$$

pour tout $\varphi \in \mathcal{D}(A)$, $\lambda \in [b,c]$ et $\mu > 0$. De cette estimation, il suit l'existence d'une constante $\mathrm{D} > 0$ satisfaisant

$$\big\|(1+|A|)^{-1}(H-\lambda-i\mu)^{-1}(1+|A|)^{-1}\big\| \le \mathrm{D}$$

uniformément en $\lambda \in [b,c]$ et $\mu > 0$. En comparant cette relation à la définition (1.5) des opérateurs H-lisses, on déduit que l'opérateur $(1+|A|)^{-1}$ est localement H-lisse sur J. De là, il suit que tout opérateur T dans $\mathcal{H}$ satisfaisant $(1+|A|)T^* \in \mathscr{B}(\mathcal{H})$ est localement H-lisse sur J. En particulier, si la différence entre hamiltoniens libre et total est égale à un produit d'opérateurs $T_1^*T_2$ avec $(1+|A|)T_j^* \in \mathscr{B}(\mathcal{H})$, alors la méthode de l'opérateur conjugué permet de prouver, via le théorème 1.3.1, l'existence locale des opérateurs d'onde.

1.4 Invariance de translation

Dans cette section, nous motivons le choix de certaines classes d'opérateurs conjugués dans le cas où l'hamiltonien non perturbé H_0 est invariant par translation le long d'une ligne de coordonnées. Nous traitons deux cas distincts correspondant d'une part aux chapitres II.2 et III.2 et d'autre part au chapitre IV.2 de ce travail. Dans le premier cas, l'opérateur H_0 consiste en le laplacien de Dirichlet négatif $-\Delta_{\mathrm{D}}^{\Omega}$ agissant dans un espace de configurations égal à (ou difféomorphe à) un guide d'ondes infini $\Omega := \Sigma \times \mathbb{R}$, où Σ est un ouvert borné et connexe dans $\mathbb{R}^{d-1}$, $d \geq 2$ (voir la figure 1.2). Dans le second

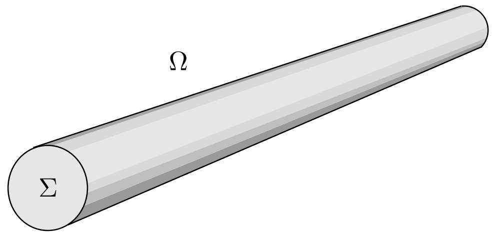


FIG. 1.2 – Exemple de guide d'ondes $\Omega = \Sigma \times \mathbb{R}$ dans $\mathbb{R}^3$

cas, l'hamiltonien H_0 consiste en l'opérateur de Dirac magnétique décrivant une particule relativiste de spin $\frac{1}{2}$ évoluant dans $\mathbb{R}^3$ en présence d'un champ magnétique de direction constante (voir la figure 1.3).

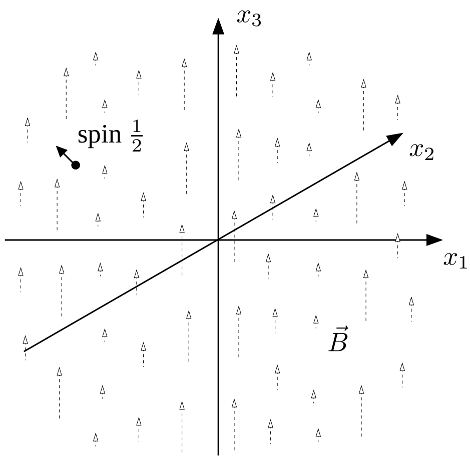


FIG. 1.3 – Particule de spin $\frac{1}{2}$ dans un champ magnétique de direction constante

Considérons le premier cas. Comme le domaine $\Omega = \Sigma \times \mathbb{R}$ est un produit direct, l'espace de Hilbert $\mathcal{H} := \mathsf{L}^2(\Omega)$ est isométrique au produit tensoriel hilbertien $\mathsf{L}^2(\Sigma) \otimes \mathsf{L}^2(\mathbb{R})$ et l'hamiltonien H_0 admet la décomposition

$$H_0 = -\Delta_{\mathrm{D}}^{\Sigma} \otimes 1 + 1 \otimes P^2, \tag{1.6}$$

où $\Delta_{\mathrm{D}}^{\Sigma}$ est le laplacien de Dirichlet dans $\mathsf{L}^2(\Sigma)$, P l'opérateur d'impulsion dans $\mathsf{L}^2(\mathbb{R})$, $\otimes$ le produit tensoriel fermé d'opérateurs et 1 les opérateurs identité. Considérons l'opérateur

$A := 1 \otimes D$, où D est le générateur du groupe unitaire des dilatations de $\mathbb{R}$:

$$(\mathrm{e}^{iD\tau}\psi)(x) := \mathrm{e}^{\tau/2}\psi(\mathrm{e}^{\tau}x), \qquad \forall \tau \in \mathbb{R},\ \psi \in \mathsf{L}^2(\mathbb{R}).$$

Comme D vérifie l'identité[5] $[iP^2, D] = 2P^2$, l'opérateur A satisfait la règle de commutation

$$[iH_0, A] = 2 \otimes P^2. \tag{1.7}$$

Par ailleurs, $\Delta_{\mathrm{D}}^{\Sigma}$ a un spectre purement discret[6] $\mathcal{T} := \{\nu_\alpha\}_{\alpha\geq 1}$ consistant en les valeurs propres $0 < \nu_1 < \nu_2 \leq \nu_3 \leq \dots$ répétées selon la multiplicité. En particulier, la mesure spectrale $E^{H_0}(\cdot)$ de H_0 admet la decompostion tensorielle [Wei80, Ex. 8.21] :

$$E^{H_0}(\cdot) = \sum_{\alpha\geq 1} \mathcal{P}_\alpha \otimes E^{P^2+\nu_\alpha}(\cdot),$$

où $\mathcal{P}_\alpha$ est la projection orthogonale 1-dimensionnelle associée à ν_α et $E^{P^2+\nu_\alpha}(\cdot)$ la mesure spectrale de $P^2 + \nu_\alpha$. Ainsi, pour tout sous-ensemble $J \subset \mathbb{R}$ ouvert et borné, on a l'égalité

$$E^{H_0}(J)[iH_0, A]E^{H_0}(J) = 2 \sum_{\alpha\in\mathbb{N}(J)} \mathcal{P}_\alpha \otimes P^2 E^{P^2+\nu_\alpha}(J), \tag{1.8}$$

où $\mathbb{N}(J) := \{\alpha \geq 1 \,:\, \sup J \geq \nu_\alpha\}$. Si $\sup J < \nu_1$, alors $E^{H_0}(J) = 0$. Dans ce cas, puisque l'inégalité

$$E^{H_0}(J)[iH_0, A]E^{H_0}(J) \geq aE^{H_0}(J)$$

est vérifiée pour tout nombre $a > 0$, on dit qu'une estimation de Mourre stricte est satisfaite pour $a \equiv +\infty$. Supposons maintenant que $\sup J \geq \nu_1$ et désignons par $\mathscr{F}$ la transformée de Fourier dans $\mathsf{L}^2(\mathbb{R})$. Alors, comme l'opérateur $1 \otimes \mathscr{F}$ est unitaire, il existe un nombre $a_J > 0$ tel que $E^{H_0}(J)[iH_0, A]E^{H_0}(J) \geq a_J E^{H_0}(J)$ si et seulement si

$$(1 \otimes \mathscr{F})E^{H_0}(J)[iH_0, A]E^{H_0}(J)(1 \otimes \mathscr{F}^{-1}) \geq a_J(1 \otimes \mathscr{F})E^{H_0}(J)(1 \otimes \mathscr{F}^{-1}). \tag{1.9}$$

En utilisant la formule (1.8), on montre aisément que l'inégalité (1.9) est vérifiée avec

$$a_J = \inf_{\lambda\in[0,\infty),\ \alpha\in\mathbb{N}(J)} 2\lambda \cdot \chi_{J-\nu_\alpha}(\lambda), \tag{1.10}$$

où $\chi_{J-\nu_\alpha}$ est la fonction caractéristique pour l'ensemble $J - \nu_\alpha$. En particulier, s'il existe un compact $K \subset (\nu_1, \infty) \setminus \mathcal{T}$ tel que $J \subset K$, alors $a_J > 0$. En conséquence, l'opérateur A est localement strictement conjugué à H_0 sur $\mathbb{R} \setminus \mathcal{T}$, *i.e.* pour chaque $\lambda \in \mathbb{R} \setminus \mathcal{T}$ il existe des nombres $\varepsilon > 0$ et $a > 0$ tels que

$$E^{H_0}(\lambda; \varepsilon)[iH_0, A]E^{H_0}(\lambda; \varepsilon) \geq aE^{H_0}(\lambda; \varepsilon),$$

où $E^{H_0}(\lambda; \varepsilon) := E^{H_0}((\lambda - \varepsilon, \lambda + \varepsilon))$.

Notons que la borne inférieure (1.10) peut-être directement obtenue en faisant appel à la théorie de l'opérateur conjugué pour les systèmes à plusieurs canaux [BG92, Eq. (3.8)]. Si les opérateurs $\mathcal{P}_\alpha \otimes (P^2 + \nu_\alpha)$ sont interprétés comme des hamiltoniens à un canal, alors H_0 peut être considéré comme un hamiltonien à plusieurs canaux car

$$H_0\varphi = \sum_{\alpha\geq 1} \mathcal{P}_\alpha \otimes (P^2 + \nu_\alpha)\varphi$$

[5] Un sens pr´ecis peut ˆetre donn´e `a tous les commutateurs ´evoqu´es dans cette section. Le caract`ere formel de la pr´esentation rel`eve simplement d'un souci de bri`evet´e.

[6] Nous renvoyons le lecteur `a [Dav95, Chap. 6] pour plus de d´etails sur le laplacien de Dirichlet.

pour tout $\varphi \in \mathcal{D}(H_0)$. Dès lors, il est naturel de ne pas pouvoir obtenir de propriétés de propagation (et donc d'estimation de Mourre) pour les états localisés en énergie autour des valeurs $\lambda \in \mathcal{T}$. C'est pourquoi les points de $\mathcal{T}$ peuvent être interprétés comme les seuils ("thresholds") pour un système physique à plusieurs canaux.

Notons encore que dans l'expression $A = 1 \otimes D$ pour l'opérateur conjugué, d'autres choix peuvent être faits pour le générateur D. Typiquement, il suffit de choisir un opérateur $\widetilde{D}$ tel que $[iP^2, \widetilde{D}] = \vartheta(P^2)$, où ϑ est une fonction strictement positive sur l'ensemble J. Ce genre de modifications permet parfois d'obtenir des résultats plus généraux, notamment concernant le principe d'absorption limite (voir le chapitre II.2).

Considérons maintenant le cas d'une particule relativiste de spin $\frac{1}{2}$ évoluant dans $\mathbb{R}^3$ en présence d'un champ magnétique de direction x_3 constante. Le système physique est décrit, dans l'espace de Hilbert $\mathcal{H} := \mathsf{L}^2(\mathbb{R}^3;\mathbb{C}^4)$, par l'opérateur de Dirac

$$H_0 := \alpha_1\Pi_1 + \alpha_2\Pi_2 + \alpha_3 P_3 + \beta m,$$

où $\beta \equiv \alpha_0, \alpha_1, \alpha_2, \alpha_3$ sont les matrices de Dirac-Pauli, $m > 0$ est la masse de la particule et $\Pi_j := -i\partial_j - a_j$ sont les générateurs des translations magnétiques avec un potentiel vecteur $\vec{a}(x_1, x_2, x_3) = (a_1(x_1, x_2), a_2(x_1, x_2), 0)$ satisfaisant $B = \partial_1 a_2 - \partial_2 a_1$. Puisque $a_3 = 0$, nous écrivons $P_3 := -i\partial_3$ au lieu de Π_3.

Notons que le point 0 n'appartient pas au spectre de H_0 car $m > 0$. Ainsi, l'opérateur H_0^{-1} appartient à $\mathscr{B}(\mathcal{H})$.

Bien que l'hamiltonien H_0 soit invariant par translation le long l'axe x_3, il n'admet pas de décomposition tensorielle du type (1.6). Cependant on peut tout de même déterminer un opérateur A tel que le commutateur $[iH_0, A]$ soit strictement positif lorsque localisé sur certains sous-ensembles du spectre de H_0. Soit Q_3 l'opérateur de multiplication dans $\mathcal{H}$ par la variable x_3. Alors on montre au chapitre IV.2 les faits suivants. L'opérateur matriciel

$$A := \tfrac{1}{2}(H_0^{-1} P_3 Q_3 + Q_3 P_3 H_0^{-1})$$

est essentiellement autoadjoint sur l'ensemble $C_0^\infty(\mathbb{R}^3;\mathbb{C}^4)$ des fonctions de $\mathbb{R}^3$ dans $\mathbb{C}^4$ infiniment différentiables et à support compact. De plus, A satisfait la règle de commutation

$$[iH_0, A] = \left(P_3 H_0^{-1}\right)^2. \tag{1.11}$$

Comme H_0 est invariant par translation le long l'axe x_3, il est décomposable dans la représentation spectrale de l'opérateur P_3. En d'autres termes, si $\mathscr{F}$ désigne la transformée de Fourier partielle dans la direction x_3, alors

$$\mathscr{F} H_0 \mathscr{F}^{-1} = \int_{\mathbb{R}}^{\oplus} \mathrm{d}\xi \, H_0(\xi),$$

où $H_0(\xi)$ est un opérateur autoajoint dans $\mathsf{L}^2(\mathbb{R}^2;\mathbb{C}^4)$ agissant comme $\alpha_1\Pi_1 + \alpha_2\Pi_2 + \alpha_3\xi + \beta m$ sur $C_0^\infty(\mathbb{R}^2;\mathbb{C}^4)$. Ce fait, plus la règle de commutation (1.11), permet d'obtenir pour chaque $\lambda \in \mathbb{R}$ l'estimation de Mourre suivante :

$$\begin{aligned}\sup_{\varepsilon>0} \sup \left\{a \in \mathbb{R} : E^{H_0}(\lambda;\varepsilon)[iH_0, A]E^{H_0}(\lambda;\varepsilon) \geq a\, E^{H_0}(\lambda;\varepsilon)\right\} \\ \geq \inf \left\{ \frac{\lambda^2 - \mu^2}{\lambda^2} \ : \ \mu \in \sigma^0_{\mathrm{sym}} \cap [0, |\lambda|] \right\},\end{aligned} \tag{1.12}$$

où $\sigma^0_{\mathrm{sym}} := \sigma\left[H_0(0)\right]$ et avec la convention que l'infimum sur un ensemble vide est égal à $+\infty$ (formellement, le numérateur dans l'expression $(\lambda^2 - \mu^2)/\lambda^2$ correspond à l'énergie

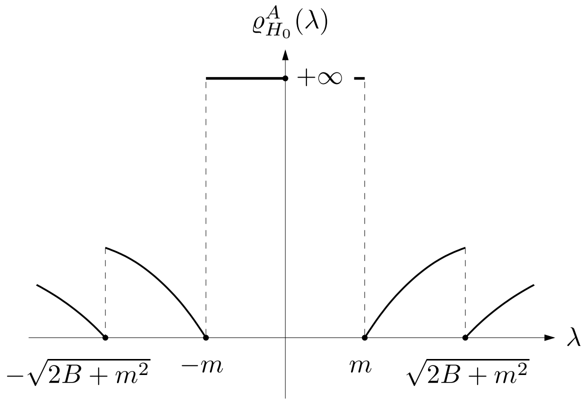


FIG. 1.4 – Schéma de la borne (1.12) (notée $\varrho^A_{H_0}(\lambda)$) lorsque B est constant et non nul, c'est-à-dire si $\sigma^0_{\mathrm{sym}} = \{\pm\sqrt{2nB+m^2}\}_{n=0,1,2,\dots}$.

cinétique associée à l'opérateur P_3^2 alors que le dénominateur correspond à l'énergie totale associée à l'opérateur H_0^2). Nous renvoyons le lecteur à la figure 1.4 pour un schéma de la borne inférieure (1.12) lorsque B est constant et non nul. En conséquence, l'opérateur A est strictement conjugué à H_0 sur $\mathbb{R} \setminus \sigma^0_{\mathrm{sym}}$, *i.e.* pour chaque $\lambda \in \mathbb{R} \setminus \sigma^0_{\mathrm{sym}}$ on a

$$\sup_{\varepsilon>0} \sup \big\{ a \in \mathbb{R} : E^{H_0}(\lambda;\varepsilon)[iH_0, A]E^{H_0}(\lambda;\varepsilon) \geq a E^{H_0}(\lambda;\varepsilon) \big\} > 0.$$

Soulignons le fait que, dans les deux cas traités, le commutateur $[iH_0, A]$ est un opérateur décomposable dans la représentation spectrale de l'opérateur d'impulsion prescrivant la direction d'invariance par translation. En effet, dans le premier cas (*cf.* (1.7)) on a :

$$(1 \otimes \mathscr{F})[iH_0, A](1 \otimes \mathscr{F}^{-1}) = \int_{\mathbb{R}}^{\oplus} \mathrm{d}\xi \, 2\xi^2,$$

où $2\xi^2$ agit dans $\mathsf{L}^2(\Sigma)$. Et dans le second cas (*cf.* (1.11)) on a :

$$\mathscr{F}[iH_0, A]\mathscr{F}^{-1} = \int_{\mathbb{R}}^{\oplus} \mathrm{d}\xi \, \xi^2 H_0(\xi)^{-2}.$$

Or, c'est précisément l'emploi de ces identités qui permet de démontrer la positivité du commutateur $[iH_0, A]$, condition indispensable pour appliquer la méthode de l'opérateur conjugué.

Deuxième partie

Temps de retard et diffusion à courte portée dans un guide d’ondes quantique

Chapitre 1

Résumé

Considérons une particule non relativiste évoluant dans $\mathbb{R}^3$ soit librement soit sous la contrainte d'une perturbation externe. Si les hamiltoniens libre H_0 et total H associés sont tels que les opérateurs d'onde $W^{\pm}$ existent et sont complets, on peut définir pour certains états φ et $r > 0$ les temps de séjour :

$$T_r^0(\varphi) := \int_{-\infty}^{\infty} \mathrm{d}t \int_{|x| \leq r} \mathrm{d}^3x \left|(\mathrm{e}^{-itH_0}\varphi)(x)\right|^2 \tag{1.1}$$

et

$$T_r(\varphi) := \int_{-\infty}^{\infty} \mathrm{d}t \int_{|x| \leq r} \mathrm{d}^3x \left|(\mathrm{e}^{-itH}W^-\varphi)(x)\right|^2 . \tag{1.2}$$

Le premier nombre est interprété comme le temps passé par l'état évoluant librement $\mathrm{e}^{-itH_0}\varphi$ dans la boule $\mathcal{B}_r := \{x \in \mathbb{R}^3 : |x| \leq r\}$, le second comme le temps passé par l'état diffusé correspondant $\mathrm{e}^{-itH}W^-\varphi$ dans la même région. Comme $\mathrm{e}^{-itH}W^-\varphi$ est asymptotiquement égal à $\mathrm{e}^{-itH_0}\varphi$ quand $t \to -\infty$ (voir la figure 1.1 de la section 1.2), la différence

$$\tau_r^{\mathrm{in}}(\varphi) := T_r(\varphi) - T_r^0(\varphi)$$

correspond au temps de retard du processus de diffusion avec état initial φ pour la boule $\mathcal{B}_r$. Le temps de retard (global) est, s'il existe, la limite de $\tau_r^{\mathrm{in}}(\varphi)$ lorsque $r \to \infty$. Si l'interaction est suffisamment à courte portée [AC87, ACS87], cette limite existe et est égale à la valeur moyenne dans l'état φ de l'opérateur de temps de retard de Eisenbud-Wigner[1].

[1] L'op´erateur de temps de retard d'Eisenbud-Wigner $\tau_{\text{E-W}}$ est l'op´erateur d´ecomposable dans la repr´esentation spectrale de H_0 donn´e formellement par la famille

$$\tau_{\text{E-W}}(\lambda) := -iS(\lambda)^* \frac{\mathrm{d}S(\lambda)}{\mathrm{d}\lambda}, \quad \lambda \in \sigma(H_0),$$

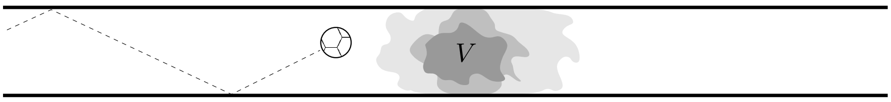
o`u $S(\cdot)$ est la matrice de diffusion.

Si le processus de diffusion associé à la paire $\{H_0, H\}$ est inélastique (typiquement, d'une nature à N corps), alors la définition du temps de retard doit être modifiée. L'argument heuristique est le suivant. Dû à la nature inélastique de l'interaction, les valeurs moyennes de l'opérateur d'impulsion dans l'état $\mathrm{e}^{-itH}W^-\varphi$ et dans l'état $\mathrm{e}^{-itH_0}\varphi$ peuvent converger vers des constantes différentes lorsque $t \to +\infty$. Ceci implique la divergence du retard (de l'avance) de l'état $\mathrm{e}^{-itH}W^-\varphi$ vis-à-vis de l'état $\mathrm{e}^{-itH_0}\varphi$. Similairement, si l'état entrant φ est remplacé par l'état sortant $S\varphi$, alors la même divergence, mais de signe opposé, survient lorsque $t \to -\infty$. Aussi, afin de compenser mutuellement ces divergences, $T_r(\varphi)$ ne doit pas être comparé au temps de séjour libre $T_r^0(\varphi)$ mais au temps de séjour libre effectif $\frac{1}{2}\left[T_r^0(\varphi) + T_r^0(S\varphi)\right]$. Nous aboutissons donc à l'expression

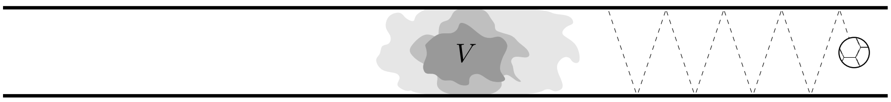
$$\tau_r(\varphi) := T_r(\varphi) - \tfrac{1}{2}\left[T_r^0(\varphi) + T_r^0(S\varphi)\right] \tag{1.3}$$

pour le temps de retard du processus de diffusion inélastique avec état initial φ pour la boule $\mathcal{B}_r$. Dans le cas de la diffusion à N corps, on peut aisément produire le pendant multi-canal de la définition (1.3) [Smi60, BO79, Mar81].

Considérons maintenant une particule non relativiste évoluant dans un guide d'ondes infini $\Omega := \Sigma \times \mathbb{R}$ de coordonnées (x', x), où Σ est un ouvert borné et connexe de $\mathbb{R}^{d-1}$, $d \geq 2$. Son évolution libre est décrite dans l'espace de Hilbert $\mathcal{H} := \mathsf{L}^2(\Omega)$ (de norme $\|\cdot\|$) par l'hamiltonien de Dirichlet $H_0 := -\Delta_{\mathrm{D}}^{\Omega}$ et son évolution perturbée par un hamiltonien H. Supposons H tel que les opérateurs d'onde $W^{\pm}$ existent et sont complets. Alors le processus de diffusion est globalement élastique mais l'énergie cinétique le long de l'axe x n'est pas conservée si l'interaction dépend de la coordonnée transverse x'. Nous renvoyons



Avant l'interaction



Après l'interaction

FIG. 1.1 – Une particule classique se déplace librement dans un tube avant et après son interaction élastique avec un potentiel V à support compact. L'énergie cinétique totale de la particule est conservée, mais sa quantité de mouvement selon l'axe du tube avant et après l'interaction diffère.

le lecteur à la figure 1.1 pour un schéma de l'analogue classique de ce phénomène. D'autre part, dans le guide d'ondes Ω, les temps de séjour (1.1) et (1.2) sont donnés par

$$T_r^0(\varphi) := \int_{-\infty}^{\infty} \mathrm{d}t\, \left\|F_r \mathrm{e}^{-itH_0}\varphi\right\|^2$$

et

$$T_r(\varphi) := \int_{-\infty}^{\infty} \mathrm{d}t\, \left\|F_r \mathrm{e}^{-itH}W^-\varphi\right\|^2,$$

où F_r est le projecteur sur l'ensemble des états localisés dans le cylindre $\Omega_r := \Sigma \times [-r, r]$. Ainsi, les temps de séjour font intervenir des régions croissant le long de l'axe x, direction selon laquelle le processus de diffusion est inélastique. Ceci explique pourquoi l'on doit faire appel à la formule (1.3) pour définir le temps de retard dans les guides d'ondes.

Dans l'article qui suit, nous étudions l'existence du temps de retard (1.3) dans les guides d'ondes ainsi que son identité avec le temps de retard d'Eisenbud-Wigner. En premier lieu, nous démontrons le critère général suivant ($\sigma_{\mathrm{p}}(H)$ dénote l'ensemble des valeurs propres de H, $\mathcal{T} = \{\nu_\alpha\}_{\alpha \geq 1}$ est défini à la section 1.4 et $\mathscr{D}_2^\Omega$ est un ensemble dense de vecteurs à support compact dans la représentation spectrale de H_0) :

Théorème 1.0.1. *Soit $\Omega := \Sigma \times \mathbb{R}$, où Σ est un ouvert borné et connexe dans $\mathbb{R}^{d-1}$, $d \geq 2$. Considérons le système de diffusion (à deux corps) dans l'espace de Hilbert $\mathcal{H} := \mathsf{L}^2(\Omega)$ avec hamiltonien libre $H_0 := -\Delta_{\mathrm{D}}^\Omega$ et hamiltonien total H. Supposons*

1. *Pour chaque $r > 0$, le projecteur F_r est localement H-lisse sur $(\nu_1, \infty) \setminus (\sigma_{\mathrm{p}}(H) \cup \mathcal{T})$.*
2. *Les opérateurs d'onde $W^\pm$ existent et sont complets.*

Soit $\varphi \in \mathscr{D}_2^\Omega$ tel que $S\varphi \in \mathscr{D}_2^\Omega$ et

$$\big\| \big(W^- - 1\big)\, \mathrm{e}^{-itH_0} \varphi \big\| \in \mathsf{L}^1((-\infty, 0), \mathrm{d}t)$$

et

$$\big\| \big(W^+ - 1\big)\, \mathrm{e}^{-itH_0} S\varphi \big\| \in \mathsf{L}^1((0, \infty), \mathrm{d}t).$$

Alors $\tau_r(\varphi)$ existe pour chaque $r > 0$ et $\tau_r(\varphi)$ converge lorsque $r \to \infty$ vers une limite finie. Si de plus la fonction $\lambda \mapsto S(\lambda)$ est fortement continûment différentiable sur un intervalle ouvert $J \subset (\nu_1, \infty)$ tel que $E^{H_0}(J)\varphi = \varphi$, alors $\lim_{r\to\infty} \tau_r(\varphi) = \langle \varphi, \tau_{\text{E-W}} \varphi \rangle$.

En utilisant le formalisme stationnaire de [Kur73] et les méthodes à commutateurs de [ABG96], nous montrons aussi quelques résultats concernant la diffusion à courte portée dans les guides d'ondes. Nous obtenons des principes d'absorption limite (qui impliquent l'existence des opérateurs d'onde) et établissons des propriétés spectrales de l'hamiltonien total. Nous prouvons un résultat sur la différentiablilité de la fonction $S(\cdot)$ en démontrant, notamment, une formule explicite pour la matrice $S(\cdot)$. Enfin, en utilisant les résultats qui précèdent, nous trouvons des conditions pour lesquelles le théorème 1.0.1 est satisfait dans le cas où la perturbation est un potentiel V borné relativement à l'hamiltonien libre H_0 :

Théorème 1.0.2. *Soit $H := H_0 + V$, où V décroît comme $|x|^{-\kappa}$, $\kappa > 4$, à l'infini. Alors il existe un ensemble dense $\mathscr{E}$ tel que, pour chaque $\varphi \in \mathscr{E}$, $\tau_r(\varphi)$ existe pour tout $r > 0$ et $\tau_r(\varphi)$ converge lorsque $r \to \infty$ vers une limite égale à $\langle \varphi, \tau_{\text{E-W}} \varphi \rangle$.*

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Chapitre 2

Time delay and short-range scattering in quantum waveguides

Abstract

Although many physical arguments account for using a modified definition of time delay in multichannel-type scattering processes, one can hardly find rigorous results on that issue in the literature. We try to fill in this gap by showing, both in an abstract setting and in a short-range case, the identity of the modified time delay and the Eisenbud-Wigner time delay in waveguides. In the short-range case we also obtain limiting absorption principles, state spectral properties of the total Hamiltonian, prove the existence of the wave operators and show an explicit formula for the S-matrix. The proofs rely on stationary and commutator methods.

2.1 Introduction and main results

This paper is concerned with time delay (defined in terms of sojourn times) in scattering theory for waveguides. Our main aim is to show that, as in N-body scattering and scattering by step potentials, one has to use a modified definition of time delay in order to prove its existence and its identity with the Eisenbud-Wigner time delay. We refer to [Mar75] for the treatment of this issue in the case of scattering with dissipative interactions.

Let us first recall the standard definition [JSM72] of time delay for an elastic two-body scattering process. Given a free Hamiltonian H_0 and a total Hamiltonian H such that the wave operators $W^{\pm}$ exist and are complete, one defines for certain states φ and $r > 0$ two sojourn times, namely :

$$T_r^0(\varphi) := \int_{-\infty}^{\infty} \mathrm{d}t \int_{|x|\le r} \mathrm{d}^3x \, \left|(\mathrm{e}^{-itH_0}\varphi)(x)\right|^2 \tag{2.1}$$

and

$$T_r(\varphi) := \int_{-\infty}^{\infty} \mathrm{d}t \int_{|x|\le r} \mathrm{d}^3x \, \left|(\mathrm{e}^{-itH}W^-\varphi)(x)\right|^2 . \tag{2.2}$$

The first number is interpreted as the time spent by the freely evolving state $\mathrm{e}^{-itH_0}\varphi$ inside the ball $\mathcal{B}_r := \{x \in \mathbb{R}^3 : |x| \le r\}$, whereas the second one is interpreted as the time spent by the associated scattering state $\mathrm{e}^{-itH}W^-\varphi$ within the same region. Since $\mathrm{e}^{-itH}W^-\varphi$ is asymptotically equal to $\mathrm{e}^{-itH_0}\varphi$ as $t \to -\infty$, the difference

$$\tau_r^{\mathrm{in}}(\varphi) := T_r(\varphi) - T_r^0(\varphi)$$

corresponds to the time delay of the scattering process with incoming state φ for the ball $\mathcal{B}_r$. The (global) time delay of the scattering process with incoming state φ is, if it exists, the limit of $\tau_r^{\mathrm{in}}(\varphi)$ as $r \to \infty$. For a suitable initial state φ and a sufficiently short-ranged interaction, it is known [AC87, ACS87] that this limit exists and is equal to the expectation value in the state φ of the Eisenbud-Wigner time delay operator.

If the scattering process associated to the pair $\{H_0, H\}$ is inelastic (typically of a N-body nature), then one has to modify the definition of time delay. The heuristic argument goes as follows. Due to the inelastic nature of the interaction, the expectation values of the momentum operator in the state $\mathrm{e}^{-itH}W^-\varphi$ and in the state $\mathrm{e}^{-itH_0}\varphi$ may converge to different constants as $t \to +\infty$. This would result in the divergence of the retardation (or advance) of the state $\mathrm{e}^{-itH}W^-\varphi$ with respect to the state $\mathrm{e}^{-itH_0}\varphi$. Similarly, if the incoming state φ is replaced by the outcoming state $S\varphi$, where S is the scattering operator, then the same divergence, but with an opposite sign, would occur as $t \to -\infty$. Therefore, in order to cancel both divergences out, $T_r(\varphi)$ should not be compared with the free sojourn time $T_r^0(\varphi)$, but with an effective free sojourn time involving both $T_r^0(\varphi)$ and $T_r^0(S\varphi)$. A symmetry argument [Mar81, Sec. V.(a)] leads naturally to the mean value $\frac{1}{2}\left[T_r^0(\varphi) + T_r^0(S\varphi)\right]$ for this effective time. Thus one ends up with the expression

$$\tau_r(\varphi) := T_r(\varphi) - \tfrac{1}{2}\left[T_r^0(\varphi) + T_r^0(S\varphi)\right] \tag{2.3}$$

for the time delay of the inelastic scattering process with incoming state φ for the ball $\mathcal{B}_r$. In the case of N-body scattering and step potential scattering, one can easily generalize the definition (2.3) to its multichannel counterpart [Smi60, BO79, Mar81].

Now consider a waveguide $\Omega := \Sigma \times \mathbb{R}$ with coordinates (x', x), where Σ is a bounded open connected set in $\mathbb{R}^{d-1}$, $d \ge 2$. Let $H_0 := -\Delta_{\mathrm{D}}^{\Omega}$ be the Dirichlet Laplacian in $\mathsf{L}^2(\Omega)$ (equipped with the norm $\|\cdot\|$). Let H be a selfadjoint perturbation of H_0 such that the wave operators $W^\pm := \mathrm{s}\text{-}\lim_{t\to\pm\infty} \mathrm{e}^{itH}\mathrm{e}^{-itH_0}$ exist and are complete (so that the scattering operator $S := (W^+)^* W^-$ is unitary). Then the associated scattering process is globally elastic, but the kinetic energy along the x-axis is not conserved if the interaction is general enough. On the other hand, the waveguide counterparts of the sojourn times (2.1) and (2.2) must be

$$T_r^0(\varphi) := \int_{-\infty}^{\infty} \mathrm{d}t \, \left\|F_r \mathrm{e}^{-itH_0}\varphi\right\|^2 \tag{2.4}$$

and

$$T_r(\varphi) := \int_{-\infty}^{\infty} \mathrm{d}t \, \left\|F_r \mathrm{e}^{-itH}W^-\varphi\right\|^2 , \tag{2.5}$$

where F_r denotes the projection onto the set of the states localized in the cylinder $\Omega_r := \Sigma \times [-r, r]$. Thus the sojourn times involve regions expanding in the x-direction, the axis along which the scattering process is inelastic. This explains why we have to use the formula (2.3) when defining time delay in waveguides. As in the N-body case, one can also write the time delay given by (2.3)–(2.5) in a multichannel way (see Remark 2.2.8).

Let us fix the notations and recall some properties of H_0 before giving a description of our results. $\otimes$ (resp. $\odot$) stands for the closed (resp. algebraic) tensor product of Hilbert spaces or of operators. Given two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, we write $\mathcal{H}_1 \subset \mathcal{H}_2$ if $\mathcal{H}_1$ is continuously embedded in $\mathcal{H}_2$ and $\mathcal{H}_1 \simeq \mathcal{H}_2$ if $\mathcal{H}_1$ and $\mathcal{H}_2$ are isometric. $\mathscr{B}(\mathcal{H}_1, \mathcal{H}_2)$ stands for the set of bounded operators from $\mathcal{H}_1$ to $\mathcal{H}_2$ with norm $\|\cdot\|_{\mathcal{H}_1 \to \mathcal{H}_2}$, and $\mathscr{B}(\mathcal{H}_1) := \mathscr{B}(\mathcal{H}_1, \mathcal{H}_1)$. $\|\cdot\|$ (resp. $\langle\cdot,\cdot\rangle$) denotes the norm (resp. scalar product) of the Hilbert space $\mathcal{H} := \mathsf{L}^2(\Omega) \simeq \mathsf{L}^2(\Sigma) \otimes \mathsf{L}^2(\mathbb{R})$. If there is no risk of confusion, the notations $\|\cdot\|$ and $\langle\cdot,\cdot\rangle$ are also used for other spaces. Q (resp. P) stands for the position (resp. momentum) operator in $\mathsf{L}^2(\mathbb{R})$. $\mathbb{N} := \{0, 1, 2, \ldots\}$ is the set of natural numbers. $\mathcal{H}^k(\Sigma)$, $k \in \mathbb{N}$, are the usual Sobolev spaces over Σ, and $\mathcal{H}^s_t(\mathbb{R}^n)$, $s, t \in \mathbb{R}$, $n \in \mathbb{N} \setminus \{0\}$, are the weighted Sobolev spaces over $\mathbb{R}^n$ [ABG96, Sec. 4.1] (with the convention that $\mathcal{H}^s(\mathbb{R}^n) := \mathcal{H}^s_0(\mathbb{R}^n)$ and $\mathcal{H}_t(\mathbb{R}^n) := \mathcal{H}^0_t(\mathbb{R}^n)$). Given a selfadjoint operator A in a Hilbert space $\mathcal{H}$, we write $E^A(\cdot)$ for the spectral measure of A and $\mathcal{D}(A)$ for the domain of A endowed with its natural graph topology. $\chi_{[-r,r]}$ is the characteristic function for the interval $[-r, r]$ and $\langle\cdot\rangle := \sqrt{1 + |\cdot|^2}$.

The Dirichlet Laplacian $-\Delta^\Sigma_{\mathrm{D}}$ in $\mathsf{L}^2(\Sigma)$ has a purely discrete spectrum $\mathcal{T} := \{\nu_\alpha\}_{\alpha \geq 1}$ consisting of eigenvalues $0 < \nu_1 < \nu_2 \leq \nu_3 \leq \ldots$ repeated according to multiplicity. In particular $-\Delta^\Sigma_{\mathrm{D}}$ admits the spectral decomposition $-\Delta^\Sigma_{\mathrm{D}} = \sum_{\alpha \geq 1} \nu_\alpha \mathcal{P}_\alpha$, where $\mathcal{P}_\alpha$ is the one-dimensional orthogonal projection associated to ν_α. The Dirichlet Laplacian $-\Delta^\Omega_{\mathrm{D}}$ can be written as $-\Delta^\Omega_{\mathrm{D}} = -\Delta^\Sigma_{\mathrm{D}} \otimes 1 + 1 \otimes P^2$, so that H_0 has a purely absolutely continuous spectrum coinciding with the interval $[\nu_1, \infty)$. Since S commutes with H_0, S can be expressed as a direct integral of unitary operators $S(\lambda)$, $\lambda \geq \nu_1$, where $S(\lambda)$ acts in the fiber at energy λ in the spectral representation of H_0 (see Section 2.2.2). $S(\lambda)$ is called the S-matrix at energy λ.

Definition 2.1.1. *Let $\sigma_{\mathrm{p}}(H)$ be the set of eigenvalues of H and $t \geq 0$, then*

$$\mathscr{D}^\Omega_t := \big\{\varphi \in \mathsf{L}^2(\Sigma) \otimes \mathcal{H}_t(\mathbb{R}) : E^{H_0}(J)\varphi = \varphi \text{ for some compact set } J \text{ in } (\nu_1, \infty) \setminus (\sigma_{\mathrm{p}}(H) \cup \mathcal{T})\big\},$$

$$\mathscr{D}^\mathbb{R}_t := \big\{\varphi \in \mathcal{H}_t(\mathbb{R}) : E^{P^2}(J)\varphi = \varphi \text{ for some compact set } J \text{ in } \mathbb{R} \setminus \{0\}\big\}.$$

It is clear that $\mathscr{D}^\mathbb{R}_t$ is dense in $\mathsf{L}^2(\mathbb{R})$ and that $\mathscr{D}^\mathbb{R}_{t_1} \subset \mathscr{D}^\mathbb{R}_{t_2}$ if $t_1 \geq t_2$. The spaces $\mathscr{D}^\Omega_t$ also satisfy $\mathscr{D}^\Omega_{t_1} \subset \mathscr{D}^\Omega_{t_2}$ if $t_1 \geq t_2$, and $\mathscr{D}^\Omega_t$ is dense in $\mathcal{H}$.

We are in a position to state our results. In Section 2.2.3, we prove the following general existence criterion. It involves the Eisenbud-Wigner time delay operator $\tau_{\text{E-W}}$, which is the decomposable operator in the spectral representation of H_0 formally defined by the family

$$\tau_{\text{E-W}}(\lambda) := -iS(\lambda)^* \frac{\mathrm{d}S(\lambda)}{\mathrm{d}\lambda}, \quad \lambda \geq \nu_1.$$

Theorem 2.1.2. *Let $\Omega := \Sigma \times \mathbb{R}$, where Σ is a bounded open connected set in $\mathbb{R}^{d-1}$, $d \geq 2$. Consider a (two-body) scattering system in the Hilbert space $\mathcal{H} := \mathsf{L}^2(\Omega)$ with free Hamiltonian $H_0 := -\Delta^\Omega_{\mathrm{D}}$ and total Hamiltonian H. Suppose that*

1. *For each $r > 0$ the projection F_r is locally H-smooth on $(\nu_1, \infty) \setminus (\sigma_{\mathrm{p}}(H) \cup \mathcal{T})$.*

2. The wave operators $W^{\pm}$ exist and are complete.

Let $\varphi \in \mathscr{D}_2^{\Omega}$ be such that $S\varphi \in \mathscr{D}_2^{\Omega}$ and

$$\left\|\left(W^{-}-1\right)\mathrm{e}^{-itH_0}\varphi\right\| \in \mathsf{L}^1((-\infty,0),\mathrm{d}t)$$

and

$$\left\|\left(W^{+}-1\right)\mathrm{e}^{-itH_0}S\varphi\right\| \in \mathsf{L}^1((0,\infty),\mathrm{d}t).$$

Then $\tau_r(\varphi)$ exists for each $r > 0$ and $\tau_r(\varphi)$ converges as $r \to \infty$ to a finite limit. If in addition the function $\lambda \mapsto S(\lambda)$ is strongly continuously differentiable on an open set $J \subset (\nu_1, \infty)$ such that $E^{H_0}(J)\varphi = \varphi$, then $\lim_{r\to\infty} \tau_r(\varphi) = \langle \varphi, \tau_{\text{E-W}}\varphi\rangle$.

Using the stationary formalism of [Kur73] and the commutator methods of [ABG96], we show in Section 2.3.1 some results concerning short-range scattering theory in waveguides. In Theorem 2.3.4, we obtain limiting absorption principles (which lead to the existence of the wave operators) and state spectral properties of the total Hamiltonian. We also prove a result on the norm differentiability of the S-matrix (Proposition 2.3.8) which relies on an explicit formula for the S-matrix (Lemma 2.3.7). In Section 2.3.2, we use the results of Section 2.3.1 to find sufficient conditions under which the hypotheses of Theorem 2.1.2 are satisfied (see Theorem 2.3.11 for the precise statement) :

Theorem 2.1.3. *Let $H := H_0 + V$, where V decays as $|x|^{-\kappa}$, $\kappa > 4$, at infinity. Then there exists a dense set $\mathscr{E}$ such that, for each $\varphi \in \mathscr{E}$, $\tau_r(\varphi)$ exists for all $r > 0$ and $\tau_r(\varphi)$ converges as $r \to \infty$ to a finite limit equal to $\langle \varphi, \tau_{\text{E-W}}\varphi\rangle$.*

Remark 2.1.4. *A comparison with the corresponding theorem [ACS87, Prop. 4] for scattering in $\mathbb{R}^d$, shows us that potentials decaying as $|x|^{-\kappa}$, $\kappa > 2$, at infinity may also be treated. This could certainly be done by adapting results on the mapping properties of the scattering operator (*e.g.*[ACS87, JN92]) to the waveguide case. However, since these properties deserve a study on their own, we prefer not to use them in the present paper.*

We finally mention Lemma 2.2.4 which establishes some regularity properties of the trace-type operator associated to the spectral transformation for H_0.

2.2 General existence of time delay in waveguides

2.2.1 Preliminaries

In the sequel we give sufficient conditions for the existence of the time delay in Ω_r. Then we show that the (global) time delay, if it exists, is expressed in terms of the limit of an auxiliary time. We start by recalling some facts which will be freely used throughout the paper.

The one-dimensional Fourier transform $\mathscr{F}$ is a topological isomorphism of $\mathcal{H}_t^s(\mathbb{R})$ onto $\mathcal{H}_s^t(\mathbb{R})$ for any $s, t \in \mathbb{R}$. Given two separable Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ one has the relation $(\mathcal{H}_1 \otimes \mathcal{H}_2)^* \simeq \mathcal{H}_1^* \otimes \mathcal{H}_2^*$ for their adjoint spaces. Furthermore, if 1 is the identity operator in $\mathcal{H}_1$ and A a selfadjoint operator in $\mathcal{H}_2$, then one has the identity $\mathcal{D}(1 \otimes A) \simeq \mathcal{H}_1 \otimes \mathcal{D}(A)$. If $\mathcal{H}_1$, $\mathcal{H}_2$, $\mathcal{K}_1$, $\mathcal{K}_2$ are Hilbert spaces and $A_i \in \mathscr{B}(\mathcal{H}_i, \mathcal{K}_i)$ ($i = 1, 2$), then $A_1 \otimes A_2 \in \mathscr{B}(\mathcal{H}_1 \otimes \mathcal{H}_2, \mathcal{K}_1 \otimes \mathcal{K}_2)$.

Remark 2.2.1. *Since $H_0 = -\Delta_{\mathrm{D}}^{\Sigma} \otimes 1 + 1 \otimes P^2$, the domain of H_0 has the following form [BG92, Sec. 3] :*

$$\mathcal{D}(H_0) = \left[\mathcal{D}(-\Delta_{\mathrm{D}}^{\Sigma}) \otimes \mathsf{L}^2(\mathbb{R})\right] \cap \left[\mathsf{L}^2(\Sigma) \otimes \mathcal{H}^2(\mathbb{R})\right].$$

The set $\mathcal{D}(H_0)$ is endowed with the intersection topology, so that it is a Hilbert. The spectral measure of H_0 admits the tensorial decomposition [Wei80, Ex. 8.21] :

$$E^{H_0}(\cdot) = \sum_{\alpha \geq 1} \mathcal{P}_\alpha \otimes E^{P^2+\nu_\alpha}(\cdot).$$

Hence the equality

$$\mathrm{e}^{itH_0} = \sum_{\alpha \geq 1} \mathcal{P}_\alpha \otimes \mathrm{e}^{it(P^2+\nu_\alpha)} \tag{2.6}$$

holds in the sense of the strong convergence. Furthermore each $\varphi \in \mathscr{D}_t^\Omega$ is a finite sum of vectors $\varphi_\alpha^\Sigma \otimes \varphi_\alpha^\mathbb{R}$, where $\varphi_\alpha^\Sigma \in \mathcal{P}_\alpha \mathsf{L}^2(\Sigma)$ and $\varphi_\alpha^\mathbb{R} \in \mathscr{D}_t^\mathbb{R}$.

For each $r > 0$, we define the auxiliary time $\tau_r^{\mathrm{free}}(\varphi)$ by

$$\tau_r^{\mathrm{free}}(\varphi) := \tfrac{1}{2}\Big\{ \int_{-\infty}^0 \mathrm{d}t \Big[\big\|F_r \mathrm{e}^{-itH_0}\varphi\big\|^2 - \big\|F_r \mathrm{e}^{-itH_0} S\varphi\big\|^2 \Big] + \int_0^\infty \mathrm{d}t \Big[\big\|F_r \mathrm{e}^{-itH_0} S\varphi\big\|^2 - \big\|F_r \mathrm{e}^{-itH_0}\varphi\big\|^2 \Big] \Big\}.$$

The supscript "free" makes reference to the fact that the formula for $\tau_r^{\mathrm{free}}(\varphi)$ involves only the free evolution of the vectors φ and $S\varphi$.

Lemma 2.2.2. *Suppose that the hypotheses 1 and 2 of Theorem 2.1.2 hold and let $r > 0$, $\varphi \in \mathscr{D}_0^\Omega$. Then*

- *(a) $\big\|F_r \mathrm{e}^{-itH_0}\varphi\big\|$ belongs to $\mathsf{L}^2(\mathbb{R}, \mathrm{d}t)$,*
- *(b) $\big\|F_r \mathrm{e}^{-itH_0} S\varphi\big\|$ belongs to $\mathsf{L}^2(\mathbb{R}, \mathrm{d}t)$,*
- *(c) $\big\|F_r \mathrm{e}^{-itH} W^- \varphi\big\|$ belongs to $\mathsf{L}^2(\mathbb{R}, \mathrm{d}t)$,*
- *(d) $\tau_r(\varphi)$ and $\tau_r^{\mathrm{free}}(\varphi)$ exist.*

Proof. Since $F_r = 1 \otimes \chi_{[-r,r]}(Q)$, the point (a) follows from Remark 2.2.1 and the local smoothness [Lav73, Thm. 1] of $\chi_{[-r,r]}(Q)$ with respect to P^2. Since S and $E^{H_0}(\cdot)$ commute, the statement (b) can be shown as (a). The point (c) follows from the intertwining relation $E^H(\cdot)W^\pm = W^\pm E^{H_0}(\cdot)$ and the fact that F_r is locally H-smooth on $(\nu_1, \infty) \setminus (\sigma_{\mathrm{p}}(H) \cup \mathcal{T})$. The last statement is a consequence of points (a), (b) and (c). □

The following result can be easily deduced from the proof of [AC87, Prop. 2].

Lemma 2.2.3. *Suppose that the hypotheses 1 and 2 of Theorem 2.1.2 hold and let $\varphi \in \mathscr{D}_0^\Omega$ be such that*

$$\big\|\big(W^- - 1\big)\,\mathrm{e}^{-itH_0}\varphi\big\| \in \mathsf{L}^1((-\infty, 0), \mathrm{d}t)$$

and

$$\big\|\big(W^+ - 1\big)\,\mathrm{e}^{-itH_0}S\varphi\big\| \in \mathsf{L}^1((0, \infty), \mathrm{d}t).$$

Then one has the equality

$$\lim_{r\to\infty} \tau_r(\varphi) = \lim_{r\to\infty} \tau_r^{\mathrm{free}}(\varphi). \tag{2.7}$$

We emphasize that the equation (2.7) should be interpreted as follows : if one of the two limits exists, then so does the other one, and the two limits are equal.

2.2.2 Spectral decomposition and trace-type operator

We now gather some results on the spectral transformation for H_0 and on the associated trace-type operator. We begin with the definition of the trace-type operator. $\mathcal{H}(\lambda)$ denotes the fibre at energy $\lambda \geq \nu_1$ in the spectral representation of H_0 :

$$\mathcal{H}(\lambda) := \bigoplus_{\alpha\in\mathbb{N}(\lambda)} \big\{\mathcal{P}_\alpha \mathsf{L}^2(\Sigma) \oplus \mathcal{P}_\alpha \mathsf{L}^2(\Sigma)\big\}\,,$$

where $\mathbb{N}(\lambda) := \{\alpha \in \mathbb{N} \setminus \{0\} : \nu_\alpha \leq \lambda\}$. Since $\mathcal{H}(\lambda)$ is naturally embedded in

$$\mathcal{H}(\infty) := \bigoplus_{\alpha\geq 1} \big\{\mathcal{P}_\alpha \mathsf{L}^2(\Sigma) \oplus \mathcal{P}_\alpha \mathsf{L}^2(\Sigma)\big\}\,,$$

we shall sometimes write $\mathcal{H}(\infty)$ instead of $\mathcal{H}(\lambda)$. For $\xi \in \mathbb{R}$, let $\gamma(\xi) : \mathscr{S}(\mathbb{R}) \to \mathbb{C}$ be the trace operator given by $\gamma(\xi)\varphi := \varphi(\xi)$. Then, for $\lambda \in (\nu_1,\infty)\setminus\mathcal{T}$, we define the trace-type operator $T(\lambda) : \mathsf{L}^2(\Sigma) \odot \mathscr{S}(\mathbb{R}) \to \mathcal{H}(\lambda)$ by

$$[T(\lambda)\varphi]_\alpha := (\lambda-\nu_\alpha)^{-1/4}\Big\{\big[\mathcal{P}_\alpha \otimes \gamma(-\sqrt{\lambda-\nu_\alpha})\big]\varphi, \big[\mathcal{P}_\alpha \otimes \gamma(\sqrt{\lambda-\nu_\alpha})\big]\varphi\Big\}. \quad (2.8)$$

In the next lemma we show some regularity properties of the operator $T(\lambda)$. The proof can be found in the appendix.

Lemma 2.2.4. *Let $t \in \mathbb{R}$. Then*

(a) For any $\lambda \in (\nu_1,\infty)\setminus\mathcal{T}$ and $s > 1/2$, the operator $T(\lambda)$ extends to an element of $\mathscr{B}\big(\mathsf{L}^2(\Sigma)\otimes\mathcal{H}^s_t(\mathbb{R}),\mathcal{H}(\infty)\big)$.

(b) For any $s > 1/2$, the function $T : (\nu_1,\infty)\setminus\mathcal{T} \to \mathscr{B}\big(\mathsf{L}^2(\Sigma)\otimes\mathcal{H}^s_t(\mathbb{R}),\mathcal{H}(\infty)\big)$ is locally Hölder continuous.

(c) For any $s > n+1/2$, $n \in \mathbb{N}$, the function $\lambda \mapsto T(\lambda)$ is n times continuously differentiable as a map from $(\nu_1,\infty)\setminus\mathcal{T}$ to $\mathscr{B}\big(\mathsf{L}^2(\Sigma)\otimes\mathcal{H}^s_t(\mathbb{R}),\mathcal{H}(\infty)\big)$.

We give now the spectral transformation for H_0 in terms of the operators $T(\lambda)$.

Proposition 2.2.5. *The mapping $\mathscr{U} : \mathcal{H} \to \int^\oplus_{[\nu_1,\infty)} \mathrm{d}\lambda\,\mathcal{H}(\lambda)$, defined by*

$$(\mathscr{U}\varphi)(\lambda) := 2^{-1/2}T(\lambda)(1\otimes\mathscr{F})\varphi \quad (2.9)$$

for all $\varphi \in \mathsf{L}^2(\Sigma)\odot\mathscr{S}(\mathbb{R})$, $\lambda \in (\nu_1,\infty)\setminus\mathcal{T}$, is unitary and

$$\mathscr{U} H_0 \mathscr{U}^* = \int^\oplus_{[\nu_1,\infty)} \mathrm{d}\lambda\,\lambda.$$

Proof. A direct calculation shows that $\|\mathscr{U}\varphi\| = \|\varphi\|$ for all $\varphi \in \mathsf{L}^2(\Sigma)\odot\mathscr{S}(\mathbb{R})$. Since $\mathsf{L}^2(\Sigma)\odot\mathscr{S}(\mathbb{R})$ is dense in $\mathcal{H}$, this implies that $\mathscr{U}$ is an isometry. Furthermore, for any $\psi \equiv \{\psi^-_\alpha(\lambda),\psi^+_\alpha(\lambda)\} \in \int^\oplus_{[\nu_1,\infty)} \mathrm{d}\lambda\,\mathcal{H}(\lambda)$, one can check that

$$\mathscr{U}^*\psi = (1\otimes\mathscr{F}^*)\,\widetilde{\psi} \qquad \text{where} \qquad \widetilde{\psi}(\cdot,\xi) := \begin{cases} \sqrt{2|\xi|}\sum_{\alpha\geq1}\psi^-_\alpha(\xi^2+\nu_\alpha) & \text{if} \quad \xi<0 \\ \sqrt{2|\xi|}\sum_{\alpha\geq1}\psi^+_\alpha(\xi^2+\nu_\alpha) & \text{if} \quad \xi\geq 0, \end{cases} \quad (2.10)$$

so that $\|\mathscr{U}^*\psi\| = \|\psi\|$. Hence $\mathscr{U}$ is unitary. The second statement follows by using (2.8) and (2.9). ☐

Since the scattering operator S commutes with H_0, it follows by Proposition 2.2.5 that S admits the direct integral decomposition

$$\mathscr{U} S \mathscr{U}^* = \int_{[\nu_1,\infty)}^{\oplus} \mathrm{d}\lambda\, S(\lambda),$$

where $S(\lambda)$ (the S-matrix at energy λ) is an operator acting unitarily in $\mathcal{H}(\lambda)$.

2.2.3 Existence theorem

In the present section we shall give the proof of Theorem 2.1.2. We first prove an asymptotic formula involving

$$D_0 := \tfrac{1}{2}\left(P^{-1}Q + QP^{-1}\right),$$

which is a well defined symmetric operator on $\mathscr{D}_1^{\mathbb{R}}$.

Proposition 2.2.6.

(a) *Suppose that the hypothesis 2 of Theorem 2.1.2 holds and let $\varphi \in \mathscr{D}_0^{\Omega}$. Then*

$$\tau_r^{\text{free}}(\varphi) = \tfrac{1}{2}\int_0^\infty \mathrm{d}t\, \big\langle S\varphi, \big[1 \otimes \big(\mathrm{e}^{itP^2}\chi_{[-r,r]}(Q)\mathrm{e}^{-itP^2} - \mathrm{e}^{-itP^2}\chi_{[-r,r]}(Q)\mathrm{e}^{itP^2}\big), S\big]\varphi\big\rangle.$$

(b) *For all $\varphi, \psi \in \mathscr{D}_2^{\mathbb{R}}$*

$$\lim_{r\to\infty}\int_0^\infty \mathrm{d}t\, \big\langle \varphi, \big[\mathrm{e}^{itP^2}\chi_{[-r,r]}(Q)\mathrm{e}^{-itP^2} - \mathrm{e}^{-itP^2}\chi_{[-r,r]}(Q)\mathrm{e}^{itP^2}\big]\psi\big\rangle = -\langle \varphi, D_0\psi\rangle. \tag{2.11}$$

(c) *Suppose that the hypothesis 2 of Theorem 2.1.2 holds and let $\varphi \in \mathscr{D}_2^{\Omega}$ be such that $S\varphi \in \mathscr{D}_2^{\Omega}$. Then*

$$\lim_{r\to\infty}\tau_r^{\text{free}}(\varphi) = -\tfrac{1}{2}\langle \varphi, S^*[1\otimes D_0, S]\varphi\rangle. \tag{2.12}$$

Proof. (a) Due to (2.6), one has the equality

$$\mathrm{e}^{itH_0}F_r\mathrm{e}^{-itH_0} = 1 \otimes \mathrm{e}^{itP^2}\chi_{[-r,r]}(Q)\mathrm{e}^{-itP^2}.$$

This together with the unitarity of the scattering operator implies the claim.

(b) (i) It is sufficient to prove (2.11) for $\varphi = \psi$, the case $\varphi \neq \psi$ being obtained by means of the polarization identity.

For any $f \in \mathsf{L}^\infty(\mathbb{R})$ and $t > 0$ one has [AJS77, Eq. (13.4)]

$$\mathrm{e}^{itP^2}f(Q)\mathrm{e}^{-itP^2} = Z_{1/4t}^* f(2tP) Z_{1/4t},$$

where $Z_\tau := \mathrm{e}^{i\tau Q^2}$. This together with the change of variables $\mu := r(2t)^{-1}$ and $\nu := (2r)^{-1}$ leads to the equality

$$\begin{aligned}\int_0^\infty \mathrm{d}t\, \big\langle \varphi, \big[\mathrm{e}^{itP^2}\chi_{[-r,r]}(Q)\mathrm{e}^{-itP^2} - \mathrm{e}^{-itP^2}\chi_{[-r,r]}(Q)\mathrm{e}^{itP^2}\big]\varphi\big\rangle \\ = \tfrac{1}{4}\int_0^\infty \frac{\mathrm{d}\mu}{\nu\mu^2}\big\langle \varphi, \big[Z_{\nu\mu}^*\chi_{[-\mu,\mu]}(P)Z_{\nu\mu} - Z_{\nu\mu}\chi_{[-\mu,\mu]}(P)Z_{\nu\mu}^*\big]\varphi\big\rangle.\end{aligned} \tag{2.13}$$

Hence the l.h.s. of (2.11) (for $\varphi = \psi$) can be written as

$$K_\infty(\varphi) := \lim_{\nu\searrow 0} \tfrac{1}{4}\int_0^\infty \frac{\mathrm{d}\mu}{\nu\mu^2}\,\big\langle\varphi,\big[Z^*_{\nu\mu}\chi_{[-\mu,\mu]}(P)Z_{\nu\mu} - \chi_{[-\mu,\mu]}(P) + \chi_{[-\mu,\mu]}(P) - Z_{\nu\mu}\chi_{[-\mu,\mu]}(P)Z^*_{\nu\mu}\big]\varphi\big\rangle. \tag{2.14}$$

(ii) To prove the statement, we shall show that one may interchange the limit and the integral in (2.14), by invoking the Lebesgue dominated convergence theorem. This will be done in (iii) below. If one assumes the result for the moment, then a direct calculation as in [AC87, Sec. 2] leads to the desired equality, that is

$$\begin{aligned}K_\infty(\varphi) &= \tfrac{1}{4}\int_0^\infty \frac{\mathrm{d}\mu}{\mu^2}\frac{\mathrm{d}}{\mathrm{d}\nu}\,\big\langle\varphi,\big[Z^*_{\nu\mu}\chi_{[-\mu,\mu]}(P)Z_{\nu\mu} - Z_{\nu\mu}\chi_{[-\mu,\mu]}(P)Z^*_{\nu\mu}\big]\,\varphi\big\rangle\Big|_{\nu=0}\\ &= -\,\langle\varphi, D_0\varphi\rangle\end{aligned}$$

if $\varphi \in \mathscr{D}_2^{\mathbb{R}}$.

(iii) It remains to prove the applicability of the Lebesgue dominated convergence theorem to (2.14). For this we rewrite (2.13) (which is equivalent to (2.14)) as

$$K_\infty(\varphi) = \lim_{\nu\searrow 0}\tfrac{1}{4}\int_0^\infty \frac{\mathrm{d}\mu}{\mu}\Big[\Big\langle\chi_{[-\mu,\mu]}(P)Z_{\nu\mu}\varphi, \frac{Z_{\nu\mu}-Z^*_{\nu\mu}}{\nu\mu}\,\varphi\Big\rangle + \Big\langle\frac{Z_{\nu\mu}-Z^*_{\nu\mu}}{\nu\mu}\,\varphi, \chi_{[-\mu,\mu]}(P)Z^*_{\nu\mu}\varphi\Big\rangle\Big]. \tag{2.15}$$

Since $\tau^{-1}(Z_\tau - Z_\tau^*)\varphi$ converges strongly to $2iQ^2\varphi$ as $\tau\to 0$, we may choose a number $\delta > 0$ such that $\|\tau^{-1}(Z_\tau - Z^*_\tau)\varphi\| \le 3\|Q^2\varphi\|$ for all $\tau\in[-\delta,\delta]$. We then have

$$\Big\|\tfrac{1}{\nu\mu}(Z_{\nu\mu}-Z^*_{\nu\mu})\varphi\Big\| \le \begin{cases}3\|Q^2\varphi\| & \text{if} \quad \nu\mu\le\delta\\ \frac{2}{\delta}\|\varphi\| & \text{if} \quad \nu\mu\ge\delta\,.\end{cases} \tag{2.16}$$

Let $\ell\in(0,1/2)$, then $|P|^{-\ell}\langle Q\rangle^{-2}$ belongs to $\mathscr{B}(\mathsf{L}^2(\mathbb{R}))$ (after exchanging the role of P and Q, this follows from the fact that $|Q|^{-\ell}$ is P^2-bounded [Amr81, Prop. 2.28]), and

$$|\mu^{-1}\xi|^\ell\chi_{[-\mu,\mu]}(\xi)\le\chi_{[-\mu,\mu]}(\xi)\le 1$$

for all $\xi\in\mathbb{R}$. Thus one has the estimate

$$\begin{aligned}\mu^{-1}\big\|\chi_{[-\mu,\mu]}(P)Z_{\pm\nu\mu}\varphi\big\| &= \mu^{\ell-1}\big\||\mu^{-1}P|^\ell\chi_{[-\mu,\mu]}(P)|P|^{-\ell}\langle Q\rangle^{-2}Z_{\pm\nu\mu}\langle Q\rangle^2\varphi\big\|\\ &\le \text{Const. }\mu^{\ell-1}\big\|\langle Q\rangle^2\varphi\big\|.\end{aligned} \tag{2.17}$$

Hence (2.16) and (2.17) imply that the integrand in (2.15) is bounded by a function in $\mathsf{L}^1_{\mathrm{loc}}((0,\infty),\mathrm{d}\mu)$, which is sufficient for applying the Lebesgue dominated convergence theorem on any finite interval $[0,\mu_0]$.

Since the case $\mu\to\infty$ can be treated as in [AC87, Sec. 2], this concludes the proof of the statement.

(c) This is a consequence of Remark 2.2.1 and points (a) and (b). ☐

Remark 2.2.7. *We know from Section 2.2.2 that $\mathcal{H}$ can be identified with the direct integral $\int^\oplus_{[\nu_1,\infty)}\mathrm{d}\lambda\,\mathcal{H}(\lambda)$, where H_0 acts as the multiplication operator by λ. So one may write $\varphi(\lambda)$ for the component of $\varphi\in\mathcal{H}$ at energy λ and $\langle\cdot,\cdot\rangle_{\mathcal{H}(\lambda)}$ for the scalar product in*

$\mathcal{H}(\lambda)$. A direct calculation using (2.8)–(2.10) shows that $1 \otimes D_0 = 2i\frac{\mathrm{d}}{\mathrm{d}\lambda}$ in the spectral representation of H_0. On the other hand $\varphi \in \mathcal{D}(1 \otimes D_0^2)$ if $\varphi \in \mathscr{D}_2^\Omega$. Therefore if $\varphi \in \mathscr{D}_2^\Omega$, then the function $\lambda \mapsto \varphi(\lambda)$ is continuously differentiable on each interval $(\nu_\alpha, \nu_{\alpha+1})$. As a consequence, if $\varphi \in \mathscr{D}_2^\Omega$ is such that $S\varphi \in \mathscr{D}_2^\Omega$, and if the function $\lambda \mapsto S(\lambda)$ is strongly continuously differentiable on the support of $\varphi(\cdot)$, then one gets from (2.12) the equalities

$$\lim_{r\to\infty} \tau_r^{\mathrm{free}}(\varphi) = -i\int_{\nu_1}^{\infty} \mathrm{d}\lambda \left\langle \varphi(\lambda), S(\lambda)^* \Big[\frac{\mathrm{d}S(\lambda)}{\mathrm{d}\lambda}\Big]\varphi(\lambda)\right\rangle_{\mathcal{H}(\lambda)} \equiv \langle \varphi, \tau_{\text{E-W}}\varphi\rangle . \quad (2.18)$$

Provided that (2.7) holds, (2.18) expresses the identity of the (global) time delay and the Eisenbud-Wigner time delay in waveguides.

Theorem 2.1.2 is a direct consequence of Lemma 2.2.2, Lemma 2.2.3, Proposition 2.2.6 and Remark 2.2.7.

Remark 2.2.8. *The S-matrix at energy λ can be written as the double sum*

$$S(\lambda) = \sum_{\beta,\alpha\in\mathbb{N}(\lambda)} S_{\beta\alpha}(\lambda),$$

where $S_{\beta\alpha}(\lambda) := [\mathscr{U}(\mathcal{P}_\beta \otimes 1)S(\mathcal{P}_\alpha \otimes 1)\mathscr{U}^*](\lambda)$. Therefore if φ_α is a vector in $(\mathcal{P}_\alpha \otimes 1)\mathcal{H}$ satisfying the hypotheses of Theorem 2.1.2, then a simple calculation shows that (2.18) is equivalent to

$$\lim_{r\to\infty} \tau^{\mathrm{free}}(\varphi_\alpha) = -i\int_{\nu_1}^{\infty} \mathrm{d}\lambda \left\langle \varphi_\alpha(\lambda), \sum_{\beta\in\mathbb{N}(\lambda)} S_{\beta\alpha}(\lambda)^* \Big[\frac{\mathrm{d}S_{\beta\alpha}(\lambda)}{\mathrm{d}\lambda}\Big]\varphi_\alpha(\lambda)\right\rangle_{\mathcal{H}(\lambda)} . \quad (2.19)$$

This equation admits a natural interpretation : if each subspace $(\mathcal{P}_\alpha \otimes 1)\mathcal{H}$ is seen as a channel Hilbert space, then (2.19) can be considered as a multichannel formulation in waveguides of the identity of the (global) time delay and the Eisenbud-Wigner time delay for an incoming state in channel α.

2.3 Time delay in waveguides : the short-range case

2.3.1 Short-range scattering in waveguides

In this section we collect some results on the scattering theory for the pair $\{H_0, H\}$ in the case $H := H_0 + V$, where V is a short-range potential satisfying the following condition :

Assumption 2.3.1. *V is a multiplication operator by a real-valued measurable function on Ω such that V defines a compact operator from $\mathcal{D}(H_0)$ to $\mathcal{H}$ and a bounded operator from $\mathsf{L}^2(\Sigma) \otimes \mathcal{H}^2(\mathbb{R})$ to $\mathsf{L}^2(\Sigma) \otimes \mathcal{H}_\kappa(\mathbb{R})$ for some $\kappa > 1$.*

By using duality, interpolation and the fact that V commutes with the operator $1 \otimes \langle Q\rangle^t$, $t \in \mathbb{R}$, one shows that V also defines a bounded operator from $\mathsf{L}^2(\Sigma) \otimes \mathcal{H}_t^{2s}(\mathbb{R})$ to $\mathsf{L}^2(\Sigma) \otimes \mathcal{H}_{t+\kappa}^{2(s-1)}(\mathbb{R})$ for any $s \in [0,1]$, $t \in \mathbb{R}$.

If V satisfies Assumption 2.3.1, then the operator H is selfadjoint on $\mathcal{D}(H) = \mathcal{D}(H_0)$, $(H + i)^{-1} - (H_0 + i)^{-1}$ is compact and $\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(H_0) = [\nu_1, \infty)$. In order to get more informations on H, we shall apply the conjugate operator method. We refer to

[ABG96] for the definitions of the regularity classes appearing in the sequel, and for more explanations on the conjugate operator method.

For $\varepsilon \in (0,1)$, we choose a function $\vartheta \in C_0^\infty((\varepsilon,\infty))$ and define $F:\mathbb{R}\to\mathbb{R}$ by

$$F(x) := \begin{cases} \frac{1}{2x}\vartheta(x^2) & \text{if} \quad x \in (-\infty,-\sqrt{\varepsilon}) \cup (\sqrt{\varepsilon},\infty) \\ 0 & \text{otherwise.} \end{cases}$$

We first introduce the operator $A_{\shortparallel} := F(P)Q + \frac{i}{2}F'(P)$ acting on $\mathscr{S}(\mathbb{R})$. $A_{\shortparallel}$ has the following properties [ABG96, Lemma 7.6.4] : $A_{\shortparallel}$ is essentially selfadjoint, the group $\{e^{i\tau A_{\shortparallel}}\}_{\tau\in\mathbb{R}}$ leaves $\mathcal{D}(-\Delta^{\mathbb{R}}) = \mathcal{H}^2(\mathbb{R})$ invariant, $-\Delta^{\mathbb{R}}$ is of class $C^\infty(A_{\shortparallel})$ and $A_{\shortparallel}$ is strictly conjugate to $-\Delta^{\mathbb{R}}$ on $(-\infty,0)\cup I_\vartheta$, where $I_\vartheta := \{u \in (\varepsilon,\infty) : \vartheta(u) = 1\}$. Now let $A := 1 \otimes A_{\shortparallel}$. It turns out that H_0 has many regularity properties with respect to A, namely (see [BG92, Sec. 3]) $\{e^{i\tau A}\}_{\tau\in\mathbb{R}}$ is a C_0-group in $\mathcal{D}(H_0)$, H_0 is of class $C^\infty(A)$ and A is strictly conjugate to H_0 on $(-\infty,\nu_1)\cup J_\vartheta$, where J_ϑ is a bounded open set in $(\nu_1,\infty)\setminus\mathcal{T}$ depending on I_ϑ. The exact nature of J_ϑ can be explicitly deduced from that of I_ϑ by using the formula [BG92, Eq. (3.8)], which relates the Mourre estimate for $-\Delta^{\mathbb{R}}$ to the Mourre estimate for H_0. In our case it is enough to note that, given any compact set K in $\mathbb{R}\setminus\mathcal{T}$, there exist $\varepsilon\in(0,1)$ and $\vartheta\in C_0^\infty((\varepsilon,\infty))$ such that K is contained in $(-\infty,\nu_1)\cup J_\vartheta$.

Now we prove that V also satisfies regularity conditions with respect to A. Given an operator B in $\mathcal{H}$ and a Hilbert space $\mathscr{G}\subset\mathcal{H}$, we write $\mathcal{D}(B;\mathscr{G}) := \{\varphi\in\mathcal{D}(B)\cap\mathscr{G} : B\varphi\in\mathscr{G}\}$ for the domain of B in $\mathscr{G}$.

Lemma 2.3.2. *Let V satisfy Assumption 2.3.1. Then*

(a) V is of class $\mathscr{C}^{1,1}(A;\mathcal{D}(H_0),\mathcal{D}(H_0)^*)$.

(b) The operators $[H_0,A]$ and $[H,A]$, which a priori only belong to $\mathscr{B}(\mathcal{D}(H_0),\mathcal{D}(H_0)^*)$, are such that $[H_0,A]\in\mathscr{B}(\mathcal{D}(H_0))$ and $[H,A]\in\mathscr{B}(\mathcal{D}(H_0),\mathcal{H})$.

Proof. (a) We use the criterion [ABG96, Thm. 7.5.8] to prove the statement. The three conditions needed for that theorem are obtained in points (i), (ii) and (iii) below.

(i) Let $\Lambda := 1\otimes\langle Q\rangle$. Since $\{e^{i\tau\langle Q\rangle}\}_{\tau\in\mathbb{R}}$ is a polynomially bounded C_0-group in $\mathcal{H}^2(\mathbb{R})$ [ABG96, Sec. 7.6.3], a direct calculation using the tensorial decomposition of H_0 (see Remark 2.2.1) shows that $\{e^{i\tau\Lambda}\}_{\tau\in\mathbb{R}}$ is a polynomially bounded C_0-group in $\mathcal{D}(H_0)$.

(ii) Since $\{e^{i\tau A}\}_{\tau\in\mathbb{R}}$ is a C_0-group in $\mathcal{D}(H_0)$, there exists $r>0$ such that $-ir$ belongs to the resolvent set of A (considered as an operator in $\mathcal{D}(H_0)$). In particular, the operator $(A+ir)^{-1} = -i\int_0^\infty d\tau\, e^{-r\tau}e^{i\tau A}$ is a homeomorphism from $\mathcal{D}(H_0)$ onto $\mathcal{D}(A;\mathcal{D}(H_0))$ (both domains being endowed with their natural graph topology). Therefore any set $\mathscr{E}$ of the form $(A+ir)^{-1}\mathscr{D}$, with $\mathscr{D}$ dense in $\mathcal{D}(H_0)$, is dense in $\mathcal{D}(A;\mathcal{D}(H_0))$. Let us take $\mathscr{D} := \{\varphi_\alpha\}\odot\mathscr{S}(\mathbb{R})$, where $\{\varphi_\alpha\}$ is the set of eigenvectors of $-\Delta_{\mathrm{D}}^{\Sigma}$ (since $H_0\restriction\mathscr{D}$ is essentially selfadjoint, $\mathscr{D}$ is dense in $\mathcal{D}(H_0)$). A vector ψ in $\mathscr{E}$ is of the form $\psi = -i\sum_{\alpha\le\mathrm{Const.}}\varphi_\alpha\otimes\int_0^\infty d\tau\, e^{-r\tau}e^{i\tau A_{\shortparallel}}\eta_\alpha$, where $(\varphi_\alpha,\eta_\alpha)\in\{\varphi_\alpha\}\times\mathscr{S}(\mathbb{R})$ and the integral converges in $\mathcal{H}^2(\mathbb{R})$. Since $\langle Q\rangle^{-2}\in\mathscr{B}\big(\mathsf{L}^2(\mathbb{R})\big)$ and $A_{\shortparallel}\eta_\alpha\in\mathscr{S}(\mathbb{R})$, the vector

$$\widetilde{\psi} := -i\sum_{\alpha\le\mathrm{Const.}}\varphi_\alpha\otimes\int_0^\infty d\tau\, e^{-r\tau}\langle Q\rangle^{-2}e^{i\tau A_{\shortparallel}}A_{\shortparallel}\eta_\alpha$$

belongs to $\mathcal{H}$. Furthermore $\widetilde{\psi} = \Lambda^{-2}A\psi$ and $\Lambda^{-2}A\psi\in\mathcal{D}(H_0)$. Since $e^{i\tau A_{\shortparallel}}\eta_\alpha\in\mathscr{S}(\mathbb{R})$ [ABG96, Prop. 4.2.4], one can use commutator expansions to get the equality

$$\big\|\langle Q\rangle^{-2}e^{i\tau A_{\shortparallel}}A_{\shortparallel}\eta_\alpha - S_1\langle Q\rangle^{-1}e^{i\tau A_{\shortparallel}}\eta_\alpha\big\|_{\mathcal{H}^2(\mathbb{R})} = 0$$

for some operator $S_1 \in \mathscr{B}\left(\mathcal{H}^2(\mathbb{R})\right)$. This implies that

$$\left\|\Lambda^{-2}A\psi - (1\otimes S_1)\Lambda^{-1}\psi\right\|_{\mathcal{D}(H_0)} = 0 \tag{2.20}$$

for $\psi \in \mathscr{E}$. Since $1\otimes S_1$ and Λ^{-1} belong to $\mathscr{B}(\mathcal{D}(H_0))$ and $\mathscr{E}$ is dense in $\mathcal{D}(A;\mathcal{D}(H_0))$, (2.20) even holds for $\psi \in \mathcal{D}(A;\mathcal{D}(H_0))$. Thus, for each $\psi \in \mathcal{D}\left(A^2;\mathcal{D}(H_0)\right)$, one gets

$$\left\|\Lambda^{-2}A^2\psi - (1\otimes S_1)\Lambda^{-1}A\psi\right\|_{\mathcal{D}(H_0)} = \left\|(\Lambda^{-2}A)A\psi - (1\otimes S_1)\Lambda^{-1}A\psi\right\|_{\mathcal{D}(H_0)} = 0.$$

Using an argument similar to the one leading to (2.20), one shows that

$$\left\|\Lambda^{-1}A\psi - (1\otimes S_2)\psi\right\|_{\mathcal{D}(H_0)} = 0$$

for each $\psi \in \mathcal{D}(A;\mathcal{D}(H_0))$ and some operator $S_2 \in \mathscr{B}\left(\mathcal{H}^2(\mathbb{R})\right)$. Therefore

$$\left\|\Lambda^{-2}A^2\psi - (1\otimes S_1S_2)\psi\right\|_{\mathcal{D}(H_0)} = 0$$

for each $\psi \in \mathcal{D}\left(A^2;\mathcal{D}(H_0)\right)$. This implies that $\Lambda^{-2}A^2 : \mathcal{D}\left(A^2;\mathcal{D}(H_0)\right) \to \mathcal{D}(H_0)$ extends to an element of $\mathscr{B}(\mathcal{D}(H_0))$.

(iii) The short-range decay of V required in [ABG96, Eq. (7.5.29)] follows from Assumption 2.3.1.

(b) We have $[H_0, A] \in \mathscr{B}(\mathcal{D}(H_0))$ because $[H_0, iA] = 1\otimes\vartheta(P^2)$ [ABG96, Lemma 7.6.4], [BG92, Sec. 3]. Since $H = H_0+V$, it remains to show that $[V, A] \in \mathscr{B}(\mathcal{D}(H_0), \mathcal{H})$. This follows by using the fact that V is bounded from $\mathsf{L}^2(\Sigma)\otimes\mathcal{H}_t^{2s}(\mathbb{R})$ to $\mathsf{L}^2(\Sigma)\otimes\mathcal{H}_{t+\kappa}^{2(s-1)}(\mathbb{R})$ for any $s\in[0,1]$, $t\in\mathbb{R}$, and the fact that A is bounded from $\mathsf{L}^2(\Sigma)\otimes\mathcal{H}_t^s(\mathbb{R})$ to $\mathsf{L}^2(\Sigma)\otimes\mathcal{H}_{t-1}^s(\mathbb{R})$ for any $s,t\in\mathbb{R}$. ☐

Since $\{e^{i\tau A}\}_{\tau\in\mathbb{R}}$ leaves $\mathcal{D}(H_0)$ invariant and H_0 is of class $C^\infty(A)$, Lemma 2.3.3.(a) implies that H is of class $\mathscr{C}^{1,1}(A)$ [ABG96, Thm. 6.3.4.(b)]. This has the following consequence.

Lemma 2.3.3. *Let V satisfy Assumption 2.3.1. Then A is conjugate to H on $(-\infty,\nu_1)\cup J_\vartheta$.*

Proof. Since H_0 and H are of class $\mathscr{C}^{1,1}(A)$, $(H+i)^{-1}-(H_0+i)^{-1}$ is compact and A is strictly conjugate to H_0 on $(-\infty,\nu_1)\cup J_\vartheta$, the claim follows by [ABG96, Thm. 7.2.9]. ☐

Now we can prove limiting absorption principles for H_0 and H, and state spectral properties of H. If $\mathscr{G}^\mu := \mathcal{D}(H_0^\mu)$, $\mu\in\mathbb{R}$, then the limiting absorption principles can be expressed in terms of the Banach space $\mathcal{K} := \left(\mathscr{G}^{-1/2}\cap\mathcal{D}(A;\mathscr{G}^{-1}), \mathscr{G}^{-1/2}\right)_{1/2,1}$ defined by real interpolation [ABG96, Chap. 2]. We emphasize that $\mathcal{K}$ contains $\mathsf{L}^2(\Sigma)\otimes\mathcal{H}_t^{-1}(\mathbb{R})$ for any $t>1/2$, which is shown in the appendix.

Theorem 2.3.4. *Let V satisfy Assumption 2.3.1. Then*

(a) H has no singularly continuous spectrum.

(b) The eigenvalues of H in $\sigma(H)\setminus\mathcal{T}$ are of finite multiplicity and can accumulate at points of $\mathcal{T}$ only.

(c) The limit $\lim_{\varepsilon\searrow 0}(H_0-\lambda\mp i\varepsilon)^{-1}$, resp. $\lim_{\varepsilon\searrow 0}(H-\lambda\mp i\varepsilon)^{-1}$, exists in the weak topology of $\mathscr{B}(\mathcal{K},\mathcal{K}^*)$ uniformly in λ on each compact subset of $\mathbb{R}\setminus\mathcal{T}$, resp. $\mathbb{R}\setminus(\sigma_{\rm p}(H)\cup\mathcal{T})$.*

Proof. The operator H is of class $\mathscr{C}^{1,1}(A)$ and A is conjugate to H on $(-\infty, \nu_1) \cup J_\vartheta$ by Lemma 2.3.4. Furtheremore, given any compact set K in $\mathbb{R} \setminus \mathcal{T}$, there exist $\varepsilon \in (0,1)$ and $\vartheta \in C_0^\infty((\varepsilon, \infty))$ such that K is contained in $(-\infty, \nu_1) \cup J_\vartheta$. Therefore the assertions (a) and (b) follow by the conjugate operator method [ABG96, Cor. 7.2.11 & Thm. 7.4.2]. Due to Lemma 2.3.3.(b) and the regularity properties of H_0 and H with respect to A, the limiting absorption principles are obtained via [ABG96, Thm. 7.5.2]. □

Corollary 2.3.5. *Let V satisfy Assumption 2.3.1. Then*

(a) If T belongs to $\mathscr{B}\left(\mathsf{L}^2(\Sigma) \otimes \mathcal{H}^1_{-t}(\mathbb{R}), \mathcal{H}\right)$ for some $t > 1/2$, then T is locally H_0-smooth (resp. H-smooth) on $\mathbb{R} \setminus \mathcal{T}$ (resp. $\mathbb{R} \setminus (\sigma_\mathrm{p}(H) \cup \mathcal{T})$).

(b) The wave operators $W^\pm$ exist and are complete.

Proof. (a) Let $\mathscr{E} := \mathsf{L}^2(\Sigma) \otimes \mathcal{H}_t^{-1}(\mathbb{R})$. Since $\mathscr{E} \subset \mathcal{D}(H_0)^*$ densely, and $\mathscr{E} \subset \mathcal{K}$, it is enough to verify the remaining hypothesis of [ABG96, Prop. 7.1.3.(b)] on $\mathscr{E}$ to prove the statement. Let $\mathscr{E}^{*\circ}$ be the closure of $\mathcal{D}(H_0)$ in $\mathscr{E}^*$, equipped with the norm of $\mathscr{E}^*$. Clearly $\mathscr{E}^{*\circ} \subset \mathscr{E}^*$. Furthermore, since $\mathcal{D}(H_0)$ is dense in $\mathscr{E}^*$, we also have $\mathscr{E}^* \subset \mathscr{E}^{*\circ}$. Therefore $\mathscr{E}^* = \mathscr{E}^{*\circ}$. By taking the adjoint, this leads to $\mathscr{E} = (\mathscr{E}^{*\circ})^*$.

(b) By the point (a), $V_1 := 1 \otimes \langle Q\rangle^{-\kappa/2} \langle P\rangle$ is locally H_0-smooth on $\mathbb{R} \setminus \mathcal{T}$ and $V_2 := (1 \otimes \langle Q\rangle^{\kappa/2} \langle P\rangle^{-1})V$ is locally H-smooth on $\mathbb{R} \setminus (\sigma_\mathrm{p}(H) \cup \mathcal{T})$. Since $\sigma_\mathrm{p}(H) \cup \mathcal{T}$ is countable and $\langle \varphi, V\psi\rangle = \langle V_1\varphi, V_2\psi\rangle$ for all $\varphi, \psi \in \mathcal{D}(H_0)$, one can conclude by applying the smooth perturbation theory [RS78, Corollary to Thm. XIII.31]. □

Under Assumption 2.3.1 one could also find optimal spaces where the analogue of the limiting absorption principles of Theorem 2.3.4.(c) holds in norm. The following particular result is sufficient for us. If $t > 1/2$, then the boundary values

$$R^{H_0}(\lambda \pm i0) := \lim_{\varepsilon \searrow 0} (H_0 - \lambda \mp i\varepsilon)^{-1}, \quad \lambda \in \mathbb{R} \setminus \mathcal{T},$$

and

$$R^H(\lambda \pm i0) := \lim_{\varepsilon \searrow 0} (H - \lambda \mp i\varepsilon)^{-1}, \quad \lambda \in \mathbb{R} \setminus (\sigma_\mathrm{p}(H) \cup \mathcal{T}),$$

exist in $\mathscr{B}\big(\mathsf{L}^2(\Sigma) \otimes \mathcal{H}_t(\mathbb{R}), \mathsf{L}^2(\Sigma) \otimes \mathcal{H}_{-t}(\mathbb{R})\big)$ (see [BGM93, Thm. 4.13]). In the rest of the section we study the norm differentiability of the function $\lambda \mapsto S(\lambda)$, which relies on the differentiability of the function $\lambda \mapsto R^H(\lambda \pm i0)$.

Lemma 2.3.6. *Let $t > n + 1/2$, $n \in \mathbb{N}$. Let V satisfy Assumption 2.3.1 with $\kappa > n + 1$. Then $\lambda \mapsto R^H(\lambda + i0)$ is n times continuously differentiable as a map from $(\nu_1, \infty) \setminus (\sigma_\mathrm{p}(H) \cup \mathcal{T})$ to $\mathscr{B}\big(\mathsf{L}^2(\Sigma) \otimes \mathcal{H}_t(\mathbb{R}), \mathsf{L}^2(\Sigma) \otimes \mathcal{H}_{-t}(\mathbb{R})\big)$.*

Proof. Since H_0 is of class $C^\infty(A)$ and $\mathsf{L}^2(\Sigma) \otimes \mathcal{H}_t(\mathbb{R}) \subset \mathcal{D}(\langle A\rangle^t)$, we have the following result [BGS, Sec. 1.7]. For each $\lambda \in (\nu_1, \infty) \setminus \mathcal{T}$ and $k \leq n$, the boundary values $\lim_{\varepsilon \searrow 0} (H_0 - \lambda \mp i\varepsilon)^{-k-1}$ exist in $\mathscr{B}\big(\mathsf{L}^2(\Sigma) \otimes \mathcal{H}_t(\mathbb{R}), \mathsf{L}^2(\Sigma) \otimes \mathcal{H}_{-t}(\mathbb{R})\big)$. Furthermore $\lambda \mapsto R^{H_0}(\lambda \pm i0)$ is k times continuously differentiable as a map from $(\nu_1, \infty) \setminus \mathcal{T}$ to $\mathscr{B}\big(\mathsf{L}^2(\Sigma) \otimes \mathcal{H}_t(\mathbb{R}), \mathsf{L}^2(\Sigma) \otimes \mathcal{H}_{-t}(\mathbb{R})\big)$ with

$$\tfrac{\mathrm{d}^k}{\mathrm{d}\lambda^k} R^{H_0}(\lambda \pm i0) = k! \lim_{\varepsilon \searrow 0} (H_0 - \lambda \mp i\varepsilon)^{-k-1}.$$

Thus one can apply the inductive method of [JN92, Lemma 4.3] to infer the result for H from the one for H_0. □

In the following lemma we prove the usual formula for the S-matrix.

Lemma 2.3.7. *Let V satisfy Assumption 2.3.1. Then for each $\lambda \in (\nu_1,\infty)\setminus(\sigma_{\rm p}(H)\cup\mathcal{T})$, one has the equality*

$$S(\lambda)=1-i\pi T(\lambda)\,(1\otimes\mathscr{F})\left[1-VR^H(\lambda+i0)\right]V\,(1\otimes\mathscr{F}^*)\,T(\lambda)^*. \tag{2.21}$$

Proof. The claim is a consequence of the stationary method [Kur73, Thm. 6.3] applied to the pair $\{H_0,H\}$. Therefore we simply verify the principal hypotheses of that theorem.

The total Hamiltonian admits the factorization $H=H_0+V_1V_2$ where V_1 is the H_0-compact operator $1\otimes\langle Q\rangle^{-\kappa/2}$ (see [KT04, Lemma 2.1]) and V_2 is the (maximal) operator associated to $1\otimes\langle Q\rangle^{\kappa/2}V$. Moreover, since $T:(\nu_1,\infty)\setminus\mathcal{T}\to\mathscr{B}\big(\mathsf{L}^2(\Sigma)\otimes\mathcal{H}^s_t(\mathbb{R}),\mathcal{H}(\infty)\big)$ is locally Hölder continuous for each $t\in\mathbb{R}$, $s>1/2$, the functions $T(\cdot;V_j):(\nu_1,\infty)\setminus\mathcal{T}\to\mathscr{B}\left(\mathcal{H},\mathcal{H}(\infty)\right)$, $j=1,2$, defined by

$$T(\lambda;V_j)\varphi:=\left(\mathscr{U}V_j^*\varphi\right)(\lambda),$$

are locally Hölder continuous. □

Finally we have the following result on the norm differentiability of the function $\lambda\mapsto S(\lambda)$.

Proposition 2.3.8. *Let V satisfy Assumption 2.3.1 with $\kappa>n+1$, $n\in\mathbb{N}$. Then $\lambda\mapsto S(\lambda)$ is n times continuously differentiable as a map from $(\nu_1,\infty)\setminus(\sigma_{\rm p}(H)\cup\mathcal{T})$ to $\mathcal{H}(\infty)$.*

Proof. Due to (2.21) and Lemmas 2.2.4.(c) and 2.3.6, all operators in the expression for $S(\lambda)$ are n times continuously norm differentiable. Then a direct calculation as in the proof of [Jen81, Thm. 3.5] implies the claim. □

2.3.2 Existence theorem

To illustrate Theorem 2.1.2, we verify in this section the existence of the (global) time delay in the case $H:=H_0+V$, where V satisfies Assumption 2.3.1 with $\kappa>4$. To begin with we prove two technical lemmas in relation with the hypotheses of Theorem 2.1.2.

Lemma 2.3.9. *If V satisfies Assumption 2.3.1 with $\kappa>2$ and $\varphi\in\mathscr{D}^\Omega_\tau$ for some $\tau>2$, then*

$$\left\|\left(W^--1\right)\mathrm{e}^{-itH_0}\varphi\right\|\in\mathsf{L}^1((-\infty,0),\mathrm{d}t) \tag{2.22}$$

and

$$\left\|\left(W^+-1\right)\mathrm{e}^{-itH_0}\varphi\right\|\in\mathsf{L}^1((0,\infty),\mathrm{d}t). \tag{2.23}$$

Proof. For $\varphi\in\mathscr{D}^\Omega_\tau$ and $t\in\mathbb{R}$, we have (see the proof of [Jen81, Lemma 4.6])

$$\left(W^--1\right)\mathrm{e}^{-itH_0}\varphi=-i\mathrm{e}^{-itH}\int_{-\infty}^t\mathrm{d}s\,\mathrm{e}^{isH}V\mathrm{e}^{-isH_0}\varphi,$$

where the integral is strongly convergent. Hence to prove (2.22) it is enough to show that

$$\int_{-\infty}^{-\delta}\mathrm{d}t\int_{-\infty}^t\mathrm{d}s\left\|V\mathrm{e}^{-isH_0}\varphi\right\|<\infty \tag{2.24}$$

for some $\delta>0$. We know from Remark 2.2.1 that $\varphi=\sum_{\alpha\le\text{Const.}}\varphi^\Sigma_\alpha\otimes\varphi^{\mathbb{R}}_\alpha$, where $\varphi^\Sigma_\alpha\in\mathcal{P}_\alpha\mathsf{L}^2(\Sigma)$ and $\varphi^{\mathbb{R}}_\alpha\in\mathscr{D}^{\mathbb{R}}_\tau$. Thus there exists $\eta\in C^\infty_0((0,\infty))$ such that $1\otimes\eta(P^2)\varphi=\varphi$.

Furthermore, if $\zeta := \min\{\kappa, \tau\}$, then $\| \langle Q\rangle^\zeta \varphi_\alpha^{\mathbb{R}}\| < \infty$ and $V(1 \otimes \langle P\rangle^{-2} \langle Q\rangle^\zeta)$ belongs to $\mathscr{B}(\mathcal{H})$ due to Assumption 2.3.1. This implies that

$$\begin{aligned}\|V\mathrm{e}^{-isH_0}\varphi\| &\le \sum_{\alpha \le \text{Const.}} \Big\| V(1 \otimes \langle P\rangle^{-2} \langle Q\rangle^\zeta) \\ &\qquad \cdot \big[\varphi_\alpha^\Sigma \otimes \langle Q\rangle^{-\zeta} \langle P\rangle^2 \eta(P^2)\mathrm{e}^{-isP^2} \langle Q\rangle^{-\zeta} \langle Q\rangle^\zeta \varphi_\alpha^{\mathbb{R}}\big]\Big\| \\ &\le \text{Const.} \| \langle Q\rangle^{-\zeta} \langle P\rangle^2 \eta(P^2)\mathrm{e}^{-isP^2} \langle Q\rangle^{-\zeta} \|.\end{aligned}$$

For each $\varepsilon > 0$, it follows from [ACS87, Lemma 9] that there exists a constant $\mathrm{c} > 0$ such that $\|V\mathrm{e}^{-isH_0}\varphi\| \le \mathrm{c}\,(1 + |s|)^{-\zeta+\varepsilon}$. Since $\zeta > 2$, this implies (2.24). The proof of (2.23) is similar. ☐

Let $\mathscr{E}$ be the finite span of vectors $\varphi \in \mathcal{H}$ of the form $\{\varphi(\lambda)\} = \{\rho(\lambda)h(\lambda)\}$ in the spectral representation of H_0, where $\rho : (\nu_1, \infty) \to \mathbb{C}$ is three times continuously differentiable and has compact support in $(\nu_1, \infty) \setminus (\sigma_{\mathrm{p}}(H) \cup \mathcal{T})$, and $\lambda \mapsto h(\lambda) \in \mathcal{H}(\lambda)$ is λ-independent on each interval $(\nu_\alpha, \nu_{\alpha+1})$. Clearly the set $\mathscr{E}$ is dense in $\mathcal{H}$. Furthermore one has the following inclusions.

Lemma 2.3.10.

(a) $\mathscr{E}$ is contained in $\mathscr{D}_3^\Omega$.

(b) Let V satisfy Assumption 2.3.1 with $\kappa > 4$. Then $S\mathscr{E}$ is contained in $\mathscr{D}_3^\Omega$.

Proof. (a) Let $\varphi \in \mathscr{E}$. It is clear that there exists a compact set J in $(\nu_1, \infty) \setminus (\sigma_{\mathrm{p}}(H) \cup \mathcal{T})$ such that $E^{H_0}(J)\varphi = \varphi$. Thus, in order to show that $\varphi \in \mathscr{D}_3^\Omega$, one has to verify that $\varphi \in \mathsf{L}^2(\Sigma) \otimes \mathcal{H}_3(\mathbb{R}) = \mathcal{D}(1 \otimes Q^3)$.

Let $\psi \in \mathsf{L}^2(\Sigma) \odot \mathscr{S}(\mathbb{R})$. Then, using (2.8)–(2.10), we obtain

$$\big[\mathscr{U}(1 \otimes Q^3)\psi\big]_\alpha(\lambda) = \{ig_\alpha^-(\lambda), -ig_\alpha^+(\lambda)\}, \tag{2.25}$$

where

$$\begin{aligned}g_\alpha^\pm(\lambda) := \tfrac{3}{8}(\lambda - \nu_\alpha)^{-3/2}(\mathscr{U}\psi)_\alpha^\pm(\lambda) + \tfrac{3}{2}(\lambda - \nu_\alpha)^{-1/2}\tfrac{\mathrm{d}}{\mathrm{d}\lambda}(\mathscr{U}\psi)_\alpha^\pm(\lambda) \\ + 18(\lambda - \nu_\alpha)^{1/2}\tfrac{\mathrm{d}^2}{\mathrm{d}\lambda^2}(\mathscr{U}\psi)_\alpha^\pm(\lambda) + 8(\lambda - \nu_\alpha)^{3/2}\tfrac{\mathrm{d}^3}{\mathrm{d}\lambda^3}(\mathscr{U}\psi)_\alpha^\pm(\lambda).\end{aligned} \tag{2.26}$$

The r.h.s. of (2.25)–(2.26) with $\psi \in \mathsf{L}^2(\Sigma) \odot \mathscr{S}(\mathbb{R})$ replaced by $\varphi \in \mathscr{E}$ defines a vector $\widetilde{\varphi}$ belonging to $\int_{[\nu_1,\infty)}^\oplus \mathrm{d}\lambda\, \mathcal{H}(\lambda)$. Thus, using partial integration for the terms involving derivatives with respect to λ, one finds that

$$\big|\big\langle(1 \otimes Q^3)\psi, \varphi\big\rangle\big| = |\langle\mathscr{U}\psi, \widetilde{\varphi}\rangle| \le \text{Const.}\|\psi\|$$

for all $\psi \in \mathsf{L}^2(\Sigma) \odot \mathscr{S}(\mathbb{R})$, $\varphi \in \mathscr{E}$. Since $(1 \otimes Q^3) \restriction \mathsf{L}^2(\Sigma) \odot \mathscr{S}(\mathbb{R})$ is essentially selfadjoint, this implies that $\varphi \in \mathcal{D}(1 \otimes Q^3)$.

(b) By Proposition 2.3.8 the function $\lambda \mapsto S(\lambda)$ is three times continuously norm differentiable. Thus the argument in point (a) with φ replaced by $S\varphi$ gives the result. ☐

Theorem 2.3.11. *Let $H := H_0 + V$, where V satisfies Assumption 2.3.1 with $\kappa > 4$. Then, for each $\varphi \in \mathscr{E}$, $\tau_r(\varphi)$ exists for all $r > 0$ and $\tau_r(\varphi)$ converges as $r \to \infty$ to a finite limit equal to $\langle\varphi, \tau_{\text{E-W}}\varphi\rangle$.*

Proof. We apply Theorem 2.1.2. The hypotheses 1 and 2 of that theorem are satisfied due to Corollary 2.3.5, and the hypotheses on $\varphi \in \mathscr{E}$ follow from Lemmas 2.3.9 and 2.3.10. Since the function $\lambda \mapsto S(\lambda)$ is strongly continuously differentiable on $(\nu_1, \infty) \setminus (\sigma_{\mathrm{p}}(H) \cup \mathcal{T})$, the proof is complete. ☐

Appendix

Proof of Lemma 2.2.4. (a) Fix $\lambda \in (\nu_1, \infty) \setminus \mathcal{T}$ and let $\varphi \in \mathsf{L}^2(\Sigma) \odot \mathscr{S}(\mathbb{R})$. Choose $f \in C_0^\infty(\mathbb{R})$ such that

$$\big[1 \otimes \gamma(\pm\sqrt{\lambda - \nu_\alpha})\big]\varphi = \big[1 \otimes \gamma(\pm\sqrt{\lambda - \nu_\alpha})\big][1 \otimes f(Q)]\varphi$$

for each $\alpha \in \mathbb{N}(\lambda)$. Then we get

$$\|T(\lambda)\varphi\|^2_{\mathcal{H}(\infty)} \leq \text{Const.} \sum_{\alpha \in \mathbb{N}(\lambda)} \Big\{ \Big\| \big[1 \otimes \gamma(-\sqrt{\lambda - \nu_\alpha}) f(Q)\big]\varphi \Big\|^2_{\mathsf{L}^2(\Sigma)} + \Big\| \big[1 \otimes \gamma(\sqrt{\lambda - \nu_\alpha}) f(Q)\big]\varphi \Big\|^2_{\mathsf{L}^2(\Sigma)} \Big\}.$$

Since $\gamma(\pm\sqrt{\lambda - \nu_\alpha})$ extends to an element of $\mathscr{B}(\mathcal{H}^s(\mathbb{R}), \mathbb{C})$ [Kur78, Thm. 2.4.2] and $f(Q)$ is bounded from $\mathcal{H}^s_t(\mathbb{R})$ to $\mathcal{H}^s(\mathbb{R})$, this implies that

$$\|T(\lambda)\varphi\|^2_{\mathcal{H}(\infty)} \leq \text{Const.} \|\varphi\|^2_{\mathsf{L}^2(\Sigma)\otimes\mathcal{H}^s_t(\mathbb{R})}.$$

(b) Let K be a compact set in $(\nu_1, \infty) \setminus \mathcal{T}$. Choose $\delta = \delta(K) > 0$ such that λ_1 and λ_2 belong to the same interval $(\nu_\alpha, \nu_{\alpha+1})$ whenever $\lambda_1, \lambda_2 \in K$ and $|\lambda_1 - \lambda_2| < \delta$. Let $\varphi \in \mathsf{L}^2(\Sigma) \odot \mathscr{S}(\mathbb{R})$. Due to the point (a), it is enough to show that there exists $\zeta > 0$ such that

$$\|\,[T(\lambda_1) - T(\lambda_2)]\,\varphi\|_{\mathcal{H}(\infty)} \leq \text{Const.} |\lambda_1 - \lambda_2|^\zeta \, \|\varphi\|_{\mathsf{L}^2(\Sigma)\otimes\mathcal{H}^s_t(\mathbb{R})} \tag{2.27}$$

if $\lambda_1, \lambda_2 \in K$ and $|\lambda_1 - \lambda_2| < \delta$.

Choose $f \in C_0^\infty(\mathbb{R} \setminus \{0\})$ such that

$$(\lambda - \nu_\alpha)^{-1/4}\big[1 \otimes \gamma(\pm\sqrt{\lambda - \nu_\alpha})\big]\varphi = \big[1 \otimes \gamma(\pm\sqrt{\lambda - \nu_\alpha})\big]\big[1 \otimes |Q|^{-1/2} f(Q)\big]\varphi$$

for each $\lambda \in K$, $\alpha \in \mathbb{N}(\sup K)$. Then we get

$$\begin{aligned}
&\|[T(\lambda_1) - T(\lambda_2)]\varphi\|^2_{\mathcal{H}(\infty)} \\
&\leq \text{Const.} \sum_{\alpha \in \mathbb{N}(\lambda_1)} \Big\{ \Big\| 1 \otimes \big[\gamma(-\sqrt{\lambda_1 - \nu_\alpha}) - \gamma(-\sqrt{\lambda_2 - \nu_\alpha})\big]\big[1 \otimes \sqrt{Q} f(Q)\big]\varphi \Big\|^2_{\mathsf{L}^2(\Sigma)} \\
&\qquad + \Big\| 1 \otimes \big[\gamma(\sqrt{\lambda_1 - \nu_\alpha}) - \gamma(\sqrt{\lambda_2 - \nu_\alpha})\big]\big[1 \otimes \sqrt{Q} f(Q)\big]\varphi \Big\|^2_{\mathsf{L}^2(\Sigma)} \Big\}.
\end{aligned}$$

Since the function $\mathbb{R} \ni \xi \mapsto \gamma(\xi) \in \mathscr{B}(\mathcal{H}^s(\mathbb{R}), \mathbb{C})$ is Hölder continuous [Kur78, Thm. 2.4.2] and $|Q|^{-1/2} f(Q)$ is bounded from $\mathcal{H}^s_t(\mathbb{R})$ to $\mathcal{H}^s(\mathbb{R})$, this implies (2.27).

(c) The proof is similar to that of [Jen81, Lemma 3.3]. □

Proof of the embedding $\mathsf{L}^2(\Sigma) \otimes \mathcal{H}^{-1}_t(\mathbb{R}) \subset \mathcal{K}$ *for any* $t > 1/2$. Since $\mathsf{L}^2(\Sigma) \otimes \mathcal{H}^{-1}(\mathbb{R}) \subset \mathscr{G}^{-1/2}$ and $\mathcal{D}(A; \mathscr{G}^{-1/2}) \subset \mathscr{G}^{-1/2} \cap \mathcal{D}(A; \mathscr{G}^{-1})$, we have

$$\big(\mathcal{D}[A; \mathsf{L}^2(\Sigma) \otimes \mathcal{H}^{-1}(\mathbb{R})], \mathsf{L}^2(\Sigma) \otimes \mathcal{H}^{-1}(\mathbb{R})\big)_{1/2,1} \subset \mathcal{K}$$

due to [ABG96, Cor. 2.6.3]. Then we obtain that

$$\big(\mathcal{D}[A; \mathsf{L}^2(\Sigma) \otimes \mathcal{H}^{-1}(\mathbb{R})], \mathsf{L}^2(\Sigma) \otimes \mathcal{H}^{-1}(\mathbb{R})\big)_{\mu,2} \subset \mathcal{K}$$

for any $\mu < 1/2$, by using [ABG96, Thm. 3.4.3.(a)]. Since $\mathsf{L}^2(\Sigma)\otimes\mathcal{H}^{-1}_1(\mathbb{R}) \subset \mathcal{D}[A; \mathsf{L}^2(\Sigma) \otimes \mathcal{H}^{-1}(\mathbb{R})]$, this leads to the embedding

$$\big(\mathsf{L}^2(\Sigma) \otimes \mathcal{H}^{-1}_1(\mathbb{R}), \mathsf{L}^2(\Sigma) \otimes \mathcal{H}^{-1}(\mathbb{R})\big)_{\mu,2} \subset \mathcal{K}$$

[ABG96, Cor. 2.6.3]. Now, by using [Aub00, Thm. 12.6.1] and [LP64, Thm. VII(I.1)], we get the isometry $\mathsf{L}^2(\Sigma)\otimes\mathcal{H}^{-1}_{1-\mu}(\mathbb{R}) \simeq \big(\mathsf{L}^2(\Sigma) \otimes \mathcal{H}^{-1}_1(\mathbb{R}), \mathsf{L}^2(\Sigma) \otimes \mathcal{H}^{-1}(\mathbb{R})\big)_{\mu,2}$. Therefore $\mathsf{L}^2(\Sigma) \otimes \mathcal{H}^{-1}_t(\mathbb{R}) \subset \mathcal{K}$ for any $t > 1/2$. □

Troisième partie

Spectre essentiel dans un guide d’ondes quantique courbe

Chapitre 1

Résumé

Considérons une particule non relativiste évoluant librement dans un guide d'ondes courbe infini $\Gamma \subset \mathbb{R}^d$, $d \geq 2$, de section transverse $\omega \subset \mathbb{R}^{d-1}$ bornée, connexe et constante. Le guide d'ondes Γ est supposé asymptotiquement droit (voir la figure 1.1). Le système physique est décrit dans l'espace de Hilbert $\mathsf{L}^2(\Gamma)$ par l'hamiltonien de Dirichlet $-\Delta_{\mathrm{D}}^{\Gamma}$.

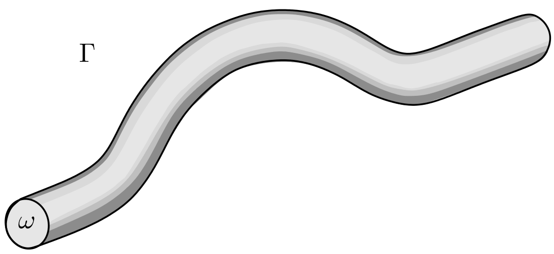

FIG. 1.1 – Exemple de guide d'ondes courbe dans $\mathbb{R}^3$

Dans l'article qui suit, nous étudions les propriétés du spectre essentiel de l'opérateur $-\Delta_{\mathrm{D}}^{\Gamma}$. Si les courbures caractérisant le guide d'ondes Γ satisfont certaines hypothèses de décroissance à l'infini, nous localisons le spectre essentiel de $-\Delta_{\mathrm{D}}^{\Gamma}$, nous prouvons que $-\Delta_{\mathrm{D}}^{\Gamma}$ ne possède pas de spectre singulier continu et nous montrons que, en dehors du spectre discret $\mathcal{T}$ de $-\Delta_{\mathrm{D}}^{\omega}$, les valeurs propres de $-\Delta_{\mathrm{D}}^{\Gamma}$ sont de multiplicité finie et ne présentent pas de points d'accumulation. La démonstration repose sur le fait que, sous certaines conditions, le domaine Γ est difféomorphe au cylindre infini $\Omega := \mathbb{R} \times \omega$. Dans ce cas, le laplacien de Dirichlet négatif $-\Delta_{\mathrm{D}}^{\Gamma}$ dans $\mathsf{L}^2(\Gamma)$ est unitairement équivalent à un opérateur elliptique dans $\mathsf{L}^2(\Omega)$ du type

$$H := -\partial_i G^{ij} \partial_j + V \tag{1.1}$$

sujet aux conditions aux bords de Dirichlet. Les dérivées partielles ∂_i font référence aux composantes de $x \in \Omega$, $G \equiv (G^{ij})$ est une fonction de Ω à valeurs dans les matrices

$d \times d$ rélles symétriques et V est un potentiel réel borné. Ainsi, pour déterminer la nature spectrale du laplacien de Dirichlet négatif $-\Delta_{\mathrm{D}}^{\Gamma}$, il suffit d'étudier le spectre de l'opérateur (1.1) correspondant.

Nous donnons maintenant une description plus détaillée de nos résultats. Considérons une courbe régulière $p \in C^{\infty}(\mathbb{R};\mathbb{R}^d)$ paramétrisée par la longueur d'arc s. Supposons que cette courbe possède un référentiel de Frenet C^{∞} approprié. Notons $\kappa_i \in C^{\infty}(\mathbb{R};\mathbb{R})$, $i \in \{1,\ldots,d-1\}$, les courbures associées. Nous construisons alors le guide d'onde Γ comme un tube infini de section ω autour de la courbe p (voir la figure 1.2). Si nous

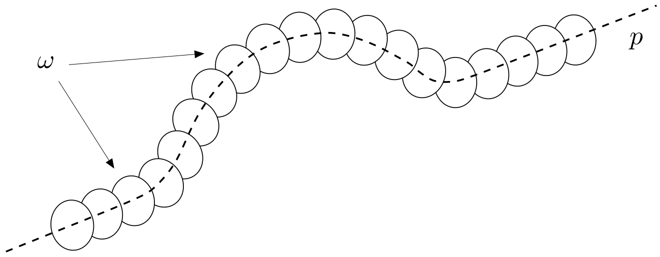

FIG. 1.2 – Exemple de guide d'ondes courbe dans $\mathbb{R}^3$ construit autour d'une courbe p

supposons que toutes les courbures κ_i s'annulent à l'infini et prescrivons certaines vitesses de décroissance, alors l'opérateur $A := 1 \otimes D$ (voir la section 1.4) est conjugué sur $\mathbb{R} \setminus \mathcal{T}$ à l'hamiltonien H (1.1) unitairement équivalent au laplacien négatif $-\Delta_{\mathrm{D}}^{\Gamma}$. De ceci découle l'existence d'un principe d'absorption limite pour H sur $\mathbb{R} \setminus \mathcal{T}$. Comme l'opérateur H et le laplacien négatif $-\Delta_{\mathrm{D}}^{\Gamma}$ sont unitairement équivalents, nous en déduisons le théorème suivant (par souci de simplicité, nous présentons le résultat dans le cas $d = 2$) :

Théorème 1.0.1 ($d = 2$). *Soit Γ comme ci-dessus pour $d = 2$ avec $\omega := (-a, a)$ pour un $a > 0$ et $\kappa := \kappa_1$. Soit $\mathcal{T}$ l'ensemble des valeurs propres de $-\Delta_{\mathrm{D}}^{\omega}$ avec $\nu_1 := \inf \mathcal{T}$. Supposons*

1. *$\kappa(s)$, $\ddot{\kappa}(s) \to 0$ quand $|s| \to \infty$,*
2. *il existe $\vartheta \in (0, 1]$ tel que $\dot{\kappa}$ et $\dddot{\kappa}$ décroissent comme $|s|^{-(1+\vartheta)}$ quand $|s| \to \infty$.*

Alors, on a

(a) *Le spectre essentiel de $-\Delta_{\mathrm{D}}^{\Gamma}$ coïncide avec l'intervalle $[\nu_1, \infty)$.*

(b) *L'opérateur $-\Delta_{\mathrm{D}}^{\Gamma}$ n'a pas de spectre singulier continu.*

(c) *Les valeurs propres de $-\Delta_{\mathrm{D}}^{\Gamma}$ dans $\mathbb{R} \setminus \mathcal{T}$ sont de multiplicité finie et ne peuvent s'accumuler qu'en les points de l'ensemble $\mathcal{T}$.*

Ce travail met en exergue la similitude qui existe entre d'une part l'évolution libre d'une particule sur une variété riemannienne courbe et d'autre part l'évolution de la même particule dans l'espace euclidien sous la contrainte d'un hamiltonien du type (1.1). En particulier, tout porte à croire que le théorème 1.0.1 doit demeurer vrai sous des hypothèses beaucoup moins contraignantes sur κ, *i.e.* des assomptions telles que l'opérateur H unitairement équivalent à $-\Delta_{\mathrm{D}}^{\Gamma}$ puisse être considéré comme une perturbation à courte portée ou à longue portée de l'opérateur $-\Delta$ dans Ω. Par contre, si κ converge vers une valeur non nulle à l'infini, la similitude mentionnée plus haut laisse supposer que le traitement perturbatif employé dans ce travail ne peut pas fournir de résultats. En effet, dans ce cas, l'opérateur H est un opérateur anisotrope[1] dont l'analyse spectrale ne peut être effectuée qu'au prix d'un changement radical de méthode [Ric05].

CE TRAVAIL A ÉTÉ EFFECTUÉ EN COLLABORATION AVEC DAVID KREJČIŘÍK, DE L'INSTITUT DE PHYSIQUE NUCLÉAIRE DE REZ. UN ARTICLE INTITULÉ *"The nature of the essential spectrum in curved quantum waveguides"* A ÉTÉ PUBLIÉ DANS *J. Phys. A : Math. Gen.* ***37*** *(2004), no. 20, 5449-5466*.

[1] Nous considérons ici qu'un opérateur de H de la forme (1.1) est anisotrope si la matrice (G^{ij}) ne converge pas vers la matrice identité vers l'infini ou si le potentiel V ne tend pas vers 0 à l'infini.

Chapitre 2

The nature of the essential spectrum in curved quantum waveguides

Abstract

We study the nature of the essential spectrum of the Dirichlet Laplacian in tubes about infinite curves embedded in Euclidean spaces. Under suitable assumptions about the decay of curvatures at infinity, we prove the absence of singular continuous spectrum and state properties of possible embedded eigenvalues. The argument is based on Mourre conjugate operator method developed for acoustic multistratified domains by Benbernou in [Ben98] and Dermenjian *et al.* in [DDI98]. As a technical preliminary, we carry out a spectral analysis for Schrödinger-type operators in straight Dirichlet tubes. We also apply the result to the strips embedded in abstract surfaces.

2.1 Introduction

A strong physical motivation to study the Dirichlet Laplacian in infinitely stretched tubular regions comes from the fact it constitutes a reasonable model for the Hamiltonian of a non-relativistic quantum particle in mesoscopic systems called *quantum waveguides* [DE95, LCM99, Hur00]. Since there exists a close relation between spectral and scattering properties of Hamiltonians, one is naturally interested in carrying out the spectral analysis of the Laplacian in order to understand the quantum dynamics in waveguides. For instance, the crucial step in most proofs of asymptotic completeness is to show that the Hamiltonian has no singular continuous spectrum [RS78]. The Laplacian in a tube has attracted considerable attention since it was shown in [EŠ89] that there may be discrete eigenvalues in curved waveguides. However, a detailed analysis of the essential part of the spectrum has been left aside up to now. The purpose of the present paper is to fill in this gap.

The usual model for a curved quantum waveguide, which we adopt in this paper, is as follows. Let $s \mapsto p(s)$ be an infinite unit-speed smooth curve in $\mathbb{R}^d$, $d \geq 2$ (the physical cases corresponding to $d = 2, 3$). Assuming that the curve possesses an appropriate smooth Frenet frame $\{e_1, \ldots, e_d\}$ (*cf.* Assumption 2.3.1), the i^{th} curvature κ_i of p, $i \in \{1, \ldots, d-1\}$, is a smooth function of the arc-length parameter $s \in \mathbb{R}$. Given a bounded open connected set ω in $\mathbb{R}^{d-1}$ with the centre of mass at the origin, we identify the configuration space Γ of the waveguide with a tube of cross-section ω about p, namely :

$$\Gamma := \mathscr{L}(\mathbb{R} \times \omega), \qquad \mathscr{L}(s, u^2, \ldots, u^d) := p(s) + u^\mu \mathcal{R}_\mu^{\ \nu}(s) e_\nu(s), \tag{2.1}$$

where μ, ν are summation indices taking values in $\{2, \ldots, d\}$ and $(\mathcal{R}_\mu^{\ \nu})$ is a family of rotation matrices in $\mathbb{R}^{d-1}$. In this paper, we choose the rotations in such a way that (s, u), with $u := (u^2, \ldots, u^d)$, are orthogonal "coordinates" (*cf.* Section 2.3.1) due to the technical simplicity. It should be stressed here that while the shape of the tube Γ is not influenced by a special choice of $(\mathcal{R}_\mu^{\ \nu})$ provided ω is circular, this may no longer be true for a general cross-section. We make the hypotheses (Assumption 2.3.3) that κ_1 is bounded, $a\|\kappa_1\|_\infty < 1$, with $a := \sup_{u\in\omega} |u|$, and Γ does not overlap itself so that the tube can be globally parameterised by (s, u). Our object of interest is the Dirichlet Laplacian associated with the tube, *i.e.* ,

$$-\Delta_{\mathrm{D}}^{\Gamma} \qquad \text{on} \qquad \mathsf{L}^2(\Gamma). \tag{2.2}$$

If p is a straight line, *i.e.* , all $\kappa_i = 0$, then Γ may be identified with the straight tube $\Omega := \mathbb{R} \times \omega$. In that case, it is easy to see that the spectrum of (2.2) is purely *absolutely continuous* and equal to the interval $[\nu_1, \infty)$, where ν_1 denotes the first eigenvalue of the Dirichlet Laplacian in the cross-section ω.

On the other hand, if p is non-trivially curved and straight asymptotically, in the sense that the curvature κ_1 vanishes at infinity, then the essential spectrum of (2.2) remains equal to $[\nu_1, \infty)$. However, there are always *discrete eigenvalues* below ν_1. When $d = 2$, the latter was proved for the first time in [EŠ89] for a rapidly decaying curvature and sufficiently small a. Numerous subsequent studies improved and generalised this initial result [GJ92, RB95, DE95, Kre03, KK, CDFK]. The generalisation to tubes of circular cross-section in $\mathbb{R}^3$ was done in [GJ92] (see also [DE95]) and the case of any dimension $d \geq 2$ and arbitrary cross-section can be found in [CDFK]. Let us also mention that the discrete spectrum may be generated by other local perturbations of the straight tube Ω (see, *e.g.*, [BGRS97, EV97, BEGK01]), but in the bent-tube case the phenomenon is of a purely quantum origin because there are no classical closed trajectories, apart from those given by a zero measure set of initial conditions in the phase space.

The main goal of the present work is a thorough analysis of the *essential spectrum* of (2.2). In particular, we find sufficient conditions which guarantee that the essential spectrum of a curved tube "does not differ too much" from the straight case (for simplicity, we present here our results only for $d = 2$, see Theorem 2.3.9 for the d-dimensional case) :

Theorem 2.1.1 (*d*=2). *Let Γ be as above for $d = 2$ ($\kappa := \kappa_1$) and $\mathcal{T} := \{n^2\nu_1\}_{n=1}^\infty$ with $\nu_1 := \pi^2/(2a)^2$ (the set of eigenvalues of the Dirichlet Laplacian in the 1-dimensional cross-section ω). Suppose*

1. $\kappa(s), \ddot{\kappa}(s) \longrightarrow 0$ *as* $|s| \to \infty$,
2. $\exists \vartheta \in (0, 1]$ *s.t.* $\dot{\kappa}(s), \dddot{\kappa}(s) = \mathcal{O}\left(|s|^{-(1+\vartheta)}\right)$.

Then

(i) $\sigma_{\rm ess}\left(-\Delta_{\rm D}^{\Gamma}\right) = [\nu_1, \infty)$,
(ii) $\sigma_{\rm sc}\left(-\Delta_{\rm D}^{\Gamma}\right) = \varnothing$,
(iii) $\sigma_{\rm p}\left(-\Delta_{\rm D}^{\Gamma}\right) \cup \mathcal{T}$ *is closed and countable,*
(iv) $\sigma_{\rm p}\left(-\Delta_{\rm D}^{\Gamma}\right) \setminus \mathcal{T}$ *is composed of finitely degenerated eigenvalues which can accumulate at points of* $\mathcal{T}$ *only*.

To prove this theorem (and the general Theorem 2.3.9), we use the conjugate operator method introduced by [Mou81] E. Mourre and lastly developed by [ABG96] W. Amrein *et al.* Notice that the set $\mathcal{T}$ plays a role analogous to the set of *thresholds* in the Mourre theory of N-body Schrödinger operators [CFKS87].

Actually, the property (i) holds true whenever the first curvature vanishes at infinity, without assuming any decay of the derivatives (they may not even exist), see [KK] for $d = 2$ and [CDFK] for the general case. Our second result (ii) can be compared only with [DEŠ95] (see also [DEM98]), where the problem of resonances is investigated for $d = 2$. Assuming that there exists $\vartheta \in (0,1]$ such that $\kappa(s), \dot\kappa(s)^2, \ddot\kappa(s) = \mathcal{O}\big(|s|^{-(1+\vartheta)}\big)$, the authors proved the absence of singular continuous spectrum as a consequence of the completeness of wave operators obtained by standard smooth perturbation methods of scattering theory. Notice that our and their results are independent. Indeed, while we need to require a faster decay of $\dot\kappa$ and also impose a condition on $\dddot\kappa$, our decay assumptions on κ and $\ddot\kappa$ are on the contrary much weaker. Our other spectral results (iii) and (iv) (and (ii) for $d \geq 3$) are new.

The organisation of this paper is as follows. In Section 2.2, we consider the Schrödinger-type operator

$$H := -\partial_i G^{ij} \partial_j + V \qquad \text{on} \qquad \mathcal{H}(\Omega) := \mathsf{L}^2(\Omega), \tag{2.3}$$

subject to Dirichlet boundary conditions, i and j being summation indices taking values in $\{1, \dots, d\}$, $G \equiv (G^{ij})$ a real symmetric matrix-valued measurable function on Ω and V the multiplication operator by a real-valued measurable function on Ω. We make Assumption 2.2.1 and Assumption 2.2.2 stated below. Adapting the approach of [Ben98, DDI98] to non-zero V and G different from a multiple of the identity, we study the nature of the essential spectrum of the operator H. In particular, we prove the absence of singular continuous spectrum and state properties of possible embedded eigenvalues. The result is contained in Theorem 2.2.18 and is of independent interest. In Section 2.3, we apply it to the case of curved tubes (2.1). Using the diffeomorphism $\mathscr{L} : \Omega \to \Gamma$ and a unitary transformation (ideas which go back to [EŠ89]), we cast the Laplacian (2.2) into a unitarily equivalent operator of the form (2.3) for which Theorem 2.2.18 can be used. The obtained spectral results can be found in Theorem 2.3.9 (the general version of Theorem 2.1.1 above). Finally, in Section 2.4, we similarly investigate the essential spectrum of the Dirichlet Laplacian in an infinite strip in an abstract two-dimensional Riemannian manifold of curvature K. The general result is contained in Theorem 2.4.4, while the case of flat strips, *i.e.* , with $K = 0$, is summarised in Theorem 2.4.5 (the latter involves the curved strips in $\mathbb{R}^2$ as a special case).

For the conjugate operator method and notation used in Section 2.2, the reader is referred to [ABG96] and particularly to short well-arranged reviews of the abstract theory in [Ben98, Sec. 2] or [DDI98, Sec. 1]. A more detailed geometric background for Section 2.3 and Section 2.4 can be found in [Kli78, CDFK] and [Gra90, Kre03], respectively.

We use the standard component notation of tensor analysis throughout the paper. In particular, the repeated indices convention is adopted henceforth, the range of indices being $1, \dots, d$ for Latin and $2, \dots, d$ for Greek. The indices are associated in a natural way with the components of $x \in \mathbb{R} \times \omega$. The partial derivative w.r.t. x^i is often denoted by a comma with the index i. The brackets $(\cdot)$ are used in order to distinguish a matrix from its coefficients. The symbols δ_{ij} and δ^{ij} are reserved for the components of the identity matrix 1.

2.2 Schrödinger-type operators in straight tubes

2.2.1 Preliminaries

Let ω be an (arbitrary) bounded open connected set in $\mathbb{R}^{d-1}$, $d \geq 2$, and consider the straight tube $\Omega := \mathbb{R} \times \omega$. Our object of interest in this section is the operator given formally by (2.3), subject to Dirichlet boundary conditions. In addition to the basic properties required for the matrix G and function V, we make the following assumptions.

Assumption 2.2.1.

1. $\exists C_\pm \in (0,\infty)$ *s.t.* $C_- 1 \leq G(x) \leq C_+ 1$ *for a.e.* $x \in \Omega$,
2. $\forall i,j \in \{1,\dots,d\}$, $\lim_{R\to\infty} \operatorname*{ess\,sup}_{x \in (\mathbb{R}\setminus[-R,R])\times\omega} \left|G^{ij}(x) - \delta^{ij}\right| = 0$,
3. $\exists \vartheta_1 \in (0,1], C \in (0,\infty)$ *s.t.* $\left(\left|G^{ij}_{,1}(x)\right|\right) \leq C\langle x^1\rangle^{-(1+\vartheta_1)} 1$ *for a.e.* $x \in \Omega$,
4. $G^{1i}_{,i} \in L^\infty(\Omega)$.

Here $\langle\cdot\rangle := \left(1 + |\cdot|^2\right)^{1/2}$ and the inequalities must be understood in the sense of matrices.

Assumption 2.2.2.

1. $V \in \mathsf{L}^\infty(\Omega)$,
2. $\lim_{R\to\infty} \operatorname*{ess\,sup}_{x \in (\mathbb{R}\setminus[-R,R])\times\omega} |V(x)| = 0$,
3. $\exists \vartheta_2 \in (0,1], C \in (0,\infty)$ *s.t.* $|V_{,1}(x)| \leq C\langle x^1\rangle^{-(1+\vartheta_2)}$ *for a.e.* $x \in \Omega$.

Let us fix some notations. We write $\mathcal{H}^\nu(\Omega)$ and $\mathcal{H}^\nu_0(\Omega)$, $\nu \in \mathbb{R}$, for the usual Sobolev spaces [Ada75]. Given two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, we denote by $\mathscr{B}(\mathcal{H}_1,\mathcal{H}_2)$, respectively $\mathcal{K}(\mathcal{H}_1,\mathcal{H}_2)$, the set of bounded, respectively compact, operators from $\mathcal{H}_1$ to $\mathcal{H}_2$. We also define $\mathscr{B}(\mathcal{H}_1) := \mathscr{B}(\mathcal{H}_1,\mathcal{H}_1)$ and $\mathcal{K}(\mathcal{H}_1) := \mathcal{K}(\mathcal{H}_1,\mathcal{H}_1)$. We denote by $\mathcal{H}_1^*$ the topological antidual of $\mathcal{H}_1$. We write $(\cdot,\cdot)$ for the inner product in $\mathcal{H}(\Omega)$ and $\|\cdot\|$ for the norm in $\mathcal{H}(\Omega)$ and $\mathscr{B}(\mathcal{H}(\Omega))$.

We now give a meaning to the formal expression (2.3). We start by introducing the sesquilinear form Q_0 on $\mathcal{H}(\Omega)$ defined by

$$Q_0(\varphi,\psi) := \left(\varphi_{,i}, \delta^{ij}\psi_{,j}\right), \qquad \varphi,\psi \in \mathcal{D}(Q_0) := \mathcal{H}^1_0(\Omega), \tag{2.4}$$

which is densely defined, symmetric, non-negative and closed. Consequently, there exists a unique self-adjoint operator H_0 associated with it, which is just the Dirichlet Laplacian $-\Delta^\Omega_{\mathrm{D}}$ on $\mathsf{L}^2(\Omega)$. We have

$$H_0\psi = -\Delta\psi, \qquad \psi \in \mathcal{D}(H_0) = \left\{\psi \in \mathcal{H}^1_0(\Omega) \,:\, \Delta\psi \in \mathcal{H}(\Omega)\right\}.$$

We consider H as an operator obtained by perturbing the free Hamiltonian H_0. Since the matrix G is uniformly positive and bounded by Assumption 2.2.1.1, the sesquilinear form

$(\varphi, \psi) \mapsto \big(\varphi_{,i}, G^{ij}\psi_{,j}\big)$ defined on $\mathcal{D}(Q_0) \times \mathcal{D}(Q_0)$ is also densely defined, symmetric, non-negative and closed. At the same time, the potential V is supposed to be bounded by Assumption 2.2.2.1, which means that the sesquilinear form Q defined by

$$Q(\varphi, \psi) := \big(\varphi_{,i}, G^{ij}\psi_{,j}\big) + (\varphi, V\psi)\,, \qquad \varphi, \psi \in \mathcal{D}(Q) := \mathcal{H}_0^1(\Omega)\,, \tag{2.5}$$

gives rise to a semi-bounded self-adjoint operator H. Using the representation theorem [Kat95, Chap. VI, Thm. 2.1] and the fact that V is bounded (recall also Assumption 2.2.1.1), one may check that

$$\mathcal{D}(H) = \big\{\psi \in \mathcal{H}_0^1(\Omega) \,:\, \partial_i G^{ij}\partial_j\psi \in \mathcal{H}(\Omega)\big\}\,,$$

where the derivatives must be interpreted in the distributional sense, and that H is acting as in (2.3) on its domain.

For any $z \in \mathbb{C} \setminus \sigma(H_0)$, respectively $z \in \mathbb{C} \setminus \sigma(H)$, let $R_0(z) := (H_0 - z)^{-1}$, respectively $R(z) := (H - z)^{-1}$.

2.2.2 Localisation of the essential spectrum

The Dirichlet Laplacian $-\Delta_{\mathrm{D}}^{\omega}$ on $\mathsf{L}^2(\omega)$, *i.e.* , the operator associated with

$$q(\varphi, \psi) := (\varphi_{,\mu}, \delta^{\mu\nu}\psi_{,\nu})\,, \qquad \varphi, \psi \in \mathcal{D}(q) := \mathcal{H}_0^1(\omega)\,,$$

has a purely discrete spectrum consisting of eigenvalues $\nu_1 < \nu_2 \leq \nu_3 \leq \ldots$ with $\nu_1 > 0$. We set $\mathcal{T} := \{\nu_n\}_{n=1}^{\infty}$. Since H_0 is naturally decoupled in the following way :

$$H_0 = -\Delta^{\mathbb{R}} \otimes 1 + 1 \otimes (-\Delta_{\mathrm{D}}^{\omega}) \qquad \text{on} \qquad \mathsf{L}^2(\mathbb{R}) \otimes \mathsf{L}^2(\omega)\,,$$

where "$\otimes$" denote the closed tensor product, 1 the identity operators on appropriate spaces and $-\Delta^{\mathbb{R}}$ the Laplacian on $\mathsf{L}^2(\mathbb{R})$, one has

$$\sigma(H_0) = \sigma_{\mathrm{ess}}(H_0) = [\nu_1, \infty). \tag{2.6}$$

In order to prove that (under our assumptions) H possesses the same essential spectrum, we need the following lemma.

Lemma 2.2.3. *Let $\varphi \in C_0^{\infty}(\mathbb{R})$ and set $\phi := \varphi \otimes 1$ on Ω. Then, as a multiplication operator, $\phi \in \mathcal{K}\big(\mathcal{D}(H_0), \mathcal{H}_0^1(\Omega)\big)$.*

Proof. Since

$$\phi = H_0^{-1/2} H_0^{1/2} \phi H_0^{-1} H_0$$

in $\mathscr{B}\big(\mathcal{D}(H_0), \mathcal{H}_0^1(\Omega)\big)$, $H_0 \in \mathscr{B}\left(\mathcal{D}(H_0), \mathcal{H}(\Omega)\right)$ and $H_0^{-1/2} \in \mathscr{B}\big(\mathcal{H}(\Omega), \mathcal{H}_0^1(\Omega)\big)$, it is enough to prove that $H_0^{1/2}\phi H_0^{-1} \in \mathcal{K}\left(\mathcal{H}(\Omega)\right)$. However,

$$\begin{aligned} H_0^{1/2}\phi H_0^{-1} &= H_0^{-1/2}\left[H_0, \phi\right] H_0^{-1} + H_0^{-1/2}\phi \\ &= -H_0^{-1/2}\left(2\phi_{,1}\partial_1 + \phi_{,11}\right) H_0^{-1} + H_0^{-1/2}\phi, \end{aligned} \tag{2.7}$$

where each term on the r.h.s. is in $\mathcal{K}\left(\mathcal{H}(\Omega)\right)$. Let us demonstrate it for the first term. Since $\partial_1 H_0^{-1} \in \mathscr{B}\left(\mathcal{H}(\Omega)\right)$, it is sufficient to prove that $H_0^{-1/2}\phi_{,1} \in \mathcal{K}\left(\mathcal{H}(\Omega)\right)$. Let $z_1 \in (-\infty, 0)$ and $z_2 \in (-\infty, \nu_1)$ be such that $z_1 + z_2 = 0$. Define $R_{\shortparallel}(z_1) := \big(-\Delta^{\mathbb{R}} - z_1\big)^{-1}$

and $R_\perp(z_2) := (-\Delta^\omega_{\mathrm{D}} - z_2)^{-1}$. Then, using some standard results on tensor products of operators [KR86, Chap. 11], one can write

$$H_0^{-1/2}\phi_{,1} = H_0^{-1/2}\big[R_{\shortparallel}^{-1/4}(z_1) \otimes R_\perp^{-1/4}(z_2)\big]\big[R_{\shortparallel}^{1/4}(z_1)\varphi_{,1} \otimes R_\perp^{1/4}(z_2)\big]$$

where $\varphi_{,1}$ is viewed as a multiplication operator in $\mathsf{L}^2(\mathbb{R})$. The third factor on the r.h.s. is in $\mathcal{K}(\mathcal{H}(\Omega))$ because $-\Delta^\omega_{\mathrm{D}}$ has a compact resolvent and $R_{\shortparallel}^{1/4}(z_1)\varphi_{,1} \in \mathcal{K}\left(\mathsf{L}^2(\mathbb{R})\right)$ by [ABG96, Thm. 4.1.3]. The remaining factors can be rewritten as

$$\Psi(X_1, X_2) := (X_1 + X_2)^{-1/2} X_1^{1/4} X_2^{1/4}$$

with $X_1 := \left(-\Delta^{\mathbb{R}} - z_1\right) \otimes 1$ and $X_2 := 1 \otimes (-\Delta^\omega_{\mathrm{D}} - z_2)$ (both self-adjoint and mutually commuting). So, one can estimate

$$\|\Psi(X_1, X_2)\| \le \sup_{x_1, x_2 \in (0,\infty)} (x_1 + x_2)^{-1/2}(x_1 x_2)^{1/4} < \infty.$$

Hence, the first term on the r.h.s. of (2.7) is in $\mathcal{K}(\mathcal{H}(\Omega))$. The argument is similar for the remaining terms. ☐

Proposition 2.2.4. *One has*
(i) $\forall z \in \mathbb{C} \setminus (\sigma(H) \cup \sigma(H_0)),\ R(z) - R_0(z) \in \mathcal{K}\big(\mathcal{H}(\Omega)\big)$,
(ii) $\sigma_{\mathrm{ess}}(H) = [\nu_1, \infty)$.

Proof. We prove (i) for some (and hence for all) value of $z \in \mathbb{C} \setminus (\sigma(H) \cup \sigma(H_0))$. Let $z \in \mathbb{C} \setminus \mathbb{R}$. Define $R_1(z) := (H_0 + V - z)^{-1}$. Then, one has

$$R(z) - R_0(z) = R(z) - R_1(z) - R_1(z) V R_0(z).$$

Let us first consider $R(z) - R_1(z)$. Knowing that H and $H_0 + V$ have the same form domain, the identity

$$R(z) - R_1(z) = -R(z)(H - H_0 - V)R_1(z)$$

holds in $\mathscr{B}\left(\mathcal{H}^{-1}(\Omega), \mathcal{H}^1_0(\Omega)\right)$. But, one has the following sequence of continuous and dense imbeddings of Hilbert spaces

$$\mathcal{D}(H) \subset \mathcal{H}^1_0(\Omega) \subset \mathcal{H}(\Omega) \subset \mathcal{H}^{-1}(\Omega) \subset \mathcal{D}(H)^*$$

which implies that $R(z)$ extends (by duality) to a homeomorphism of $\mathcal{D}(H)^*$ onto $\mathcal{H}(\Omega)$. Thus, since $R_1(z)$ is also a homeomorphism from $\mathcal{H}(\Omega)$ onto $\mathcal{D}(H_0)$, $R(z) - R_1(z) \in \mathcal{K}(\mathcal{H}(\Omega))$ if and only if $H - H_0 - V \in \mathcal{K}(\mathcal{D}(H_0), \mathcal{D}(H)^*)$. For all $n \in \mathbb{N} \setminus \{0\}$, let $\varphi_n \in C_0^\infty(\mathbb{R})$ be such that $0 \le \varphi_n \le 1$ and

$$\varphi_n(x^1) = \begin{cases} 1 & \text{if} \quad |x^1| \le n \\ 0 & \text{if} \quad |x^1| \ge n + 1. \end{cases}$$

Set $\phi_n := \varphi_n \otimes 1$ on Ω and

$$K_n \psi := -\partial_i F^{ij} \phi_n \partial_j \psi, \qquad \psi \in \mathcal{D}(H_0),$$

where $(F^{ij}) := (G^{ij} - \delta^{ij})$. Clearly, $H - H_0 - V, K_n \in \mathscr{B}(\mathcal{D}(H_0), \mathcal{D}(H)^*)$ and

$$\begin{aligned}
&\|K_n - (H - H_0 - V)\|_{\mathscr{B}(\mathcal{D}(H_0),\mathcal{D}(H)^*)} \\
&\equiv \sup_{\psi\in\mathcal{D}(H_0),\|\psi\|_{\mathcal{D}(H_0)}=1} \left\| \left(1+H^2\right)^{-1/2} \left[-\partial_i F^{ij} (\phi_n - 1) \partial_j\right] \psi \right\| \\
&\leq \sup_{\psi\in\mathcal{D}(H_0),\|\psi\|_{\mathcal{D}(H_0)}=1} \sum_{j=1}^{d} \left\| \left(1+H^2\right)^{-1/2} \partial_i \right\| \left\| F^{ij} (\phi_n - 1)\right\|_\infty \|\psi\|_{\mathcal{H}_0^1(\Omega)} \xrightarrow[n\to\infty]{} 0,
\end{aligned}$$

where we have used the fact that $\mathcal{D}(H_0) \subset \mathcal{H}_0^1(\Omega)$ continuously and Assumption 2.2.1.2 in the final step. So, it only remains to show that $K_n \in \mathcal{K}(\mathcal{D}(H_0), \mathcal{D}(H)^*)$. After a commutation, one gets in $\mathscr{B}(\mathcal{D}(H_0), \mathcal{D}(H)^*)$

$$K_n = -\partial_i F^{ij} \partial_j \phi_n + \partial_i F^{i1} \phi_{n,1}$$

where ϕ_n, $\phi_{n,1}$ are seen as multiplication operators in $\mathcal{H}(\Omega)$. It is clear that both $\partial_i F^{ij} \partial_j$ and $\partial_i F^{i1}$ are in $\mathscr{B}\left(\mathcal{H}_0^1(\Omega), \mathcal{D}(H)^*\right)$. Moreover, ϕ_n and $\phi_{n,1}$ are in $\mathcal{K}\left(\mathcal{D}(H_0), \mathcal{H}_0^1(\Omega)\right)$ by Lemma 2.2.3. Thus, $K_n \in \mathcal{K}(\mathcal{D}(H_0), \mathcal{D}(H)^*)$ so that $R(z) - R_1(z) \in \mathcal{K}(\mathcal{H}(\Omega))$. Using similar arguments, one can also prove that the $R_1(z) V \phi_n R_0(z)$ is compact and converges to $R_1(z) V R_0(z)$ in $\mathscr{B}(\mathcal{H}(\Omega))$ due to Assumption 2.2.2.2. This implies that $R_1(z) V R_0(z) \in \mathcal{K}(\mathcal{H}(\Omega))$.
(ii) It is a direct consequence of (i), (2.6) and Weyl's theorem [RS78, Thm. XIII.14]. ☐

Remark 2.2.5. *Notice that* Assumptions 2.2.1.3, 2.2.1.4 *and* 2.2.2.3 *are not used in the proof of* Proposition 2.2.4.

2.2.3 Nature of the essential spectrum

This part is devoted to a more detailed analysis of the essential spectrum of H. In particular, we show that the singular continuous spectrum is empty. The strategy adapted from [Ben98] is the following. Firstly, we construct a dilation operator A such that $H_0 \in C^\infty(A)$ and $H \in C^{1+\vartheta}(A)$ with $\vartheta := \min\{\vartheta_1, \vartheta_2\} \in (0,1]$ (see [ABG96], [Ben98, Sec. 2] or [DDI98, Sec. 1] for definitions of the spaces involved here and in the sequel). Secondly, we prove that A is *strictly conjugate* (in Mourre's sense) to H_0 on $\mathbb{R}\setminus\mathcal{T}$. Finally, since $R(i) - R_0(i)$ is compact by the first claim of Proposition 2.2.4 and both H and H_0 are of class $C_u^1(A) \supseteq C^{1+\vartheta}(A) \supseteq C^\infty(A)$, it follows that A is conjugate to H on $\mathbb{R}\setminus\mathcal{T}$ as well.

The dilation operator

Let q^1 be the multiplication operator by the coordinate x^1 in $\mathcal{H}(\Omega)$. Let

$$A := \tfrac{1}{2}\left(q^1 p_1 + p_1 q^1\right) \qquad \text{with} \qquad p_1 := -i\partial_1 \tag{2.8}$$

be the dilation operator in $\mathcal{H}(\Omega)$ w.r.t. x^1, *i.e.* , the self-adjoint extension of the operator defined by the expression (2.8) with $C_0^\infty(\Omega)$ as initial domain. Define $A_{\shortparallel}$ as the self-adjoint operator in $\mathsf{L}^2(\mathbb{R})$ such that $A = A_{\shortparallel} \otimes 1$.

Remark 2.2.6. *The group* $\left\{e^{iAt}\right\}_{t\in\mathbb{R}}$ *leaves invariant* $\mathcal{H}_0^1(\Omega)$. *Indeed, using the natural isomorphism* $\mathcal{H}_0^1(\Omega) \simeq \mathcal{H}^1(\mathbb{R}) \otimes \mathcal{H}_0^1(\omega)$, *one can write*

$$\forall t \in \mathbb{R}, \qquad e^{iAt}\mathcal{H}_0^1(\Omega) = \left(e^{iA_{\shortparallel}t}\mathcal{H}^1(\mathbb{R})\right) \otimes \mathcal{H}_0^1(\omega).$$

Then, the affirmation follows from the fact [ABG96, Prop. 4.2.4] *that* $\mathcal{H}^1(\mathbb{R})$ *is stable under* $\big\{\mathrm{e}^{iA_{\shortparallel}t}\big\}_{t\in\mathbb{R}}$.

In order to deal with the commutator $i\,[H,A]$, we need the following family of operators

$$\big\{p_1(\varepsilon) := p_1(1+i\varepsilon p_1)^{-1}\big\}_{\varepsilon>0}\,, \tag{2.9}$$

which regularises the momentum operator p_1 :

Lemma 2.2.7. *One has*

(i) $\{p_1(\varepsilon)\}_{\varepsilon>0} \subset \mathscr{B}\big(\mathcal{H}(\Omega)\big)$,

(ii) $\{p_1(\varepsilon)\}_{\varepsilon>0}$ *is uniformly bounded in* $\mathscr{B}\big(\mathcal{H}^1(\Omega),\mathcal{H}(\Omega)\big)$ *and* s-$\lim_{\varepsilon\to 0} p_1(\varepsilon) = p_1$ *in* $\mathscr{B}\big(\mathcal{H}^1(\Omega),\mathcal{H}(\Omega)\big)$,

(iii) $\forall\varepsilon>0,\ [p_1(\varepsilon),q_1] = -i(1+i\varepsilon p_1)^{-2}$ *in* $\mathscr{B}(\mathcal{H}(\Omega))$,

(iv) $\forall\varepsilon>0,\ p_1(\varepsilon)\mathcal{H}^1_0(\Omega)\subset\mathcal{H}^1_0(\Omega)$.

Proof. The first three assertions are established in [Ben98, Lemma 4.1]. Consequently, it only remains to prove the last statement. Using the isomorphism mentioned in Remark 2.2.6, one can write

$$\forall\varepsilon>0,\qquad p_1(\varepsilon)\mathcal{H}^1_0(\Omega) = -i\varepsilon^{-1}\big\{\big[1+i\varepsilon^{-1}(p_1-i\varepsilon^{-1})^{-1}\big]\mathcal{H}^1(\mathbb{R})\big\}\otimes\mathcal{H}^1_0(\omega),$$

where p_1 on the r.h.s. must be viewed as an operator acting in $\mathsf{L}^2(\mathbb{R})$. With this last relation, it is clear that $\mathcal{H}^1_0(\Omega)$ is left invariant by the family $\{p_1(\varepsilon)\}_{\varepsilon>0}$. □

We also need the following density result for the set $\mathcal{D}(H)_c := \{\psi\in\mathcal{D}(H) : \mathrm{supp}(\psi)$ is compact$\}$.

Lemma 2.2.8. *One has*

(i) $\mathcal{D}(H)_c$ *is dense in* $\mathcal{D}(H)$,

(ii) $\mathcal{D}(H)_c$ *is dense in* $\mathcal{H}^1_0(\Omega)$.

Proof. (i) We are inspired by [DDI98, Lemma 2.1]. Let $\psi\in\mathcal{D}(H)$. Define $\varphi_0\in C_0^\infty(\mathbb{R})$ such that

$$\varphi_0(x^1) = \begin{cases} 1 & \text{if} \quad |x^1|\le 1\\ 0 & \text{if} \quad |x^1|\ge 2.\end{cases}$$

Let $n\in\mathbb{N}$. Set $\varphi_n(x^1) := \varphi_0(x^1/(n+1))$ for $x^1\in\mathbb{R}$ and $\phi_n := \varphi_n\otimes 1$ on Ω. Then, $\phi_n\psi\in\mathcal{H}^1_0(\Omega)$, $\lim_{n\to\infty}\phi_n\psi=\psi$ in $\mathcal{H}(\Omega)$ and

$$H\phi_n\psi = \phi_n H\psi - 2\phi_{n,1}G^{1j}\psi_{,j} - \phi_{n,11}G^{11}\psi - \phi_{,1}G^{1i}_{\ \ ,i}\psi \tag{2.10}$$

in the sense of distributions. Using the fact that $\mathrm{supp}(\phi_n)$ is compact, Assumption 2.2.1.1 and Assumption 2.2.1.4, one has $\phi_n\psi\in\mathcal{D}(H)_\mathrm{c}$. Moreover, as a consequence of (2.10) and the property

$$\forall k\in\mathbb{N},\ \forall x\in\Omega,\qquad \partial_1^k\phi_n(x) = (n+1)^{-k}\varphi_0^{(k)}(x^1/(n+1)),$$

one also has $\lim_{n\to\infty} H\phi_n\psi = H\psi$ in $\mathcal{H}(\Omega)$.

(ii) Using point (i) and the fact that $\mathcal{D}(H)\subset\mathcal{H}^1_0(\Omega)$ continuously and densely, one gets the following embeddings

$$\mathcal{H}^1_0(\Omega) = \overline{\overline{\mathcal{D}(H)_\mathrm{c}}^{\mathcal{D}(H)}}^{\mathcal{H}^1_0(\Omega)} \subseteq \overline{\overline{\mathcal{D}(H)_\mathrm{c}}^{\mathcal{H}^1_0(\Omega)}}^{\mathcal{H}^1_0(\Omega)} = \overline{\mathcal{D}(H)_\mathrm{c}}^{\mathcal{H}^1_0(\Omega)} \subseteq \mathcal{H}^1_0(\Omega)$$

which, in particular, imply that $\mathcal{D}(H)_\mathrm{c}$ is dense in $\mathcal{H}^1_0(\Omega)$. □

Now, we can compute the commutator $i\,[H,A]$.

Proposition 2.2.9. *The sesquilinear form $\mathcal{Q}$ on $\mathcal{H}(\Omega)$ defined by*

$$\mathcal{Q}(\varphi,\psi) := i\left[(H\varphi, A\psi) - (A\varphi, H\psi)\right], \qquad \varphi,\psi \in \mathcal{D}(\mathcal{Q}) := \mathcal{D}(H)\cap\mathcal{D}(A),$$

is continuous on $\mathcal{D}(H)_{\mathrm{c}}$ for the topology induced by $\mathcal{H}^1_0(\Omega)$. Moreover,

$$i\,[H,A] = -\partial_j G^{1j}\partial_1 - \partial_1 G^{1j}\partial_j + \partial_i q^1 G^{ij}_{,1}\partial_j - q^1 V_{,1} \tag{2.11}$$

as operators in $\mathscr{B}\left(\mathcal{H}^1_0(\Omega), \mathcal{H}^{-1}(\Omega)\right)$.

Proof. Let $\varphi,\psi \in \mathcal{D}(H)_c$. Using the identity $A = q^1 p_1 - \frac{i}{2}$ valid on $\mathcal{D}(H)_c \subset \mathcal{D}(A)$, we have

$$\begin{aligned}\mathcal{Q}(\varphi,\psi) &= i\left[(H\varphi, A\psi) - (A\varphi, H\psi)\right]\\ &= (\varphi, H\psi) + i\left[\left(-\partial_i G^{ij}\partial_j\varphi, q^1 p_1\psi\right) - \left(q^1 p_1\varphi, -\partial_i G^{ij}\partial_j\psi\right)\right]\\ &\quad + \left(V\varphi, q^1\psi_{,1}\right) + \left(q^1\varphi_{,1}, V\psi\right).\end{aligned}$$

In order to justify the subsequent integration by parts, we employ the family (2.9). Since ψ has a compact support and belongs to $\mathcal{H}^1_0(\Omega)$, it follows by using properties (iii) and (iv) of Lemma 2.2.7 that $q^1 p_1(\varepsilon)\psi \in \mathcal{H}^1_0(\Omega)$ for all $\varepsilon > 0$. So, we can write

$$\begin{aligned}\left(-\partial_i G^{ij}\partial_j\varphi, q^1 p_1\psi\right) &= \lim_{\varepsilon\to 0}\left(-\partial_i G^{ij}\partial_j\varphi, q^1 p_1(\varepsilon)\psi\right)\\ &= \lim_{\varepsilon\to 0}\left(\varphi_{,j}, G^{ij}\partial_i q^1 p_1(\varepsilon)\psi\right)\\ &= -i\left(\varphi_{,j}, G^{1j}\psi_{,1}\right) + \lim_{\varepsilon\to 0}\left(\varphi_{,i}, G^{ij} q^1 p_1(\varepsilon)\psi_{,j}\right)\end{aligned}$$

and similarly for the integral

$$\left(q^1 p_1\varphi, -\partial_i G^{ij}\partial_j\psi\right) = i\left(\varphi_{,1}, G^{1j}\psi_{,j}\right) + \lim_{\varepsilon\to 0}\left(p_1(\varepsilon)^*\varphi_{,i}, q^1 G^{ij}\psi_{,j}\right).$$

Since

$$\begin{aligned}\lim_{\varepsilon\to 0}\left(p_1(\varepsilon)^*\varphi_{,i}, q^1 G^{ij}\psi_{,j}\right) &= \lim_{\varepsilon\to 0}\left(\varphi_{,i}, p_1(\varepsilon) q^1 G^{ij}\psi_{,j}\right)\\ &= -i\left[\left(\varphi_{,i}, G^{ij}\psi_{,j}\right) + \left(\varphi_{,i}, q^1 G^{ij}_{,1}\psi_{,j}\right)\right]\\ &\quad + \lim_{\varepsilon\to 0}\left(\varphi_{,i}, q^1 G^{ij} p_1(\varepsilon)\psi_{,j}\right),\end{aligned}$$

and

$$\left(q^1\varphi_{,1}, V\psi\right) = -\left(\varphi, \partial_1 q^1 V\psi\right) = -(\varphi, V\psi) - \left(\varphi, q^1 V_{,1}\psi\right) - \left(\varphi, q^1 V\psi_{,1}\right),$$

we finally obtain that

$$\mathcal{Q}(\varphi,\psi) = \left(\varphi_{,j}, G^{1j}\psi_{,1}\right) + \left(\varphi_{,1}, G^{1j}\psi_{,j}\right) - \left(\varphi_{,i}, q^1 G^{ij}_{,1}\psi_{,j}\right) - \left(\varphi, q^1 V_{,1}\psi\right). \tag{2.12}$$

This implies that $\mathcal{Q}$ restricted to $\mathcal{D}(H)_{\mathrm{c}}$ is continuous for the topology induced by $\mathcal{H}^1_0(\Omega)$. Now, $\mathcal{D}(H)_{\mathrm{c}}$ is dense in $\mathcal{H}^1_0(\Omega)$ by Lemma 2.2.8.(ii). Thus, $\mathcal{Q}$ defines (by continuous extension) an operator in $\mathscr{B}(\mathcal{H}^1_0(\Omega), \mathcal{H}^{-1}(\Omega))$, which we shall denote $i\,[H,A]$. Furthermore, using (2.12), we obtain (2.11) in $\mathscr{B}(\mathcal{H}^1_0(\Omega), \mathcal{H}^{-1}(\Omega))$. □

Strict Mourre estimate for the free Hamiltonian

Now we prove that H_0 is of class $C^\infty(A)$ and A strictly conjugate to it on $\mathbb{R}\setminus\mathcal{T}$. So, let us first recall the following definition [ABG96, Sec. 7.2.1 & 7.2.2] :

Definition 2.2.10. *Let A, H be self-adjoint operators in a Hilbert space $\mathcal{H}$ with H of class $C^1(A)$. Furthermore, if $S,T\in\mathscr{B}(\mathcal{H})$, we write $S\gtrsim T$ if there exists $K\in\mathcal{K}(\mathcal{H})$ so that $S\geq T+K$. Then, $\forall\lambda\in\mathbb{R}$,*

$$\varrho_H^A(\lambda):=\sup\left\{a\in\mathbb{R}\,:\,\exists\varepsilon>0\ \textit{s.t.}\ \ E^H(\lambda;\varepsilon)i\,[H,A]\,E^H(\lambda;\varepsilon)\geq aE^H(\lambda;\varepsilon)\right\},$$
$$\widetilde{\varrho}_H^A(\lambda):=\sup\left\{a\in\mathbb{R}\,:\,\exists\varepsilon>0\ \textit{s.t.}\ \ E^H(\lambda;\varepsilon)i\,[H,A]\,E^H(\lambda;\varepsilon)\gtrsim aE^H(\lambda;\varepsilon)\right\}$$

where $E^H(\lambda;\varepsilon):=E^H((\lambda-\varepsilon,\lambda+\varepsilon))$ designates the spectral projection of H for the interval $(\lambda-\varepsilon,\lambda+\varepsilon)$.

We also need the following natural generalisation of [BG92, Thm. 3.4].

Theorem 2.2.11. *Let H_1, H_2 be two self-adjoint, bounded from below operators in the Hilbert spaces $\mathcal{H}_1,\mathcal{H}_2$. Assume that $A_\jmath$, $\jmath=1,2$, is a self-adjoint operator in $\mathcal{H}_\jmath$ such that $H_\jmath$ is of class $C^k(A_\jmath)$, $k\in(\mathbb{N}\setminus\{0\})\cup\{+\infty\}$. Let $H:=H_1\otimes 1+1\otimes H_2$ and $A:=A_1\otimes 1+1\otimes A_2$, which are self-adjoint operators in $\mathcal{H}_1\otimes\mathcal{H}_2$. Then H is of class $C^k(A)$ and $\forall\lambda\in\mathbb{R}$:*

$$\varrho_H^A(\lambda)=\inf_{\lambda=\lambda_1+\lambda_2}\left[\varrho_{H_1}^{A_1}(\lambda_1)+\varrho_{H_2}^{A_2}(\lambda_2)\right].$$

Corollary 2.2.12. *$H_0\in C^\infty(A)$ and*

$$\forall\lambda\in\mathbb{R},\qquad \varrho_{H_0}^A(\lambda)=\begin{cases}2\rho(\lambda) & \textit{if}\quad \lambda\geq\nu_1\\ +\infty & \textit{if}\quad\lambda<\nu_1,\end{cases}\tag{2.13}$$

where $\rho(\lambda):=\lambda-\sup\{\zeta\in\mathcal{T}\,:\,\zeta\leq\lambda\}$ is strictly positive on $\mathbb{R}\setminus\mathcal{T}$.

Proof. $A_1:=A_{\shortparallel}$, $A_2:=0$ are self-adjoint in $\mathsf{L}^2(\mathbb{R})$, respectively $\mathsf{L}^2(\omega)$. $H_1:=p_1^2$, $H_2:=-\Delta_{\mathrm{D}}^\omega$ are self-adjoint, bounded from below in $\mathsf{L}^2(\mathbb{R})$, respectively $\mathsf{L}^2(\omega)$. Clearly, [ABG96, Ex. 6.2.8] $p_1^2\in C^\infty(A_{\shortparallel})$ and $-\Delta_{\mathrm{D}}^\omega\in C^\infty(0)$. The first part of the claim and (2.13) then follows from Theorem 2.2.11. The expression for $\rho(\lambda)$ is a direct consequence of the respective behaviours of [ABG96, Sec. 7.2.1] $\varrho_{p_1^2}^{A_{\shortparallel}}$ and $\varrho_{-\Delta_{\mathrm{D}}^\omega}^0$:

$$\begin{bmatrix}\varrho_{p_1^2}^{A_{\shortparallel}}(\lambda_1)\\ \varrho_{-\Delta_{\mathrm{D}}^\omega}^0(\lambda_2)\end{bmatrix}=\begin{cases}\begin{bmatrix}2\lambda_1\\+\infty\end{bmatrix} & \text{if}\quad\begin{bmatrix}\lambda_1\geq 0\\ \lambda_1<0\end{bmatrix}\\[2ex] \begin{bmatrix}0\\+\infty\end{bmatrix} & \text{if}\quad\begin{bmatrix}\lambda_2\in\mathcal{T}\\ \lambda_2\in\mathbb{R}\setminus\mathcal{T}\end{bmatrix}.\end{cases}$$

□

Regularity of the Hamiltonian

In order to prove the regularity of H, we need two technical lemmas.

Lemma 2.2.13. $\forall z\in\mathbb{R}\setminus\sigma(H)$, $\forall\vartheta\leq 1$, *one has*

(i) $\left[R(z), \langle q^1\rangle^\vartheta\right] \in \mathscr{B}\left(\mathcal{H}(\Omega), \mathcal{H}_0^1(\Omega)\right)$,
(ii) $\forall i \in \{1,\dots,d\}$, $\left[R(z), \langle q^1\rangle^\vartheta\right]\partial_i \in \mathscr{B}\left(\mathcal{H}(\Omega), \mathcal{H}_0^1(\Omega)\right)$.

This is established by adapting the proof of [Ben98, Lemma 4.3] while next Lemma follows from the use of [Ben98, Proof of Prop. 4.2].

Lemma 2.2.14. *Let $S \in \mathscr{B}(\mathcal{H}(\Omega))$ be self-adjoint and $\vartheta \in (0,1]$, then*

$$\langle q^1\rangle^\vartheta S \in \mathscr{B}\left(\mathcal{H}(\Omega), \mathcal{H}^\vartheta(\mathbb{R}) \otimes \mathsf{L}^2(\omega)\right) \implies S \in C^\vartheta(A).$$

(Note that the proof involves principally two facts. First, $S \in \mathscr{B}\left(\mathcal{H}(\Omega), \mathcal{D}(|A|^\vartheta)\right)$ implies $S \in C^\vartheta(A)$. Second, the continuous imbedding $\mathcal{H}^\vartheta_\vartheta(\mathbb{R}) \subseteq \mathcal{D}(|A_{\shortparallel}|^\vartheta)$, which follows by real interpolation [ABG96, Sec. 2.7] from the continuous imbedding $\mathcal{H}^1_1(\mathbb{R}) \subseteq \mathcal{D}(|A_{\shortparallel}|)$.)

Remark 2.2.15. *The facts that $i\,[H,A] \in \mathscr{B}\left(\mathcal{H}_0^1(\Omega), \mathcal{H}^{-1}(\Omega)\right)$ and that $\mathcal{H}_0^1(\Omega)$ is stable under $\{\mathrm{e}^{iAt}\}_{t\in\mathbb{R}}$ imply* [ABG96, Sec. 6.3] *that $H \in C^1(A)$.*

Proposition 2.2.16. $\exists\vartheta \in (0,1]$ *such that* $H \in C^{1+\vartheta}(A)$.

Proof. We show that each term appearing in the expression for $B := i\,[H,A]$ is at least of class $C^\gamma(A)$ for a certain $\gamma \in (0,1]$.

Consider first $B_1 := -\partial_j G^{j1}\partial_1 - \partial_1 G^{1j}\partial_j$. An explicit calculation (analogous to that of the proof of Proposition 2.2.9) implies that

$$i\,[B_1, A] = -2\partial_1 G^{11}\partial_1 - \partial_1 G^{1j}\partial_j - \partial_j G^{j1}\partial_1 + \partial_j q^1 G^{j1}_{,1}\partial_1 + \partial_1 q^1 G^{1j}_{,1}\partial_j$$

as operators in $\mathscr{B}(\mathcal{H}_0^1(\Omega), \mathcal{H}^{-1}(\Omega))$. Thus, $B_1 \in C^1(A)$ by Remark 2.2.15.

Let $z \in \mathbb{R}\setminus\sigma(H)$. As a consequence of the fact that $H \in C^1(A)$, one can interpret $i\,[A, R(z)]$ as the product of [ABG96, Sec. 6.2.2] three bounded operators, *viz.* $R(z) : \mathcal{H}(\Omega) \to \mathcal{D}(H)$, $B : \mathcal{D}(H) \to \mathcal{D}(H)^*$ and $R(z) : \mathcal{D}(H)^* \to \mathcal{H}(\Omega)$. Thus, using Proposition 2.2.9, one can write as an operator identity in $\mathscr{B}(\mathcal{H}(\Omega))$

$$\begin{aligned} i\,[A, R(z)] = R(z)BR(z) = R(z)B_1R(z) &+ R(z)\partial_i q^1 G^{ij}_{,1}\partial_j R(z) \\ &- R(z)q^1 V_{,1}R(z). \end{aligned}$$

Since the first term has already been shown to be bounded, it is enough to prove that the second and third terms on the r.h.s. are of class $C^\gamma(A)$ for some $\gamma \in (0,1]$.

We employ Lemma 2.2.14 with $\vartheta := \min\{\vartheta_1, \vartheta_2\}$ in order to deal with both terms. Using some commutation relations, we get

$$\begin{aligned} \langle q^1\rangle^\vartheta R(z)\partial_i q^1 G^{ij}_{,1}\partial_j R(z) = R(z)\partial_i &\langle q^1\rangle^\vartheta q^1 G^{ij}_{,1}\partial_j R(z) \\ &- \left[R(z), \langle q^1\rangle^\vartheta\right]\partial_i q^1 G^{ij}_{,1}\partial_j R(z) \\ &- R(z)\left[\partial_i, \langle q^1\rangle^\vartheta\right] q^1 G^{ij}_{,1}\partial_j R(z). \end{aligned}$$

Under Assumption 2.2.1.3, the first term on the r.h.s. is in $\mathscr{B}(\mathcal{H}(\Omega), \mathcal{H}_0^1(\Omega))$. The second and the last one are in $\mathscr{B}(\mathcal{H}(\Omega), \mathcal{H}_0^1(\Omega))$ by Lemma 2.2.13.(ii) and the boundedness of $\langle q^1\rangle^\vartheta_{,1}$, respectively. Moreover,

$$\langle q^1\rangle^\vartheta R(z)q^1V_{,1}R(z) = R(z)\langle q^1\rangle^\vartheta q^1 V_{,1}R(z) + \left[\langle q^1\rangle^\vartheta, R(z)\right] q^1 V_{,1}R(z)$$

is in $\mathscr{B}\left(\mathcal{H}(\Omega), \mathcal{H}_0^1(\Omega)\right)$ by Assumption 2.2.2.3 and Lemma 2.2.13.(i). Thus, all the terms in the expression of B are at least of class $C^\vartheta(A)$. This implies the claim. □

The main result

Proposition 2.2.17. $\forall\lambda \in \mathbb{R}\setminus\mathcal{T},\ \widetilde{\varrho}_H^A(\lambda) > 0.$

Proof. Corollary 2.2.12 and Proposition 2.2.16 imply that both H_0 and H are of class $C_u^1(A)$. Furthermore, $R(i) - R_0(i)$ is compact by Proposition 2.2.4, with the result that $\widetilde{\varrho}_H^A = \widetilde{\varrho}_{H_0}^A$ due to [ABG96, Thm. 7.2.9]. Finally, since [ABG96, Prop. 7.2.6] $\widetilde{\varrho}_{H_0}^A \geq \varrho_{H_0}^A$, we can conclude using Corollary 2.2.12. □

Summing up, we result in the following spectral properties of H.

Theorem 2.2.18. *Let ω be a bounded open connected set in $\mathbb{R}^{d-1}$, $d \geq 2$, and denote by $\mathcal{T}$ the set of eigenvalues of $-\Delta_D^\omega$. Let H be the operator* (2.3) *with $\Omega := \mathbb{R}\times\omega$, subject to Dirichlet boundary conditions, and satisfying* Assumptions 2.2.1 *and* 2.2.2. *Then*

(i) $\sigma_{\mathrm{ess}}(H) = [\kappa,\infty)$, *where* $\kappa := \inf\mathcal{T}$,

(ii) $\sigma_{\mathrm{sc}}(H) = \varnothing$,

(iii) $\sigma_{\mathrm{p}}(H)\cup\mathcal{T}$ *is closed and countable*,

(iv) $\sigma_{\mathrm{p}}(H)\setminus\mathcal{T}$ *is composed of finitely degenerated eigenvalues, which can accumulate at the points of $\mathcal{T}$ only*,

Proof. The claim (i) is included in Proposition 2.2.4. Since A is conjugate to H on $\mathbb{R}\setminus\mathcal{T}$ by Proposition 2.2.17, the assertions (ii)–(iv) follow by the abstract conjugate operator method [ABG96, Thm. 7.4.2]. □

To conclude this section, let us remark that Assumptions 2.2.1.3 and 2.2.2.3 could be weakened. Firstly, we recall that the situation with $V = 0$ and $G = \rho\mathbb{1}$, ρ being a real-valued function greater than a strictly positive constant, is investigated in [Ben98, DDI98] where the authors admit local singularities of ρ. More specifically, one assumes that $\rho = \rho_{\mathrm{s}} + \rho_\ell$, where ρ_ℓ is the part satisfying a condition analogous to Assumption 2.2.1.3, while ρ_{s} need not be differentiable. (In [Ben98], $\mathrm{supp}(\rho_{\mathrm{s}})$ is assumed to be compact. The result of [DDI98] is better in the sense that ρ_s is only supposed to be a short-range perturbation there. However, this requires strengthening of the condition analogous to Assumption 2.2.1.2 about the decay of ρ at infinity.) Secondly, the optimal conditions one has to impose on the potential of a Schrödinger operator are known [BGM93, ABG96].

2.3 Curved tubes

In this part, we use Theorem 2.2.18 in order to find geometric sufficient conditions which guarantee that the spectral results of the theorem hold true for curved tubes.

2.3.1 Geometric preliminaries

The reference curve

Given $d \geq 2$, let $p : \mathbb{R} \to \mathbb{R}^d$ be a regular unit-speed smooth (*i.e.* , C^∞-smooth) curve satisfying the following hypothesis.

Assumption 2.3.1. *There exists a collection of d smooth mappings $e_i : \mathbb{R} \to \mathbb{R}^d$ with the following properties :*

1. $\forall i,j \in \{1,\dots,d\}, \forall s \in \mathbb{R},\ e_i(s)\cdot e_j(s) = \delta_{ij}$,

2. $\forall i \in \{1,\dots,d-1\}$, $\forall s \in \mathbb{R}$, *the* $i^{\rm th}$ *derivative* $p^{(i)}(s)$ *of* $p(s)$ *lies in the span of* $e_1(s),\dots,e_i(s)$,
3. $e_1 = \dot{p}$,
4. $\forall s \in \mathbb{R}$, $\{e_1(s),\dots,e_d(s)\}$ *has the positive orientation*,
5. $\forall i \in \{1,\dots,d-1\}$, $\forall s \in \mathbb{R}$, $\dot{e}_i(s)$ *lies in the span of* $e_1(s),\dots,e_{i+1}(s)$.

Here and in the sequel, " $\cdot$ " denotes the inner product in $\mathbb{R}^d$.

Remark 2.3.2. *A vector field with the property 1 is called a* moving frame *along* p *and it is a* Frenet frame *if it satisfies 2 in addition,* cf. [Kli78, Sec. 1.2]. *A sufficient condition to ensure the existence of the frame of* Assumption 2.3.1 *is to require that* [Kli78, Prop. 1.2.2], *for all* $s \in \mathbb{R}$, *the vectors* $\dot{p}(s), p^{(2)}(s), \dots, p^{(d-1)}(s)$ *are linearly independent. This is always satisfied if* $d = 2$. *However, we do not assume* a priori *the above non-degeneracy condition for* $d \geq 3$ *because it excludes the curves such that, for some open* $I \subseteq \mathbb{R}$, $p \restriction I$ *lies in a lower-dimensional subspace of* $\mathbb{R}^d$.

The properties of $\{e_1,\dots,e_d\}$ summarised in Assumption 2.3.1 yield [Kli78, Sec. 1.3] the Serret-Frenet formulae,

$$\dot{e}_i = \mathcal{K}_i^{\ j} e_j \tag{2.14}$$

with $\mathcal{K} \equiv \left(\mathcal{K}_i^{\ j}\right)$ being a skew-symmetric $d \times d$ matrix defined by

$$\mathcal{K} := \begin{pmatrix} 0 & \kappa_1 & & \mathbf{0} \\ -\kappa_1 & \ddots & \ddots & \\ & \ddots & \ddots & \kappa_{d-1} \\ \mathbf{0} & & -\kappa_{d-1} & 0 \end{pmatrix}. \tag{2.15}$$

Here κ_i is called the $i^{\rm th}$ *curvature* of p. Under our Assumption 2.3.1, the curvatures are smooth functions of the arc-length parameter $s \in \mathbb{R}$.

The appropriate moving frame

In this subsection, we introduce another moving frame along p, which better reflects the geometry of the curve, and will be used later to define a tube about it. We shall refer to it as the *Tang frame* because it is a natural generalisation of the Tang frame known from the theory of 3-dimensional waveguides [TG89, GJ92, DE95]. Our construction follows the generalisation introduced in [CDFK].

Let the $(d-1)\times(d-1)$ matrix $(\mathcal{R}_\mu^{\ \nu})$ be defined by the system of differential equations

$$\dot{\mathcal{R}}_\mu^{\ \nu} + \mathcal{R}_\mu^{\ \alpha}\mathcal{K}_\alpha^{\ \nu} = 0 \tag{2.16}$$

with $(\mathcal{R}_\mu^{\ \nu}(s_0))$ being a rotation matrix in $\mathbb{R}^{d-1}$ for some $s_0 \in \mathbb{R}$ as initial condition, *i.e.* ,

$$\det\left(\mathcal{R}_\mu^{\ \nu}(s_0)\right) = 1 \qquad \text{and} \qquad \delta_{\alpha\beta}\mathcal{R}_\mu^{\ \alpha}(s_0)\mathcal{R}_\nu^{\ \beta}(s_0) = \delta_{\mu\nu}. \tag{2.17}$$

The solution of (2.16) exists and is smooth by standard arguments in the theory of differential equations (*cf.* [Kur86, Sec. 4]). Furthermore, the conditions (2.17) are satisfied for *all* $s_0 \in \mathbb{R}$. Indeed, by means of Liouville's formula [Kur86, Thm. 4.7.1] and $\mathrm{tr}(\mathcal{K}) = 0$, one checks that $\det\big(\mathcal{R}_\mu^{\ \nu}\big) = 1$ identically, while the validity of the second condition for all $s_0 \in \mathbb{R}$ is obtained via the skew-symmetry of $\mathcal{K}$:

$$\big(\delta_{\alpha\beta}\mathcal{R}_\mu^{\ \alpha}\mathcal{R}_\nu^{\ \beta}\big)^{\cdot} = -\mathcal{R}_\mu^{\ \alpha}\big(\delta_{\gamma\beta}\mathcal{K}_\alpha^{\ \gamma} + \delta_{\alpha\gamma}\mathcal{K}_\beta^{\ \gamma}\big)\mathcal{R}_\nu^{\ \beta} = 0.$$

We set

$$\mathcal{R} \equiv \big(\mathcal{R}_i^{\ j}\big) := \begin{pmatrix} 1 & 0 \\ 0 & \big(\mathcal{R}_\mu^{\ \nu}\big) \end{pmatrix}$$

and introduce the Tang frame as the moving frame $\{\tilde{e}_1, \dots, \tilde{e}_d\}$ along p defined by

$$\tilde{e}_i := \mathcal{R}_i^{\ j} e_j. \tag{2.18}$$

Combining (2.14) with (2.16), one easily finds

$$\dot{\tilde{e}}_1 = \kappa_1 e_2 \qquad \text{and} \qquad \dot{\tilde{e}}_\mu = \mathcal{R}_\mu^{\ \alpha}\mathcal{K}_\alpha^{\ 1} e_1 = -\kappa_1 \mathcal{R}_\mu^{\ 2} e_1. \tag{2.19}$$

The interest of the Tang frame will appear in the following subsection.

The tube

Let ω be a bounded open connected set in $\mathbb{R}^{d-1}$. Without loss of generality, we assume that ω is translated so that its centre of mass is at the origin. Let $\Omega := \mathbb{R} \times \omega$ be a straight tube. We define the curved tube Γ of the same cross-section ω about p as the image of the mapping

$$\mathscr{L} : \Omega \to \mathbb{R}^d, \qquad \big(s, u^2, \dots, u^d\big) \mapsto p(s) + \tilde{e}_\mu(s) u^\mu, \tag{2.20}$$

i.e. , $\Gamma := \mathscr{L}(\Omega)$.

As already mentioned in Introduction, the shape of the curved tube Γ of cross-section ω about p depends on the choice of rotations $(\mathcal{R}_\mu^{\ \nu})$ in (2.18), unless ω is rotation invariant. As usual in the theory of quantum waveguides (see, *e.g.*, [DE95, CDFK]), we restrict ourselves to the technically most advantageous choice determined by (2.16), *i.e.* , when the cross-section ω rotates along p w.r.t. the Tang frame (another choice can be found in [EFK04]).

We write $u \equiv (u^2, \dots, u^d)$, define $a := \sup_{u\in\omega} |u|$ and always assume

Assumption 2.3.3.

1. $\kappa_1 \in \mathsf{L}^\infty(\mathbb{R})$ *and* $a\|\kappa_1\|_\infty < 1$,
2. Γ *does not overlap itself*.

Then, the mapping $\mathscr{L} : \Omega \to \Gamma$ is a diffeomorphism. Indeed, by virtue of the inverse function theorem, the first condition guarantees that it is a local diffeomorphism which is global through the injectivity induced by the second condition. Consequently, $\mathscr{L}^{-1}$ determines a system of global (*geodesic* or *Fermi*) “coordinates” (s, u). At the same time, the tube Γ can be identified with the Riemannian manifold (Ω, g), where $g \equiv (g_{ij})$ is the metric tensor induced by the immersion (2.20), that is $g_{ij} := \mathscr{L}_{,i} \cdot \mathscr{L}_{,j}$. The formulae (2.19) yield

$$g = \operatorname{diag}\big(h^2, 1, \dots, 1\big) \qquad \text{with} \qquad h(s,u) := 1 + u^\mu \mathcal{R}_\mu^{\ \alpha}(s)\mathcal{K}_\alpha^{\ 1}(s). \tag{2.21}$$

Note that the metric tensor (2.21) is diagonal due to our special choice of the “transverse” frame $\{\tilde{e}_2, \dots, \tilde{e}_d\}$, which is the advantage of the Tang frame.

We set $|g| := \det(g) = h^2$, which defines through $\mathrm{d}v := h(s,u)\,\mathrm{d}s\,\mathrm{d}u$ the volume element of Γ ; here $\mathrm{d}u$ denotes the $(d-1)$-dimensional Lebesgue measure in ω.

Remark 2.3.4 (Low-dimensional examples). *When $d = 2$, the cross-section ω is just the interval $(-a, a)$, the curve p has only one curvature $\kappa := \kappa_1$, the rotation matrix $(\mathcal{R}_\mu^{\ \nu})$ equals (the scalar) 1 and*

$$h(s, u) = 1 - \kappa(s)u.$$

If $d = 3$, it is convenient to make the Ansatz

$$\left(\mathcal{R}_\mu^{\ \nu}\right) = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix},$$

where α is a real-valued differentiable function. Then, it is easy to see that (2.16) *reduces to the differential equation $\dot{\alpha} = \tau$, where τ is the torsion of p,* i.e. , *one puts $\kappa := \kappa_1$ and $\tau := \kappa_2$. Choosing α as an integral of τ, we can write*

$$h(s, u) = 1 - \kappa(s)\left[u^2 \cos\alpha(s) + u^3 \sin\alpha(s)\right].$$

Remark 2.3.5 (On Assumption 2.3.3). *If p were a compact embedded curve, then* Assumption 2.3.3 *could always be achieved for sufficiently small a. In general, however, one cannot exclude self-intersections of the tube using the local geometry of an embedded curve p only. One way to avoid this disadvantage would be to consider (Ω, g) as an abstract Riemannian manifold where only the curve p is embedded in $\mathbb{R}^d$. Nonetheless, in the present paper, we prefer to assume* Assumption 2.3.3.2 a priori *because Γ does not have a physical meaning if it is self-intersecting. Finding global geometric conditions on p ensuring the validity of* Assumption 2.3.3.2 *is an interesting question, which is beyond the scope of the present paper, however.*

2.3.2 The Laplacian

Our object of interest is the Dirichlet Laplacian (2.2), with Γ defined by (2.20). We construct it as follows. Using the diffeomorphism (2.20), we identify the Hilbert space $\mathsf{L}^2(\Gamma)$ with $\mathsf{L}^2(\Omega, \mathrm{d}v)$ and consider on the latter the Dirichlet form

$$\widetilde{Q}(\varphi, \psi) := \int_\Omega \overline{\varphi_{,i}} g^{ij} \psi_{,j} \, \mathrm{d}v, \qquad \varphi, \psi \in \mathcal{D}(\widetilde{Q}) := \mathcal{H}_0^1(\Omega, \mathrm{d}v), \tag{2.22}$$

where $(g^{ij}) := g^{-1}$. The form $\widetilde{Q}$ is clearly densely defined, non-negative, symmetric and closed on its domain. Consequently, there exists a unique non-negative self-adjoint operator $\widetilde{H}$ satisfying $\mathcal{D}(\widetilde{H}) \subset \mathcal{D}(\widetilde{Q})$ associated with $\widetilde{Q}$.We have

$$\widetilde{H}\psi = -|g|^{-1/2} \partial_i |g|^{1/2} g^{ij} \partial_j \psi, \tag{2.23}$$

$$\psi \in \mathcal{D}(\widetilde{H}) = \left\{\psi \in \mathcal{H}_0^1(\Omega, \mathrm{d}v) \, : \, \partial_i |g|^{1/2} g^{ij} \partial_j \psi \in \mathsf{L}^2(\Omega, \mathrm{d}v)\right\}. \tag{2.24}$$

That is, $\widetilde{H}$ is the Laplacian (2.2) expressed in the coordinates (s, u).

In order to apply Theorem 2.2.18, we transform $\widetilde{H}$ into a unitarily equivalent operator H of the form (2.3) acting on the Hilbert space $\mathcal{H}(\Omega) := \mathsf{L}^2(\Omega)$, without the additional weight $|g|^{1/2}$ in the volume element. This is achieved by means of the unitary mapping $\mathcal{U} : \mathsf{L}^2(\Omega, \mathrm{d}v) \to \mathcal{H}(\Omega), \psi \mapsto |g|^{1/4}\psi$. Defining $H := \mathcal{U}\widetilde{H}\mathcal{U}^{-1}$, one has

$$H\psi = -|g|^{-1/4} \partial_i |g|^{1/2} g^{ij} \partial_j |g|^{-1/4} \psi, \tag{2.25}$$

$$\psi \in \mathcal{D}(H) = \left\{\psi \in \mathcal{H}_0^1(\Omega) \, : \, \partial_i |g|^{1/2} g^{ij} \partial_j |g|^{-1/4} \psi \in \mathsf{L}^2(\Omega)\right\}. \tag{2.26}$$

Commuting $|g|^{-1/4}$ with the gradient components in the expression for H, we obtain on $\mathcal{D}(H)$

$$H = -\partial_i g^{ij} \partial_j + V\,, \tag{2.27}$$

where

$$V := -\frac{5}{4}\frac{(h_{,1})^2}{h^4} + \frac{1}{2}\frac{h_{,11}}{h^3} - \frac{1}{4}\frac{\delta^{\mu\nu} h_{,\mu} h_{,\nu}}{h^2} + \frac{1}{2}\frac{\delta^{\mu\nu} h_{,\mu\nu}}{h}. \tag{2.28}$$

Actually, (2.27) with (2.28) is a general formula valid for any smooth metric of the form $g = \mathrm{diag}(h^2, 1, \dots, 1)$. In our special case with h given by (2.21), we find that $h_{,\mu\nu} = 0$, $\delta^{\mu\nu} h_{,\mu} h_{,\nu} = \delta^{\alpha\beta} \mathcal{K}_\alpha^{\ 1} \mathcal{K}_\beta^{\ 1}$ by (2.17), while (2.16) gives

$$\begin{aligned} h_{,1}(\cdot, u) &= u^\mu \mathcal{R}_\mu^{\ \alpha} \big(\dot{\mathcal{K}}_\alpha^{\ 1} - \mathcal{K}_\alpha^{\ \beta} \mathcal{K}_\beta^{\ 1}\big), \\ h_{,11}(\cdot, u) &= u^\mu \mathcal{R}_\mu^{\ \alpha} \big(\ddot{\mathcal{K}}_\alpha^{\ 1} - \dot{\mathcal{K}}_\alpha^{\ \beta} \mathcal{K}_\beta^{\ 1} - 2\mathcal{K}_\alpha^{\ \beta} \dot{\mathcal{K}}_\beta^{\ 1} + \mathcal{K}_\alpha^{\ \beta} \mathcal{K}_\beta^{\ \gamma} \mathcal{K}_\gamma^{\ 1}\big). \end{aligned} \tag{2.29}$$

2.3.3 Results

It remains to impose decay conditions on the curvatures of p (and their derivatives) in order that the operator (2.27) satisfies Assumption 2.2.1 and Assumption 2.2.2.

Let us first consider the more general situation where the matrix (g^{ij}) is equal to $\mathrm{diag}(h^{-2}, 1, \dots, 1)$ with the explicit dependence of h on s and u not specified. One shows that it is sufficient to impose the following hypotheses.

Assumption 2.3.6. *Uniformly for $u \in \omega$,*

1. $h(s,u) \longrightarrow 1$ *as* $|s| \to \infty$,
2. $h_{,11}(s,u)$, $(\delta^{\mu\nu} h_{,\mu} h_{,\nu})(s,u)$, $\delta^{\mu\nu} h_{,\mu\nu}(s,u) \longrightarrow 0$ *as* $|s| \to \infty$,
3. $\exists \vartheta \in (0,1]$ *s.t.*

$$h_{,1}(s,u),\ h_{,111}(s,u),\ (\delta^{\mu\nu} h_{,\mu} h_{,\nu})_{,1}(s,u),\ \delta^{\mu\nu} h_{,1\mu\nu}(s,u) = \mathcal{O}\big(|s|^{-(1+\vartheta)}\big).$$

Indeed, the first hypothesis supplies Assumption 2.2.1.2, while Assumption 2.2.1.1 is fulfilled due to basic Assumption 2.3.3. Next, since h is a smooth function, Assumption 2.3.6.2 together with the behaviour of $h_{,1}$ in Assumption 2.3.6.3 are sufficient to ensure both Assumption 2.2.2.1 and Assumption 2.2.2.2. It is also clear that the asymptotic behaviour of $h_{,1}$ in Assumption 2.3.6.3 supplies Assumption 2.2.1.3. Assumption 2.2.1.4 holds true due to Assumption 2.2.1.3 and the particular form of (g^{ij}). It remains to check Assumption 2.2.2.3. This is easily done by calculating the derivative of the potential (2.28) :

$$\begin{aligned} V_{,1} = {} & 5\frac{(h_{,1})^3}{h^5} - 4\frac{h_{,1} h_{,11}}{h^4} + \frac{h_{,111}}{2h^3} \\ & + \frac{\delta^{\mu\nu}}{2}\left(\frac{h_{,1} h_{,\mu} h_{,\nu}}{h^3} - \frac{h_{,1} h_{,\mu\nu} + h_{,1\mu} h_{,\nu}}{h^2} + \frac{h_{,1\mu\nu}}{h}\right). \end{aligned}$$

With h given by (2.21), we find in addition to (2.29) that $h_{,1\mu\nu} = 0$ and

$$\begin{aligned} (\delta^{\mu\nu} h_{,\mu} h_{,\nu})_{,1} &= 2\delta^{\alpha\beta} \dot{\mathcal{K}}_\alpha^{\ 1} \mathcal{K}_\beta^{\ 1} \\ h_{,111}(\cdot, u) &= u^\mu \mathcal{R}_\mu^{\ \alpha} \big(\dddot{\mathcal{K}}_\alpha^{\ 1} - \ddot{\mathcal{K}}_\alpha^{\ \beta} \mathcal{K}_\beta^{\ 1} - 3\mathcal{K}_\alpha^{\ \beta} \ddot{\mathcal{K}}_\beta^{\ 1} - 3\dot{\mathcal{K}}_\alpha^{\ \beta} \dot{\mathcal{K}}_\beta^{\ 1} + \dot{\mathcal{K}}_\alpha^{\ \beta} \mathcal{K}_\beta^{\ \gamma} \mathcal{K}_\gamma^{\ 1} \\ & \qquad + 2\mathcal{K}_\alpha^{\ \beta} \dot{\mathcal{K}}_\beta^{\ \gamma} \mathcal{K}_\gamma^{\ 1} + 3\mathcal{K}_\alpha^{\ \beta} \mathcal{K}_\beta^{\ \gamma} \dot{\mathcal{K}}_\gamma^{\ 1} - \mathcal{K}_\alpha^{\ \beta} \mathcal{K}_\beta^{\ \gamma} \mathcal{K}_\gamma^{\ \delta} \mathcal{K}_\delta^{\ 1}\big). \end{aligned}$$

Since $|u^\mu \mathcal{R}_\mu^{\ \alpha}| < a$, Assumption 2.3.6 holds true provided we impose the following conditions on the curvatures

Assumption 2.3.7.

1. $\forall \alpha \in \{2, \ldots, d\},\ \mathcal{K}_\alpha^{\ 1}(s),\ \ddot{\mathcal{K}}_\alpha^{\ 1}(s) \longrightarrow 0$ *as* $|s| \to \infty$,
2. $\forall \alpha, \beta \in \{2, \ldots, d\},\ \mathcal{K}_\alpha^{\ \beta},\ \dot{\mathcal{K}}_\alpha^{\ 2} \in L^\infty(\mathbb{R})$,
3. $\exists \vartheta \in (0, 1]$ *s.t.* $\forall \alpha \in \{2, \ldots, d\}$,

$$\dot{\mathcal{K}}_\alpha^{\ 1}(s),\ \dddot{\mathcal{K}}_\alpha^{\ 1}(s),\ \mathcal{K}_\alpha^{\ 2}(s),\ \ddot{\mathcal{K}}_\alpha^{\ 2}(s),\ \big(\dot{\mathcal{K}}_\alpha^{\ \beta}\mathcal{K}_\beta^{\ 2}\big)(s),\ \big(\mathcal{K}_\alpha^{\ \beta}\dot{\mathcal{K}}_\beta^{\ 2}\big)(s) = \mathcal{O}\big(|s|^{-(1+\vartheta)}\big).$$

Remark 2.3.8. *These conditions reduce to those of* Theorem 2.1.1 *provided* $d = 2$*. When* $d = 3$*, it is sufficient to assume the conditions of* Theorem 2.1.1 *for the first curvature, and* $\dot{\kappa}_2 \in L^\infty(\mathbb{R})$ *and* $\kappa_2(s), \ddot{\kappa}_2(s) = \mathcal{O}\left(|s|^{-(1+\vartheta)}\right)$ *for some* $\vartheta \in (0, 1]$.

We conclude this section by applying Theorem 2.2.18.

Theorem 2.3.9. *Let* Γ *be a tube defined via* (2.20) *about a smooth infinite curve embedded in* $\mathbb{R}^d$*. Suppose* Assumptions 2.3.1, 2.3.3 *and* 2.3.7*. Then all the spectral results* (i)–(iv) *of* Theorem 2.2.18 *hold true for the Dirichlet Laplacian on* $\mathsf{L}^2(\Gamma)$.

2.4 Curved strips on surfaces

In this final section, we investigate the situation where the ambient space is a general Riemannian manifold instead of the Euclidean space $\mathbb{R}^d$. We restrict ourselves to $d = 2$, *i.e.* , Γ is a strip around an infinite curve in an (abstract) two-dimensional surface. We refer to [Kre03] for basic spectral properties of $-\Delta_{\mathrm{D}}^{\Gamma}$ and geometric details.

2.4.1 Preliminaries

Let $\mathcal{A}$ be a smooth connected complete non-compact two-dimensional Riemannian manifold of bounded Gauss curvature K. Let $p : \mathbb{R} \to \mathcal{A}$ be a smooth unit-speed curve embedded in $\mathcal{A}$ with (geodesic) curvature κ and denote by $n : \mathbb{R} \to T_{p(\cdot)}\mathcal{A}$ a smooth unit normal vector field along p. Given $a > 0$, we consider the straight strip $\Omega := \mathbb{R} \times (-a, a)$ and define a curved strip Γ of same width over p as a a-tubular neighbourhood of p in $\mathcal{A}$ by

$$\Gamma := \mathscr{L}(\Omega), \qquad \text{where} \qquad \mathscr{L} : (s, u) \mapsto \exp_{p(s)}(un(s)). \tag{2.30}$$

Note that $s \mapsto \mathscr{L}(s, u)$ traces the curves parallel to p at a fixed distance $|u|$, while the curve $u \mapsto \mathscr{L}(s, u)$ is a unit-speed geodesic orthogonal to p for any fixed s. We always assume

Assumption 2.4.1. $\mathscr{L} : \Omega \to \Gamma$ *is a diffeomorphism,*

Then $\mathscr{L}^{-1}$ determines a system of Fermi "coordinates" (s, u), *i.e.* , the geodesic coordinates based on p. The metric tensor of Γ in these coordinates acquires [Gra90, Sec. 2.4] the diagonal form

$$g(s, u) = \operatorname{diag}\left(h^2(s, u), 1\right), \tag{2.31}$$

where h is a smooth function satisfying the Jacobi equation

$$h_{,22} + Kh = 0 \qquad \text{with} \qquad \begin{cases} h(\cdot, 0) = 1 \\ h_{,2}(\cdot, 0) = -\kappa. \end{cases} \tag{2.32}$$

Here K and κ are considered as functions of the Fermi coordinates (the sign of κ being uniquely determined up to the re-parameterisation $s \mapsto -s$ or the choice of n). The determinant of the metric tensor, $|g| := \det(g) = h^2$, defines through $\mathrm{d}v := h(s,u)\mathrm{d}s\mathrm{d}u$ the area element of the strip.

Assuming that the metric g is uniformly elliptic in the sense that

Assumption 2.4.2. $\exists c_\pm \in (0,\infty)$ *s.t.* $\forall (s,u) \in \Omega,\ c_- \leq h(s,u) \leq c_+$

holds true, the Dirichlet Laplacian corresponding to Γ can be defined in the same way as in Section 2.3.2, *i.e.* , as the operator $\widetilde{H}$ associated with the form (2.22), satisfying (2.23). At the same time, we may introduce the unitarily equivalent operator H on $\mathsf{L}^2(\Omega)$ given by (2.25) and satisfying (2.27) with (2.28).

Remark 2.4.3. *If* Assumption 2.4.2 *holds true, then the inverse function theorem together with* (2.32) *yield that* Assumption 2.4.1 *is satisfied for all sufficiently small* a *provided the strip* Γ *does not overlap itself.* Assumption 2.4.2 *is satisfied, for instance, if* Γ *is a sufficiently thin strip on a ruled surface,* cf. [Kre03, Sec. 7].

2.4.2 Results

In view of the more general approach in the beginning of Section 2.3.3, we see that Assumption 2.3.6 (with $d = 2$) guarantees Assumptions 2.2.1 and 2.2.2 also in the present case. Applying Theorem 2.2.18, we obtain, with $\mathcal{T} = \{n^2\nu_1\}_{n=1}^\infty$ where $\nu_1 := \pi^2/(2a)^2$, the following result

Theorem 2.4.4. *Let* Γ *be a tubular neighbourhood of radius* $a > 0$ *about a smooth infinite curve, which is embedded in a smooth connected complete non-compact surface of bounded curvature. Suppose* Assumptions 2.4.1, 2.4.2 *and* 2.3.6*. Then all the spectral results* (i)–(iv) *of* Theorem 2.2.18 *hold true for the Dirichlet Laplacian on* $\mathsf{L}^2(\Gamma)$.

Assume now that the strip is *flat* in the sense of [Kre03], *i.e.* , the curvature K is equal to zero everywhere on Γ. Then the Jacobi equation (2.32) has the explicit solution (*cf.* (2.21) for $d = 2$)

$$h(s,u) = 1 - \kappa(s)u \tag{2.33}$$

and Assumption 2.3.6 can be replaced by some conditions on the decay of the curvature κ at infinity, namely, we adopt Assumption 2.3.7 with $\kappa_1 \equiv \kappa$ and $\mathcal{K}_\mu^\nu = 0$ (*cf.* the assumptions of Theorem 2.1.1). At the same time, it easy to see that Assumption 2.4.1 and 2.4.2 are satisfied if Assumption 2.3.3 holds true.

Theorem 2.4.5 (Flat strips). *Let* Γ *be a tubular neighbourhood of radius* $a > 0$ *about a smooth infinite curve of curvature* κ*, which is embedded in a smooth connected complete non-compact surface of bounded curvature* K *such that* $K \restriction \Gamma = 0$*. Suppose* Assumption 2.3.3 *and*

1. $\kappa(s), \ddot{\kappa}(s) \longrightarrow 0$ *as* $|s| \to \infty$,
2. $\exists \vartheta \in (0,1]$ *s.t.* $\dot{\kappa}(s), \dddot{\kappa}(s) = \mathcal{O}\left(|s|^{-(1+\vartheta)}\right)$.

Then, all the spectral results (i)–(iv) *of* Theorem 2.2.18 *hold true for the Dirichlet Laplacian on* $\mathsf{L}^2(\Gamma)$.

Quatrième partie

Opérateur de Dirac avec champ magnétique

Chapitre 1

Résumé

Considérons une particule relativiste de masse $m > 0$ et de spin $\frac{1}{2}$ évoluant dans $\mathbb{R}^3$ en présence d'un champ magnétique variable de direction constante. En vertu des équations de Maxwell, il est possible de choisir sans perte de généralité un référentiel orthonormé dans lequel le champ magnétique prend la forme suivante : $\vec{B}(x_1, x_2, x_3) = (0, 0, B(x_1, x_2))$. Le système physique est alors décrit dans l'espace de Hilbert $\mathcal{H} := \mathsf{L}^2(\mathbb{R}^3; \mathbb{C}^4)$ par l'opérateur de Dirac

$$H_0 := \alpha_1 \Pi_1 + \alpha_2 \Pi_2 + \alpha_3 P_3 + \beta m,$$

où $\beta \equiv \alpha_0, \alpha_1, \alpha_2, \alpha_3$ sont les matrices de Dirac-Pauli et $\Pi_j := -i\partial_j - a_j$ sont les générateurs des translations magnétiques avec un potentiel vecteur

$$\vec{a}(x_1, x_2, x_3) = (a_1(x_1, x_2), a_2(x_1, x_2), 0) \tag{1.1}$$

satisfaisant $B = \partial_1 a_2 - \partial_2 a_1$. Puisque $a_3 = 0$, nous écrivons $P_3 := -i\partial_3$ au lieu de Π_3.

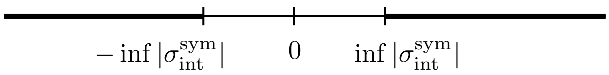

FIG. 1.1 – Spectre de H_0

Dans l'article qui suit, nous étudions la stabilité des propriétés spectrales de H_0 sous l'effet de perturbations dues à l'ajout d'un potentiel matriciel V. Si V satisfait certaines hypothèses de décroissance à l'infini, nous démontrons un principe d'absorption limite pour l'hamiltonien perturbé $H := H_0 + V$. Nous en déduisons l'existence d'opérateurs d'onde locaux ainsi que l'absence de spectre singulier et la finitude du spectre ponctuel de H dans certains sous-ensembles de $\mathbb{R}$. Les sous-ensembles en question correspondent aux trous spectraux dans le spectre symétrisé de l'opérateur $H^0 := \sigma_1 \Pi_1 + \sigma_2 \Pi_2 + \sigma_3 m$ agissant dans $\mathsf{L}^2(\mathbb{R}^2; \mathbb{C}^2)$, où σ_j sont les matrices de Pauli. Le spectre symétrisé $\sigma_{\rm sym}^0$

de H^0 est la réunion des spectres de H^0 et $-H^0$ [1]. L'opérateur H^0 peut être interprété comme un hamiltonien interne au système. Nous renvoyons le lecteur à la figure 1.1 pour un schéma du spectre de H_0 et à la figure 1.2 pour un schéma des spectres $\sigma(H)$ et σ^0_{sym} dans le cas où le champ magnétique B est constant et non nul. Dans le cas où le champ

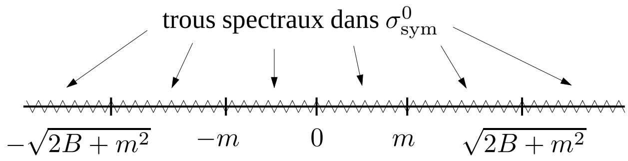

FIG. 1.2 – Si B est constant et non nul, alors $\sigma^0_{\mathrm{sym}} = \{\pm\sqrt{2nB+m^2}\}_{n=0,1,2,\ldots}$. Le trait en zig-zag représente le spectre (indéterminé) de l'opérateur H.

magnétique tend vers 0 à l'infini, le spectre essentiel de H_0 est égal à l'union des intervalles $(-\infty,-m]$ et $[m,\infty)$ [Tha92, Thm. 7.7] et la différence des résolvantes de H_0 et H est compacte[2]. Le spectre essentiel de l'hamiltonien perturbé H est donc aussi égal à l'union $(-\infty,-m]\cup[m,\infty)$. En particulier, l'ensemble des valeurs propres de H dans $\mathbb{R}\setminus\sigma^0_{\mathrm{sym}}$ (forcément inclu dans $(-m,m)$) n'est composé que de valeurs propres isolées et de multiplicité finie. En conséquence, notre approche ne fournit pas d'informations pertinentes.

Nous donnons maintenant une description plus précise de nos résultats. Considérons un champ magnétique $\vec{B}$ continu de la forme $\vec{B}=(0,0,B(x_1,x_2))$. Soit $\vec{a}$ un potentiel vecteur vérifiant (1.1) obtenu, par exemple, en utilisant la jauge transverse. Soit V une application bornée de $\mathbb{R}^3$ à valeurs dans les matrices 4×4 hermitiennes. Nous supposons que le potentiel V s'annule à l'infini et imposons une certaine vitesse de décroissance dans la direction x_3. Aucune vitesse de décroissance n'est prescrite dans les directions orthogonales x_1 et x_2. Nous montrons alors que l'opérateur matriciel

$$A := \tfrac{1}{2}(H_0^{-1}P_3Q_3 + Q_3P_3H_0^{-1})$$

est essentiellement autoadjoint sur $C_0^\infty(\mathbb{R}^3;\mathbb{C}^4)$ et conjugué à l'hamiltonien H sur $\mathbb{R}\setminus\sigma^0_{\mathrm{sym}}$. De ceci découle l'existence d'un principe d'absorption limite sur $\mathbb{R}\setminus\sigma^0_{\mathrm{sym}}$. Les résultats suivants sont obtenus comme corollaires :

(a) Les valeurs propres de H dans $\mathbb{R}\setminus\sigma^0_{\mathrm{sym}}$ sont de multiplicité finie et ne peuvent s'accumuler qu'en les points de l'ensemble σ^0_{sym}.

(b) L'opérateur H n'a pas de spectre singulier continu dans $\mathbb{R}\setminus\sigma^0_{\mathrm{sym}}$.

(c) Supposons qu'il existe un nombre $s>1$ tel que $|Q_3|^sV$ soit borné. Alors pour chaque ensemble ouvert $J\subset\mathbb{R}\setminus\big(\sigma^0_{\mathrm{sym}}\cup\sigma_{\mathrm{p}}(H)\big)$, les opérateurs d'onde locaux

$$\text{s-}\lim_{t\to\pm\infty} e^{itH_0}e^{-itH}E^H(J)$$

existent et leurs images sont égales à $E^{H_0}(J)\mathcal{H}$, où $E^H(\cdot)$ et $E^{H_0}(\cdot)$ sont les mesures spectrales de H et H_0.

[1] Dans la section 1.4, nous avons défini l'ensemble σ^0_{sym} comme le spectre de la composante $H_0(0)$ de l'opérateur H_0 dans la représentation spectrale de l'opérateur P_3. Les deux définitions sont équivalentes, *i.e.*

$$\sigma^0_{\mathrm{sym}} = \sigma(H^0)\cup\sigma(-H^0) = \sigma[H_0(0)].$$

[2] Nous renvoyons le lecteur à [Tha92, Sec. 4.3.4] pour plus de détails sur les questions de compacité relative et d'invariance du spectre essentiel dans le cas des perturbations de l'opérateur de Dirac libre.

L'intérêt de cette étude réside dans le fait que le champ magnétique initial est quelconque ; hormis l'hypothèse de continuité, aucune restriction n'est imposée à la fonction $B : \mathbb{R}^2 \to \mathbb{R}$. La démarche ne dépend donc pas explicitement du choix du champ magnétique si ce n'est pour le calcul de l'ensemble σ^0_{sym}. Dans le cas où B est constant et non nul, le principe d'absorption limite obtenu est sensiblement plus général que ceux démontrés dans certains travaux récents. Pour des champs magnétiques plus arbitraires, nos résultats semblent nouveaux.

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Chapitre 2

On perturbations of Dirac operators with variable magnetic field of constant direction

Abstract

We carry out the spectral analysis of matrix valued perturbations of 3-dimensional Dirac operators with variable magnetic field of constant direction. Under suitable assumptions on the magnetic field and on the pertubations, we obtain a limiting absorption principle, we prove the absence of singular continuous spectrum in certain intervals and state properties of the point spectrum. Various situations, for example when the magnetic field is constant, periodic or diverging at infinity, are covered. The importance of an internal-type operator (a 2-dimensional Dirac operator) is also revealed in our study. The proofs rely on commutator methods.

2.1 Introduction and main results

We consider a relativistic spin-$\frac{1}{2}$ particle evolving in $\mathbb{R}^3$ in presence of a variable magnetic field of constant direction. By virtue of the Maxwell equations, we may assume with no loss of generality that the magnetic field has the form $\vec{B}(x_1, x_2, x_3) = \big(0, 0, B(x_1, x_2)\big)$. So the unperturbed system is described, in the Hilbert space $\mathsf{L}^2(\mathbb{R}^3; \mathbb{C}^4)$, by the Dirac operator

$$H_0 := \alpha_1 \Pi_1 + \alpha_2 \Pi_2 + \alpha_3 P_3 + \beta m,$$

where $\beta \equiv \alpha_0, \alpha_1, \alpha_2, \alpha_3$ are the usual Dirac-Pauli matrices, m is the strictly positive mass of the particle and $\Pi_j := -i\partial_j - a_j$ are the generators of the magnetic translations with a vector potential $\vec{a}(x_1, x_2, x_3) = (a_1(x_1, x_2), a_2(x_1, x_2), 0)$ that satisfies $B = \partial_1 a_2 - \partial_2 a_1$. Since $a_3 = 0$, we have written $P_3 := -i\partial_3$ instead of Π_3.

In this paper we study the stability of certain parts of the spectrum of H_0 under matrix valued perturbations V. More precisely, if V satisfies some natural hypotheses, we shall prove the absence of singular continuous spectrum and the finiteness of the point spectrum of $H := H_0 + V$ in intervals of $\mathbb{R}$ corresponding to gaps in the symmetrized spectrum of the operator $H^0 := \sigma_1\Pi_1 + \sigma_2\Pi_2 + \sigma_3 m$ in $\mathsf{L}^2(\mathbb{R}^2; \mathbb{C}^2)$. The matrices σ_j are the Pauli matrices and the symmetrized spectrum σ^0_{sym} of H^0 is the union of the spectra of H^0 and $-H^0$. We stress that our analysis does not require any restriction on the behaviour of the magnetic field at infinity. Nevertheless, the pertinence of our work depends on a certain property of the internal-type operator H^0 ; namely, the size and the number of gaps in σ^0_{sym}. We refer to [BS99], [Dan99], [GM93], [HNW89] and [Tha92] for various results on the spectrum of H^0, especially in the situations of physical interest, for example when B is constant, periodic or diverges at infinity.

Technically, this work relies on commutator methods initiated by E. Mourre [Mou81] and extensively developed in [ABG96]. For brevity we shall constantly refer to the latter reference for notations and definitions. Our choice of a conjugate operator enables us to treat Dirac operators with general magnetic fields provided they point in a constant direction. On the other hand, as already put into evidence in [GM01], the use of a conjugate operator with a matrix structure has a few "rather awkward consequences" for long-range perturbations. We finally mention that this study is the counterpart for Dirac operators of [MP00], where only Schrödinger operators are considered. Unfortunately, the intrinsic structure of the Dirac equation prevents us from using the possible magnetic anisotropy to control the perturbations (see Remark 2.3.2 for details).

We give now a more precise description of our results. For simplicity we impose the continuity of the magnetic field and avoid perturbations with local singularities. Hence we assume that B is a $C(\mathbb{R}^2; \mathbb{R})$-function and choose any vector potential $\vec{a} = (a_1, a_2, 0) \in C(\mathbb{R}^2; \mathbb{R}^3)$, *e.g.* the one obtained by means of the transversal gauge [Tha92]. The definitions below concern the admissible perturbations. In the long-range case, we restrict them to the scalar type in order not to impose unsatisfactory constraints. In the sequel, $\mathscr{B}_{\text{h}}(\mathbb{C}^4)$ stands for the set of 4×4 hermitian matrices, and $\|\cdot\|$ denotes the norm of the Hilbert space $\mathcal{H} := \mathsf{L}^2(\mathbb{R}^3; \mathbb{C}^4)$ as well as the norm of $\mathscr{B}(\mathcal{H})$, the set of bounded linear operators on $\mathcal{H}$. $\mathbb{N} := \{0, 1, 2, \ldots\}$ is the set of natural numbers. ϑ is an arbitrary $C^\infty\big([0,\infty)\big)$-function such that $\vartheta = 0$ near 0 and $\vartheta = 1$ near infinity. Q_j is the multiplication operator by the coordinate x_j in $\mathcal{H}$, and the expression $\langle\cdot\rangle$ corresponds to $\sqrt{1 + (\cdot)^2}$.

Definition 2.1.1. *Let V be a multiplication operator by an element of $\mathsf{L}^\infty\big(\mathbb{R}^3; \mathscr{B}_{\text{h}}(\mathbb{C}^4)\big)$.*

(a) V is small at infinity *if* $\lim_{r\to\infty} \Big\| \vartheta\Big(\frac{\langle Q\rangle}{r}\Big) V \Big\| = 0$,

(b) V is short-range *if* $\int_1^\infty \Big\| \vartheta\Big(\frac{\langle Q_3\rangle}{r}\Big) V \Big\| \,\mathrm{d}r < \infty$,

(c) Let V_L be in $C^1(\mathbb{R}^3; \mathbb{R})$ with $x \mapsto \langle x_3\rangle(\partial_j V_L)(x)$ in $\mathsf{L}^\infty(\mathbb{R}^3; \mathbb{R})$ for $j = 1, 2, 3$, then $V := V_L$ is long-range *if*

$$\int_1^\infty \Big\| \vartheta\Big(\frac{\langle Q_3\rangle}{r}\Big) \langle Q_3\rangle (\partial_j V) \Big\| \,\frac{\mathrm{d}r}{r} < \infty \qquad \textit{for} \qquad j = 1, 2, 3.$$

Note that Definitions 2.1.1.(b) and 2.1.1.(c) differ from the standard ones : the decay rate is imposed only in the x_3 direction.

We are in a position to state our results. Let $\mathcal{D}(\langle Q_3\rangle)$ denote the domain of $\langle Q_3\rangle$ in $\mathcal{H}$, then the limiting absorption principle for H is expressed in terms of the Banach space

$\mathcal{G} := \big(\mathcal{D}(\langle Q_3\rangle), \mathcal{H}\big)_{1/2,1}$ defined by real interpolation [ABG96]. For convenience, we recall that $\mathcal{D}(\langle Q_3\rangle^s)$ is contained in $\mathcal{G}$ for each $s > 1/2$.

Theorem 2.1.2. *Assume that B is in $C(\mathbb{R}^2;\mathbb{R})$, and that V belongs to $\mathsf{L}^\infty\big(\mathbb{R}^3;\mathscr{B}_\mathrm{h}(\mathbb{C}^4)\big)$, is small at infinity and can be written as the sum of a short-range and a long-range matrix valued function. Then*

(a) The point spectrum of the operator H in $\mathbb{R}\setminus\sigma^0_\mathrm{sym}$ is composed of eigenvalues of finite multiplicity and with no accumulation point in $\mathbb{R}\setminus\sigma^0_\mathrm{sym}$.
(b) The operator H has no singular continuous spectrum in $\mathbb{R}\setminus\sigma^0_\mathrm{sym}$.
(c) The limits $\lim_{\varepsilon\to+0}\langle\psi,(H-\lambda\mp i\varepsilon)^{-1}\psi\rangle$ exist for each $\psi\in\mathcal{G}$, uniformly in λ on each compact subset of $\mathbb{R}\setminus\{\sigma^0_\mathrm{sym}\cup\sigma_\mathrm{pp}(H)\}$.

The limiting absorption principle (c), together with the inclusions mentioned before the theorem, lead to locally H-smooth operators. They imply the existence of local wave operators.

Corollary 2.1.3. *Let V belong to $\mathsf{L}^\infty\big(\mathbb{R}^3;\mathscr{B}_\mathrm{h}(\mathbb{C}^4)\big)$ and be small at infinity. Assume there exists some $s > 1$ such that $\langle Q_3\rangle^s V\in\mathscr{B}(\mathcal{H})$. Then for each open set $J\subset\mathbb{R}\setminus\{\sigma^0_\mathrm{sym}\cup\sigma_\mathrm{pp}(H)\}$, the local wave operators* s-$\lim_{t\to\pm\infty} e^{itH_0}e^{-itH}E^H(J)$ *exist and their ranges are equal to $E^{H_0}(J)\mathcal{H}$, where E^H and E^{H_0} are the spectral measures of H and H_0 respectively.*

Remark 2.1.4. *H_0-bounded perturbations (with relative bound less than one) may also be treated with some slight adaptations of Definition 2.1.1. In particular Coulomb-type potentials and Zeeman effect [Hac93] could be considered for certain magnetic fields and vector potentials. However, to our knowledge, there is not any explicit class of H_0-bounded perturbations for arbitrary continuous magnetic fields. For this reason, we concentrate on bounded potentials V only, and thus present a simplified version of a more general, and more complicated, perturbation theory.*

The above statements seem to be new for such a general magnetic field. In the special but important case of a nonzero constant magnetic field B_0, the admissible perturbations introduced in Definition 2.1.1 are more general than those allowed in [Yok01]. We stress that in this situation σ^0_sym is equal to $\{\pm\sqrt{2nB_0+m^2} : n\in\mathbb{N}\}$, which implies that there are plenty of gaps where our analysis gives results. On the other hand, if $B(x_1,x_2)\to 0$ as $|(x_1,x_2)|\to\infty$, our treatment gives no information since both $(-\infty,-m]$ and $[m,\infty)$ belong to σ^0_sym. We finally mention the paper [BC02] for a related work on perturbations of magnetic Dirac operators.

2.2 Mourre estimate for the operator H_0

2.2.1 Preliminaries

Let us start by recalling some known results. The operator H_0 is essentially self-adjoint on $\mathscr{D} := C_0^\infty(\mathbb{R}^3;\mathbb{C}^4)$ [Che77, Thm. 2.1]. Its spectrum is symmetric with respect to 0 and does not contain the interval $(-m,m)$ [Tha92, Cor. 5.14]. Thus the subset $H_0\mathscr{D}$ is dense in $\mathcal{H}$ since $\mathscr{D}$ is dense in $\mathcal{D}(H_0)$ (endowed with the graph topology) and H_0 is a homeomorphism from $\mathcal{D}(H_0)$ onto $\mathcal{H}$.

We now introduce a suitable representation of the Hilbert space $\mathcal{H}$. We consider the partial Fourier transformation

$$\mathscr{F} : \mathscr{D} \to \int_{\mathbb{R}}^{\oplus} \mathcal{H}_{12}\, \mathrm{d}\xi, \qquad (\mathscr{F}\psi)(\xi) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{e}^{-i\xi x_3} \psi(\cdot, x_3)\, \mathrm{d}x_3, \tag{2.1}$$

where $\mathcal{H}_{12} := \mathsf{L}^2(\mathbb{R}^2; \mathbb{C}^4)$. This map extends uniquely to a unitary operator from $\mathcal{H}$ onto $\int_{\mathbb{R}}^{\oplus} \mathcal{H}_{12}\, \mathrm{d}\xi$, which we denote by the same symbol $\mathscr{F}$. As a first application, one obtains the following direct integral decomposition of H_0 :

$$\mathscr{F} H_0 \mathscr{F}^{-1} = \int_{\mathbb{R}}^{\oplus} H_0(\xi)\, \mathrm{d}\xi,$$

where $H_0(\xi)$ is a self-adjoint operator in $\mathcal{H}_{12}$ acting as $\alpha_1 \Pi_1 + \alpha_2 \Pi_2 + \alpha_3 \xi + \beta m$ on $C_0^\infty(\mathbb{R}^2; \mathbb{C}^4)$. In the following remark we draw the connection between the operator $H_0(\xi)$ and the operator H^0 introduced in Section 2.1. It reveals the importance of the internal-type operator H^0 and shows why its negative $-H_0$ also has to be taken into account.

Remark 2.2.1. *The operator $H_0(0)$ acting on $C_0^\infty(\mathbb{R}^2; \mathbb{C}^4)$ is unitarily equivalent to the direct sum operator $\begin{pmatrix} m & \Pi_- \\ \Pi_+ & -m \end{pmatrix} \oplus \begin{pmatrix} m & \Pi_+ \\ \Pi_- & -m \end{pmatrix}$ acting on $C_0^\infty(\mathbb{R}^2; \mathbb{C}^2) \oplus C_0^\infty(\mathbb{R}^2; \mathbb{C}^2)$, where $\Pi_\pm := \Pi_1 \pm i\Pi_2$. Now, these two matrix operators act in $\mathsf{L}^2(\mathbb{R}^2; \mathbb{C}^2)$ and are essentially self-adjoint on $C_0^\infty(\mathbb{R}^2; \mathbb{C}^2)$ [Che77, Thm. 2.1]. However, the first one is nothing but H^0, while the second one is unitarily equivalent to $-H^0$ (this can be obtained by means of the abstract Foldy-Wouthuysen transformation [Tha92, Thm. 5.13]). Therefore $H_0(0)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^2; \mathbb{C}^4)$ and*

$$\sigma[H_0(0)] = \sigma(H^0) \cup \sigma(-H^0) \equiv \sigma^0_{\mathrm{sym}}.$$

Moreover, there exists a relation between $\sigma[H_0(\xi)]$ and σ^0_{sym}. Indeed, for $\xi \in \mathbb{R}$ fixed, one can show that $H_0(\xi)^2 = H_0(0)^2 + \xi^2$ on $\mathcal{D}\big(H_0(\xi)^2\big) = \mathcal{D}\big(H_0(0)^2\big)$, so that

$$\sigma[H_0(\xi)^2] = \sigma[H_0(0)^2 + \xi^2] = \big(\sigma[H_0(0)]\big)^2 + \xi^2 = (\sigma^0_{\mathrm{sym}})^2 + \xi^2, \tag{2.2}$$

where the spectral theorem has been used for the second equality. Since the spectrum of $H_0(\xi)$ is symmetric with respect to 0 [Tha92, Cor. 5.14], it follows that

$$\sigma[H_0(\xi)] = -\sqrt{(\sigma^0_{\mathrm{sym}})^2 + \xi^2} \,\cup\, \sqrt{(\sigma^0_{\mathrm{sym}})^2 + \xi^2}.$$

Define $\mu_0 := \inf |\sigma^0_{\mathrm{sym}}|$ (which is bigger or equal to m because H^0 has no spectrum in $(-m, m)$ [Tha92, Cor. 5.14]). Then from the direct integral decomposition of H_0, one readily gets

$$\sigma(H_0) = (-\infty, -\mu_0] \cup [\mu_0, +\infty). \tag{2.3}$$

We conclude the section by giving two technical lemmas in relation with the operator H_0^{-1}. Proofs can be found in an appendix.

Lemma 2.2.2. *(a) For each $n \in \mathbb{N}$, $H_0^{-n}\mathscr{D}$ belongs to $\mathcal{D}(Q_3)$,*

(b) $P_3 H_0^{-1}$ is a bounded self-adjoint operator equal to $H_0^{-1} P_3$ on $\mathcal{D}(P_3)$. In particular, $H_0^{-1}\mathcal{H}$ belongs to $\mathcal{D}(P_3)$.

One may observe that, given a $C^1(\mathbb{R}; \mathbb{C})$-function f with f' bounded, the operator $f(Q_3)$ is well-defined on $\mathcal{D}(Q_3)$. Thus $f(Q_3) H_0^{-n} \mathscr{D}$ is a subset of $\mathcal{H}$ for each $n \in \mathbb{N}$. The preceding lemma and the following simple statement are constantly used in the sequel.

Lemma 2.2.3. *Let f be in $C^1(\mathbb{R};\mathbb{C})$ with f' bounded, and $n \in \mathbb{N}$. Then*
(a) $iH_0^{-1}f(Q_3) - if(Q_3)H_0^{-1}$ is equal to $-H_0^{-1}\alpha_3 f'(Q_3)H_0^{-1}$ on $H_0^{-n}\mathscr{D}$,
(b) $P_3H_0^{-1}f(Q_3) - f(Q_3)P_3H_0^{-1}$ is equal to $i(P_3H_0^{-1}\alpha_3 - 1)f'(Q_3)H_0^{-1}$ on $\mathscr{D}$.

Both right terms belong to $\mathscr{B}(\mathcal{H})$. For shortness we shall denote them by $[iH_0^{-1}, f(Q_3)]$ and $[P_3H_0^{-1}, f(Q_3)]$ respectively.

2.2.2 The conjugate operator

The aim of the present section is to define an appropriate operator conjugate to H_0. To begin with, one observes that $Q_3P_3H_0^{-1}\mathscr{D} \subset \mathcal{H}$ as a consequence of Lemma 2.2.2. In particular, the formal expression

$$A := \tfrac{1}{2}(H_0^{-1}P_3Q_3 + Q_3P_3H_0^{-1}) \tag{2.4}$$

leads to a well-defined symmetric operator on $\mathscr{D}$.

Proposition 2.2.4. *The operator A is essentially self-adjoint on $\mathscr{D}$ and its closure is essentially self-adjoint on any core for $\langle Q_3\rangle$.*

Proof. The claim is a consequence of Nelson's criterion of essential self-adjointness [RS78, Thm. X.37] applied to the triple $\{\langle Q_3\rangle, A, \mathscr{D}\}$. Let us simply verify the two hypotheses of that theorem. By using Lemmas 2.2.2 and 2.2.3, one first obtains that for all $\psi \in \mathscr{D}$:

$$\|A\psi\| = \left\|\left(P_3H_0^{-1}Q_3 - \tfrac{1}{2}\left[P_3H_0^{-1}, Q_3\right]\right)\psi\right\| \leq \textsc{c}\,\|\langle Q_3\rangle\psi\|$$

for some constant $\textsc{c} > 0$ independent of ψ. Then, for all $\psi \in \mathscr{D}$ one has :

$$\begin{aligned}\langle A\psi, \langle Q_3\rangle\psi\rangle - \langle\langle Q_3\rangle\psi, A\psi\rangle &= i\,\mathsf{Im}\left\langle Q_3\psi, \left[P_3H_0^{-1}, \langle Q_3\rangle\right]\psi\right\rangle \\ &= i\,\mathsf{Re}\left\langle\left(\alpha_3P_3H_0^{-1} - 1\right)Q_3\psi, Q_3\langle Q_3\rangle^{-1}H_0^{-1}\psi\right\rangle.\end{aligned}$$

A few more commutator calculations, using again Lemma 2.2.3 with $f(Q_3) = \langle Q_3\rangle^{1/2}$, lead to the following result : for all $\psi \in \mathscr{D}$, there exists a constant $\textsc{d} > 0$ independent of ψ such that

$$|\,\langle A\psi, \langle Q_3\rangle\,\psi\rangle - \langle\langle Q_3\rangle\,\psi, A\psi\rangle\,| \leq \textsc{d}\left\|\,\langle Q_3\rangle^{\frac{1}{2}}\,\psi\right\|^2.$$

□

As far as we know, the operator (2.4) has never been employed before for the study of magnetic Dirac operators. In [Yok01], a slightly different conjugate operator has been introduced for Dirac operators with constant magnetic field, namely

$$A = \tfrac{1}{2}U_{\text{FW}}^{-1}\left(\langle P_3\rangle^{-1}P_3Q_3 + Q_3P_3\langle P_3\rangle^{-1}\right)\beta\,U_{\text{FW}},$$

where U_{FW} is the Foldy-Wouthuysen transformation that diagonalizes H_0. Though this operator could also be used in our more general context, it presents the major drawback of making the perturbation theory somewhat more complicated.

2.2.3 Strict Mourre estimate for H_0

We now gather some results on the regularity of H_0 with respect to A. We recall that $\mathcal{D}(H_0)^*$ is the adjoint space of $\mathcal{D}(H_0)$ and that one has the continuous dense embeddings $\mathcal{D}(H_0) \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{D}(H_0)^*$, where $\mathcal{H}$ is identified with its adjoint through the Riesz isomorphism.

Proposition 2.2.5.

(a) The quadratic form $\mathcal{D}(A) \ni \psi \mapsto \langle H_0^{-1}\psi, iA\psi\rangle - \langle A\psi, iH_0^{-1}\psi\rangle$ *extends uniquely to the bounded form defined by the operator* $-H_0^{-1}(P_3H_0^{-1})^2H_0^{-1} \in \mathscr{B}(\mathcal{H})$*.*

(b) The group $\{e^{itA}\}_{t\in\mathbb{R}}$ *leaves* $\mathcal{D}(H_0)$ *invariant.*

(c) The quadratic form

$$\mathcal{D}(A) \ni \psi \mapsto \langle H_0^{-1}(P_3H_0^{-1})^2H_0^{-1}\psi, iA\psi\rangle - \langle A\psi, iH_0^{-1}(P_3H_0^{-1})^2H_0^{-1}\psi\rangle, \tag{2.5}$$

extends uniquely to a bounded form on $\mathcal{H}$*.*

In the framework of [ABG96], the statements of (a) and (c) mean that H_0 is of class $C^1(A)$ and $C^2(A)$ respectively.

Proof. (a) For any $\psi \in \mathscr{D}$, one gets

$$\begin{aligned} 2\left(\langle H_0^{-1}\psi, iA\psi\rangle - \langle A\psi, iH_0^{-1}\psi\rangle\right) &= \langle [iH_0^{-1}, Q_3]\psi, P_3H_0^{-1}\psi\rangle \\ &\quad + \langle P_3H_0^{-1}\psi, [iH_0^{-1}, Q_3]\psi\rangle \qquad (2.6)\\ &= -\langle H_0^{-1}\psi, (\alpha_3P_3H_0^{-1} + H_0^{-1}\alpha_3P_3)H_0^{-1}\psi\rangle, \qquad (2.7)\end{aligned}$$

where we have used Lemmas 2.2.2 and 2.2.3 . Furthermore, one has

$$H_0^{-1}\alpha_3 = -\alpha_3H_0^{-1} + 2H_0^{-1}P_3H_0^{-1} \tag{2.8}$$

as an operator identity in $\mathscr{B}(\mathcal{H})$. When inserting (2.8) into (2.6), one obtains the equality

$$\langle H_0^{-1}\psi, iA\psi\rangle - \langle A\psi, iH_0^{-1}\psi\rangle = -\langle \psi, H_0^{-1}(P_3H_0^{-1})^2H_0^{-1}\psi\rangle. \tag{2.9}$$

Since $\mathscr{D}$ is a core for A, the statement is obtained by density. We shall write $[iH_0^{-1}, A]$ for the bounded extension of the quadratic form $\mathcal{D}(A) \ni \psi \mapsto \langle H_0^{-1}\psi, iA\psi\rangle - \langle A\psi, iH_0^{-1}\psi\rangle$.

(b) Since $\mathcal{D}(H_0)$ is not explicitly known, one has to invoke an abstract result in order to show the invariance. Let $[iH_0, A]$ be the operator in $\mathscr{B}(\mathcal{D}(H_0), \mathcal{D}(H_0)^*)$ associated with the unique extension to $\mathcal{D}(H_0)$ of the quadratic form $\psi \mapsto \langle H_0\psi, iA\psi\rangle - \langle A\psi, iH_0\psi\rangle$ defined for all $\psi \in \mathcal{D}(H_0) \cap \mathcal{D}(A)$. Then $\mathcal{D}(H_0)$ is invariant under $\{e^{itA}\}_{t\in\mathbb{R}}$ if H_0 is of class $C^1(A)$ and if $[iH_0, A]\mathcal{D}(H_0) \subset \mathcal{H}$ [GG99, Lemma 2]. From equation (2.9) and [ABG96, Eq. 6.2.24], one obtains the following equalities valid in form sense on $\mathcal{H}$:

$$-H_0^{-1}(P_3H_0^{-1})^2H_0^{-1} = \left[iH_0^{-1}, A\right] = -H_0^{-1}\left[iH_0, A\right]H_0^{-1}.$$

Thus $[iH_0, A]$ and $(P_3H_0^{-1})^2$ are equal as operators in $\mathscr{B}(\mathcal{D}(H_0), \mathcal{D}(H_0)^*)$. But since the latter belongs to $\mathscr{B}(\mathcal{H})$, $[iH_0, A]\mathcal{D}(H_0)$ is included in $\mathcal{H}$.

(c) The boundedness on $\mathscr{D}$ of the quadratic form (2.5) follows by inserting (2.4) into the r.h.s. term of (2.5) and by applying repeatedly Lemma 2.2.3 with $f(Q_3) = Q_3$. Then one concludes by using the density of $\mathscr{D}$ in $\mathcal{D}(A)$. ☐

From now on we shall simply denote the closure in $\mathcal{H}$ of $[iH_0, A]$ by $T = (P_3H_0^{-1})^2 \in \mathscr{B}(\mathcal{H})$. One interest of this operator is that $\mathscr{F}T\mathscr{F}^{-1}$ is boundedly decomposable [Cho70, Prop. 3.6], more precisely :

$$\mathscr{F}T\mathscr{F}^{-1} = \int_{\mathbb{R}}^{\oplus} T(\xi)\,\mathrm{d}\xi \qquad \text{with} \qquad T(\xi) = \xi^2H_0(\xi)^{-2} \in \mathscr{B}(\mathcal{H}_{12}).$$

In the following definition, we introduce two functions giving the optimal value to a Mourre-type inequality. Remark that slight modifications have been done with regard to the usual definition [ABG96, Sec. 7.2.1].

Definition 2.2.6. *Let H be a self-adjoint operator in a Hilbert space $\mathcal{H}$ and assume that S is a symmetric operator in $\mathscr{B}\big(\mathcal{D}(H),\mathcal{D}(H)^*\big)$. Let $E^H(\lambda;\varepsilon) := E^H\big((\lambda-\varepsilon,\lambda+\varepsilon)\big)$ be the spectral projection of H for the interval $(\lambda-\varepsilon,\lambda+\varepsilon)$. Then, for all $\lambda\in\mathbb{R}$ and $\varepsilon>0$, we set*

$$\begin{aligned}\varrho_H^S(\lambda;\varepsilon) &:= \sup\big\{a\in\mathbb{R}\ :\ E^H(\lambda;\varepsilon)SE^H(\lambda;\varepsilon)\geq aE^H(\lambda;\varepsilon)\big\}\,,\\ \varrho_H^S(\lambda) &:= \sup_{\varepsilon>0}\varrho_H^S(\lambda;\varepsilon).\end{aligned}$$

Let us make three observations : the inequality $\varrho_H^S(\lambda;\varepsilon')\leq\varrho_H^S(\lambda;\varepsilon)$ holds whenever $\varepsilon'\geq\varepsilon$, $\varrho_H^S(\lambda)=+\infty$ if λ does not belong to the spectrum of H, and $\varrho_H^S(\lambda)\geq 0$ for all $\lambda\in\mathbb{R}$ if $S\geq 0$. We also mention that in the case of two self-adjoint operators H and A in $\mathcal{H}$, with H of class $C^1(A)$ and $S:=[iH,A]$, the function $\varrho_H^S(\cdot)$ is equal to the function $\varrho_H^A(\cdot)$ defined in [ABG96, Eq. 7.2.4].

Taking advantage of the direct integral decomposition of H_0 and T, one obtains for all $\lambda\in\mathbb{R}$ and $\varepsilon>0$:

$$\varrho_{H_0}^T(\lambda;\varepsilon) = \operatorname*{ess\,inf}_{\xi\in\mathbb{R}}\varrho_{H_0(\xi)}^{T(\xi)}(\lambda;\varepsilon). \tag{2.10}$$

Now we can deduce a lower bound for $\varrho_{H_0}^T(\cdot)$.

Proposition 2.2.7. *One has*

$$\varrho_{H_0}^T(\lambda)\geq\inf\left\{\frac{\lambda^2-\mu^2}{\lambda^2}\ :\ \mu\in\sigma_{\rm sym}^0\cap[0,|\lambda|]\right\} \tag{2.11}$$

with the convention that the infimum over an empty set is $+\infty$.

Proof. We first consider the case $\lambda\geq 0$.

(i) Recall from (2.3) that $\mu_0\equiv\inf|\sigma_{\rm sym}^0| = \inf\{\sigma(H_0)\cap[0,+\infty)\}$. Thus, for $\lambda\in[0,\mu_0)$ the l.h.s. term of (2.11) is equal to $+\infty$, since λ does not belong to the spectrum of H_0. Hence (2.11) is satisfied on $[0,\mu_0)$.

(ii) If $\lambda\in\sigma_{\rm sym}^0$, then the r.h.s. term of (2.11) is equal to 0. However, since T is positive, $\varrho_{H_0}^T(\lambda)\geq 0$. Hence the relation (2.11) is again satisfied.

(iii) Let $0<\varepsilon<\mu_0<\lambda$. Direct computations using the explicit form of $T(\xi)$ and the spectral theorem for the operator $H_0(\xi)$ show that for ξ fixed, one has

$$\varrho_{H_0(\xi)}^{T(\xi)}(\lambda;\varepsilon) = \inf\left\{\frac{\xi^2}{\rho^2}\ :\ \rho\in(\lambda-\varepsilon,\lambda+\varepsilon)\cap\sigma[H_0(\xi)]\right\}\geq\frac{\xi^2}{(\lambda+\varepsilon)^2}. \tag{2.12}$$

On the other hand one has $\varrho_{H_0(\xi)}^{T(\xi)}(\lambda;\varepsilon)=+\infty$ if $(\lambda-\varepsilon,\lambda+\varepsilon)\cap\sigma[H_0(\xi)]=\varnothing$, and a fortiori

$$\varrho_{H_0(\xi)}^{T(\xi)}(\lambda;\varepsilon)=+\infty\qquad\text{if}\qquad\big((\lambda-\varepsilon)^2,(\lambda+\varepsilon)^2\big)\cap\sigma[H_0(\xi)^2]=\varnothing.$$

Thus, by taking into account equation (2.10), (2.12), the previous observation and relation (2.2), one obtains that

$$\varrho_{H_0}^T(\lambda;\varepsilon)\geq\operatorname{ess\,inf}\left\{\frac{\xi^2}{(\lambda+\varepsilon)^2}\ :\ \xi^2\in\big((\lambda-\varepsilon)^2,(\lambda+\varepsilon)^2\big)-(\sigma_{\rm sym}^0)^2\right\}. \tag{2.13}$$

Suppose now that $\lambda\notin\sigma_{\rm sym}^0$, define $\mu:=\sup\{\sigma_{\rm sym}^0\cap[0,\lambda]\}$ and choose $\varepsilon>0$ such that $\mu<\lambda-\varepsilon$. Then the inequality (2.13) implies that

$$\varrho_{H_0}^T(\lambda;\varepsilon)\geq\frac{(\lambda-\varepsilon)^2-\mu^2}{(\lambda+\varepsilon)^2}.$$

Hence the relation (2.11) follows from the above formula when $\varepsilon \to 0$.

For $\lambda < 0$, similar arguments lead to the inequality

$$\varrho^T_{H_0}(\lambda) \geq \inf\left\{\frac{\lambda^2 - \mu^2}{\lambda^2} \,:\, \mu \in \sigma^0_{\mathrm{sym}} \cap [\lambda, 0]\right\}.$$

The claim is then a direct consequence of the symmetry of σ^0_{sym} with respect to 0. □

The above proposition implies that we have a strict Mourre estimate, *i.e.* $\varrho^T_{H_0}(\cdot) > 0$, on $\mathbb{R} \setminus \sigma^0_{\mathrm{sym}}$. Moreover it is not difficult to prove that $\varrho^T_{H_0}(\lambda) = 0$ whenever $\lambda \in \sigma^0_{\mathrm{sym}}$. It follows that the conjugate operator A does not allow to get spectral informations on H_0 in the subset σ^0_{sym}.

2.3 Mourre estimate for the perturbed Hamiltonian

In the sequel, we consider the self-adjoint operator $H := H_0 + V$ with a potential V that belongs to $\mathsf{L}^\infty\big(\mathbb{R}^3; \mathscr{B}_{\mathrm{h}}(\mathbb{C}^4)\big)$. The domain of H is equal to the domain $\mathcal{D}(H_0)$ of H_0. We first give a result on the difference of the resolvents $(H - z)^{-1} - (H_0 - z)^{-1}$ and, as a corollary, we obtain the localization of the essential spectrum of H.

Proposition 2.3.1. *Assume that V is small at infinity. Then for all $z \in \mathbb{C} \setminus \big(\sigma(H) \cup \sigma(H_0)\big)$ the difference $(H - z)^{-1} - (H_0 - z)^{-1}$ is a compact operator. It follows in particular that $\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(H_0)$.*

Proof. Since V is bounded and small at infinity, it is enough to check that H_0 is locally compact [Tha92, Sec. 4.3.4]. However, the continuity of $\vec{a}$ implies that $\mathcal{D}(H_0) \subset \mathcal{H}^{1/2}_{\mathrm{loc}}$ [BP94, Thm. 1.3]. Hence the statement follows by usual arguments. □

Remark 2.3.2. *In the study of an analogous problem for Schrödinger operators [MP00], the authors prove a result similar to Proposition 2.3.1 without assuming that the perturbation is small at infinity (it only has to be small with respect to B in a suitable sense). Their proof mainly relies on the structural inequalities $H_{\mathrm{Sch}} := \Pi_1^2 + \Pi_2^2 + P_3^2 \geq \pm B$. In the Dirac case, the counterpart of these turn out to be*

$$H_0^2 \geq 2B \cdot \mathrm{diag}(0, 1, 0, 1) \qquad \textit{and} \qquad H_0^2 \geq -2B \cdot \mathrm{diag}(1, 0, 1, 0),$$

where $\mathrm{diag}(\cdots)$ stands for a diagonal matrix. If we assume that the magnetic field is bounded from below, the first inequality enables us to treat pertubations of the type $\mathrm{diag}(V_1, V_2, V_3, V_4)$ with V_2, V_4 small with respect to the magnetic field and V_1, V_3 small at infinity in the original sense. If the magnetic field is bounded from above, the second inequality has to be used and the role of V_2, V_4 and V_1, V_3 are interchanged. However the unnatural character of these perturbations motivated us not to include their treatment in this paper.

In order to obtain a limiting absorption principle for H, one has to invoke some abstract results. An optimal regularity condition of H with respect to A has to be satisfied. We refer to [ABG96, Chap. 5] for the definitions of $\mathscr{C}^{1,1}(A)$ and $\mathscr{C}^{1,1}(A; \mathcal{D}(H_0), \mathcal{D}(H_0)^*)$, and for more explanations on regularity conditions.

Proposition 2.3.3. *Let V be a short-range or a long-range potential. Then H is of class $\mathscr{C}^{1,1}(A)$.*

Proof. Since $\{e^{itA}\}_{t\in\mathbb{R}}$ leaves $\mathcal{D}(H) = \mathcal{D}(H_0)$ invariant, it is equivalent to prove that H belongs to $\mathscr{C}^{1,1}(A; \mathcal{D}(H_0), \mathcal{D}(H_0)^*)$ [ABG96, Thm. 6.3.4.(b)]. But in Proposition 2.2.5.(c), it has already been shown that H_0 is of class $C^2(A)$, so that H_0 is of class $\mathscr{C}^{1,1}(A; \mathcal{D}(H_0), \mathcal{D}(H_0)^*)$. Thus it is enough to prove that V belongs to $\mathscr{C}^{1,1}(A; \mathcal{D}(H_0), \mathcal{D}(H_0)^*)$. In the short-range case, we shall use [ABG96, Thm. 7.5.8], which implies that V belongs to $\mathscr{C}^{1,1}(A; \mathcal{D}(H_0), \mathcal{D}(H_0)^*)$. The conditions needed for that theorem are obtained in points (i) and (ii) below. In the long-range case, the claim follows by [ABG96, Thm. 7.5.7], which can be applied because of points (i), (iii), (iv) and (v) below.

(i) We first check that $\{e^{it\langle Q_3\rangle}\}_{t\in\mathbb{R}}$ is a polynomially bounded C_0-group in $\mathcal{D}(H_0)$ and in $\mathcal{D}(H_0)^*$. Lemma 2.2.3.(a) (with $n = 0$ and $f(Q_3) = \langle Q_3\rangle$) implies that H_0 is of class $C^1(\langle Q_3\rangle)$. Furthermore, by an argument similar to that given in part (b) of the proof of Proposition 2.2.5, one shows that $\{e^{it\langle Q_3\rangle}\}_{t\in\mathbb{R}}$ leaves $\mathcal{D}(H_0)$ invariant. Since $H_0 e^{it\langle Q_3\rangle} - e^{it\langle Q_3\rangle}H_0$, defined on $\mathscr{D}$, extends continuously to the operator $t\alpha_3 Q_3\langle Q_3\rangle^{-1}e^{it\langle Q_3\rangle} \in \mathscr{B}(\mathcal{H})$, one gets that $\|e^{it\langle Q_3\rangle}\|_{\mathscr{B}(\mathcal{D}(H_0))} \leq$ Const.$\langle t\rangle$ for all $t \in \mathbb{R}$, *i.e.* the polynomial bound of the C_0-group in $\mathcal{D}(H_0)$. By duality, $\{e^{it\langle Q_3\rangle}\}_{t\in\mathbb{R}}$ extends to a polynomially bounded C_0-group in $\mathcal{D}(H_0)^*$ [ABG96, Prop. 6.3.1]. The generators of these C_0-groups are densely defined and closed in $\mathcal{D}(H_0)$ and in $\mathcal{D}(H_0)^*$ respectively; both are simply denoted by $\langle Q_3\rangle$.

(ii) Since $\{e^{itA}\}_{t\in\mathbb{R}}$ leaves $\mathcal{D}(H_0)$ invariant, one may also consider the C_0-group in $\mathcal{D}(H_0)$ obtained by restriction and the C_0-group in $\mathcal{D}(H_0)^*$ obtained by extension. The generator of each of these C_0-groups will be denoted by A. Let $\mathcal{D}\big(A; \mathcal{D}(H_0)\big) := \{\varphi \in \mathcal{D}(H_0)\cap\mathcal{D}(A) \,:\, A\varphi \in \mathcal{D}(H_0)\}$ be the domain of A in $\mathcal{D}(H_0)$, and let $\mathcal{D}\big(A^2; \mathcal{D}(H_0)\big) := \{\varphi \in \mathcal{D}(H_0) \cap \mathcal{D}(A^2) \,:\, A\varphi, A^2\varphi \in \mathcal{D}(H_0)\}$ be the domain of A^2 in $\mathcal{D}(H_0)$. We now check that $\langle Q_3\rangle^{-1}A$ and $\langle Q_3\rangle^{-2}A^2$, defined on $\mathcal{D}\big(A; \mathcal{D}(H_0)\big)$ and on $\mathcal{D}\big(A^2; \mathcal{D}(H_0)\big)$ respectively, extend to operators in $\mathscr{B}\big(\mathcal{D}(H_0)\big)$. After some commutator calculations performed on $\mathscr{D}$ and involving Lemma 2.2.3, one first obtains that $\langle Q_3\rangle^{-1}A$ and $\langle Q_3\rangle^{-2}A$ are respectively equal on $\mathscr{D}$ to some operators S_1 and $S_2\langle Q_3\rangle^{-1}$ in $\mathscr{B}(\mathcal{H})$, where S_1 and S_2 are polynomials in H_0^{-1}, $P_3H_0^{-1}$, α_3 and $f(Q_3)$ for bounded functions f with bounded derivatives. Since $\mathscr{D}$ is a core for A, these equalities even hold on $\mathcal{D}(A)$. Hence one has on $\mathcal{D}(A^2)$:

$$\langle Q_3\rangle^{-2}A^2 = \big(\langle Q_3\rangle^{-2}A\big)\, A = S_2\langle Q_3\rangle^{-1}A = S_2S_1\,.$$

In consequence, $\langle Q_3\rangle^{-1}A$ and $\langle Q_3\rangle^{-2}A^2$ are equal on $\mathcal{D}(A)$ and on $\mathcal{D}(A^2)$ respectively, to operators expressed only in terms of H_0^{-1}, $P_3H_0^{-1}$, α_3 and $f(Q_3)$ for bounded functions f with bounded derivatives. Moreover, one easily observes that these operators and their products belong to $\mathscr{B}\big(\mathcal{D}(H_0)\big)$. Thus, it follows that $\langle Q_3\rangle^{-1}A$ and $\langle Q_3\rangle^{-2}A^2$ are equal on $\mathcal{D}\big(A; \mathcal{D}(H_0)\big)$ and on $\mathcal{D}\big(A^2; \mathcal{D}(H_0)\big)$ respectively to some operators belonging to $\mathscr{B}\big(\mathcal{D}(H_0)\big)$.

(iii) By duality, the operator $(\langle Q_3\rangle^{-1}A)^*$ belongs to $\mathscr{B}\big(\mathcal{D}(H_0)^*\big)$. Now, for $\psi \in \mathcal{D}(H_0)^*$ and $\varphi \in \mathcal{D}\big(A; \mathcal{D}(H_0)\big)$, one has

$$\langle(\langle Q_3\rangle^{-1}A)^*\psi, \varphi\rangle = \langle\psi, \langle Q_3\rangle^{-1}A\varphi\rangle = \langle\langle Q_3\rangle^{-1}\psi, A\varphi\rangle, \tag{2.14}$$

where $\langle\cdot,\cdot\rangle$ denotes the duality between $\mathcal{D}(H_0)$ and $\mathcal{D}(H_0)^*$. Since $\langle Q_3\rangle^{-1}$ is a homeomorphism from $\mathcal{D}(H_0)^*$ to the domain of $\langle Q_3\rangle$ in $\mathcal{D}(H_0)^*$, it follows from (2.14) that the domain of $\langle Q_3\rangle$ in $\mathcal{D}(H_0)^*$ is included in the domain of A in $\mathcal{D}(H_0)^*$ (the adjoint of the operator A in $\mathcal{D}(H_0)$ is equal to the operator $-A$ in $\mathcal{D}(H_0)^*$).

(iv) The inequality $r\,\|(\langle Q_3\rangle + ir)^{-1}\|_{\mathscr{B}(\mathcal{D}(H_0)^*)} \leq$ Const. for all $r > 0$ is obtained from relation (2.16), given in the proof of Lemma 2.2.3, with $f(Q_3) = (\langle Q_3\rangle + ir)^{-1}$.

(v) Assume that V is a long-range (scalar) potential. Then the following equality holds in form sense on $\mathscr{D}$:

$$2\,[iV,A] = -Q_3(\partial_3 V)H_0^{-1} - H_0^{-1}Q_3(\partial_3 V) + \left[iV,H_0^{-1}\right]Q_3P_3 + P_3Q_3\left[iV,H_0^{-1}\right], \tag{2.15}$$

with $\left[iV,H_0^{-1}\right] = \sum_{j=1}^3 H_0^{-1}\alpha_j(\partial_j V)H_0^{-1}$. Using Lemma 2.2.3.(a), one gets that the last two terms in (2.15) are equal in form sense on $\mathscr{D}$ to

$$2\,\mathsf{Re}\sum_{j=1}^3 H_0^{-1}\alpha_j Q_3(\partial_j V)P_3H_0^{-1} - 2\,\mathsf{Im}\sum_{j=1}^3 H_0^{-1}\alpha_j(\partial_j V)H_0^{-1}\alpha_3P_3H_0^{-1}.$$

It follows that $[iV,A]$, defined in form sense on $\mathscr{D}$, extends continuously to an operator in $\mathscr{B}(\mathcal{H})$. Now let ϑ be as in Definition 2.1.1. Then a direct calculation using the explicit form of $[iV,A]$ obtained above implies that

$$\left\|\vartheta\Big(\frac{\langle Q_3\rangle}{r}\Big)\,[iV,A]\right\| \le \mathsf{C}\sum_{j=1}^3\left\|\vartheta\Big(\frac{\langle Q_3\rangle}{r}\Big)\langle Q_3\rangle(\partial_j V)\right\| + \frac{\mathsf{D}}{r}$$

for all $r>0$ and some positive constants C and D. □

As a direct a consequence, one obtains that

Lemma 2.3.4. *If V satisfies the hypotheses of Theorem 2.1.2, then A is conjugate to H on $\mathbb{R}\setminus\sigma^0_{\rm sym}$.*

Proof. Proposition 2.3.3 implies that both H_0 and H are of class $\mathscr{C}^{1,1}(A)$. Furthermore, the difference $(H+i)^{-1}-(H_0+i)^{-1}$ is compact by Proposition 2.3.1, and $\varrho^T_{H_0}>0$ on $\mathbb{R}\setminus\sigma^0_{\rm sym}$ due to Proposition 2.2.7. Hence the claim follows by [ABG96, Thm. 7.2.9 & Prop. 7.2.6]. □

We can finally give the proof of Theorem 2.1.2.

Proof of Theorem 2.1.2. Since A is conjugate to H on $\mathbb{R}\setminus\sigma^0_{\rm sym}$ by Lemma 2.3.4, the assertions (a) and (b) follow by the abstract conjugate operator method [ABG96, Cor. 7.2.11 & Thm. 7.4.2].

The limiting absorption principle directly obtained via [ABG96, Thm. 7.4.1] is expressed in terms of some interpolation space, associated with $\mathcal{D}(A)$, and of its adjoint. Since both are not standard spaces, one may use [ABG96, Prop. 7.4.4] for the Friedrichs couple $(\mathcal{D}(\langle Q_3\rangle),\mathcal{H})$ to get the statement (c). In order to verify the hypotheses of that proposition, one has to check that for each $z\in\mathbb{C}\setminus\sigma(H)$ the inclusion $(H-z)^{-1}\mathcal{D}(\langle Q_3\rangle)\subset\mathcal{D}(A)$ holds. However, since $\mathcal{D}(\langle Q_3\rangle)$ is included in $\mathcal{D}(A)$ by Proposition 2.2.4, it is sufficient to prove that for each $z\in\mathbb{C}\setminus\sigma(H)$ the operator $(H-z)^{-1}$ leaves $\mathcal{D}(\langle Q_3\rangle)$ invariant. Since $\mathcal{D}(H)=\mathcal{D}(H_0)$ is left invariant by the group $\{e^{it\langle Q_3\rangle}\}_{t\in\mathbb{R}}$ (see Proposition 2.3.3 (i)) one easily gets from [ABG96, Thm. 6.3.4.(a)] that H is of class $C^1(\langle Q_3\rangle)$, which implies the required invariance of $\mathcal{D}(\langle Q_3\rangle)$ [ABG96, Thm. 6.2.10.(b)]. □

Appendix

Proof of Lemma 2.2.2. (a) Let φ, ψ be in $\mathscr{D}$. Using the transformation (2.1), one gets

$$\left\langle H_0^{-n}\varphi, Q_3\psi\right\rangle = \int_{\mathbb{R}}\left\langle H_0(\xi)^{-n}(\mathscr{F}\varphi)(\xi),(i\partial_\xi\mathscr{F}\psi)(\xi)\right\rangle_{\mathcal{H}_{12}}\mathrm{d}\xi.$$

Now the map $\mathbb{R} \ni \xi \mapsto H_0(\xi)^{-n} \in \mathscr{B}(\mathcal{H}_{12})$ is norm differentiable with its derivative equal to $-\sum_{j=1}^{n} H_0(\xi)^{-j}\alpha_3 H_0(\xi)^{j-n-1}$. Hence $\{\partial_\xi[H_0(\xi)^{-n}(\mathscr{F}\varphi)(\xi)]\}_{\xi\in\mathbb{R}}$ belongs to $\int_{\mathbb{R}}^{\oplus} \mathcal{H}_{12}\,\mathrm{d}\xi$. Thus one can perform an integration by parts (with vanishing boundary contributions) and obtain

$$\langle H_0^{-n}\varphi, Q_3\psi\rangle = \int_{\mathbb{R}} \langle i\partial_\xi[H_0(\xi)^{-n}(\mathscr{F}\varphi)(\xi)], (\mathscr{F}\psi)(\xi)\rangle_{\mathcal{H}_{12}}\,\mathrm{d}\xi.$$

It follows that $|\langle H_0^{-n}\varphi, Q_3\psi\rangle| \le \text{Const.}\,\|\psi\|$ for all $\psi \in \mathscr{D}$. Since Q_3 is essentially self-adjoint on $\mathscr{D}$, this implies that $H_0^{-n}\varphi$ belongs to $\mathcal{D}(Q_3)$.

(b) The boundedness of $P_3 H_0^{-1}$ is a consequence of the estimate

$$\operatorname*{ess\,sup}_{\xi\in\mathbb{R}} \|\xi H_0(\xi)^{-1}\|_{\mathscr{B}(\mathcal{H}_{12})} = \operatorname*{ess\,sup}_{\xi\in\mathbb{R}} \left\| \frac{|\xi|}{[H_0(0)^2+\xi^2]^{1/2}} \right\|_{\mathscr{B}(\mathcal{H}_{12})} < \infty$$

and of the direct integral formalism [Cho70, Prop. 3.6 & 3.7]. The remaining assertions follow by standard arguments. □

Proof of Lemma 2.2.3. (a) One first observes that the following equality holds on $\mathscr{D}$:

$$iH_0^{-1}f(Q_3)H_0 = -H_0^{-1}\alpha_3 f'(Q_3) + if(Q_3). \tag{2.16}$$

Now, for $\varphi,\psi \in \mathscr{D}$ and $\eta \in H_0^{-n}\mathscr{D}$, one has

$$\begin{aligned}
&\langle\varphi, iH_0^{-1}f(Q_3)\eta\rangle - \langle\varphi, if(Q_3)H_0^{-1}\eta\rangle\\
&= \langle\varphi, iH_0^{-1}f(Q_3)H_0\psi\rangle + \langle\varphi, iH_0^{-1}f(Q_3)(\eta - H_0\psi)\rangle - \langle\bar f(Q_3)\varphi, iH_0^{-1}\eta\rangle\\
&= -\langle\varphi, H_0^{-1}\alpha_3 f'(Q_3)H_0^{-1}\eta\rangle - \langle\varphi, H_0^{-1}\alpha_3 f'(Q_3)H_0^{-1}(H_0\psi-\eta)\rangle\\
&\quad + \langle\bar f(Q_3)\varphi, iH_0^{-1}(H_0\psi - \eta)\rangle + \langle\bar f(Q_3)H_0^{-1}\varphi, i(\eta - H_0\psi)\rangle,
\end{aligned}$$

where we have used (2.16) in the last equality for the term $\langle\varphi, iH_0^{-1}f(Q_3)H_0\psi\rangle$. Hence there exists a constant C (depending on φ) such that

$$|\langle\varphi, iH_0^{-1}f(Q_3)\eta\rangle - \langle\varphi, if(Q_3)H_0^{-1}\eta\rangle + \langle\varphi, H_0^{-1}\alpha_3 f'(Q_3)H_0^{-1}\eta\rangle| \le \mathrm{C}\,\|\eta - H_0\psi\|.$$

Then the statement is a direct consequence of the density of $H_0\mathscr{D}$ and $\mathscr{D}$ in $\mathcal{H}$.

(b) This is a simple corollary of the point (a). □

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