

**Commutator methods
in spectral and scattering theory**

THÈSE

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Résumé

0.1 Prologue

Supposons que l'on désire étudier l'évolution dans l'espace tridimensionnel d'une particule élémentaire sans spin, ni autre structure interne, soumise à un potentiel externe borné V . Les principes de la mécanique quantique nous dictent que la description d'un tel système s'effectue au moyen de l'espace de Hilbert $\mathcal{H} = L^2(\mathbb{R}^3)$, l'état de la particule étant représenté au temps $t = 0$ par un élément ψ de celui-ci. L'évolution temporelle de la particule est alors régie par le groupe unitaire $\{e^{-iHt}\}_{t \in \mathbb{R}}$ avec l'opérateur de Schrödinger H , modélisant l'interaction entre celle-ci et le milieu ambiant, défini par l'expression $-\Delta + V(Q)$. Par analogie avec la situation classique, le Laplacien Δ correspond à (moins) l'énergie cinétique de la particule ; sa forme exacte est donnée par la somme des dérivées secondes : $\Delta = \sum_{j=1}^3 \frac{\partial^2}{\partial x_j^2}$. Le potentiel V agit comme un opérateur de multiplication, d'où la notation $V(Q)$. Soulignons que l'opérateur de Schrödinger H , appelé également Hamiltonien, encode toute l'information relative au système considéré.

La théorie spectrale s'intéresse à la nature du spectre de H , en d'autres mots à la nature du sous-ensemble de \mathbb{R} qui sous-tend le calcul fonctionnel associé à cet opérateur. Elle permet notamment de déterminer l'existence ainsi que l'énergie des possibles états liés du système. Ces états correspondent à des particules qui seraient essentiellement piégées dans une région finie de l'espace. La théorie spectrale donne également une vague information sur la diffusion des particules non liées au système. Cette information peut être obtenue en étudiant le spectre singulier continu et le spectre absolument continu de H et en différentiant alors les états respectifs.

La théorie de la diffusion se concentre sur l'étude du groupe unitaire $\{e^{-iHt}\}_{t \in \mathbb{R}}$ engendré par H . En particulier, elle tente de donner une description asymptotique aussi précise et simple que possible de l'orbite $\{e^{-iHt} \psi\}_{t \in \mathbb{R}}$ dans l'espace de Hilbert \mathcal{H} . Plus précisément, pour un état $\psi \in \mathcal{H}$ donné au temps $t = 0$, un de ses buts est de déterminer un opérateur H_0 essentiellement plus simple que H ainsi qu'un élément ψ_0 de \mathcal{H} tel que la différence

$$e^{-iHt} \psi - e^{-iH_0 t} \psi_0 \tag{1}$$

ait une norme de plus en plus petite pour un temps t devenant de plus en plus grand.

Une méthode introduite déjà dans les années 60 [Pu], et continuellement développée depuis lors, est d'une grande aide pour l'étude des théories spectrale et de la

diffusion de H . Appelée *méthode des commutateurs* ou *méthode de l'opérateur conjugué*, cette technique consiste en l'introduction d'un nouvel opérateur A agissant sur \mathcal{H} en demandant une certaine compatibilité entre H et A . Plus précisément, si H satisfait des conditions de régularité par rapport à A , régularité exprimée en termes de la résolvante de H et du groupe unitaire $\{e^{-iAt}\}_{t \in \mathbb{R}}$, et si le commutateur $[iH, A]$ est un opérateur strictement positif lorsque localisé dans une région J du spectre de H , alors de précieuses informations spectrales sur H dans J peuvent être déduites. Si de plus l'opérateur A est suffisamment comparable avec les opérateurs de position $\{Q_j\}_{j=1}^3$ (opérateurs de multiplication par les variables $\{x_j\}_{j=1}^3$), des informations sur la localisation de la particule évoluant sous l'action du groupe $\{e^{-iHt}\}_{t \in \mathbb{R}}$ dans l'espace tridimensionnel sont accessibles.

De nombreuses autres informations sur l'opérateur H peuvent être obtenues grâce à la méthode de l'opérateur conjugué. Notons que celle-ci a été en fait élaborée dans un cadre essentiellement abstrait, sans référence à une situation particulière comme celle d'une particule évoluant dans \mathbb{R}^3 introduite ci-dessus, et dans une recherche constante de généralité. Dès lors, son domaine d'applicabilité est très vaste et très varié. Nous exposerons dans la section suivante les différents aspects de cette théorie utilisés au cours de ce travail.

Dans cette thèse, nous regroupons trois travaux ayant en commun l'utilisation de la méthode des commutateurs. Les situations considérées ainsi que les résultats obtenus sont cependant de nature très différente. Chacun de ces travaux correspond à un chapitre, autosuffisant et indépendant des deux autres. Les notations, adaptées à la problématique considérée, sont introduites dans chaque chapitre et ne peuvent être extrapolées d'une partie du présent travail à une autre. Relevons que l'ordre de la lecture des différents travaux peut être choisi en fonction de l'intérêt du lecteur.

La suite de cette introduction consiste en un développement succinct de la théorie de l'opérateur conjugué ainsi qu'en de brefs résumés simplifiés de chacune des trois parties composant le corps de cette thèse.

0.2 La méthode de l'opérateur conjugué

Les ingrédients essentiels

Considérons un opérateur autoadjoint H agissant dans un espace de Hilbert \mathcal{H} , le produit scalaire et la norme de celui-ci étant notés respectivement $\langle \cdot, \cdot \rangle$ et $\|\cdot\|$. Nous désignons par $D(H)$ le domaine de H et le munissons de la topologie naturelle issue du produit scalaire suivant : $\langle \psi, \psi' \rangle_{D(H)} := \langle \psi, \psi' \rangle + \langle H\psi, H\psi' \rangle$ pour tout $\psi, \psi' \in D(H)$. L'espace ainsi défini est un nouvel espace de Hilbert, continûment et densément plongé dans \mathcal{H} . L'adjoint de cet espace est noté $D(H)^*$. En identifiant \mathcal{H} avec son propre adjoint par l'isomorphisme de Riesz, nous obtenons la suite de plongements continus et denses :

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

Soit A un second opérateur autoadjoint agissant dans \mathcal{H} . L'application suivante joue un rôle prépondérant pour définir la *régularité* de H par rapport à A :

$$\mathbb{R} \ni t \mapsto e^{iAt}(H - i)^{-1}e^{-iAt} \in \mathcal{B}(\mathcal{H}),$$

où $\mathcal{B}(\mathcal{H})$ désigne l'ensemble des opérateurs linéaires bornés sur \mathcal{H} . La condition minimale que nous allons considérer par la suite est de demander que cette application soit fortement différentiable. Nous disons dans ce cas que H est de classe $C^1(A)$. De façon équivalente, cela revient à demander le commutateur $[(H - i)^{-1}, A]$, défini au sens des formes sur le domaine $D(A)$ de A , s'étende continûment à un opérateur borné sur \mathcal{H} . Plus explicitement, il suffit qu'il existe une constante $d < \infty$ telle que

$$|\langle (H + i)^{-1}\psi, A\psi \rangle - \langle A\psi, (H - i)^{-1}\psi \rangle| \leq d\|\psi\|^2$$

pour tout $\psi \in D(A)$. Sous cette hypothèse, l'égalité fondamentale suivante est vérifiée au sens des formes sur \mathcal{H} pour tout nombre complexe z n'appartenant pas au spectre de H :

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

Le commutateur $[H, A]$ désigne l'opérateur appartenant à $\mathcal{B}(D(H), D(H)^*)^1$ associé à l'unique extension à $D(H)$ de la forme quadratique $\psi \mapsto \langle H\psi, A\psi \rangle - \langle A\psi, H\psi \rangle$ définie pour tout $\psi \in D(A) \cap D(H)$.

Les objets introduits jusqu'à maintenant sont les éléments essentiels pour la méthode de l'opérateur conjugué. A savoir : l'opérateur autoadjoint H que l'on désire étudier ainsi qu'un second opérateur autoadjoint A tel que H soit de classe $C^1(A)$. L'ingrédient suivant qu'il faut introduire est une certaine notion de positivité de l'expression $[iH, A]$ lorsque localisée dans le spectre de H .

Pour tout intervalle ouvert J de \mathbb{R} , soit $E(J)$ le projecteur spectral de H sur J . Sous l'hypothèse que H est de classe $C^1(A)$, l'expression $E(J)[iH, A]E(J)$ est un opérateur bien défini et borné sur \mathcal{H} . Il existe alors des nombres réels a tels que

$$E(J)[iH, A]E(J) \geq aE(J). \quad (2)$$

La valeur maximale de a telle que cette inégalité soit vérifiée est notée θ (qui dépend de l'intervalle J). Il sera particulièrement important par la suite de considérer les intervalles de \mathbb{R} sur lesquels cette valeur θ est strictement positive.

Nous allons maintenant esquisser comment des résultats spectraux peuvent être obtenus à partir du cadre introduit ci-dessus. Nous enchaînerons ensuite avec des résultats relatifs à la théorie de la diffusion.

Dans la théorie spectrale

Il est bien connu que si λ est une valeur appartenant au spectre de H , alors $(H - \lambda - i\mu)^{-1}$ ne peut pas avoir de limite dans $\mathcal{B}(\mathcal{H})$ pour $\mu \rightarrow +0$. En revanche, la limite

$$\lim_{\mu \rightarrow +0} \langle \psi, (H - \lambda - i\mu)^{-1}\psi \rangle \quad (3)$$

¹la notation $\mathcal{B}(\mathcal{G}, \mathcal{G}')$ désigne l'ensemble des opérateurs linéaires bornés de \mathcal{G} dans \mathcal{G}' .

pourrait exister pour certains ψ de \mathcal{H} . Si pour tous λ dans un ensemble ouvert J de \mathbb{R} et pour tous ψ 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 . Il s'ensuivra notamment que le spectre de H dans cet ensemble J est purement absolument continu.

A la fin des années 70, Mourre remarqua que l'existence d'une valeur strictement positive θ telle que l'expression (2) soit vérifiée avec $a = \theta$, ainsi que quelques conditions techniques supplémentaires, conduisaient à l'existence d'un principe d'absorption limite. On parle d'ailleurs depuis lors d'une estimation de Mourre stricte lorsque (2) est satisfaite pour une valeur θ strictement positive. Suite à ses publications ([Mo1], [Mo2]) de nombreux travaux apparurent afin de restreindre les conditions techniques supplémentaires et d'obtenir la convergence (3) pour le plus grand ensemble de vecteurs ψ . Ces différents travaux culminèrent avec la parution de [ABG] qui donne l'unique condition supplémentaire ainsi que les espaces optimaux pour formuler un principe d'absorption limite le plus général possible.

Toutes les démonstrations de l'existence de la limite (3) pour des vecteurs ψ adéquats sont relativement compliquées et ne peuvent malheureusement être expliquées en quelques phrases. Même dans le cas très simple où H est de classe $C^1(A)$ et $[iH, A] = H$, la preuve repose sur des techniques d'inégalités différentielles non banales. Afin d'illustrer ces techniques, nous donnons les arguments qui permettent d'obtenir un principe d'absorption limite dans ce cas. Relevons que dans cet exemple (trop!) simple, les conditions techniques supplémentaires sont automatiquement satisfaites. En effet, les commutateurs successifs $[[iH, A], A]$, $[[[iH, A], A], A]$, \dots sont tous égaux à H . Il n'y a donc pas de conditions supplémentaires à imposer pour les contrôler. De plus, si $J = (b, c)$ avec $0 < b < c$, la relation (2) est satisfaite pour la valeur strictement positive de a égale à b . Si $b < c < 0$, il suffit de considérer l'opérateur $-A$ pour obtenir également une valeur de a strictement positive. Du fait de la simplicité de l'exemple présenté, l'implémentation, généralement subtile, de l'inégalité de Mourre stricte dans la démonstration du principe d'absorption limite ne transparaît malheureusement pas dans les arguments qui suivent.

Un principe d'absorption limite

Nous montrons dans l'exemple mentionné ci-dessus que si ψ appartient au domaine $D(A)$ de A , alors la limite (3) existe. Pour tout nombre complexe z n'appartenant pas au spectre $\sigma(H)$ de H , nous désignons par $R(z)$ l'expression $(H - z)^{-1}$, et posons $F(z) := \langle \psi, R(z)\psi \rangle$. La technique standard utilisée pour prouver l'existence de $\lim_{\mu \rightarrow +0} F(\lambda + i\mu)$ est de démontrer l'estimation : $\int_0^1 \left| \frac{d}{d\mu} F(\lambda + i\mu) \right| d\mu < \infty$.

Des égalités $\frac{d}{dz} R(z) = R(z)^2$ et

$$[iR(z), A] = -R(z)[iH, A]R(z) = -R(z)HR(z) = -R(z) - zR(z)^2,$$

nous obtenons la relation suivante :

$$\frac{d}{dz} F(z) = -\frac{1}{z} \langle R(\bar{z})\psi, iA\psi \rangle - \frac{1}{z} \langle iA\psi, R(z)\psi \rangle - \frac{1}{z} F(z), \quad (4)$$

le commutateur $[iR(z), A]$ pouvant s'ouvrir car ψ appartient à $D(A)$ par hypothèse.

Observons maintenant que pour $z = \lambda + i\mu$ avec $\mu > 0$, nous avons

$$\|R(z)\psi\|^2 = \langle \psi, R(\bar{z})R(z)\psi \rangle = \frac{1}{2i\mu} \langle \psi, \{R(z) - R(\bar{z})\}\psi \rangle = \frac{1}{\mu} \operatorname{Im} F(z), \quad (5)$$

et de façon similaire $\|R(\bar{z})\psi\|^2 = \frac{1}{\mu} \operatorname{Im} F(z)$. En insérant les égalités ainsi obtenues $\|R(z)\psi\| = \|R(\bar{z})\psi\| = \mu^{-1/2} [\operatorname{Im} F(z)]^{1/2}$ dans la relation (4), nous générons, en supposant $\lambda \neq 0$, l'inégalité différentielle :

$$\left| \frac{d}{d\mu} F(\lambda + i\mu) \right| \leq \frac{1}{|\lambda|} \{2\|A\psi\| + \|\psi\|\} \mu^{-1/2} |F(\lambda + i\mu)|^{1/2}. \quad (6)$$

Avec les hypothèses $\mu > 0$ et $\psi \neq 0$, il suit de (5) que $F(\lambda + i\mu) \neq 0$. Les deux membres de (6) peuvent ainsi être divisés par $|F(\lambda + i\mu)|^{1/2}$, d'où nous tirons :

$$\left| \frac{d}{d\mu} F(\lambda + i\mu)^{1/2} \right| \equiv \frac{1}{2} |F(\lambda + i\mu)^{-1/2} \frac{d}{d\mu} F(\lambda + i\mu)| \leq \frac{1}{2|\lambda|} \{2\|A\psi\| + \|\psi\|\} \mu^{-1/2}.$$

L'intégration de cette inégalité donne alors une estimation valable pour $0 < \mu \leq 1$:

$$|F(\lambda + i\mu)|^{1/2} \leq |F(\lambda + i)|^{1/2} + \frac{1}{|\lambda|} \{2\|A\psi\| + \|\psi\|\}.$$

En insérant cette estimation dans le membre droit de la relation (6), il en résulte finalement que pour tout $\delta > 0$, il existe une constante $d < \infty$ telle que

$$\left| \frac{d}{d\mu} F(\lambda + i\mu) \right| \leq \frac{d}{\mu^{1/2}} \{\|\psi\|^2 + \|A\psi\|^2\}, \quad (7)$$

pour tout $|\lambda| \geq \delta$ et $0 < \mu < 1$.

Nous avons ainsi obtenu l'estimation $\int_0^1 \left| \frac{d}{d\mu} F(\lambda + i\mu) \right| d\mu < \infty$, uniformément en λ sur tout compact de \mathbb{R} ne comprenant pas 0. Il s'ensuit que la limite (3) existe pour tous les éléments de $D(A)$, uniformément en λ sur tout compact de \mathbb{R} ne comprenant pas 0. Cet ensemble de vecteurs étant dense dans \mathcal{H} , un principe d'absorption limite pour H sur $\mathbb{R} \setminus \{0\}$ a été démontré .

De nombreuses améliorations peuvent être apportées à la preuve proposée ci-dessus afin d'obtenir un plus grand nombre de vecteurs tels que la limite (3) existe pour chacun de ceux-ci. Nous renvoyons le lecteur à l'introduction du chapitre 7 de [ABG] ou à l'article [BG] pour une exposition des différentes techniques menant à ce type d'améliorations. Il est également essentiel de généraliser la démonstration pour dépasser le cadre trop restreint de la condition $[iH, A] = H$. L'idée de Mourre a été de modifier la résolvante de l'opérateur H en y ajoutant un terme supplémentaire. Plus précisément, en considérant la famille des opérateurs

$$G_\varepsilon(\lambda + i\mu) := (H - \lambda - i(\mu + \varepsilon[iH, A]))^{-1}$$

avec $\varepsilon \in [0, 1]$, et en jouant astucieusement entre les différents paramètres, il est possible d'étendre les arguments précédents à des situations où il n'existe pas d'expression

simple pour $[iH, A]$, pour autant que le signe de cet opérateur soit bien défini dans un voisinage de λ (et le même que le signe de μ). La condition de Mourre stricte est la concrétisation de cette idée lorsque le cas $\mu > 0$ est considéré.

La condition supplémentaire de régularité à imposer à H est donnée par la relation (2.1)². Un principe d'absorption limite général est énoncé dans le Théorème 7.4.1 de [ABG], sous l'hypothèse additionnelle que le spectre de H ne soit pas tout \mathbb{R} , ce qui sera vérifié dans nos applications. Une version plus élaborée de ce résultat qui ne requiert pas cette hypothèse additionnelle est proposée dans le Théorème 7.5.4 de ce même livre.

Un principe d'absorption limite sera utilisé dans les chapitres 1 et 2 de cette thèse pour étudier la nature du spectre de certains opérateurs H . Bien qu'un cadre abstrait existe, la démonstration d'un tel principe demeure une tâche complexe. Pour ce faire, il nous faudra notamment déterminer un opérateur conjugué A adéquat et démontrer les propriétés requises de régularité de H par rapport à A . Le nom de la méthode s'en trouvera justifié : méthode des commutateurs. En effet, de nombreux commutateurs, parfois subtils, devront être calculés ou estimés. En outre, l'ensemble des vecteurs pour lesquels la limite (3) existe est généralement obtenu en termes de certains espaces d'interpolation entre le domaine de A et l'espace de Hilbert \mathcal{H} . Si l'opérateur conjugué est lui-même compliqué, cet ensemble peut ne plus être compréhensible. Il est alors essentiel d'isoler un sous-ensemble suffisamment grand de ces vecteurs qui admettent une interprétation plus aisée. Le chapitre 1 est une illustration idéale des difficultés pouvant intervenir lors de l'élaboration d'un principe d'absorption limite.

La continuité absolue du spectre

A partir d'un principe d'absorption limite pour H obtenu sur un ensemble ouvert J , il est aisé de démontrer que le spectre de l'opérateur H sur J est purement absolument continu. Vu l'importance de ce résultat et l'utilisation ultérieure que nous en faisons, nous donnons la démonstration de cette implication.

Soit J un ensemble ouvert de \mathbb{R} sur lequel un principe d'absorption limite pour H a été démontré, et $[b, c]$ inclus dans J avec $b < c$. Nous avons donc que pour certains $\psi \in \mathcal{H}$ la limite $\lim_{\mu \rightarrow +0} \langle \psi, R(\lambda + i\mu)\psi \rangle$ existe, uniformément en λ pour $b \leq \lambda \leq c$. Nous rappelons que les projecteurs spectraux de H peuvent être obtenus à partir de sa résolvante, plus précisément :

$$E((b, c)) + \frac{1}{2}E(\{b\}) + \frac{1}{2}E(\{c\}) = w - \lim_{\mu \rightarrow +0} \frac{1}{\pi} \int_b^c \operatorname{Im} R(\lambda + i\mu) d\lambda,$$

où la limite doit être prise dans le sens faible. Ce résultat est appelé *la formule de Stone*. Il s'ensuit naturellement l'estimation :

$$\frac{1}{c-b} \|E((b, c))\psi\|^2 \leq \sup_{b < \lambda < c} \sup_{\mu > 0} \frac{1}{\pi} |\langle \psi, R(\lambda + i\mu)\psi \rangle| \quad (8)$$

²Le premier numéro correspond au chapitre de cette thèse dans lequel une équation porte ce numéro.

où le membre droit de (8) est fini par hypothèse. De cette inégalité, valable pour tout $[b, c] \subset J$, nous tirons l'absolue continuité sur l'ensemble J de la mesure de Borel $\{\|E(B)\psi\|^2\}_B$ associée à ψ .

Puisque l'ensemble \mathcal{D} des vecteurs ψ pour lesquels la limite (3) existe, avec l'uniformité requise en λ , est dense dans \mathcal{H} , alors l'ensemble $E(J)\mathcal{D}$ sera également dense dans le sous-espace spectral $E(J)\mathcal{H}$. La conséquence en est la continuité absolue du spectre de H dans l'ensemble J .

Au vu de ce qui précède, une remarque s'impose d'elle-même. Pour obtenir la continuité absolue de la mesure $\{\|E(B)\psi\|^2\}_B$, il n'est pas nécessaire de demander l'existence de la limite (3). Il est suffisant de demander l'existence de la limite

$$\lim_{\mu \rightarrow +0} \langle \psi, \operatorname{Im} R(\lambda + i\mu)\psi \rangle. \quad (9)$$

Le principe d'absorption limite présenté auparavant peut donc être adapté pour ne démontrer que l'existence de (9) au lieu de (3). On parle alors d'un principe d'absorption limite généralisé.

Une estimation de Mourre non stricte

Avant d'expliquer comment des résultats de la théorie de la diffusion peuvent également être obtenus à partir du cadre introduit au début de cette section, nous faisons une remarque sur une variante moins forte de l'estimation (2). Dans certaines situations, il est plus facile de vérifier une estimation de Mourre non stricte. Pour un intervalle ouvert J de \mathbb{R} , il s'agit de montrer l'existence d'une valeur a strictement positive ainsi que d'un opérateur compact K dans \mathcal{H} tels que l'inégalité

$$E(J)[iH, A]E(J) \geq aE(J) + K$$

soit satisfaite.

Les résultats spectraux issus de cette estimation sont un peu moins forts que dans le cas d'une estimation de Mourre stricte mais demeurent très intéressants. Grosso modo, il n'est plus possible de conclure à l'absolue continuité du spectre de H dans J , mais à son absolue continuité en dehors de quelques possibles valeurs propres de H qui sont alors forcément de multiplicité finie. C'est plus précisément ce genre de résultats que nous allons obtenir dans le chapitre 1 ainsi que dans la première partie du chapitre 2.

Dans la théorie de la diffusion

Dans le cadre de la théorie de la diffusion, une estimation de Mourre stricte s'avère également très utile, mais il n'existe pas pour le moment de théorie abstraite aussi solide que dans le cadre spectral pour implanter cette inégalité. De nombreux calculs relatifs à des propriétés de propagation de l'état $e^{-iHt}\psi$ en font usage, et il n'est dès lors pas possible de tous les mentionner. Cependant, nous citerons deux types distincts d'emploi de la méthode de l'opérateur conjugué. Le premier, le plus classique,

n'apparaît que de façon sous-jacente dans la deuxième partie du chapitre 2. Nous ne nous y attarderons donc guère. En revanche, le second est un ingrédient essentiel dans la démonstration de la complétude asymptotique du modèle présenté dans le chapitre 2 et tout le chapitre 3 y est consacré. Une mise en contexte sera donc proposée.

Les opérateurs H -lisses

Nous montrons comment apparaît naturellement une certaine classe d'opérateurs à partir d'un principe d'absorption limite et présentons leur intérêt pour la théorie de la diffusion. Indirectement, ces opérateurs sont les sous-produits de l'estimation de Mourre qui a servi à obtenir le principe d'absorption limite.

Nous avons obtenu précédemment et dans un exemple particulier un principe d'absorption limite pour H sur un sous-ensemble ouvert J de \mathbb{R} ; l'ensemble des vecteurs pour lesquels la limite (3) existait n'étant rien d'autre que le domaine $D(A)$ de l'opérateur conjugué. De plus, il suit de (7) que pour tout $\delta > 0$, il existe une constante d telle que la relation

$$|\langle \psi, R(\lambda + i\mu)\psi \rangle| \leq d\{\|\psi\|^2 + \|A\psi\|^2\}$$

soit vérifiée pour tout $\psi \in D(A)$, $|\lambda| \geq \delta$ et $\mu > 0$.

Ces faits sont en réalité très généraux. Supposons qu'un principe d'absorption limite ait été obtenu pour H sur un sous-ensemble ouvert J de \mathbb{R} à partir d'une estimation de Mourre sur J , alors l'ensemble des vecteurs, pour lesquels la limite (3) existe, comprend toujours $D(A)$. En fait, $D(|A|^\nu)$ pour tout $\nu > \frac{1}{2}$ est même compris dans cet ensemble. De plus, si $[b, c]$ est inclus dans J , il existe une constante d , dépendante de b et c , telle que pour tout $\psi \in D(A)$, $\lambda \in [b, c]$ et $\mu > 0$:

$$|\langle \psi, R(\lambda + i\mu)\psi \rangle| \leq d\{\|\psi\|^2 + \|A\psi\|^2\}.$$

De cette estimation on obtient alors l'existence d'une constante $d' < \infty$ satisfaisant

$$\|(1 + |A|)^{-1}R(\lambda + i\mu)(1 + |A|)^{-1}\| \leq d', \quad (10)$$

uniformément en $\lambda \in [b, c]$ et en $\mu > 0$, relation qui est à la base des développements qui suivent.

En effet, nous rappelons qu'un opérateur T fermé sur \mathcal{H} , avec $D(H) \subset D(T)$, est dit localement H -lisse sur J si pour tout intervalle $[b, c] \subset J$, il existe une constante $d < \infty$ telle que l'inégalité

$$\|T \operatorname{Im} R(\lambda + i\mu)T^*\| \leq d$$

soit vérifiée pour tout $\lambda \in [b, c]$ et $0 < \mu < 1$. En utilisant la relation

$$\operatorname{Im} R(\lambda + i\mu) = \frac{1}{2} \int_{-\infty}^{\infty} e^{i\lambda t} e^{-iHt - \mu|t|} dt,$$

on peut montrer que l'opérateur T est localement H -lisse sur J si et seulement si pour tout intervalle $[b, c] \subset J$, il existe une constante $d < \infty$ telle que

$$\int_{-\infty}^{\infty} \|Te^{-iHt}\psi\|^2 dt \leq d\|\psi\|^2$$

pour tous ψ satisfaisant $E([b, c])\psi = \psi$.

Ces opérateurs sont très utiles dans le cadre de la théorie de la diffusion pour la raison suivante :

Théorème *Soit H_1, H_2 deux opérateurs autoadjoints sur \mathcal{H} , et J un sous-ensemble ouvert de \mathbb{R} . Nous notons par E_j la mesure spectrale de H_j . Supposons que pour tout $\psi_j \in D(H_j)$ la relation $\langle H_1\psi_1, \psi_2 \rangle - \langle \psi_1, H_2\psi_2 \rangle = \langle T_1\psi_1, T_2\psi_2 \rangle$ est vérifiée, où T_j est un opérateur localement H_j -lisse sur J . Alors la limite forte*

$$W(H_1, H_2; J) := s - \lim_{t \rightarrow \infty} e^{iH_1 t} e^{-iH_2 t} E_2(J)$$

existe, est une isométrie partielle de $E_2(J)\mathcal{H}$ sur $E_1(J)\mathcal{H}$ et satisfait $W(H_1, H_2; J)^ = W(H_2, H_1; J)$.*

En comparant la relation (10) à la définition des opérateurs H -lisses, nous constatons immédiatement que l'opérateur $(1 + |A|)^{-1}$ est H -lisse. En plus de donner des informations sur la nature du spectre de H , un principe d'absorption limite fournit donc toute une classe d'opérateurs H -lisses qui peuvent ensuite être utilisés pour des résultats de diffusion, comme indiqué dans le théorème ci-dessus.

La vitesse minimale

Comme le nom l'indique, l'idée principale d'un type de résultats obtenus dans le cadre de la théorie de la diffusion est de prouver la propagation dans un certain milieu et avec une certaine vitesse minimale de l'état $e^{-iHt}\psi$. Ce milieu peut être l'espace n -dimensionnel, mais également un espace des configurations, un espace de phase ou le spectre de l'opérateur conjugué. Une inégalité de Mourre stricte semble essentielle dans toutes les démonstrations de vitesse minimale élaborées jusqu'à maintenant. Des conditions supplémentaires de régularité de H par rapport à A s'ajoutent à la condition minimale $C^1(A)$ en fonction de la forme du résultat escompté.

Nous commençons par rappeler deux résultats classiques de propagation des états avant de parler plus spécifiquement de la vitesse minimale. Précisons que leur démonstration ne fait pas intervenir la notion d'opérateur conjugué.

Supposons que B appartienne à $\mathcal{B}(\mathcal{H})$ et que le produit $B(H - i)^{-1}$ soit un opérateur compact sur \mathcal{H} . Nous désignons par $\mathcal{H}_c(H)$ le sous-espace continu de \mathcal{H} par rapport à H , c'est-à-dire le sous-espace de \mathcal{H} orthogonal au sous-espace engendré par les vecteurs propres de H . Alors pour tous vecteurs $\psi \in \mathcal{H}_c(H)$, les relations suivantes sont satisfaites (RAGE Theorem) :

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \|B e^{-iHt}\psi\|^2 dt = 0 \quad \text{et} \quad \lim_{T \rightarrow \infty} \frac{1}{T} \int_{-T}^0 \|B e^{-iHt}\psi\|^2 dt = 0. \quad (11)$$

Notons que si ψ appartient au sous-espace absolument continu $\mathcal{H}_{ac}(H)$ de \mathcal{H} par rapport à H , alors un résultat plus fort est vérifié, à savoir : $\|B e^{-iHt}\psi\| \rightarrow 0$ pour $t \rightarrow \pm\infty$.

En supposant maintenant que $\mathcal{H} = L^2(\mathbb{R}^n)$ et que l'opérateur H soit localement

compact, un cas particulier de (11) est l'affirmation bien connue

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \|\chi(|Q| \leq R) e^{-iHt} \psi\|^2 dt = 0 \quad \forall R \in (0, \infty),$$

où $\chi(|Q| \leq R)$ est l'opérateur de multiplication correspondant à la fonction caractéristique sur la boule centrée à l'origine et de rayon égale à R . L'interprétation de ce résultat est que tout $\psi \in \mathcal{H}_c(H)$ disparaît en moyenne temporelle de toute région finie de l'espace des configurations.

Dans le cadre particulier $\mathcal{H} = L^2(\mathbb{R}^n)$, le deuxième résultat classique est le suivant. Supposons que pour un certain $\psi \in \mathcal{H}$ et pour tout $R \in (0, \infty)$ la majoration suivante est satisfaite :

$$\int_{-\infty}^{\infty} \|\chi(|Q| \leq R) e^{-iHt} \psi\|^2 dt < \infty.$$

Le vecteur ψ appartient alors à $\mathcal{H}_{ac}(H)$ [Si]. L'interprétation est : si le temps de séjour de l'état $e^{-iHt} \psi$ dans toute région bornée de l'espace est fini, alors l'état ψ doit appartenir à $\mathcal{H}_{ac}(H)$.

Il est clair que dans les deux résultats rappelés ci-dessus, une certaine propagation a lieu. Sous l'évolution engendrée par H les états ψ partent de toute région finie de l'espace, mais comment et à quelle vitesse ? Cette notion de vitesse de propagation est non seulement naturelle mais également essentielle pour d'autres résultats profonds de la théorie de la diffusion.

L'exemple le plus simple où une notion de vitesse minimale est facilement calculable et compréhensible est celui d'une particule libre évoluant dans l'espace \mathbb{R}^n , voir [HSS]. Soit \mathcal{H} l'espace de Hilbert $L^2(\mathbb{R}^n)$ et $H := -\Delta$ l'opérateur de Schrödinger correspondant à cette situation. Soit ψ un élément de \mathcal{H} tel que sa transformée de Fourier soit lisse et à support à l'extérieur d'une boule centrée à l'origine et de rayon $v > 0$. Alors pour tout $m \in \mathbb{N}$, il existe une constante c_m telle que

$$\|\chi(|Q| \leq vt) e^{-iHt} \psi\|^2 \leq c_m t^{-m} \quad \text{pour } t \rightarrow \infty. \quad (12)$$

Ainsi la probabilité de présence de l'état $e^{-iHt} \psi$ dans une boule centrée à l'origine et de rayon croissant à la vitesse v tend vers 0 pour t tendant vers l'infini. La propagation a donc lieu à une vitesse supérieure à la vitesse minimale v . Notons que ce calcul a été possible car le groupe d'évolution $\{e^{-iHt}\}_{t \in \mathbb{R}}$ est connu dans ce cas simple.

Si la particule considérée est soumise à un potentiel externe borné V , le groupe d'évolution $\{e^{-iHt}\}_{t \in \mathbb{R}}$ avec $H := -\Delta + V(Q)$ n'est plus connu explicitement et l'approche utilisée ci-dessus devient caduque. L'estimation de Mourre stricte va maintenant prendre toute son importance. Suivant [HSS], nous donnons quelques arguments heuristiques mettant en évidence le rôle de l'estimation (2) dans la recherche d'une vitesse minimale.

Le cadre est toujours $\mathcal{H} = L^2(\mathbb{R}^n)$ et $H = -\frac{1}{2}\Delta + V(Q)$. Nous avons dû légèrement modifier la normalisation de la partie cinétique afin d'obtenir un résultat au plus proche de l'intuition. L'opérateur conjugué est le générateur du groupe des dilatations, à savoir $A := \frac{1}{2}(P \cdot Q + Q \cdot P)$, avec P_j l'opérateur autoadjoint dans \mathcal{H} donné par $-i \frac{\partial}{\partial j}$

sur les fonctions une fois continûment différentiables. Nous supposons que H est de classe $C^1(A)$ et qu'il existe un intervalle ouvert J de \mathbb{R} tel que $E(J)[iH, A]E(J) \geq \theta E(J)$ pour $\theta > 0$. Soit $\psi \in \mathcal{H}$ avec $\|\psi\| = 1$ et telle que $E(J)\psi = \psi$, c'est-à-dire que le support spectral de ψ est contenu dans J . Les calculs qui suivent ne sont que formels, les questions relatives aux domaines des différents opérateurs non bornés ne sont pas abordées. Formellement nous avons

$$\frac{d}{dt} \langle e^{-iHt} \psi, \frac{1}{2} Q^2 e^{-iHt} \psi \rangle = \langle e^{-iHt} \psi, A e^{-iHt} \psi \rangle.$$

De l'égalité

$$\frac{d}{dt} \langle e^{-iHt} \psi, A e^{-iHt} \psi \rangle = \langle e^{-iHt} \psi, [iH, A] e^{-iHt} \psi \rangle,$$

nous tirons alors que

$$\frac{d^2}{dt^2} \langle e^{-iHt} \psi, \frac{1}{2} Q^2 e^{-iHt} \psi \rangle \geq \theta.$$

Par intégration, il s'ensuit l'estimation

$$\langle e^{-iHt} \psi, Q^2 e^{-iHt} \psi \rangle \geq \theta t^2 + O(t) \quad \text{pour } t \geq 0.$$

Ce résultat, bien que purement formel, nous dit que la valeur moyenne de l'observable $e^{iHt} Q^2 e^{-iHt}$ pour l'état ψ diverge en fonction du temps comme θt^2 . Ceci n'est évidemment qu'une vague notion de vitesse minimale, mais l'intérêt de ce calcul est de montrer comment une inégalité de Mourre stricte peut intervenir dans une estimation de propagation.

Jusqu'à maintenant, les résultats abstraits de vitesse minimale étaient épars et pas toujours très généraux, la majeure partie n'ayant pas été élaborés dans un cadre abstrait mais en vue d'une application particulière, principalement pour le problème à N-corps. Les exceptions notoires à cette règle sont la Proposition 4.4.1 de [GL] ainsi que l'article [HSS]. Nous avons donc voulu essayer de remédier à cette lacune et d'isoler les constituants essentiels d'une démonstration de vitesse minimale dans le cadre abstrait introduit au début de cette section. Le chapitre 3 est entièrement consacré à cette problématique, les deux références mentionnées ayant inspiré chacune une partie de ce travail. Le principal résultat donne la propagation de l'état $e^{-iHt}\psi$ avec une vitesse minimale reliée à la constante θ de l'inégalité de Mourre stricte, cette propagation ayant lieu dans le spectre de l'opérateur conjugué. Nous renvoyons le lecteur au résumé du chapitre 3 pour un énoncé du résultat abstrait ainsi que pour son application pour les opérateurs de Schrödinger. De façon générale, si l'espace de Hilbert \mathcal{H} est $L^2(\mathbb{R}^n)$ et si l'opérateur conjugué A est comparable, dans un sens vague, avec les opérateurs Q_j et P_j , une vitesse minimale de propagation dans l'espace de phase ou dans l'espace des configurations pourra-t-être extraite du résultat abstrait.

Par rapport à la théorie spectrale, la théorie de la diffusion souffre encore d'un manque d'homogénéité, et les nombreux résultats connus sont généralement trop spécifiques à une problématique donnée. Il en découle une difficulté à prédire l'utilisation optimale de l'inégalité de Mourre stricte ainsi que les conditions de régularité de H par rapport à A réellement utiles. Il n'est certainement pas trop audacieux de dire que dans le cadre de la théorie de la diffusion, la méthode des commutateurs mérite encore beaucoup d'attention et peut potentiellement fournir encore de nombreux résultats.

0.3 L'opérateur de Dirac avec champ magnétique

Considérons une particule élémentaire relativiste de masse $m \neq 0$ et de spin $\frac{1}{2}$ évoluant dans l'espace tridimensionnel en présence d'un champ magnétique variable mais de direction constante. Sans perte de généralité et grâce aux équations de Maxwell, il est possible de choisir un référentiel orthonormé tel que dans celui-ci le champ magnétique prenne la forme suivante : $\vec{B}(x_1, x_2, x_3) = (0, 0, B(x_1, x_2))$. Le système est alors décrit dans l'espace de Hilbert $L^2(\mathbb{R}^3; \mathbb{C}^4)$ 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 les opérateurs $\Pi_j := -i\partial_j - a_j(Q_1, Q_2)$ sont les générateurs des translations magnétiques pour un potentiel vecteur

$$\vec{a}(x_1, x_2, x_3) = (a_1(x_1, x_2), a_2(x_1, x_2), 0) \quad (13)$$

satisfaisant $B = \partial_1 a_2 - \partial_2 a_1$. La troisième composante du potentiel vecteur étant nulle, nous avons écrit $P_3 := -i\partial_3$ au lieu de Π_3 .

Dans ce travail, nous étudions la stabilité de la nature du spectre de H_0 sous l'effet de perturbations dues à l'ajout d'un potentiel matriciel V . Plus précisément, si ce dernier satisfait certaines hypothèses sur sa décroissance à l'infini, nous vérifions un principe d'absorption limite, et montrons de la sorte l'absence de spectre singulier continu et la finitude du spectre ponctuel de $H := H_0 + V(Q)$ dans des intervalles de \mathbb{R} . Ces intervalles 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 $L^2(\mathbb{R}^2; \mathbb{C}^2)$. Les matrices σ_j désignent les matrices de Pauli et le spectre symétrisé σ_{sym}^0 de H^0 est la réunion des spectres de H^0 et de $-H^0$. Il est intéressant de constater l'apparition naturelle de l'opérateur H^0 comme une sorte d'opérateur interne à notre système.

Avant d'énoncer plus précisément les résultats obtenus, considérons l'exemple suivant : le champ magnétique est constant dans tout l'espace et prend une valeur $B_0 \neq 0$. Dans ce cas, il est bien connu que l'ensemble σ_{sym}^0 est égal à l'ensemble des valeurs $\pm\sqrt{2nB_0 + m^2}$ avec $n = 0, 1, 2, \dots$. Il s'ensuit que la portée de notre analyse est très grande dans cet exemple vu l'importance des trous spectraux. En revanche, pour un champ magnétique tendant vers 0 à l'infini, les intervalles $(-\infty, -m]$ et $[m, \infty)$ appartiennent à σ_{sym}^0 et notre étude ne fournit donc aucune information intéressante.

Plus généralement, soit \vec{B} un champ magnétique continu pointant dans la troisième direction d'un repère orthonormé et dépendant des deux autres variables. Nous choisissons un potentiel vecteur continu \vec{a} de la forme indiquée dans (13), par exemple celui obtenu dans la jauge transverse. Soit encore V une application bornée de \mathbb{R}^3 à valeurs dans les matrices 4×4 hermitiennes. Nous demandons que le potentiel V s'annule à l'infini et lui imposons une certaine vitesse de décroissance dans la troisième direction. La vitesse de décroissance du potentiel dans les deux autres directions n'est pas imposée et pourrait être extrêmement lente.

L'opérateur conjugué considéré est formellement donné par l'expression

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

Une estimation de Mourre stricte est démontrée sur les sous-ensembles de \mathbb{R} qui n'appartiennent pas à σ_{sym}^0 , puis un principe d'absorption limite est vérifié sur ces mêmes intervalles. Les résultats suivants sont obtenus comme corollaires :

- (a) le spectre ponctuel de H en dehors de σ_{sym}^0 est composé de valeurs propres de multiplicité finie et ne pouvant s'accumuler qu'en des valeurs appartenant à σ_{sym}^0 ,
- (b) l'opérateur H n'a pas de spectre singulier continu dans $\mathbb{R} \setminus \sigma_{\text{sym}}^0$.

L'intérêt de ce travail réside dans le fait que le champ magnétique initial est quelconque; nous ne lui avons imposé aucune restriction, excepté en demandant sa continuité. La démarche ne dépend donc pas explicitement du choix du champ magnétique, mais celui-ci intervient évidemment dans le calcul de σ_{sym}^0 . Dans le cas du champ magnétique constant et non nul, le principe d'absorption limite obtenu améliore sensiblement certains résultats récents. Pour des champs magnétiques plus généraux, nos résultats semblent nouveaux.

Ce travail a été effectué en collaboration avec Rafael Tiedra de Aldecoa, de l'Université de Genève. Un article intitulé On Perturbations of Dirac operators with variable magnetic field of constant direction correspondant au chapitre 1 de cette thèse paraîtra dans Journal of Mathematical Physics.

0.4 L'anisotropie cartésienne

Considérons des opérateurs de Schrödinger $H = -\Delta + V(Q)$ dans l'espace de Hilbert $L^2(\mathbb{R}^n)$ avec des potentiels V présentant une *anisotropie cartésienne*. La caractéristique de ces potentiels est de posséder des limites asymptotiques séparément pour chaque variable. Un exemple particulièrement simple dans l'espace \mathbb{R}^2 est obtenu en prenant $V(x_1, x_2) = V_1(x_1)V_2(x_2)$ pour deux fonctions réelles continues V_j telles que

$$\lim_{x_j \rightarrow \pm\infty} V_j(x_j) = c_j^\pm.$$

L'analyse de ces opérateurs s'inscrit dans le cadre plus ambitieux de l'étude des opérateurs de Schrödinger à potentiels anisotropes, c'est-à-dire des potentiels qui ne décroissent pas vers 0 à l'infini. L'intérêt plus particulier porté aux *potentiels cartésiens* réside dans le fait qu'il est possible de mener à bien une analyse spectrale et une théorie de la diffusion quasi exhaustives pour les opérateurs de Schrödinger correspondants. De plus, la facile interprétation géométrique des différents phénomènes apparaissant lors de leur étude peut stimuler l'élaboration d'une théorie plus générale.

Dans ce résumé du chapitre 2, nous allons nous concentrer sur l'exemple bidimensionnel très simple mentionné ci-dessus et expliciter sur cet exemple les résultats obtenus dans ce travail. Soulignons que le cas n -dimensionnel, avec n quelconque, est traité dans le corps du texte et que des potentiels cartésiens beaucoup plus généraux sont étudiés.

Pour $j = 1, 2$, considérons les opérateurs $H_{j\pm} := -\Delta + c_k^\pm V_j(Q_j)$, avec $k \in \{1, 2\}$ mais $k \neq j$, dits *opérateurs asymptotiques*. Nous considérons également les opérateurs $H^{j\pm} := -\Delta_j + c_k^\pm V_j(Q_j)$ agissant sur $L^2(\mathbb{R}_j)$, dits *opérateurs internes*. Notons que l'indice j dans \mathbb{R}_j correspond à l'indice de la variable x_j de \mathbb{R}^2 . Il est essentiel de remarquer que les opérateurs asymptotiques se décomposent en des opérateurs internes et des Hamiltoniens libres, par exemple :

$$H_{2\pm} = -\Delta_1 \otimes 1 + 1 \otimes H^{2\pm}$$

dans la représentation de l'espace de Hilbert $L^2(\mathbb{R}_1) \otimes L^2(\mathbb{R}_2)$. Pour $H = -\Delta + V_1(Q_1)V_2(Q_2)$, notons encore $\tau(H)$, l'ensemble *des seuils*, la réunion des valeurs propres des quatre opérateurs internes ainsi que des quatre valeurs $c_1^+ c_2^+$, $c_1^+ c_2^-$, $c_1^- c_2^+$ et $c_1^- c_2^-$. L'ensemble $\kappa(H)$ *des valeurs critiques* de H est composé des valeurs propres de H ainsi que des valeurs de $\tau(H)$. Les différents objets introduits dans ce paragraphe vont être utilisés pour énoncer certains résultats relatifs à l'analyse spectrale de H et à sa théorie de la diffusion.

Il est connu que le spectre essentiel $\sigma_{\text{ess}}(H)$ de H est égal à l'union des spectres des opérateurs asymptotiques. Cependant, vu que ceux-ci sont décomposables, une estimation plus précise peut être obtenue : $\sigma_{\text{ess}}(H) = [\sigma_0, \infty)$ où σ_0 est la plus petite valeur appartenant à l'un des spectres des opérateurs internes. De plus, supposons que les fonctions V_j tendent vers leurs limites asymptotiques de façon à courte portée, c'est-à-dire plus rapidement que $d(1 + |x|)^{-(1+\varepsilon)}$ avec $d, \varepsilon > 0$. Cette hypothèse sur la vitesse de convergence sera tacitement prise en compte dans la suite de ce résumé. Nous démontrons alors que les ensembles $\tau(H)$ et $\kappa(H)$ sont des ensembles dénombrables fermés, et que les valeurs propres de H n'appartenant pas à $\tau(H)$ sont de multiplicité finie et ne peuvent s'accumuler qu'en des valeurs appartenant à $\tau(H)$. Quant au spectre de H , nous montrons qu'il ne comporte pas de composante singulièrement continue.

Avant de donner quelques résultats précis sur la théorie de la diffusion de l'opérateur H , une brève discussion heuristique s'impose. Par analogie classique, supposons que notre potentiel $V = V_1 V_2$ ait été réalisé dans un matériau solide et qu'une bille idéale puisse se mouvoir sur cette surface bidimensionnelle. A priori, les possibles comportements asymptotiques de cette bille se présentent sous trois formes distinctes : la bille reste localisée dans une région finie de la surface, la bille s'échappe dans la direction d'un "coin" où le potentiel devient asymptotiquement constant et prend une des quatre valeurs $c_1^+ c_2^+$, $c_1^+ c_2^-$, $c_1^- c_2^+$ ou $c_1^- c_2^-$, la bille se retrouve piégée dans une vallée parallèle à l'un des axes et ne peut essentiellement se déplacer plus que dans la direction de cette vallée. En d'autres mots, la bille peut soit être piégée par le système, soit être asymptotiquement libre, soit encore être libre dans une direction mais piégée dans une autre.

Il est clair que ces différents comportements asymptotiques doivent se retrouver d'une façon ou d'une autre dans la description asymptotique de $e^{-iHt}\psi$ pour tout vecteur ψ de $L^2(\mathbb{R}^2)$. Une différentiation des états en fonction de leur comportement asymptotique va donc être nécessaire. Pour ce faire, nous allons effectuer une partition de l'espace des états, l'espace de Hilbert $L^2(\mathbb{R}^2)$, en regroupant les vecteurs qui auront une évolution asymptotique similaire sous l'action du groupe unitaire $\{e^{-iHt}\}_{t \in \mathbb{R}}$. Par

exemple, nous allons mettre ensemble tous les états qui partiront asymptotiquement dans le coin du premier quadrant de \mathbb{R}^2 et qui devraient ainsi avoir une évolution asymptotique régie par l'opérateur $-\Delta + c_1^+ c_2^+$.

Une des manières d'effectuer cette classification est, dans un premier temps, de définir la famille *des opérateurs vitesse asymptotique* \mathcal{P}_j pour $j = 1, 2$. Ceux-ci sont obtenus par leur calcul fonctionnel continu conjoint, à savoir

$$f(\mathcal{P}) = s - \lim_{t \rightarrow +\infty} e^{iHt} f\left(\frac{Q}{2t}\right) e^{-iHt} \quad (14)$$

pour toutes les fonctions f définies sur \mathbb{R}^2 et s'annulant à l'infini. Ce calcul fonctionnel est ensuite étendu à un ensemble plus grand de fonctions comprenant notamment les fonctions caractéristiques. Dans un deuxième temps, les projecteurs spectraux conjoints correspondant à certaines parties de \mathbb{R}^2 vont effectuer la partition de $L^2(\mathbb{R}^2)$ souhaitée.

Afin de ne pas allonger inutilement ce résumé, nous ne considérons que deux parties emblématiques de \mathbb{R}^2 . Pour exemple, soit $E_{++}(\mathcal{P})$ et $E_{+0}(\mathcal{P})$ les projecteurs spectraux de \mathcal{P} correspondant aux sous-ensembles $\{(x_1, x_2) \mid x_1 > 0, x_2 > 0\}$ et $\{(x_1, 0) \mid x_1 > 0\}$ de \mathbb{R}^2 . Alors, les sous-espaces $E_{++}(\mathcal{P})\mathcal{H}$ et $E_{+0}(\mathcal{P})\mathcal{H}$ sont constitués respectivement des états qui partent asymptotiquement dans le coin du premier quadrant et des états piégés dans les vallées parallèles à l'axe e_1 et partant asymptotiquement vers la droite. Relevons encore, non sans un certain plaisir, que le sous-espace $E_{00}(\mathcal{P})\mathcal{H}$, correspondant au sous-ensemble $\{(0, 0)\}$ de \mathbb{R}^2 , est égal au sous-espace engendré par les vecteurs propres de H . Autrement dit, les vecteurs de \mathcal{H} qui ont une vitesse asymptotique nulle sont les états liés du système. Il est important de noter que cette dernière affirmation ne repose pas uniquement sur l'existence de la vitesse asymptotique, une démonstration de vitesse minimale doit intervenir.

La dernière étape de cette construction consiste à montrer que pour tout vecteur fixé ψ de $E_{++}(\mathcal{P})\mathcal{H}$, respectivement de $E_{+0}(\mathcal{P})\mathcal{H}$, il est possible de déterminer un vecteur ψ_0 de \mathcal{H} tel que

$$\lim_{t \rightarrow \infty} \|e^{-iHt} \psi - e^{-i(-\Delta + c_1^+ c_2^+)t} \psi_0\| = 0,$$

respectivement

$$\lim_{t \rightarrow \infty} \|e^{-iHt} \psi - e^{-iH_{2+t}} \psi_0\| = 0.$$

La forme exacte des opérateurs d'onde permettant de déterminer ψ_0 à partir de ψ est donnée dans le corps du texte.

Comme une description asymptotique analogue à celle exposée ci-dessus existe pour n'importe quel vecteur de $\mathcal{H}_c(H)$, on dit que l'on a obtenu la complétude asymptotique. La théorie spectrale et la théorie de la diffusion ont ainsi pu être menées à leur terme pour le modèle cartésien.

Au niveau algébrique

Le chapitre 2 est le plus conséquent de cette thèse, de nombreux résultats pour le modèle cartésien y ayant été démontrés. En plus des techniques introduites auparavant

pour obtenir un principe d'absorption limite ou un résultat de vitesse minimale, nous avons eu recours à des méthodes algébriques dont nous présentons brièvement la philosophie. Ces méthodes ont été introduites en analyse spectrale principalement par Georgescu et ses collaborateurs pour l'étude des systèmes anisotropes.

Considérons une C^* -sous-algèbre \mathcal{A} de l'ensemble des fonctions bornées et uniformément continues sur \mathbb{R}^n . Nous demandons que cette algèbre soit stable sous les translations de \mathbb{R}^n , c'est-à-dire que si φ appartient à \mathcal{A} , alors $\varphi(\cdot + x) \in \mathcal{A}$ pour tout $x \in \mathbb{R}^n$. L'idée sous-jacente en introduisant cette algèbre est de modéliser un certain type d'anisotropie, les fonctions de cette algèbre étant des représentants (lisses) des potentiels V que nous désirons analyser (par exemple les potentiels cartésiens).

Par le Théorème de Gelfand, \mathcal{A} est isomorphe à une algèbre $C_0(\mathcal{X})$, où \mathcal{X} est un espace localement compact et $C_0(\mathcal{X})$ est l'ensemble des fonctions continues sur \mathcal{X} qui tendent vers 0 à l'infini. Notons que si \mathcal{A} est uniale, alors \mathcal{X} est un espace compact, et que si $C_0(\mathbb{R}^n)$ est inclus dans \mathcal{A} , alors \mathbb{R}^n peut être plongé continûment et injectivement dans \mathcal{X} . De plus, l'invariance de \mathcal{A} sous les translations de \mathbb{R}^n induit une action continue de \mathbb{R}^n sur \mathcal{X} .

L'étude des parties fermées de \mathcal{X} qui sont stables sous l'action des translations de \mathbb{R}^n est une des clés de l'analyse spectrale et de la diffusion des opérateurs de Schrödinger $H := -\Delta + V(Q)$ avec $V \in \mathcal{A}$. En effet, ce sont ces sous-ensembles de \mathcal{X} qui indiquent les Hamiltoniens asymptotiques permettant de calculer le spectre essentiel de H , voir [GI2] ou [Ma2]. Mais ces mêmes opérateurs sont également des candidats idéaux pour la théorie de la diffusion. Encore faut-il réussir à montrer qu'ils jouent vraiment le rôle endossé par H_0 dans (1) pour certains vecteurs ψ de \mathcal{H} ?

Ce programme a été complètement réalisé pour le cas cartésien. L'ensemble \mathcal{X} en relation avec l'anisotropie cartésienne est introduit dans la Section 2.1 et l'étude des parties fermées invariantes est effectuée dans la Section 2.3. C'est finalement dans la Section 2.6 que l'importance du rôle des Hamiltoniens asymptotiques est démontré pour la théorie de la diffusion.

Les observables de propagation

L'existence de la vitesse asymptotique (14) a été une pièce essentielle dans la démarche pour obtenir la complétude asymptotique du modèle cartésien. Notons que sa démonstration a précédé celle de la vitesse minimale et qu'elle ne repose pas sur une inégalité de type Mourre (il devrait même être possible de prouver l'existence d'une vitesse asymptotique dans un cadre abstrait beaucoup plus général que celui présenté dans ce chapitre). La technique utilisée pour obtenir ce résultat est celle des observables de propagation développée pour le problème à N-corps principalement par Enss, Sigal, Soffer, Graf, Dereziński et Gérard.

Considérons l'application

$$[1, \infty) \ni t \mapsto \Phi(t) \in \mathcal{B}(\mathcal{H}), \quad (15)$$

appelée *observable de propagation*. L'observable Φ est dite bornée s'il existe une constante $d < \infty$ telle que $\|\Phi(t)\| \leq d$ pour tous $t \in [1, \infty)$. Typiquement, on va

chercher à montrer pour une observable bornée Φ l'existence de la limite forte

$$s - \lim_{t \rightarrow \infty} e^{iHt} \Phi(t) e^{-iHt}. \quad (16)$$

Supposons que l'application (15) soit bornée et différentiable en norme avec une dérivée bornée, on peut alors définir sa *dérivée de Heisenberg* $[\mathbf{D}\Phi](t)$ donnée pour tous $\psi, \psi' \in D(H)$ par l'expression :

$$\langle \psi, [\mathbf{D}\Phi](t) \psi' \rangle := i \langle H\psi, \Phi(t) \psi' \rangle - i \langle \psi, \Phi(t) H \psi' \rangle + \langle \psi, \frac{d}{dt} \Phi(t) \psi' \rangle.$$

Cette définition apparaît naturellement en remarquant que pour tous $\psi, \psi' \in D(H)$:

$$\frac{d}{dt} \langle \psi, e^{iHt} \Phi(t) e^{-iHt} \psi' \rangle = \langle \psi, e^{iHt} [\mathbf{D}\Phi](t) e^{-iHt} \psi' \rangle.$$

Pour une observable de propagation Φ bornée et différentiable en norme avec une dérivée bornée, nous donnons une condition suffisante pour démontrer l'existence de la limite $s - \lim_{t \rightarrow \infty} e^{iHt} \Phi(t) e^{-iHt}$. Supposons qu'il existe une seconde observable de propagation bornée B , satisfaisant $\int_1^\infty \|B(t) e^{-iHt} \psi\|^2 dt \leq c \|\psi\|^2$ pour $c < \infty$ et tous $\psi \in D(H)$, telle que

$$|\langle \psi, [\mathbf{D}\Phi](t) \psi \rangle| \leq \|B(t) \psi\|^2$$

pour tous $\psi \in D(H)$ et $t \geq 1$. Alors la limite (16) existe. Un énoncé plus général de cette affirmation ainsi que sa démonstration sont proposés dans le Lemme 2.6.4.

L'utilité de ce résultat va dépendre de notre capacité à vérifier la condition imposée à l'observable de propagation B . L'observation suivante de Sigal et Soffer va s'avérer particulièrement utile dans ce contexte. Supposons qu'il existe une troisième observable de propagation Φ' bornée et différentiable en norme avec une dérivée bornée telle que

$$\langle \psi, [\mathbf{D}\Phi'](t) \psi \rangle \geq \langle \psi, B^*(t) B(t) \psi \rangle \quad \forall t \geq 1 \text{ et } \psi \in D(H).$$

Il existe alors une constante $c < \infty$ telle que $\int_1^\infty \|B(t) e^{-iHt} \psi\|^2 dt \leq c \|\psi\|^2$ pour tous ψ appartenant à $D(H)$. A nouveau, un énoncé plus général est donné dans le Lemme 2.6.3.

En utilisant les versions plus élaborées de ces deux résultats (Lemmes 2.6.3 et 2.6.4) pour des observables de propagation de plus en plus astucieuses, il est possible de démontrer l'existence de la vitesse asymptotique (14). La section 2.6, une des plus techniques de cette thèse, est basée presque exclusivement sur ce jeu de recherches de bonnes observables de propagation.

Un article intitulé Spectral and Scattering Theory for Schrödinger Operators with Cartesian Anisotropy correspondant au chapitre 2 de cette thèse paraîtra dans Publ. RIMS, Kyoto Univ.

0.5 La vitesse minimale

Considérons un espace de Hilbert \mathcal{H} ainsi que l'ensemble $\mathcal{B}(\mathcal{H})$ des opérateurs linéaires bornés sur \mathcal{H} . La notation $\|\cdot\|$ est utilisée non seulement pour la norme des vecteurs de l'espace de Hilbert mais également pour la norme des éléments de $\mathcal{B}(\mathcal{H})$. Soit H et A deux opérateurs autoadjoints agissant sur \mathcal{H} . Nous supposons que H est de classe $C_u^1(A)$, c'est-à-dire que l'application

$$\mathbb{R} \ni t \rightarrow e^{iAt}(H-i)^{-1}e^{-iAt} \in \mathcal{B}(\mathcal{H}) \quad (17)$$

est dérivable en norme. Nous demandons également que l'inégalité

$$E(J)[iH, A]E(J) \geq \theta E(J)$$

soit vérifiée pour un intervalle ouvert J de \mathbb{R} et une valeur de θ strictement positive. Il est important de souligner que la condition de régularité entre H et A est très faible, à peine plus forte que la condition minimale pour donner un sens à l'expression $E(J)[iH, A]E(J)$. Soit encore deux nombres réels a et t . Dans la première partie de ce travail, nous démontrons que pour toutes les fonctions réelles lisses η à support dans J et pour tout $v < \theta$, l'estimation suivante est vérifiée :

$$\|\chi(A \leq a + vt)e^{-iHt}\eta(H)\chi(A \geq a)\| \rightarrow 0 \quad \text{pour } t \rightarrow \infty \quad (18)$$

uniformément en a . Les symboles $\chi(A \leq c)$ et $\chi(A \geq c)$ désignent les projecteurs spectraux de A sur les intervalles $(-\infty, c]$ et $[c, \infty)$.

L'expression (18) donne une information sur la localisation de l'évolution e^{-iHt} dans le spectre de l'opérateur A . Ce genre d'estimation n'est pas nouveau ; des estimations analogues sont utilisées depuis longtemps dans la théorie de la diffusion, notamment pour des questions relatives à la complétude asymptotique. Cependant, le présent travail a le mérite d'avoir affaibli les hypothèses de compatibilité entre H et A à un niveau encore inégalé, le domaine d'applicabilité de l'estimation (18) s'en trouvant alors considérablement élargi.

La deuxième partie de ce travail est dédiée à la transformation de ce résultat abstrait en une version directement applicable pour certains opérateurs de Schrödinger dans l'espace de Hilbert $\mathcal{H} = L^2(\mathbb{R}^n)$. Considérons pour H l'opérateur $-\Delta + V(Q)$ ayant pour domaine le second espace de Sobolev sur \mathbb{R}^n , et pour A le générateur du groupe des dilatations dans \mathcal{H} . Les hypothèses suivantes sont toujours demandées : H est de classe $C_u^1(A)$ et l'inégalité $E(J)[iH, A]E(J) \geq \theta E(J)$ est vérifiée pour un intervalle ouvert J de \mathbb{R} et pour $\theta > 0$. Nous démontrons alors qu'il existe une valeur strictement positive v_{\min} et un ensemble dense de vecteurs ψ dans le sous-espace spectral $E(J)\mathcal{H}$ de \mathcal{H} tel que pour tout $v < v_{\min}$, l'estimation suivante est vérifiée :

$$\|\chi(|Q| \leq vt)e^{-iHt}\psi\| \rightarrow 0 \quad \text{pour } t \rightarrow \infty. \quad (19)$$

L'interprétation physique de ce résultat a déjà été donnée dans le paragraphe suivant (12), pour mémoire : la probabilité de trouver l'état $e^{-iHt}\psi$ dans une boule centrée à l'origine et dont le rayon croît à la vitesse v tend vers 0 pour le temps

t tendant vers l'infini. La différence majeure entre les relations (12) et (19) est le contrôle sur la vitesse de décroissance : très bien maîtrisé dans un cas, sans aucun contrôle dans l'autre. La raison en est la régularité de H par rapport à l'opérateur conjugué : $C^\infty(A)$ dans le premier cas (c'est-à-dire l'application (17) est infiniment différentiable), et uniquement $C_u^1(A)$ dans le second.

Ce travail soulève finalement une question encore sans réponse. L'estimation (19) semble indiquer l'absence de spectre singulier continu pour l'opérateur H . En effet, pour certains vecteurs ψ appartenant au sous-espace correspondant au spectre singulier continu de H , la probabilité de trouver l'état $e^{-iHt}\psi$ dans tout ensemble compact de \mathbb{R}^n pourrait ne pas tendre vers 0 pour t tendant vers l'infini. Cette affirmation est basée sur les résultats cités après les relations (11). Or l'existence d'une vitesse minimale de propagation est en opposition flagrante avec ce phénomène. Cependant, les résultats obtenus dans ce travail ne permettent pour le moment pas de confirmer l'hypothèse de l'absence de spectre singulier continu. Ce constat n'a rien de surprenant : la nature d'un spectre est une information issue de la théorie spectrale, théorie essentiellement statique, alors que (19) est un sous-produit d'une théorie dynamique. La question mentionnée demeure toutefois intéressante en relation avec la condition de régularité $C_u^1(A)$. Effectivement, cette dernière est actuellement insuffisante pour toutes les démonstrations connues d'absence de spectre singulier continu. En particulier, elle est plus faible que la condition minimale mentionnée auparavant pour formuler un principe d'absorption limite.

Un article intitulé Minimal escape velocities for unitary evolution groups correspondant au chapitre 3 de cette thèse paraîtra dans Annales Henri Poincaré.

Chapitre 1

Dirac operators with variable magnetic field

1.1 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 $\vec{B}(x_1, x_2, x_3) = (0, 0, B(x_1, x_2))$. In the Hilbert space $L^2(\mathbb{R}^3; \mathbb{C}^4)$, the unperturbed system is described 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 $L^2(\mathbb{R}^2; \mathbb{C}^2)$. The matrices σ_j are the Pauli matrices and the symmetrized spectrum σ_{sym}^0 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_{sym}^0 . We refer to [BS], [Da], [GMo], [HNW] and [Th] 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 [Mo1] and extensively developed in [ABG]. 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 arbitrary magnetic fields provided they point in a constant direction. On the other hand, as already put into evidence in [GMa], 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 [MP], 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 1.3.2 for details).

We give now a more precise description of our results. For simplicity we impose some smoothness on 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 [Th]. 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, $\mathbf{M}_h(\mathbb{C}^4)$ stands for the set of 4×4 hermitian matrices and $\|\cdot\|$ denotes the norm of the Hilbert space $\mathcal{H} := L^2(\mathbb{R}^3; \mathbb{C}^4)$ as well as the norm of $\mathcal{B}(\mathcal{H})$, the set of bounded linear operators on \mathcal{H} . $\mathbb{N} := \{0, 1, 2, \dots\}$ is the set of natural numbers. ϑ is an arbitrary $C^\infty([0, \infty))$ -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 1.1.1. *Let V be a multiplication operator in \mathcal{H} associated with an element of $L^\infty(\mathbb{R}^3; \mathbf{M}_h(\mathbb{C}^4))$.*

$$(a) \ V \text{ is small at infinity if } \lim_{r \rightarrow \infty} \left\| \vartheta\left(\frac{\langle Q \rangle}{r}\right) V \right\| = 0,$$

$$(b) \ V \text{ is short-range if } \int_1^\infty \left\| \vartheta\left(\frac{\langle Q_3 \rangle}{r}\right) V \right\| dr < \infty,$$

(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 $L^\infty(\mathbb{R}^3; \mathbb{R})$ for $j = 1, 2, 3$, then $V := V_L I_4$ is long-range if*

$$\int_1^\infty \left\| \vartheta\left(\frac{\langle Q_3 \rangle}{r}\right) \langle Q_3 \rangle (\partial_j V) \right\| \frac{dr}{r} < \infty \quad \text{for } j = 1, 2, 3.$$

Note that Definitions 1.1.1.(b) and 1.1.1.(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 $\mathcal{K} := (\mathcal{D}(\langle Q_3 \rangle), \mathcal{H})_{1/2, 1}$ defined by real interpolation [ABG]. For convenience, we recall that $\mathcal{D}(\langle Q_3 \rangle^s)$ is contained in \mathcal{K} for each $s > 1/2$.

Theorem 1.1.2. *Assume that B belongs to $C(\mathbb{R}^2; \mathbb{R})$ and that $V : \mathbb{R}^3 \rightarrow \mathbf{M}_h(\mathbb{C}^4)$ is bounded, 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 $\mathbb{R} \setminus \sigma_{\text{sym}}^0$ is composed of eigenvalues of finite multiplicity and with no accumulation point in $\mathbb{R} \setminus \sigma_{\text{sym}}^0$.*

- (b) The operator H has no singular continuous spectrum in $\mathbb{R} \setminus \sigma_{\text{sym}}^0$.
- (c) The limits $\lim_{\varepsilon \rightarrow +0} \langle \psi, (H - \lambda \mp i\varepsilon)^{-1} \psi \rangle$ exist for each $\psi \in \mathcal{K}$, uniformly in λ on each compact subset of $\mathbb{R} \setminus \{\sigma_{\text{sym}}^0 \cup \sigma_{\text{pp}}(H)\}$.

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 1.1.1 are more general than those allowed in [Yo]. We stress that in this situation σ_{sym}^0 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 $|B(x_1, x_2)| \rightarrow 0$ as $|(x_1, x_2)| \rightarrow \infty$, our treatment gives no information since both $(-\infty, -m]$ and $[m, \infty)$ belong to σ_{sym}^0 . We finally mention the paper [BC] for a related work on perturbations of magnetic Dirac operators.

1.2 A Mourre estimate for the unperturbed operator

Preliminaries

Let us start by recalling some known results. The operator H_0 is essentially self-adjoint on $\mathcal{D} := C_0^\infty(\mathbb{R}^3; \mathbb{C}^4)$ [Che, Thm. 2.1]. Its spectrum is symmetric with respect to 0 and does not contain the interval $(-m, m)$ [Th, Cor. 5.14]. Thus the operator H_0^{-1} belongs to $\mathcal{B}(\mathcal{H})$, and its range is equal to $\mathcal{D}(H_0)$. Moreover, the subset $H_0\mathcal{D}$ is dense in \mathcal{H} since \mathcal{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

$$\mathcal{F} : \mathcal{D} \rightarrow \int_{\mathbb{R}}^{\oplus} \mathcal{H}_{12} \, d\xi, \quad (\mathcal{F}\psi)(\xi) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-i\xi x_3} \psi(\cdot, x_3) \, dx_3, \quad (1.1)$$

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

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

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 1.1. 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 1.2.1. *The operator $H_0(0)$ acting on $\mathcal{D}_{12} := C_0^\infty(\mathbb{R}^2; \mathbb{C}^4)$ is unitarily equivalent to the 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 $L^2(\mathbb{R}^2; \mathbb{C}^2)$ and are essentially self-adjoint on $C_0^\infty(\mathbb{R}^2; \mathbb{C}^2)$ [Che, 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 [Th, Thm. 5.13]). Therefore $H_0(0)$ is essentially self-adjoint on \mathcal{D}_{12} and

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

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

$$\sigma[H_0(\xi)^2] = \sigma[H_0(0)^2 + \xi^2] = (\sigma[H_0(0)])^2 + \xi^2 = (\sigma_{\text{sym}}^0)^2 + \xi^2, \quad (1.2)$$

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

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

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

$$\sigma(H_0) = (-\infty, -\mu_0] \cup [\mu_0, +\infty). \quad (1.3)$$

The rest of the section is devoted to two technical lemmas in relation with the operator H_0^{-1} .

Lemma 1.2.2. (a) For each $n \in \mathbb{N}$, $H_0^{-n}\mathcal{D}$ belongs to $\mathcal{D}(Q_3)$,

(b) $P_3H_0^{-1}$ 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 $\mathcal{D}(P_3)$.

Proof. (a) Let $\varphi, \psi \in \mathcal{D}$. Using the transformation (1.1), one gets

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

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

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

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

(b) The boundedness of $P_3H_0^{-1}$ is a consequence of the estimate

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

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

One may observe that, given a $C^1(\mathbb{R}; \mathbb{C})$ -function f with f' bounded, the operator $f(Q_3) \equiv f(Q_3)I_4$ is well-defined on $\mathcal{D}(Q_3)$. Thus $f(Q_3)H_0^{-n}\mathcal{D}$ 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 1.2.3. *Let f be in $C^1(\mathbb{R}; \mathbb{C})$ with f' bounded, and $n \in \mathbb{N}$. Then*

$$(a) \quad iH_0^{-1}f(Q_3) - if(Q_3)H_0^{-1} \text{ is equal to } -H_0^{-1}\alpha_3f'(Q_3)H_0^{-1} \text{ on } H_0^{-n}\mathcal{D},$$

$$(b) \quad P_3H_0^{-1}f(Q_3) - f(Q_3)P_3H_0^{-1} \text{ is equal to } i(P_3H_0^{-1}\alpha_3 - 1)f'(Q_3)H_0^{-1} \text{ on } \mathcal{D}.$$

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

Proof. (a) One first observes that the following equality holds on \mathcal{D} :

$$iH_0^{-1}f(Q_3)H_0 = -H_0^{-1}\alpha_3f'(Q_3) + if(Q_3). \quad (1.4)$$

Now, for $\varphi, \psi \in \mathcal{D}$ and $\eta \in H_0^{-n}\mathcal{D}$, one has

$$\begin{aligned} & \langle \varphi, iH_0^{-1}f(Q_3)\eta \rangle - \langle \varphi, if(Q_3)H_0^{-1}\eta \rangle \\ &= \langle \varphi, iH_0^{-1}f(Q_3)H_0\psi \rangle + \langle \varphi, iH_0^{-1}f(Q_3)(\eta - H_0\psi) \rangle - \langle \bar{f}(Q_3)\varphi, iH_0^{-1}\eta \rangle \\ &= -\langle \varphi, H_0^{-1}\alpha_3f'(Q_3)H_0^{-1}\eta \rangle - \langle \varphi, H_0^{-1}\alpha_3f'(Q_3)H_0^{-1}(H_0\psi - \eta) \rangle \\ & \quad + \langle \bar{f}(Q_3)\varphi, iH_0^{-1}(H_0\psi - \eta) \rangle + \langle \bar{f}(Q_3)H_0^{-1}\varphi, i(\eta - H_0\psi) \rangle, \end{aligned}$$

where we have used (1.4) 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

$$|\langle \varphi, iH_0^{-1}f(Q_3)\eta \rangle - \langle \varphi, if(Q_3)H_0^{-1}\eta \rangle + \langle \varphi, H_0^{-1}\alpha_3f'(Q_3)H_0^{-1}\eta \rangle| \leq C\|\eta - H_0\psi\|.$$

Then the statement is a direct consequence of the density of $H_0\mathcal{D}$ and \mathcal{D} in \mathcal{H} .

(b) This is a corollary of the previous result. \square

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 $Q_3P_3H_0^{-1}\mathcal{D} \subset \mathcal{H}$ as a consequence of Lemma 1.2.2. In particular, the formal expression

$$A := \frac{1}{2}(H_0^{-1}P_3Q_3 + Q_3P_3H_0^{-1}) \quad (1.5)$$

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

Proposition 1.2.4. *The operator A is essentially self-adjoint on \mathcal{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 [RS, Thm. X.37] applied to the triple $\{\langle Q_3 \rangle, A, \mathcal{D}\}$. By using Lemmas 1.2.2 and 1.2.3, one first obtains that for all $\psi \in \mathcal{D}$:

$$\|A\psi\| = \|(P_3 H_0^{-1} Q_3 - \frac{1}{2} [P_3 H_0^{-1}, Q_3]) \psi\| \leq c \|\langle Q_3 \rangle \psi\|$$

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

$$\begin{aligned} \langle A\psi, \langle Q_3 \rangle \psi \rangle - \langle \langle Q_3 \rangle \psi, A\psi \rangle &= i \operatorname{Im} \langle Q_3 \psi, [P_3 H_0^{-1}, \langle Q_3 \rangle] \psi \rangle \\ &= i \operatorname{Re} \langle (\alpha_3 P_3 H_0^{-1} - 1) Q_3 \psi, Q_3 \langle Q_3 \rangle^{-1} H_0^{-1} \psi \rangle. \end{aligned}$$

A few more commutator calculations, using again Lemma 1.2.3 with $f(Q_3) = \langle Q_3 \rangle^{1/2}$, lead to the following result: for all $\psi \in \mathcal{D}$, there exists a constant $D > 0$ independent of ψ such that

$$|\langle A\psi, \langle Q_3 \rangle \psi \rangle - \langle \langle Q_3 \rangle \psi, A\psi \rangle| \leq D \|\langle Q_3 \rangle^{\frac{1}{2}} \psi\|^2. \quad \square$$

As far as we know, the matrix conjugate operator (1.5) has never been employed before for the study of magnetic Dirac operators.

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 1.2.5. (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 $-H_0^{-1}(P_3 H_0^{-1})^2 H_0^{-1} \in \mathcal{B}(\mathcal{H})$,

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

(c) *The quadratic form*

$$\mathcal{D}(A) \ni \psi \mapsto \langle H_0^{-1}(P_3 H_0^{-1})^2 H_0^{-1} \psi, iA\psi \rangle - \langle A\psi, iH_0^{-1}(P_3 H_0^{-1})^2 H_0^{-1} \psi \rangle, \quad (1.6)$$

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

In the framework of [ABG], 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 $\psi \in \mathcal{D}$, one gets

$$\begin{aligned} &2 (\langle H_0^{-1} \psi, iA\psi \rangle - \langle A\psi, iH_0^{-1} \psi \rangle) \\ &= \langle [iH_0^{-1}, Q_3] \psi, P_3 H_0^{-1} \psi \rangle + \langle P_3 H_0^{-1} \psi, [iH_0^{-1}, Q_3] \psi \rangle \end{aligned} \quad (1.7)$$

$$= -\langle H_0^{-1} \psi, (\alpha_3 P_3 H_0^{-1} + H_0^{-1} \alpha_3 P_3) H_0^{-1} \psi \rangle, \quad (1.8)$$

where we have used Lemmas 1.2.2 and 1.2.3 . Furthermore, one has

$$H_0^{-1}\alpha_3 = -\alpha_3 H_0^{-1} + 2H_0^{-1}P_3H_0^{-1} \quad (1.9)$$

as an operator identity in $\mathcal{B}(\mathcal{H})$. When inserting (1.9) into (1.7), one obtains the equality

$$\langle H_0^{-1}\psi, iA\psi \rangle - \langle A\psi, iH_0^{-1}\psi \rangle = -\langle \psi, H_0^{-1}(P_3H_0^{-1})^2H_0^{-1}\psi \rangle. \quad (1.10)$$

Since \mathcal{D} is a core for A , the statement is obtained by density. We shall write $[iH_0^{-1}, A]$ for the extension.

(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 $\mathcal{B}(\mathcal{D}(H_0), \mathcal{D}(H_0)^*)$ 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 $[iH_0, A]\mathcal{D}(H_0) \subset \mathcal{H}$ [GG, Lemma 2]. From equation (1.10) and [ABG, Eq. 6.2.24], one obtains the following equalities valid in form sense on \mathcal{H} :

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

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

(c) The boundedness on \mathcal{D} of the quadratic form (1.6) follows by inserting (1.5) into the r.h.s. term of (1.6) and by applying repeatedly Lemma 1.2.3 with $f(Q_3) = Q_3$. Then one concludes by using the density of \mathcal{D} in $\mathcal{D}(A)$. \square

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

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

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 [ABG, Sec. 7.2.1].

Definition 1.2.6. *Let H be a self-adjoint operator in a Hilbert space \mathcal{H} and assume that S is a symmetric operator in $\mathcal{B}(\mathcal{D}(H), \mathcal{D}(H)^*)$. Let $E^H(\lambda; \varepsilon) := E^H((\lambda - \varepsilon, \lambda + \varepsilon))$ 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*

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

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 [ABG, 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 $\varepsilon > 0$:

$$\varrho_{H_0}^T(\lambda; \varepsilon) = \operatorname{ess\,inf}_{\xi \in \mathbb{R}} \varrho_{H_0(\xi)}^{T(\xi)}(\lambda; \varepsilon). \quad (1.11)$$

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

Proposition 1.2.7. *One has*

$$\varrho_{H_0}^T(\lambda) \geq \inf \left\{ \frac{\lambda^2 - \mu^2}{\lambda^2} : \mu \in \sigma_{\text{sym}}^0 \cap [0, |\lambda|] \right\} \quad (1.12)$$

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

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

(i) Recall from (1.3) that $\mu_0 \equiv \inf |\sigma_{\text{sym}}^0| = \inf \{\sigma(H_0) \cap [0, +\infty)\}$. Thus, for $\lambda \in [0, \mu_0)$ the l.h.s. term of (1.12) is equal to $+\infty$, since λ does not belong to the spectrum of H_0 . Hence (1.12) is satisfied on $[0, \mu_0)$.

(ii) If $\lambda \in \sigma_{\text{sym}}^0$, then the r.h.s. term of (1.12) is equal to 0. However, since T is positive, $\varrho_{H_0}^T(\lambda) \geq 0$. Hence the relation (1.12) 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 $\rho \in \mathbb{R}$ and ξ fixed, one has

$$\varrho_{H_0(\xi)}^{T(\xi)}(\lambda; \varepsilon) = \inf \left\{ \frac{\xi^2}{\rho^2} : \rho \in (\lambda - \varepsilon, \lambda + \varepsilon) \cap \sigma[H_0(\xi)] \right\} \geq \frac{\xi^2}{(\lambda + \varepsilon)^2}. \quad (1.13)$$

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

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

Thus, by taking into account equation (1.11), (1.13), the previous observation and relation (1.2), one obtains that

$$\varrho_{H_0}^T(\lambda; \varepsilon) \geq \operatorname{ess\,inf} \left\{ \frac{\xi^2}{(\lambda + \varepsilon)^2} : \xi^2 \in ((\lambda - \varepsilon)^2, (\lambda + \varepsilon)^2) - (\sigma_{\text{sym}}^0)^2 \right\}. \quad (1.14)$$

Suppose now that $\lambda \notin \sigma_{\text{sym}}^0$, define $\mu := \sup \{\sigma_{\text{sym}}^0 \cap [0, \lambda]\}$ and choose $\varepsilon > 0$ such that $\mu < \lambda - \varepsilon$. Then the inequality (1.14) implies that

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

Hence the relation (1.12) follows from the above formula when $\varepsilon \rightarrow 0$.

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

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

The claim is then a direct consequence of the symmetry of σ_{sym}^0 with respect to 0. \square

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

1.3 On the perturbed Hamiltonian

In the sequel, we consider the self-adjoint operator $H := H_0 + V$ with a potential V that belongs to $L^\infty(\mathbb{R}^3; \mathbf{M}_h(\mathbb{C}^4))$. 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 1.3.1. *Assume that V is small at infinity. Then for all $z \in \mathbb{C} \setminus (\sigma(H) \cup \sigma(H_0))$ the difference $(H - z)^{-1} - (H_0 - z)^{-1}$ is a compact operator. It follows in particular that $\sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(H_0)$.*

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

Remark 1.3.2. *In the study of an analogous problem for Schrödinger operators [MP], the authors prove a result similar to Proposition 1.3.1 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 $H_{\text{Sch}} := \Pi_1^2 + \Pi_2^2 + P_3^2 \geq \pm B$. In the Dirac case, the counterpart of these turn out to be*

$$H_0^2 \geq 2B \cdot \text{diag}(0, 1, 0, 1) \quad \text{and} \quad H_0^2 \geq -2B \cdot \text{diag}(1, 0, 1, 0),$$

where $\text{diag}(\dots)$ stands for a diagonal matrix. If we assume that the magnetic field is bounded from below, the first inequality enables us to treat perturbations of the type $\text{diag}(V_1, V_2, V_3, V_4)$ 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. For the definitions of $\mathcal{C}^{1,1}(A)$ and $\mathcal{C}^{1,1}(A; \mathcal{D}(H_0), \mathcal{D}(H_0)^*)$, and for more explanations on regularity conditions, we refer to [ABG, Chap. 5].

Proposition 1.3.3. *Let V be a short-range or a long-range potential. Then H is of class $\mathcal{C}^{1,1}(A)$.*

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 $\mathcal{C}^{1,1}(A; \mathcal{D}(H_0), \mathcal{D}(H_0)^*)$ [ABG, Thm. 6.3.4.(b)]. But in Proposition 1.2.5.(c), it has already been shown that H_0 is of class $C^2(A)$, so that H_0 is of class $\mathcal{C}^{1,1}(A; \mathcal{D}(H_0), \mathcal{D}(H_0)^*)$. Thus it is enough to prove that V belongs to $\mathcal{C}^{1,1}(A; \mathcal{D}(H_0), \mathcal{D}(H_0)^*)$. In the short-range case, we shall use [ABG, Thm. 7.5.8], which implies that V belongs to $\mathcal{C}^{1,1}(A; \mathcal{D}(H_0), \mathcal{D}(H_0)^*)$. The conditions needed for that theorem are obtained in points (i) and (ii) below. In the long-range case, the claim follows by [ABG, 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 1.2.3.(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 1.2.5, 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 \mathcal{D} , extends continuously to the operator $t\alpha_3 Q_3 \langle Q_3 \rangle^{-1} e^{it\langle Q_3 \rangle} \in \mathcal{B}(\mathcal{H})$, one gets that $\|e^{it\langle Q_3 \rangle}\|_{\mathcal{B}(\mathcal{D}(H_0))} \leq \text{Const.} \cdot |t|$ 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 $\mathcal{D}(H_0)^*$. 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 obtained by restriction to $\mathcal{D}(H_0)$ and then the C_0 -group in $\mathcal{D}(H_0)^*$ obtained by duality. The generator of each of these C_0 -groups will be denoted by A . Let $\mathcal{D}(A; \mathcal{D}(H_0)) := \{\varphi \in \mathcal{D}(H_0) \cap \mathcal{D}(A) : A\varphi \in \mathcal{D}(H_0)\}$ be the domain of A in $\mathcal{D}(H_0)$, and let $\mathcal{D}(A^2; \mathcal{D}(H_0)) := \{\varphi \in \mathcal{D}(H_0) \cap \mathcal{D}(A^2) : A\varphi, A^2\varphi \in \mathcal{D}(H_0)\}$ 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 $\mathcal{D}(A; \mathcal{D}(H_0))$ and on $\mathcal{D}(A^2; \mathcal{D}(H_0))$ respectively, extend to operators in $\mathcal{B}(\mathcal{D}(H_0))$. After some commutator calculations performed on \mathcal{D} and involving Lemma 1.2.3, one first obtains that $\langle Q_3 \rangle^{-1}A$ and $\langle Q_3 \rangle^{-2}A^2$ are respectively equal on \mathcal{D} to some operators S_1 and $S_2 \langle Q_3 \rangle^{-1}$ in $\mathcal{B}(\mathcal{H})$, where S_1 and S_2 are polynomials in H_0^{-1} , $P_3 H_0^{-1}$, α_3 and $f(Q_3)$ for bounded functions f with bounded derivatives. Since \mathcal{D} is a core for A , these equalities even hold on $\mathcal{D}(A)$. Hence one has on $\mathcal{D}(A^2)$:

$$\langle Q_3 \rangle^{-2}A^2 = (\langle Q_3 \rangle^{-2}A)A = S_2 \langle Q_3 \rangle^{-1}A = S_2 S_1.$$

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} , $P_3 H_0^{-1}$, 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 $\mathcal{B}(\mathcal{D}(H_0))$. Thus, it follows that $\langle Q_3 \rangle^{-1}A$ and $\langle Q_3 \rangle^{-2}A^2$ are equal on $\mathcal{D}(A; \mathcal{D}(H_0))$ and on $\mathcal{D}(A^2; \mathcal{D}(H_0))$ respectively to some operators belonging to $\mathcal{B}(\mathcal{D}(H_0))$.

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

$$\langle (\langle Q_3 \rangle^{-1}A)^* \psi, \varphi \rangle = \langle \psi, \langle Q_3 \rangle^{-1}A\varphi \rangle = \langle \langle Q_3 \rangle^{-1}\psi, A\varphi \rangle, \quad (1.15)$$

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 (1.15) 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 $r \|(\langle Q_3 \rangle + ir)^{-1}\|_{\mathcal{B}(\mathcal{D}(H_0)^*)} \leq \text{Const.}$ for all $r > 0$ is obtained from relation (1.4) 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 \mathcal{D} :

$$2[iV, A] = -Q_3(\partial_3 V)H_0^{-1} - H_0^{-1}Q_3(\partial_3 V) + [iV, H_0^{-1}]Q_3P_3 + P_3Q_3[iV, H_0^{-1}], \quad (1.16)$$

with $[iV, H_0^{-1}] = \sum_{j=1}^3 H_0^{-1}\alpha_j(\partial_j V)H_0^{-1}$. Using Lemma 1.2.3.(a), one gets that the last two terms in (1.16) are equal in form sense on \mathcal{D} to

$$2\text{Re} \sum_{j=1}^3 H_0^{-1}\alpha_j Q_3(\partial_j V)P_3H_0^{-1} - 2\text{Im} \sum_{j=1}^3 H_0^{-1}\alpha_j(\partial_j V)H_0^{-1}\alpha_3 P_3H_0^{-1}.$$

It follows that $[iV, A]$, defined in form sense on \mathcal{D} , extends continuously to an operator in $\mathcal{B}(\mathcal{H})$. Now let ϑ be as in Definition 1.1.1. Then a direct calculation using the explicit form of $[iV, A]$ obtained above implies that

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

for all $r > 0$ and some positive constants c and D . \square

As a direct consequence, one obtains that

Lemma 1.3.4. *If V satisfies the hypotheses of Theorem 1.1.2, then A is conjugate to H on $\mathbb{R} \setminus \sigma_{\text{sym}}^0$.*

Proof. Proposition 1.3.3 implies that both H_0 and H are of class $\mathcal{C}^{1,1}(A)$. Furthermore, the difference $(H + i)^{-1} - (H_0 + i)^{-1}$ is compact by Proposition 1.3.1, and $\varrho_{H_0}^T > 0$ on $\mathbb{R} \setminus \sigma_{\text{sym}}^0$ due to Proposition 1.2.7. Hence the claim follows by [ABG, Thm. 7.2.9 & Prop. 7.2.6]. \square

We can finally give the proof of Theorem 1.1.2.

Proof of Theorem 1.1.2. Since A is conjugate to H on $\mathbb{R} \setminus \sigma_{\text{sym}}^0$ by Lemma 1.3.4, the assertions (a) and (b) follow by the abstract conjugate operator method [ABG, Cor. 7.2.11 & Thm. 7.4.2].

The limiting absorption principle directly obtained via [ABG, 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 [ABG, 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 1.2.4, 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. Now, since $\mathcal{D}(H) = \mathcal{D}(H_0)$ is left invariant by the group $\{e^{it(Q_3)}\}_{t \in \mathbb{R}}$ (see Proposition 1.3.3 (i)) one easily gets from [ABG, Thm. 6.3.4.(a)] that H is of class $C^1(\langle Q_3 \rangle)$, which implies the required invariance of $\mathcal{D}(\langle Q_3 \rangle)$ [ABG, Thm. 6.2.10.(b)]. \square

Chapitre 2

Schrödinger operators with Cartesian anisotropy

2.1 Introduction

In this paper we shall be interested in the spectral and scattering theory of some anisotropic Schrödinger operators $H = -\Delta + V$ in the Hilbert space $L^2(\mathbb{R}^n)$. A general theory for highly anisotropic potentials is still lacking, but various partial approaches are already well developed. The most famous one, and best achieved, is with no doubt the N-body problem (see [PSS], [FH1], [SS1] and [DG]). Let us also mention [GI2] and [Ma1] for the spectral analysis of general anisotropic systems, [DS] for the scattering theory for systems with different spatial asymptotics on the left and right, and [HS] and references therein for a thorough analysis of Schrödinger operators with potentials independent of $|x|$. Here another type of anisotropy is considered. It is called *cartesian* since the potentials V admit limits at infinity separately for each variable. For the corresponding operators, the spectral and scattering theory can be completely achieved. Moreover, since our approach to the propagation properties of states is close to intuition, we expect that it could stimulate the development of a general theory.

Let us illustrate our framework with a simple example. We consider the operator $H = -\Delta + V$ in $L^2(\mathbb{R}^2)$, with $V(x_1, x_2) = V_1(x_1)V_2(x_2)$, and for $j \in \{1, 2\}$, V_j is a continuous real function defined on \mathbb{R} which has limits c_j^\pm at $\pm\infty$ and converges to these limits in a short-range way. We call asymptotic Hamiltonians the operators $H_{j\pm} = -\Delta + c_k^\pm V_j$, with $j, k \in \{1, 2\}$ but $j \neq k$, and internal Hamiltonians the operators $H^{j\pm} = -\Delta_j + c_k^\pm V_j$ acting in $L^2(\mathbb{R})$. Then the essential spectrum of H is the union of the spectra of the four asymptotic Hamiltonians. The eigenvalues of the internal Hamiltonians and the numbers $c_1^+ c_2^+, c_1^+ c_2^-, c_1^- c_2^+, c_1^- c_2^-$ compose the set of thresholds. If the critical set $\kappa(H)$ is defined as the set of these thresholds and of the eigenvalues of H , we prove a Mourre estimate and deduce a limiting absorption principle on $\mathbb{R} \setminus \kappa(H)$, and thus get the absence of singularly continuous spectrum. For the scattering, let us make some heuristic discussion and get some physical intuition. Consider a state in the absolutely continuous subspace of $L^2(\mathbb{R}^2)$

with respect to H propagating into the positive quadrant of \mathbb{R}^2 . We can expect that its asymptotic evolution is governed by the operator $-\Delta + c_1^+ c_2^+$, and thus this state will be asymptotically free. But there might also exist some infinite valley parallel to one of the axis which could trap some scattering states. And such states would then behave asymptotically like guided waves.

This variety of possible outcomes for the asymptotic evolution is one of the reasons for the complexity of the analysis of anisotropic systems. In order to predict the asymptotic behaviour of a given scattering state, one has to know roughly its asymptotic localization. It seems to us that the right concept for obtaining this information is the *asymptotic velocity*. In the previous example, the asymptotic velocity of the asymptotically free state points out in the positive quadrant, while for the asymptotically guided state, the asymptotic velocity has a zero component. Such characteristics will be used for classifying the scattering states.

Let us briefly describe our mathematical tools. For the spectral analysis, we mainly use the method of the conjugate operator in the algebraic framework developed by W.O. Amrein, A. Boutet de Monvel and V. Georgescu [ABG]. In this approach, the main object of the theory is a C^* -subalgebra \mathfrak{C} of the set of bounded linear operators in some Hilbert space \mathcal{H} . This C^* -algebra is closely related to the anisotropy. The operators H under consideration are then self-adjoint operators in \mathcal{H} affiliated to \mathfrak{C} , *i.e.* the resolvent $(H - z)^{-1}$ belongs to \mathfrak{C} for any complex number z with non-zero imaginary part. We also rely upon the recent idea that a class of functions defined on \mathbb{R}^n having a certain type of anisotropy is associated with a compactification of \mathbb{R}^n , the one on which all these functions admit a continuous extension. We refer to [AMP], [GI2] and to [Ma1], [Ma2] of M. Măntoiu for motivations, for some general principles and in particular for the use of crossed products in relation with spectral analysis. For the scattering theory, the strategy of J. Dereziński and C. Gérard exposed in [DG], Sections 6.6 and 6.7, is followed. Various propagation estimates are proved with the help of some propagation observables and with a partition of unity inspired by the paper of G.M. Graf [Gr]. The notions of minimal and maximal velocities are introduced and the asymptotic velocity is used for the definition of the wave operators and the proof of asymptotic completeness.

In the sequel we shall consider potentials V such that $\lim_{x_j \rightarrow \pm\infty} V(\cdot)$ exist for each $j \in \{1, \dots, n\}$ in a suitable sense, and call them *cartesian potentials*. This leads to a natural n -dimensional generalization of certain situations considered in [DS] and [GI1]. The underlying compactification of \mathbb{R}^n is the cartesian product of n copies of the two-point compactification $\overline{\mathbb{R}} := \{-\infty\} \sqcup \mathbb{R} \sqcup \{+\infty\}$ of \mathbb{R} . Hence let us define $\overline{\mathbb{R}}^n := \overline{\mathbb{R}}_1 \times \dots \times \overline{\mathbb{R}}_n$ (the indexation corresponds to that of the variables) endowed with the product topology, and let $C(\overline{\mathbb{R}}^n)$ denote the algebra of continuous complex functions on $\overline{\mathbb{R}}^n$. This algebra is naturally identified with a subalgebra of $BC_u(\mathbb{R}^n)$, the bounded uniformly continuous complex functions on \mathbb{R}^n . The precise definition of cartesian potentials is given in Definition 2.4.3. However, let us already mention that any real element of $C(\overline{\mathbb{R}}^n)$ is a smooth cartesian potential.

We introduce some notations which are needed for the statement of our results. Let \mathcal{L} be the set of all multi-indexes $\alpha = \{\alpha_j\}_{j=1}^n$ with α_j taking values in $\{-1, 0, 1\}$.

There exists a one-to-one relation between \mathcal{L} and all generalized hypersurfaces of an n -dimensional hypercube. Indeed, the hypersurface $\overline{\mathbb{R}}^\alpha := \overline{\mathbb{R}}_1^{\alpha_1} \times \cdots \times \overline{\mathbb{R}}_n^{\alpha_n}$ (with the convention that $\overline{\mathbb{R}}_j^0 = \overline{\mathbb{R}}_j$ and $\overline{\mathbb{R}}_j^{\pm 1} = \{\pm\infty_j\}$) is a generalized face of $\overline{\mathbb{R}}^n$. Endowed with the induced topology, its interior is clearly isomorphic to $\mathbb{R}^\alpha := \prod_{\{j|\alpha_j=0\}} \mathbb{R}_j$ or to $\{0\}$. We symbolize by $|\alpha|$ the dimension of the vector space \mathbb{R}^α . For $|\alpha| \neq 0$, let \mathcal{H}_α denote the Hilbert space $L^2(\mathbb{R}^\alpha)$ and let \mathcal{H}_α^2 be the usual Sobolev space of order two on \mathbb{R}^α . This space is the domain of the Laplace operator $\Delta^\alpha := \sum_{\{j|\alpha_j=0\}} \Delta_j$. If $\alpha = o := (0, \dots, 0)$ the familiar notations are kept: $\mathbb{R}^o = \mathbb{R}^n$, $\mathcal{H}_o = \mathcal{H}$, $\mathcal{H}_o^2 = \mathcal{H}^2$ and $\Delta^o = \Delta$. In the special cases $|\alpha| = 0$, meaning that $\overline{\mathbb{R}}^\alpha$ is a corner of the hypercube, we take by convention $\mathcal{H}_\alpha = \mathcal{H}_\alpha^2 = \mathbb{C}$.

For any function $V \in C(\overline{\mathbb{R}}^n)$, its restriction V^α to the hypersurface $\overline{\mathbb{R}}^\alpha$ is identified with an element of $BC_u(\mathbb{R}^\alpha)$. One notices that the expression $V^\alpha(x)$ with $x \in \mathbb{R}^n$ has an unambiguous meaning. Indeed, the algebra $BC_u(\mathbb{R}^\alpha)$ is canonically identified with a subalgebra of $BC_u(\mathbb{R}^n)$, its elements depending only on the variables x_j for which $\alpha_j = 0$. More generally, for any cartesian potential V the restriction V^α of V to the hypersurface $\overline{\mathbb{R}}^\alpha$ also exists in a generalized sense (*cf.* Definition 2.4.3). Thus we may set $H_\alpha := -\Delta + V^\alpha$ and $H^\alpha := -\Delta^\alpha + V^\alpha$, the former being a self-adjoint operator in \mathcal{H} with domain \mathcal{H}^2 and the latter a self-adjoint operator in \mathcal{H}_α with domain \mathcal{H}_α^2 . Let $\sigma_p(\cdot)$ denote the point spectrum of any self-adjoint operator. With the *cartesian Hamiltonian* $H \equiv H^o = -\Delta + V$, one associates two special sets: the set of thresholds $\tau(H) = \cup_{\alpha \neq o} \sigma_p(H^\alpha)$, and $\kappa(H) = \cup_{\alpha \in \mathcal{L}} \sigma_p(H^\alpha)$, the critical set of H .

In order to give a precise description of the spectrum $\sigma(H)$ of H , some regularity of the potential with respect to the generator A of dilations has to be imposed. We refer to Section 2.2 for the description of this regularity (including the definition of the class $C^{1,1}(A)$) and to Section 2.5 for its compatibility with the cartesian anisotropy. If \mathcal{G} is a Banach space, its norm is written $\|\cdot\|_{\mathcal{G}}$. The weighted Sobolev space \mathcal{H}_t^s is the closure of the Schwartz space on \mathbb{R}^n with respect to the norm $\|\cdot\|_{\mathcal{H}_t^s} = \|(1+P^2)^{s/2}(1+Q^2)^{t/2}\cdot\|$, where $P_j := -i\nabla_j$, $j \in \{1, \dots, n\}$, are the components of the momentum operator and Q_j is the operator of multiplication by the variable x_j . If $t = 0$, we simply omit this index.

Theorem 2.1.1. *Let $H = -\Delta + V$ with V a cartesian potential. Then*

$$i) \quad \sigma_{\text{ess}}(H) = [\min_{|\alpha|=n-1} \inf \sigma(H^\alpha), \infty).$$

Furthermore, if V is of class $C^{1,1}(A)$, with A the generator of dilations, then

ii) $\tau(H)$ and $\kappa(H)$ are closed countable sets, the eigenvalues of H not belonging to $\tau(H)$ are of finite multiplicity and can accumulate only at points of $\tau(H)$,

iii) H has no singularly continuous spectrum,

iv) for each $\delta > 0$, there exists $c < \infty$ such that $|\langle \varphi, (H - \lambda \pm i\mu)^{-1} \varphi \rangle| \leq c \|\varphi\|_{\mathcal{H}_{1/2+\delta}^{-1}}^2$ for all $\varphi \in \mathcal{H}_{1/2+\delta}^{-1}$ and uniformly in λ on each compact subset of $\mathbb{R} \setminus \kappa(H)$ and in $\mu > 0$.

We mention that there exists a slightly stronger version of the limiting absorption principle in terms of Besov spaces [ABG]. For reasons of simplicity we do not take this improvement into account.

Let us recall that the asymptotic velocity \mathcal{P} for a system described by H is obtained as the limit $\lim_{t \rightarrow +\infty} e^{iHt} \frac{Q}{2t} e^{-iHt}$ in a suitable sense. Since the limit $t \rightarrow -\infty$ is completely similar, we do not consider it. We denote by \mathcal{P}_α the asymptotic velocity obtained for H_α . The following partition of \mathbb{R}^n is useful for the description of the different possible outcomes of the asymptotic evolution. For each $\alpha \in \mathcal{L}$, we define

$$Z_\alpha := \{x \in \mathbb{R}^n \mid x_j = 0 \text{ if } \alpha_j = 0 \text{ and } \alpha_j x_j > 0 \text{ if } \alpha_j \neq 0\}.$$

We shall prove that for $\alpha \neq o$, the elements of \mathcal{H} with support of their asymptotic velocity on Z_α have an asymptotic evolution governed by the Hamiltonian H_α . For this purpose, we roughly impose that the potential V approaches its limits at infinity in a short-range way. A more precise condition is given in Section 2.7, equation (2.22).

If C is an m -tuple of commuting self-adjoint operators (m a positive integer), we denote by $E_\Xi(C)$ its spectral projection corresponding to the subset $\Xi \subset \mathbb{R}^m$. We also use the notation $E_p(B)$ for the orthogonal projection on the subspace spanned by the eigenvectors of a self-adjoint operator B .

Theorem 2.1.2. *Let V be a cartesian potential of class $C^{1,1}(A)$ satisfying (2.22), with A the generator of dilations. Then for each $\alpha \in \mathcal{L}$,*

- i) *the operator $\Omega_\alpha^+ := s\text{-}\lim_{t \rightarrow +\infty} e^{iHt} e^{-iH_\alpha t} E_{Z_\alpha}(\mathcal{P}_\alpha)$ exists, and its range $\text{Ran } \Omega_\alpha^+$ is equal to $E_{Z_\alpha}(\mathcal{P})\mathcal{H}$,*
- ii) *if $\beta \neq \alpha$, then $\text{Ran } \Omega_\beta^+$ is orthogonal to $\text{Ran } \Omega_\alpha^+$; furthermore the direct sum $\bigoplus_{\beta \neq o} \text{Ran } \Omega_\beta^+$ spans the absolutely continuous subspace of \mathcal{H} with respect to H ,*
- iii) *if \mathcal{H} is identified with $\left(\bigotimes_{\{j|\alpha_j \neq 0\}} L^2(\mathbb{R}_j) \right) \otimes \mathcal{H}_\alpha$, the spectral projection $E_{Z_\alpha}(\mathcal{P}_\alpha)$ is equal to $\left(\bigotimes_{\{j|\alpha_j \neq 0\}} E_{\{y \in \mathbb{R}|\alpha_j y > 0\}}(P_j) \right) \otimes E_p(H^\alpha)$.*

Let us notice that the projections $E_{Z_\alpha}(\mathcal{P})$ correspond to the projections $P^+(E)$ conjectured in the Introduction of [DS]. In relation with this result, we mention the recent work of Y. Dermenjian and V. Ifimie in the case of perturbed stratified media [DI]. Their results are comparable but the anisotropy they consider is less general than ours since it is a short-range perturbation of a L^∞ -function which depends only on the variable x_n and admits limits as $x_n \rightarrow \pm\infty$.

In Section 2.2 we describe the algebraic framework and some generalities on the regularity of H with respect to the conjugate operator. The algebra related to the cartesian anisotropy is introduced in Section 2.3, where its rich internal structure is investigated. It already gives some informations on the essential spectrum. In order to deal with non-smooth potentials, some technicalities are needed. Section 2.4 is devoted to this purpose. Definition 2.4.3 contains the description of a generalized class of cartesian potentials, which includes $C(\overline{\mathbb{R}^n})$. The affiliation of the corresponding

cartesian Hamiltonians to the mentioned algebra is proved. The Mourre estimate and the limiting absorption principle are elaborated in Section 2.5, where the proof of Theorem 2.1.1 is given. The last two sections are dedicated to the scattering theory. Section 2.6 deals with the asymptotic velocity \mathcal{P} and some of its properties. In Section 2.7, we use it to construct the wave operators and to prove Theorem 2.1.2.

We end the Introduction with two observations. The first one concerns the relationship between cartesian and N-body Hamiltonians. Although our approach for the spectral and scattering theory of the former is similar to that developed for the latter, potentials which are both cartesian and of N-body type are very special cases of cartesian potentials and of N-body potentials. Indeed, in the formalism of generalized N-body systems (see Section 5.1 of [DG]) such potentials correspond to a system related to a finite semilattice of subspaces of \mathbb{R}^n which satisfy some orthogonality relations; on the other hand, as cartesian potentials, they must converge to zero (in a suitable sense) except in the vicinity of some subspaces of \mathbb{R}^n of lower dimensions. The second observation is that the difficulties due to the anisotropy already appear in two dimensions, a situation which is easily visualized. Therefore this model is, undoubtedly, of pedagogical interest. For convenience, we have included some relevant examples of cartesian potentials in Sections 2.4, 2.5 and 2.7.

2.2 The algebraic framework

Let us consider a self-adjoint operator H in a Hilbert space \mathcal{H} . The spectrum and the essential spectrum of H can be expressed in terms of its continuous functional calculus:¹

$$\begin{aligned}\sigma(H) &= \{\lambda \in \mathbb{R} \mid \text{if } \eta \in C_0(\mathbb{R}) \text{ and } \eta(\lambda) \neq 0, \text{ then } \eta(H) \neq 0\}, \\ \sigma_{\text{ess}}(H) &= \{\lambda \in \mathbb{R} \mid \text{if } \eta \in C_0(\mathbb{R}) \text{ and } \eta(\lambda) \neq 0, \text{ then } \eta(H) \notin \mathcal{K}(\mathcal{H})\}.\end{aligned}$$

If \mathfrak{C} is a C^* -subalgebra of $\mathcal{B}(\mathcal{H})$, then H is said to be *affiliated to* \mathfrak{C} if $\eta(H) \in \mathfrak{C}$ for all $\eta \in C_0(\mathbb{R})$. A sufficient condition is that $(H - z)^{-1} \in \mathfrak{C}$ for some $z \in \mathbb{C} \setminus \sigma(H)$.

The above situation is a special case of the following more abstract framework:

Definition 2.2.1. *i) A self-adjoint observable affiliated to a C^* -algebra \mathfrak{C} is a functional calculus taking value in \mathfrak{C} , i.e. a $*$ -morphism $H : C_0(\mathbb{R}) \rightarrow \mathfrak{C}$. The notation $\eta(H)$ will be used instead of $H(\eta)$.*

ii) The spectrum $\sigma(H)$ of the observable H is the set of real values λ such that, whenever $\eta \in C_0(\mathbb{R})$ and $\eta(\lambda) \neq 0$, then $\eta(H) \neq 0$.

iii) If $\pi : \mathfrak{C} \rightarrow \mathfrak{C}'$ is a $$ -morphism between two C^* -algebras and H is a self-adjoint observable affiliated to \mathfrak{C} , then $\pi(H) : C_0(\mathbb{R}) \rightarrow \mathfrak{C}'$, given by $\eta(\pi(H)) :=$*

¹If m and k are positive integers, we denote by $C_0(\mathbb{R}^m)$ the set of all continuous complex functions on \mathbb{R}^m converging to zero at infinity, and by $C_c^k(\mathbb{R}^m)$ the subset of $C_0(\mathbb{R}^m)$ of k times continuously differentiable functions of compact support. For any Hilbert spaces \mathcal{H} and \mathcal{G} , $\mathcal{B}(\mathcal{H}, \mathcal{G})$ denotes the Banach space of bounded linear operators from \mathcal{H} to \mathcal{G} , $\mathcal{B}(\mathcal{H}) := \mathcal{B}(\mathcal{H}, \mathcal{H})$ and $\mathcal{K}(\mathcal{H})$ is the ideal of compact operators in \mathcal{H} .

$\pi(\eta(H))$, is a self-adjoint observable affiliated to \mathfrak{C}' . We call it the image of H through π .

In the sequel we shall simply write morphism for $*$ -morphism between two C^* -algebras.

We recall some definitions related to the Mourre estimate and refer to [ABG] for details and a self-contained presentation. Let $\{W_t\}_{t \in \mathbb{R}}$ be the unitary group in \mathcal{H} generated by a self-adjoint operator A . For any $B \in \mathcal{B}(\mathcal{H})$, we write $B \in C^1(A)$ if the mapping $\mathbb{R} \ni t \mapsto W_{-t} B W_t \in \mathcal{B}(\mathcal{H})$ is strongly C^1 . If this mapping is C^1 in norm we write $B \in C_u^1(A)$. By assuming that $B \in C^1(A)$, we give a rigorous sense to the commutator $[B, iA] \in \mathcal{B}(\mathcal{H})$.

A self-adjoint operator H in \mathcal{H} is of class $C^1(A)$ (resp. $C_u^1(A)$) if $(H - z)^{-1} \in C^1(A)$ (resp. $(H - z)^{-1} \in C_u^1(A)$) for some, and then for all, $z \in \mathbb{C} \setminus \sigma(H)$. Let \mathcal{G} be the domain of H endowed with the graph norm and assume that it is left invariant by the group $\{W_t\}_{t \in \mathbb{R}}$. We denote by \mathcal{G}^* its dual space and by $\{W_t^*\}_{t \in \mathbb{R}}$ the standard C_0 -group obtained by duality from the action of the group restricted to \mathcal{G} . Then H is of class $C^1(A)$ if and only if the mapping $\mathbb{R} \ni t \mapsto W_t^* H W_t \in \mathcal{B}(\mathcal{G}, \mathcal{G}^*)$ is strongly C^1 (see [ABG], Theorem 6.3.4). In this case, the commutator $[H, iA]$ belongs unambiguously to $\mathcal{B}(\mathcal{G}, \mathcal{G}^*)$.

With any H of class $C^1(A)$, one associates the functions ϱ_H^A and $\tilde{\varrho}_H^A$ defined on \mathbb{R} with values in $(-\infty, \infty]$ by

$$\begin{aligned} \varrho_H^A(\lambda) &= \sup\{a \in \mathbb{R} \mid \exists \eta \in C_c^\infty(\mathbb{R}) \text{ s.t. } \eta(\lambda) \neq 0 \text{ and} \\ &\quad a\eta^2(H) \leq \eta(H)[H, iA]\eta(H)\}, \\ \tilde{\varrho}_H^A(\lambda) &= \sup\{a \in \mathbb{R} \mid \exists \eta \in C_c^\infty(\mathbb{R}) \text{ and } K \in \mathcal{K}(\mathcal{H}) \text{ s.t. } \eta(\lambda) \neq 0 \\ &\quad \text{and } a\eta^2(H) + K \leq \eta(H)[H, iA]\eta(H)\}. \end{aligned}$$

Some properties of these functions will be quoted later on (Proposition 2.5.3). The Mourre set of H with respect to A is $\mu^A(H) := \{\lambda \in \mathbb{R} \mid \varrho_H^A(\lambda) > 0\}$. Since the work of Mourre ([Mo1], [Mo2]), it is known that H has nice spectral properties on this set. In particular H has no eigenvalue in $\mu^A(H)$ and, under an additional regularity assumption, a limiting absorption principle can be stated on it. This additional condition is as follows: for some, and then for all, $z \in \mathbb{C} \setminus \sigma(H)$,

$$\int_0^1 \|W_{-t}(H - z)^{-1}W_t + W_t(H - z)^{-1}W_{-t} - 2(H - z)^{-1}\| \frac{dt}{t^2} < \infty. \quad (2.1)$$

If this condition is satisfied, H is said to be of class $C^{1,1}(A)$. Assuming the invariance of \mathcal{G} under each W_t , an equivalent requirement (see Theorem 6.3.4 of [ABG]) is that

$$\int_0^1 \|W_t^* H W_t + W_{-t}^* H W_{-t} - 2H\|_{\mathcal{G} \rightarrow \mathcal{G}^*} \frac{dt}{t^2} < \infty,$$

where $\|\cdot\|_{\mathcal{G} \rightarrow \mathcal{G}^*}$ is the norm of $\mathcal{B}(\mathcal{G}, \mathcal{G}^*)$.

In our applications, H is equal to $-\Delta + V$ in $\mathcal{H} = L^2(\mathbb{R}^n)$ with domain \mathcal{H}^2 , the Sobolev space of order two on \mathbb{R}^n . The unitary group $\{W_t\}_{t \in \mathbb{R}}$ is the group of

dilations, which leaves \mathcal{H}^2 invariant. Since $W_t^* \Delta W_t = e^{2t} \Delta$, an easy calculation shows that the operator $-\Delta$ satisfies the $C^{1,1}(A)$ -condition. Hence H is of class $C^{1,1}(A)$ if V is Δ -bounded with relative bound less than one and is of class $C^{1,1}(A)$. We still recall some definitions related to this condition in such a setting.

Definition 2.2.2. *Let $U : \mathcal{H}^2 \rightarrow \mathcal{H}$ be a linear symmetric operator.*

- i) *We say that U is a Mourre potential if the sesquilinear form $[[U, A], A]$ defined on the Schwartz space on \mathbb{R}^n is continuous for the topology induced by \mathcal{H}^2 .*
- ii) *We say that U is a long-range potential if $[U, A] \in \mathcal{B}(\mathcal{H}^2, \mathcal{H}^{-1})$ and if there exists a function $\xi \in C^\infty(\mathbb{R}^n)$ with $\xi(x) = 0$ if $|x| \leq 1$ and $\xi(x) = 1$ if $|x| \geq 2$ such that*

$$\int_1^\infty \left\| \xi \left(\frac{Q}{r} \right) [U, A] \right\|_{\mathcal{H}^2 \rightarrow \mathcal{H}^{-1}} \frac{dr}{r} < \infty.$$

- iii) *We say that U is a short-range potential if $\int_1^\infty \left\| \xi \left(\frac{Q}{r} \right) U \right\|_{\mathcal{H}^2 \rightarrow \mathcal{H}} dr < \infty$ for some $\xi \in C^\infty(\mathbb{R}^n)$ such that $\xi(x) = 0$ if $|x| \leq 1$ and $\xi(x) = 1$ if $|x| \geq 2$.*

It is shown in [ABG] that in all three cases, U is of class $C^{1,1}(A)$. These definitions are useful in order to construct examples of cartesian potentials of this class. We shall make some remarks on this point at the end of Section 2.5.

2.3 The Cartesian algebra and the essential spectrum

In this section, we study the *cartesian algebra* \mathfrak{C} which characterizes in some sense the Hamiltonians under consideration. Its properties will be extensively used in our later proofs. Let us first observe that \mathcal{L} is naturally endowed with the structure of a finite semilattice, with largest element $o : \beta \leq \alpha$ if $\overline{\mathbb{R}}^\beta \subset \overline{\mathbb{R}}^\alpha$. $\beta < \alpha$ means strict ordering, and we write $\beta \triangleleft \alpha$ if $\beta < \alpha$ and $\overline{\mathbb{R}}^\beta \subset \overline{\mathbb{R}}^\gamma \subset \overline{\mathbb{R}}^\alpha$ implies that either $\gamma = \beta$ or $\gamma = \alpha$. For $j \in \{1, \dots, n\}$, let $(\beta - \alpha)_j$ be equal to $\beta_j - \alpha_j$. One has equivalently that $\beta \leq \alpha$ if, whenever $\alpha_j \neq 0$, then $\beta_j = \alpha_j$, and that $\beta \triangleleft \alpha$ if and only if $\beta \leq \alpha$ and there is exactly one value of j such that $(\beta - \alpha)_j \neq 0$. One also notices that $|\alpha|$ is equal to $n - \sum_{j=1}^n |\alpha_j|$.

In the sequel, we shall make some abuses of notation: $\overline{\mathbb{R}}^\alpha$ will denote either a hypersurface of $\overline{\mathbb{R}}^n$ or the isomorphic cartesian product of $\overline{\mathbb{R}}_j$ for all $\alpha_j = 0$ (a $|\alpha|$ -dimensional hypercube). Similarly, $C(\overline{\mathbb{R}}^\alpha)$ will be viewed either as a C^* -algebra on its own, or as a subalgebra of $C(\overline{\mathbb{R}}^n)$ with elements depending only on the variables x_j for which $\alpha_j = 0$. However, in every case, the context should suppress the ambiguity.

Before defining \mathfrak{C} , we summarize some easy properties of the abelian algebra $C(\overline{\mathbb{R}}^n)$. For each $\alpha \in \mathcal{L}$, let us show the invariance of the hypersurface $\overline{\mathbb{R}}^\alpha$ under the natural action \mathcal{U}^α of \mathbb{R}^n on $\overline{\mathbb{R}}^n$ by translations. For $y \in \mathbb{R}$, let $U_y : \overline{\mathbb{R}} \rightarrow \overline{\mathbb{R}}$ with $U_y(z) = z + y$ if $z \in \mathbb{R}$ and $U_y(\pm\infty) = \pm\infty$, be the extension to $\overline{\mathbb{R}}$ of the translation by y on \mathbb{R} . Since $\overline{\mathbb{R}}^n$ equals $\overline{\mathbb{R}}_1 \times \dots \times \overline{\mathbb{R}}_n$, the action of the group on $\overline{\mathbb{R}}^n$ can be defined componentwise: $[\mathcal{U}_x^\alpha(z)]_j = U_{x_j}(z_j)$ for any $z \in \overline{\mathbb{R}}^n$ and $x \in \mathbb{R}^n$. But

$\{-\infty\}$, $\{+\infty\}$ and $\overline{\mathbb{R}}$ are invariant under each homeomorphism U_y , and therefore $\overline{\mathbb{R}}^\alpha$ is invariant. Consequently, each subalgebra $C(\overline{\mathbb{R}}^\alpha)$ of $C(\overline{\mathbb{R}}^n)$ is stable under the action of translations. Indeed, the group \mathcal{U}^o of homeomorphisms induces a representation of the translation group by $*$ -automorphisms of $C(\overline{\mathbb{R}}^\alpha)$: for $f \in C(\overline{\mathbb{R}}^\alpha)$, $x \in \mathbb{R}^n$ and $z \in \overline{\mathbb{R}}^\alpha$, $(\mathcal{U}_x^o(f))(z) = f(\mathcal{U}_x^o(z))$. In particular, it implies the stability of $C(\overline{\mathbb{R}}^n)$ under \mathcal{U}^o , and similarly the stability of the C^* -algebra $C(\overline{\mathbb{R}}^\alpha)$ under \mathcal{U}^α , where \mathcal{U}^α is the corresponding action of \mathbb{R}^α on $\overline{\mathbb{R}}^\alpha$.

For each subalgebra $C(\overline{\mathbb{R}}^\alpha)$ of $C(\overline{\mathbb{R}}^n)$, there exists a morphism

$$\pi_\alpha : C(\overline{\mathbb{R}}^n) \ni f \mapsto \pi_\alpha(f) \equiv f^\alpha \in C(\overline{\mathbb{R}}^\alpha)$$

given by restriction of f to the hypersurface $\overline{\mathbb{R}}^\alpha$. This morphism is covariant since the relation $\pi_\alpha \circ \mathcal{U}_x^o = \mathcal{U}_x^o \circ \pi_\alpha$ is satisfied for all $x \in \mathbb{R}^n$. Let $C_0(\mathbb{R}^n)$ be identified with the ideal of functions in $C(\overline{\mathbb{R}}^n)$ which are null on the boundary $\overline{\mathbb{R}}^n \setminus \mathbb{R}^n$. A certain direct sum of morphisms π_α has an important feature: $\bigoplus_{\alpha \ll o} \pi_\alpha : C(\overline{\mathbb{R}}^n) \rightarrow \bigoplus_{\alpha \ll o} C(\overline{\mathbb{R}}^\alpha)$ is a covariant morphism with kernel equal to $C_0(\mathbb{R}^n)$. Thus there exists a natural injective morphism

$$\pi : C(\overline{\mathbb{R}}^n)/C_0(\mathbb{R}^n) \hookrightarrow \bigoplus_{\alpha \ll o} C(\overline{\mathbb{R}}^\alpha). \quad (2.2)$$

We now identify $C(\overline{\mathbb{R}}^\alpha)$ with the subalgebra of $\mathcal{B}(\mathcal{H}_\alpha)$ consisting of all multiplication operators $f(Q)$ with $f \in C(\overline{\mathbb{R}}^\alpha)$. $C_0(\mathbb{R}^{\alpha*})$ denotes the set of operators $h(P) := \mathcal{F}_\alpha^* h(Q) \mathcal{F}_\alpha$ with $h \in C_0(\mathbb{R}^\alpha)$ and where \mathcal{F}_α is the Fourier transform in \mathcal{H}_α (we have identified the dual of \mathbb{R}^α with \mathbb{R}^α itself). A few elements from the theory of crossed products are used in the sequel. We refer to [GI2], Sections 3 and 4 for an overview on this subject in relation with spectral analysis. This reference includes some precise definitions and all the required results.

One defines $\mathfrak{C}^\alpha := \langle C(\overline{\mathbb{R}}^\alpha) \cdot C_0(\mathbb{R}^{\alpha*}) \rangle$, the norm closure in $\mathcal{B}(\mathcal{H}_\alpha)$ of the set of finite sums of the form $f_1(Q)h_1(P) + \dots + f_N(Q)h_N(P)$ with $f_k \in C(\overline{\mathbb{R}}^\alpha)$ and $h_k \in C_0(\mathbb{R}^\alpha)$. It is shown in [GI2], Theorem 4.1, that \mathfrak{C}^α is a C^* -algebra; the stability of $C(\overline{\mathbb{R}}^\alpha)$ under \mathcal{U}^α is here essential. Moreover, this algebra is isomorphic to the crossed product $C(\overline{\mathbb{R}}^\alpha) \rtimes \mathbb{R}^\alpha$, which is defined abstractly in terms of the action of translations on $C(\overline{\mathbb{R}}^\alpha)$. In the special case $\alpha = o$, we simply set $\mathfrak{C} := \mathfrak{C}^o$. We shall give in Lemma 2.4.1 another description of this C^* -algebra in terms of suitable limits at infinity. We also mention the following known relations:

$$\mathcal{K}(\mathcal{H}) = \langle C_0(\mathbb{R}^n) \cdot C_0(\mathbb{R}^{n*}) \rangle \cong C_0(\mathbb{R}^n) \rtimes \mathbb{R}^n. \quad (2.3)$$

Due to the embedding of $C(\overline{\mathbb{R}}^\alpha)$ into $C(\overline{\mathbb{R}}^n)$ and its stability under \mathcal{U}^o , one may form $\langle C(\overline{\mathbb{R}}^\alpha) \cdot C_0(\mathbb{R}^{n*}) \rangle$, which is a C^* -subalgebra of \mathfrak{C} isomorphic to $C(\overline{\mathbb{R}}^\alpha) \rtimes \mathbb{R}^n$. Let $\mathbb{R}^{\alpha^\perp}$ denote the orthogonal complement of \mathbb{R}^α in \mathbb{R}^n . Proposition 2.4 of [Ta] asserts that $C(\overline{\mathbb{R}}^\alpha) \rtimes \mathbb{R}^n$ is isomorphic to $[C \rtimes \mathbb{R}^{\alpha^\perp}] \otimes [C(\overline{\mathbb{R}}^\alpha) \rtimes \mathbb{R}^\alpha]$. Hence, if \mathcal{H} is identified with $L^2(\mathbb{R}^{\alpha^\perp}) \otimes \mathcal{H}_\alpha$, the C^* -algebra $\langle C(\overline{\mathbb{R}}^\alpha) \cdot C_0(\mathbb{R}^{n*}) \rangle$ of bounded operators in \mathcal{H} is isomorphic to the C^* -algebra $C_0(\mathbb{R}^{\alpha^\perp*}) \otimes \mathfrak{C}^\alpha$ of bounded operators in $L^2(\mathbb{R}^{\alpha^\perp}) \otimes \mathcal{H}_\alpha$.

Since the morphism π_α is covariant, there exists a unique morphism

$$\Pi_\alpha : \langle C(\overline{\mathbb{R}}^n) \cdot C_0(\mathbb{R}^{n*}) \rangle \rightarrow \langle C(\overline{\mathbb{R}}^\alpha) \cdot C_0(\mathbb{R}^{n*}) \rangle$$

such that $\Pi_\alpha[f(Q)h(P)] = f^\alpha(Q)h(P)$ for each $f \in C(\overline{\mathbb{R}^n})$ and each $h \in C_0(\mathbb{R}^n)$. Furthermore, since $C_0(\mathbb{R}^n)$ is a stable ideal of $C(\overline{\mathbb{R}^n})$, the general theory of crossed products gives the canonical isomorphism:

$$[C(\overline{\mathbb{R}^n}) \rtimes \mathbb{R}^n]/[C_0(\mathbb{R}^n) \rtimes \mathbb{R}^n] \cong [C(\overline{\mathbb{R}^n})/C_0(\mathbb{R}^n)] \rtimes \mathbb{R}^n.$$

Using (2.2), (2.3) and some isomorphisms introduced above, one obtains:

$$\begin{aligned} \mathfrak{C}/\mathcal{K}(\mathcal{H}) &\cong [C(\overline{\mathbb{R}^n})/C_0(\mathbb{R}^n)] \rtimes \mathbb{R}^n \\ &\hookrightarrow [\oplus_{\alpha < o} C(\overline{\mathbb{R}^\alpha})] \rtimes \mathbb{R}^n \cong \oplus_{\alpha < o} [C(\overline{\mathbb{R}^\alpha}) \rtimes \mathbb{R}^n] \\ &\cong \oplus_{\alpha < o} \langle C(\overline{\mathbb{R}^\alpha}) \cdot C_0(\mathbb{R}^{n*}) \rangle. \end{aligned} \quad (2.4)$$

The resulting injective morphism is denoted by Π . But if Θ is the canonical surjection $\mathfrak{C} \rightarrow \mathfrak{C}/\mathcal{K}(\mathcal{H})$, then $\Pi \circ \Theta = \oplus_{\alpha < o} \Pi_\alpha$. Assume now that H is a self-adjoint observable affiliated to \mathfrak{C} . Then $\sigma_{\text{ess}}(H)$ is equal to $\sigma[\Theta(H)]$, where $\Theta(H)$ is the image of H in the Calkin algebra. Since an injective morphism preserves the spectrum, we have:

$$\sigma_{\text{ess}}(H) = \sigma\left(\Pi(\Theta(H))\right) = \sigma\left(\oplus_{\alpha < o} \Pi_\alpha(H)\right) = \bigcup_{\alpha < o} \sigma(\Pi_\alpha(H)), \quad (2.5)$$

the last equality being valid because the spectrum of an observable affiliated to a finite direct sum is the union of the spectra of its components. Let us mention that some similar results were already obtained in [Ma1].

2.4 Cartesian Hamiltonians

Schrödinger operators $-\Delta + V$ in $L^2(\mathbb{R}^n)$ affiliated to the C^* -algebra \mathfrak{C} are called *cartesian*. If V is a real element of $C(\overline{\mathbb{R}^n})$, the corresponding Hamiltonian is cartesian. This is easily seen by using the Neumann series

$$(-\Delta + V - z)^{-1} = \sum_{k=0}^{\infty} (-\Delta - z)^{-1} [V(z + \Delta)^{-1}]^k$$

which is norm convergent for $|\Im z|$ large enough. In order to deal with non-smooth potentials, several technical results have to be obtained. This section is entirely devoted to this question.

In the sequel, we shall often use some non-decreasing functions ξ in $C^\infty(\mathbb{R})$ satisfying $\xi(y) = 0$ if $y \leq 1$ and $\xi(y) = 1$ if $y \geq 2$. For reasons that will become obvious already in the next lemma, we call them *asymptotic localization functions*. Let us say that a bounded operator B is *semi-compact* if $\zeta(Q)B$ is compact for all $\zeta \in C_0(\mathbb{R}^n)$. We recall that for each $\alpha < o$, there exists exactly one j such that $\alpha_j \neq 0$. Hence $\alpha \cdot Q$ means $\alpha_j Q_j$ and therefore $\xi(\alpha \cdot Q)$ is well-defined for any function ξ on \mathbb{R} . We start with a new description of \mathfrak{C} .

Lemma 2.4.1. *i) Each operator in \mathfrak{C} is semi-compact.*

ii) A semi-compact operator B belongs to \mathfrak{C} if and only if there exist an asymptotic localization function ξ and a family $\{B_\alpha\}_{\alpha \ll o}$ such that $B_\alpha \in \langle C(\overline{\mathbb{R}}^\alpha) \cdot C_0(\mathbb{R}^{n*}) \rangle$ and $\lim_{r \rightarrow \infty} \left\| \xi \left(\alpha \cdot \frac{Q}{r} \right) (B - B_\alpha) \right\| = 0$. Moreover, each operator B_α is unique and equal to $\Pi_\alpha(B)$.

Proof. a) By using (2.3) one observes that the product $\zeta(Q)[f(Q)h(P)]$ belongs to $\mathcal{K}(\mathcal{H})$ for any $\zeta, h \in C_0(\mathbb{R}^n)$ and any $f \in C(\overline{\mathbb{R}}^n)$. Since \mathfrak{C} is the norm closure of the vector space generated by products of the form $f(Q)h(P)$ and since $\mathcal{K}(\mathcal{H})$ is norm closed, $\zeta(Q)B$ is compact for any $\zeta \in C_0(\mathbb{R}^n)$ and any $B \in \mathfrak{C}$. This proves i).

b) We now check the “only if” part of ii). Consider $f \in C(\overline{\mathbb{R}}^n)$ and $\alpha \in \mathcal{L}$. Let us observe that $f = f^\alpha + (f - f^\alpha)$, where $f^\alpha \in C(\overline{\mathbb{R}}^\alpha)$ and $(f - f^\alpha)$ belongs to the ideal J_α of functions of $C(\overline{\mathbb{R}}^n)$ which are equal to zero on the hypersurface $\overline{\mathbb{R}}^\alpha$. So, one has $C(\overline{\mathbb{R}}^n) = C(\overline{\mathbb{R}}^\alpha) + J_\alpha$, and J_α is nothing but the kernel of the morphism π_α of the previous section. By Corollary 3.1 of [GI2], one gets

$$\mathfrak{C} = \langle C(\overline{\mathbb{R}}^\alpha) \cdot C_0(\mathbb{R}^{n*}) \rangle + \langle J_\alpha \cdot C_0(\mathbb{R}^{n*}) \rangle,$$

where $\langle J_\alpha \cdot C_0(\mathbb{R}^{n*}) \rangle$ is the kernel of the morphism Π_α . Now for any $B \in \mathfrak{C}$, we set $B_\alpha := \Pi_\alpha(B) \in \langle C(\overline{\mathbb{R}}^\alpha) \cdot C_0(\mathbb{R}^{n*}) \rangle$; then $B - B_\alpha$ is an element of $\langle J_\alpha \cdot C_0(\mathbb{R}^{n*}) \rangle$. If $\alpha \ll o$, it is easy to see that for any asymptotic localization function ξ , $\left\{ 1 - \xi \left(\alpha \cdot \frac{Q}{r} \right) \right\}_{r \geq 1}$ is an approximate unit for this ideal and thus $\lim_{r \rightarrow \infty} \left\| \xi \left(\alpha \cdot \frac{Q}{r} \right) (B - B_\alpha) \right\| = 0$.

c) To prove the “if” part in ii), let us introduce a partition of unity adapted to the anisotropy. Set $\xi_0(y) := 1 - \xi(y) - \xi(-y)$ for $y \in \mathbb{R}$, and for $x \in \mathbb{R}^n$ set $\xi_\alpha(x) := \prod_{\{j|\alpha_j \neq 0\}} \xi(\alpha_j x_j) \prod_{\{k|\alpha_k = 0\}} \xi_0(x_k)$. For $\varepsilon > 0$, there exists $r' > 0$ such that for all $r \geq r'$ and all $\alpha \ll o$, $\left\| \xi \left(\alpha \cdot \frac{Q}{r} \right) (B - B_\alpha) \right\| < \frac{\varepsilon}{2(3^n - 1)}$. For each $\alpha \ll o$, there exists $N_\alpha < \infty$, $f_k^\alpha \in C(\overline{\mathbb{R}}^\alpha)$ and $h_k^\alpha \in C_0(\mathbb{R}^n)$ such that $\|B_\alpha - \sum_{k=1}^{N_\alpha} f_k^\alpha(Q)h_k^\alpha(P)\| < \frac{\varepsilon}{2(3^n - 1)}$. Finally, for each $\beta \neq o$, choose $\alpha(\beta)$ such that $\alpha(\beta) \ll o$ and $\beta \leq \alpha(\beta)$. Since $\xi_\beta(Q) \leq \xi(\alpha(\beta) \cdot Q) \leq 1$ and since \mathcal{L} contains 3^n elements, one obtains

$$\left\| B - \xi_o \left(\frac{Q}{r'} \right) B - \sum_{\beta \neq o} \sum_{k=1}^{N_{\alpha(\beta)}} \xi_\beta \left(\frac{Q}{r'} \right) f_k^{\alpha(\beta)}(Q) h_k^{\alpha(\beta)}(P) \right\| < \varepsilon.$$

By semi-compactness of B , $\xi_o \left(\frac{Q}{r'} \right) B$ belongs to $\mathcal{K}(\mathcal{H})$, and hence to \mathfrak{C} ; and each term in the sum belongs to \mathfrak{C} by construction. Since \mathfrak{C} is norm closed, one gets that $B \in \mathfrak{C}$.

d) For each $\alpha \ll o$, the uniqueness of B_α is shown by proving the following statement: if C belongs to $\langle C(\overline{\mathbb{R}}^\alpha) \cdot C_0(\mathbb{R}^{n*}) \rangle$ and satisfies $\lim_{r \rightarrow \infty} \left\| \xi \left(\alpha \cdot \frac{Q}{r} \right) C \right\| = 0$, then $C = 0$. To see this, assume that $C \neq 0$ and for simplicity let us fix $\alpha = (1, 0, \dots, 0)$. Choose $\varphi \in \mathcal{H}$ such that $\|\varphi\| = 1$ and $C\varphi \neq 0$. By hypothesis, there exists $r \geq 1$ such that $\left\| \xi \left(\frac{Q_1}{r} \right) C \right\| < \frac{1}{2} \|C\varphi\|$, and so $\left\| \xi \left(\frac{Q_1}{r} \right) C e^{-iyP_1} \varphi \right\| < \frac{1}{2} \|C\varphi\|$ for each $y \in \mathbb{R}$. But, since all elements of $\langle C(\overline{\mathbb{R}}^\alpha) \cdot C_0(\mathbb{R}^{n*}) \rangle$ commute with the unitary operator

e^{-iyP_1} ($y \in \mathbb{R}$), one has $\left\| \xi \left(\frac{Q_1}{r} \right) C e^{-iyP_1} \varphi \right\| = \left\| \xi \left(\frac{Q_1}{r} + \frac{y}{r} \right) C \varphi \right\| \rightarrow \|C\varphi\|$ as $y \rightarrow \infty$, a contradiction with the preceding inequality. Hence $C = 0$. \square

Lemma 2.4.2. *Let H be a self-adjoint operator in \mathcal{H} with domain $D(H)$ and assume that for each $\alpha \ll o$, there exists a self-adjoint operator H_α in \mathcal{H} , affiliated to $\langle C(\overline{\mathbb{R}}^\alpha) \cdot C_0(\mathbb{R}^{n^*}) \rangle$, with domain equal to $D(H)$. Assume also that for some asymptotic localization function ξ and each $\alpha \ll o$,*

$$\lim_{r \rightarrow \infty} \left\| \xi \left(\alpha \cdot \frac{Q}{r} \right) (H - H_\alpha) \right\|_{D(H) \rightarrow \mathcal{H}} = 0.$$

Then H is affiliated to \mathfrak{C} and $\Pi_\alpha(H) = H_\alpha$ (in the sense of Definition 2.2.1).

Proof. Set $R := (H - z)^{-1}$ and $R_\alpha := (H_\alpha - z)^{-1}$ for any fixed $z \in \mathbb{C} \setminus \mathbb{R}$ and each $\alpha \ll o$. Since H_α is affiliated to the subalgebra $\langle C(\overline{\mathbb{R}}^\alpha) \cdot C_0(\mathbb{R}^{n^*}) \rangle$ of \mathfrak{C} , R_α belongs to \mathfrak{C} and thus is semi-compact, cf. *i*) of Lemma 2.4.1. Then R is semi-compact since for any $\zeta \in C_0(\mathbb{R}^n)$, $\zeta(Q)R_\alpha \in \mathcal{K}(\mathcal{H})$ and $R_\alpha^{-1}R$ is bounded by the closed graph theorem [Ka].

Furthermore,

$$\left\| \xi \left(\alpha \cdot \frac{Q}{r} \right) (R - R_\alpha) \right\| \leq c \left\{ \left\| \xi \left(\alpha \cdot \frac{Q}{r} \right) (H - H_\alpha) R \right\| + \left\| \left[\xi \left(\alpha \cdot \frac{Q}{r} \right), R_\alpha \right] \right\| \right\}$$

where $c = \max\{\|R_\alpha\|, \|(H - H_\alpha)R\|\}$. The first term on the r.h.s. goes to 0 as $r \rightarrow \infty$ by hypothesis. For the second term, one has to use the isomorphism $\langle C(\overline{\mathbb{R}}^\alpha) \cdot C_0(\mathbb{R}^{n^*}) \rangle \cong C_0(\mathbb{R}^{\alpha^+}) \otimes \mathfrak{C}^\alpha$ introduced in Section 2.3 and either Lemma 3.4 of [GI1] or a commutator expansion for terms of the form $\left[\xi \left(\alpha \cdot \frac{Q}{r} \right), g(\alpha \cdot P) \right]$ with $g \in C_0(\mathbb{R}^{\alpha^+})$. It then follows that $\lim_{r \rightarrow \infty} \left\| \left[\xi \left(\alpha \cdot \frac{Q}{r} \right), R_\alpha \right] \right\| = 0$, and the affiliation of H to \mathfrak{C} is obtained with Lemma 2.4.1 and the observation made before Definition 2.2.1.

We have thus obtained that $\Pi_\alpha((H - z)^{-1}) = (H_\alpha - z)^{-1}$ for all $z \in \mathbb{C} \setminus \mathbb{R}$. The last statement of the lemma follows from the density in $C_0(\mathbb{R})$ of the vector space generated by the set of functions $\{(\cdot - z)^{-1} \mid z \in \mathbb{C} \setminus \mathbb{R}\}$. \square

We now give the general definition of the potentials under consideration, and we shall prove in Proposition 2.4.5 the affiliation to \mathfrak{C} for the corresponding Schrödinger operators. One notices that if V belongs to $C(\overline{\mathbb{R}}^n)$, the functions V^α introduced in the following definition are nothing but the restrictions of V to the hypersurfaces $\overline{\mathbb{R}}^\alpha$.

Definition 2.4.3. *A Borel function $V : \mathbb{R}^n \rightarrow \mathbb{R}$ is a cartesian potential (relative to \mathcal{L}) if there exists a collection of Borel functions $\{V^\alpha\}_{\alpha \in \mathcal{L}}$, with $V^o \equiv V$ and $V^\alpha : \mathbb{R}^\alpha \rightarrow \mathbb{R}$, such that for each $\alpha \in \mathcal{L}$:*

- i) $V^\alpha(Q)$ is Δ^α -bounded with relative bound less than one,*
- ii) $\lim_{r \rightarrow \infty} \left\| \xi \left((\beta - \alpha) \cdot \frac{Q}{r} \right) (V^\alpha(Q) - V^\beta(Q)) \right\|_{\mathcal{H}_\alpha^2 \rightarrow \mathcal{H}_\alpha} = 0$ for each $\beta \ll \alpha$ and some asymptotic localization function ξ .*

The second condition means that for each $\alpha \in \mathcal{L}$, the function V^α defined on \mathbb{R}^α approaches its asymptotic limits V^β with $\beta \triangleleft \alpha$ in the norm $\|\cdot\|_{\mathcal{H}_\alpha^2 \rightarrow \mathcal{H}_\alpha}$. Let us observe that Lemma 9.4.8 of [ABG] implies that if V is a cartesian potential, then $V^\alpha(Q)$ is Δ -bounded with relative bound less than one, and *ii*) is also fulfilled with the norm $\|\cdot\|_{\mathcal{H}^2 \rightarrow \mathcal{H}}$ instead of the norm $\|\cdot\|_{\mathcal{H}_\alpha^2 \rightarrow \mathcal{H}_\alpha}$. We give a rather general example of such potentials.

Example 2.4.4. Let V_1 be a bounded real function on \mathbb{R}^n such that for each $\alpha \triangleleft o$, there exists $V^\alpha \in L^\infty(\mathbb{R}^\alpha)$ satisfying

$$\lim_{r \rightarrow \infty} \sup_{x \in \mathbb{R}^n} \left| \xi \left(\alpha \cdot \frac{x}{r} \right) (V_1(x) - V^\alpha(x)) \right| = 0$$

for some asymptotic localization function ξ . Let $V_2(Q)$ be a Δ -bounded operator (relative bound less than one) such that $\lim_{r \rightarrow \infty} \left\| \xi \left(\frac{|Q|}{r} \right) V_2(Q) \right\|_{\mathcal{H}^2 \rightarrow \mathcal{H}} = 0$. Then $V^o := V_1 + V_2$ is a cartesian potential. Indeed, let $\beta \in \mathcal{L}$ with $|\beta| = n - 2$ and let α, α' be the only two distinct elements of \mathcal{L} such that $\beta \triangleleft \alpha$ and $\beta \triangleleft \alpha'$. Let $j, j' \in \{1, \dots, n\}$ be such that $(\beta - \alpha)_j \neq 0$ and $(\beta - \alpha')_{j'} \neq 0$. Then one can check that $\{V^\alpha|_{x_j = \beta_j n}\}_{n \in \mathbb{N}}$ and $\{V^{\alpha'}|_{x_{j'} = \beta_{j'} n}\}_{n \in \mathbb{N}}$ are two Cauchy sequences in $L^\infty(\mathbb{R}^\beta)$ which converge to the same element (denoted V^β). Both requirements of Definition 2.4.3 are now clearly satisfied for $\alpha = o$ and for each $\alpha \triangleleft o$. The same procedure can then be applied again in order to construct successively V^β for all $\beta \in \mathcal{L}$ and to check that the conditions of Definition 2.4.3 are satisfied.

For the next proof and some later uses, we introduce the semilattice $\mathcal{L}^\alpha := \{\beta \in \mathcal{L} \mid \beta \leq \alpha\}$.

Proposition 2.4.5. *Assume that V is a cartesian potential. Then $H = -\Delta + V$ is a cartesian Hamiltonian and $\Pi_\alpha(H) = -\Delta + V^\alpha$ for each $\alpha \in \mathcal{L}$.*

Proof. Since the proof is performed by induction over the lattice \mathcal{L} , let us first introduce some notations. For each $\alpha \in \mathcal{L}$ and each $\beta \leq \alpha$, let

$$\pi_\beta^\alpha : C(\overline{\mathbb{R}}^\alpha) \ni f \mapsto \pi_\beta^\alpha(f) \in C(\overline{\mathbb{R}}^\beta)$$

be the covariant morphism given by restriction of f to the hypersurface $\overline{\mathbb{R}}^\beta$, and let Π_β^α be the unique morphism $\mathfrak{C}^\alpha \rightarrow \langle C(\overline{\mathbb{R}}^\beta) \cdot C_0(\mathbb{R}^{\alpha*}) \rangle$ satisfying $\Pi_\beta^\alpha[f(Q)h(P)] = \pi_\beta^\alpha(f)(Q)h(P)$ for each $f \in C(\overline{\mathbb{R}}^\alpha)$ and each $h \in C_0(\mathbb{R}^\alpha)$. If $\alpha = o$, then Π_β^α is just Π_β . In this setting, the statement of the proposition reads: if V^α is a cartesian potential relative to the lattice \mathcal{L}^α , then $H^\alpha = -\Delta^\alpha + V^\alpha$ is affiliated to \mathfrak{C}^α and $\Pi_\beta^\alpha(H^\alpha) = -\Delta^\alpha + V^\beta$ for each $\beta \in \mathcal{L}^\alpha$.

Let us notice that for each $\alpha \in \mathcal{L}$, V^α is a cartesian potential relative to the lattice \mathcal{L}^α . In the special case $|\alpha| = 0$, V^α is a real number, $H^\alpha = V^\alpha$ and H^α is clearly affiliated to \mathfrak{C}^α , which is simply \mathbb{C} . For any fixed α , $|\alpha| \neq 0$, we may now assume that the assertions of the proposition are proved for each H^β with $\beta \triangleleft \alpha$ and we prove it for H^α . With no loss of generality and for simplicity of notations, we choose $\alpha = o$.

So assume that for each $\beta < o$, H^β is affiliated to \mathfrak{C}^β . Let $j \in \{1, \dots, n\}$ such that $\beta_j \neq 0$. Then the operator $-\Delta_j \otimes I + I \otimes H^\beta$ in $L^2(\mathbb{R}_j) \otimes \mathcal{H}_\beta$ is affiliated to the C^* -algebra $C_0(\mathbb{R}_j^*) \otimes \mathfrak{C}^\beta$ (see [ABG], Section 8.2.3). Furthermore, if we identify $L^2(\mathbb{R}_j) \otimes \mathcal{H}_\beta$ with \mathcal{H} , then the operator $-\Delta_j \otimes I + I \otimes H^\beta$ is equal to $-\Delta + V^\beta$, which is thus affiliated to $\langle C(\overline{\mathbb{R}}^\beta) \cdot C_0(\mathbb{R}^{n*}) \rangle$, cf. Section 2.3. Hence $H_\beta = -\Delta + V^\beta$ is a self-adjoint operator in \mathcal{H} of domain \mathcal{H}^2 and affiliated to $\langle C(\overline{\mathbb{R}}^\beta) \cdot C_0(\mathbb{R}^{n*}) \rangle$. But H is also a self-adjoint operator with domain \mathcal{H}^2 and

$$\left\| \xi \left(\beta \cdot \frac{Q}{r} \right) (H - H_\beta) \right\|_{\mathcal{H}^2 \rightarrow \mathcal{H}} = \left\| \xi \left(\beta \cdot \frac{Q}{r} \right) (V(Q) - V^\beta(Q)) \right\|_{\mathcal{H}^2 \rightarrow \mathcal{H}} \rightarrow 0 \text{ as } r \rightarrow \infty$$

(ξ is the asymptotic localization function introduced in Definition 2.4.3). By invoking Lemma 2.4.2 one gets that H is affiliated to \mathfrak{C} and that $\Pi_\beta(H) = H_\beta$ for each $\beta < o$.

The general case $\Pi_\gamma(H) = H_\gamma$ for all $\gamma \leq o$ is obtained by taking into account the trivial equality $\Pi_\gamma = \Pi_\gamma \circ \Pi_\beta$ for $\gamma \leq \beta$, the identification of the morphisms Π_γ on $\langle C(\overline{\mathbb{R}}^\beta) \cdot C_0(\mathbb{R}^{n*}) \rangle$ and $I \otimes \Pi_\gamma^\beta$ on $C_0(\mathbb{R}^{\beta+\ast}) \otimes \mathfrak{C}^\beta$, and by using the assumption $\Pi_\gamma^\beta(H^\beta) = -\Delta^\beta + V^\gamma$. \square

2.5 The Mourre estimate

The strategy for obtaining the results announced in this title is similar to that developed for the N-body problem. The analogy is possible mainly because of the rich internal structure of \mathfrak{C} and its compatibility with the unitary group $\{W_t\}_{t \in \mathbb{R}}$ of dilations in \mathcal{H} (Lemma 2.5.1). More precisely, we consider $\{W_t = e^{2iAt}\}_{t \in \mathbb{R}}$ with self-adjoint generator $A = \frac{1}{4} \sum_{j=1}^n (P_j Q_j + Q_j P_j)$. Let us observe that $[\Delta, iA] = \Delta$, and recall that this group leaves \mathcal{H}^2 invariant. Each W_t induces an automorphism \mathcal{W}_t of $\mathcal{B}(\mathcal{H})$, namely $\mathcal{W}_t[B] = W_{-t} B W_t$ for $B \in \mathcal{B}(\mathcal{H})$.

Lemma 2.5.1. *For each $t \in \mathbb{R}$, \mathcal{W}_t leaves the C^* -algebra \mathfrak{C} invariant; for each $\alpha \in \mathcal{L}$, $\mathcal{W}_t \circ \Pi_\alpha = \Pi_\alpha \circ \mathcal{W}_t$ on \mathfrak{C} .*

Proof. For $f \in C(\overline{\mathbb{R}}^n)$ and $h \in C_0(\mathbb{R}^n)$, one has $\mathcal{W}_t[f(Q)h(P)] = f(e^{-t}Q)h(e^tP)$. It is now easy to verify that $(\mathcal{W}_t \circ \Pi_\alpha)[f(Q)h(P)] = (\Pi_\alpha \circ \mathcal{W}_t)[f(Q)h(P)]$. Since \mathfrak{C} is the norm closure of the vector space generated by such products, \mathfrak{C} is invariant and \mathcal{W}_t and Π_α commute on \mathfrak{C} . \square

The next lemma contains two results which are analogous to the statements of Lemma 9.4.3 and Theorem 8.4.3 of [ABG]. The compatibility of the structure of \mathfrak{C} with the dilation group is essential. One observes that

$$A = \frac{1}{4} \sum_{\{j|\alpha_j=0\}} (P_j Q_j + Q_j P_j) + \frac{1}{4} \sum_{\{j|\alpha_j \neq 0\}} (P_j Q_j + Q_j P_j) \equiv A^\alpha + A^{\alpha^\perp},$$

where A^α (resp. A^{α^\perp}) is the generator of dilations in \mathbb{R}^α (resp. $\mathbb{R}^{\alpha^\perp}$).

Lemma 2.5.2. *Let V be a cartesian potential such that $H = -\Delta + V$ is of class $C_u^1(A)$. Then:*

- i) for each $\alpha \in \mathcal{L}$, H_α is of class $C_u^1(A)$ and H^α is of class $C_u^1(A^\alpha)$,*
- ii) one has $\tilde{\varrho}_H^A = \min_{\alpha < o} \varrho_{H_\alpha}^A$.*

The proof of *i)* can be performed by rewriting the proof of Lemma 9.4.3 of [ABG] in our formalism. The statement *ii)* is obtained by taking into account the injective morphism (2.4), together with our Lemma 2.5.1 and Proposition 8.3.5 of [ABG].

Let us now recall two important results in Mourre theory which are expressed in terms of the functions ϱ and $\tilde{\varrho}$. Proofs can be found in Section 7.2 of [ABG].

Proposition 2.5.3. *Let H be a self-adjoint operator of class $C^1(A)$.*

- i) If $\tilde{\varrho}_H^A(\lambda) > 0$ for some $\lambda \in \mathbb{R}$, then λ has a neighbourhood in which there is at most a finite number of eigenvalues of H , each of finite multiplicity.*
- ii) One has $\varrho_H^A(\lambda) = \tilde{\varrho}_H^A(\lambda)$ unless λ is an eigenvalue of H and $\tilde{\varrho}_H^A(\lambda) > 0$, in which case $\varrho_H^A(\lambda) = 0$.*

The next statement contains the Mourre estimate, which is the main result of this section.

Proposition 2.5.4. *Assume that V is a cartesian potential and that $H = -\Delta + V$ is of class $C_u^1(A)$. Then $\tau(H)$ and $\kappa(H)$ are closed countable sets, the eigenvalues of H outside $\tau(H)$ are of finite multiplicity and can accumulate only at points belonging to $\tau(H)$, and $\mu^A(H)$ is equal to $\mathbb{R} \setminus \kappa(H)$. Moreover, for each $\lambda \in \mathbb{R}$,*

$$\tilde{\varrho}_H^A(\lambda) = \inf\{\lambda - \mu \mid \mu \in \tau(H), \mu \leq \lambda\}$$

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

Proof. a) We begin with some preliminary observations. One notices that for each $\alpha \in \mathcal{L}$, $\tau(H^\alpha) = \cup_{\beta < \alpha} \sigma_p(H^\beta)$ and $\kappa(H^\alpha) = \cup_{\beta \leq \alpha} \sigma_p(H^\beta)$ are countable sets. Furthermore, if $\tilde{\varrho}_{H^\alpha}^A(\lambda) > 0$ for all $\lambda \in \mathbb{R} \setminus \tau(H^\alpha)$, then $\sigma_p(H^\alpha)$ can only accumulate at points of $\tau(H^\alpha)$, since otherwise it would contradict *i)* of Proposition 2.5.3. Since $\kappa(H^\alpha)$ is equal to $\tau(H^\alpha) \cup \sigma_p(H^\alpha)$, this implies that if $\tau(H^\alpha)$ is closed and $\tilde{\varrho}_{H^\alpha}^A(\lambda) > 0$ for all $\lambda \in \mathbb{R} \setminus \tau(H^\alpha)$, then $\kappa(H^\alpha)$ is also closed.

b) The proof is going to be performed by induction over \mathcal{L} . We have already noticed that for each $\alpha \in \mathcal{L}$, V^α is a cartesian potential relative to \mathcal{L}^α and H^α is of class $C_u^1(A^\alpha)$. First, for $|\alpha| = 0$, H^α is equal to the real number V^α , $\tau(H^\alpha) = \emptyset$ and $\kappa(H^\alpha) = \{V^\alpha\}$. Moreover, $\tilde{\varrho}_{H^\alpha}^0(\lambda) = +\infty$ for all $\lambda \in \mathbb{R}$, while $\varrho_{H^\alpha}^0(V^\alpha) = 0$ and $\varrho_{H^\alpha}^0(\lambda) = +\infty$ for $\lambda \neq V^\alpha$. The proposition is thus verified in this special case. Next, for any fixed α , $|\alpha| \neq 0$, we assume that the assertions of the proposition are proved for each H^β with $\beta < \alpha$ and we prove it for H^α . For simplicity but with no loss of generality, we choose $\alpha = o$.

c) We start by determining $\varrho_{H_\beta}^A$ for each $\beta \ll o$. If $j \in \{1, \dots, n\}$ such that $\beta_j \neq 0$, then H_β is equal to $-\Delta_j \otimes I + I \otimes H^\beta$. The ϱ -function for operators of this form is extensively studied in [ABG], Theorem 8.3.6 :

$$\varrho_{H_\beta}^A(\lambda) = \inf_{\lambda_1 + \lambda_2 = \lambda} \left\{ \varrho_{H^\beta}^{A^\beta}(\lambda_1) + \varrho_{-\Delta_j}^{A^{\beta^\perp}}(\lambda_2) \right\}.$$

But $\varrho_{-\Delta_j}^{A^{\beta^\perp}}(\lambda_2) = \infty$ if $\lambda_2 < 0$ and $\varrho_{-\Delta_j}^{A^{\beta^\perp}}(\lambda_2) = \lambda_2$ if $\lambda_2 \geq 0$, and hence $\varrho_{H_\beta}^A(\lambda) = \inf_{\mu \leq \lambda} \left\{ \varrho_{H^\beta}^{A^\beta}(\mu) + (\lambda - \mu) \right\}$. By assumption, $\tilde{\varrho}_{H^\beta}^{A^\beta}(\lambda) = \inf\{\lambda - \mu \mid \mu \in \tau(H^\beta), \mu \leq \lambda\}$, and so $\tilde{\varrho}_{H^\beta}^{A^\beta}$ is zero on $\tau(H^\beta)$ and strictly positive on $\mathbb{R} \setminus \tau(H^\beta)$ (since $\tau(H^\beta)$ is assumed to be closed). Thus, in view of *ii*) of Proposition 2.5.3, $\varrho_{H^\beta}^{A^\beta}(\lambda) = 0$ if $\lambda \in \kappa(H^\beta)$ and $\varrho_{H^\beta}^{A^\beta}(\lambda) = \tilde{\varrho}_{H^\beta}^{A^\beta}(\lambda)$ elsewhere. From these relations one easily finds that $\varrho_{H_\beta}^A(\lambda) = \inf\{\lambda - \mu \mid \mu \in \kappa(H^\beta), \mu \leq \lambda\}$ for each $\beta \ll o$.

d) By using the result of c) and *ii*) of Lemma 2.5.2, one gets that $\tilde{\varrho}_H^A(\lambda) = \inf\{\lambda - \mu \mid \mu \in \tau(H), \mu \leq \lambda\}$, because $\cup_{\beta \ll o} \kappa(H^\beta) = \cup_{\beta \ll o} [\cup_{\gamma \leq \beta} \sigma_p(H^\gamma)] = \tau(H)$. Since $\tau(H)$ is a finite union of closed sets, it is closed. Hence $\tilde{\varrho}_H^A$ is strictly positive outside $\tau(H)$ and zero on $\tau(H)$, so that one may apply the result of a) with $\alpha = o$. By taking into account the statement *ii*) of Proposition 2.5.3, one sees that $\varrho_H^A(\lambda) = 0$ if $\lambda \in \kappa(H)$ and $\varrho_H^A(\lambda) > 0$ if $\lambda \notin \kappa(H)$. Hence $\mu^A(H) = \mathbb{R} \setminus \kappa(H)$. \square

Collecting the results obtained so far, we can now prove Theorem 2.1.1. We mention that if the operator H is of class $C^{1,1}(A)$, the $C_u^1(A)$ -condition of Proposition 2.5.4 is fulfilled.

Proof of Theorem 2.1.1. Since the potential V is Δ -bounded (with relative bound less than one) and is of class $C^{1,1}(A)$, H is of class $C^{1,1}(A)$. From (2.5), one has $\sigma_{\text{ess}}(H) = \cup_{\alpha \ll o} \sigma(H_\alpha)$. But $\sigma(H_\alpha) = [\inf \sigma(H^\alpha), \infty)$ because $H_\alpha = -\Delta_j \otimes I + I \otimes H^\alpha$ for j such that $\alpha_j \neq 0$, *cf.* [RS]. This implies *i*). *ii*) is part of Proposition 2.5.4. *iv*) results from our Proposition 2.5.4 and Proposition 7.4.6 of [ABG]. Finally, *iii*) is a well-known consequence of *iv*). \square

In order to ascertain that the $C^{1,1}(A)$ -condition is not too restrictive with respect to the cartesian anisotropy, let us indicate two examples of cartesian potentials of class $C^{1,1}(A)$.

Example 2.5.5. For any cartesian potential \tilde{V} , we consider the following approximation V_m of \tilde{V} . Let m be any positive number and ξ an asymptotic localization function. Set $\xi_0(y) := 1 - \xi(y) - \xi(-y)$ for $y \in \mathbb{R}$ and

$$\xi_\alpha(x) := \prod_{\{j \mid \alpha_j \neq 0\}} \xi(\alpha_j x_j) \prod_{\{k \mid \alpha_k = 0\}} \xi_0(x_k)$$

for $x \in \mathbb{R}^n$ and $\alpha \in \mathcal{L}$. We now define $V_m(x) := \sum_{\alpha \in \mathcal{L}} \xi_\alpha \left(\frac{x}{m} \right) \tilde{V}^\alpha(x)$ for $x \in \mathbb{R}^n$. Some calculations show that V_m is a Mourre potential (*cf.* Definition 2.2.2) and that

$\lim_{m \rightarrow \infty} \|\tilde{V}(Q) - V_m(Q)\|_{\mathcal{H}^2 \rightarrow \mathcal{H}} = 0$. Let V be equal to $V_m + V_{\text{LR}} + V_{\text{SR}}$, with V_{LR} (V_{SR}) a long-range (short-range) potential satisfying the additional condition

$$\lim_{r \rightarrow \infty} \left\| \xi \left(\frac{|Q|}{r} \right) (V_{\text{LR}}(Q) + V_{\text{SR}}(Q)) \right\|_{\mathcal{H}^2 \rightarrow \mathcal{H}} = 0.$$

Then V is a cartesian potential of class $C^{1,1}(A)$.

Example 2.5.6. Let V_j be a bounded function on \mathbb{R}_j having limits as $x_j \rightarrow \pm\infty$ and converging to these limits in a short-range or long-range way. Then $V := \prod_{j=1}^n V_j$ is a cartesian potential of class $C^{1,1}(A)$. To check this assertion, we first observe that if U is a self-adjoint operator in \mathcal{H}_α of class $C^{1,1}(A^\alpha)$ for some $\alpha \in \mathcal{L}$, then U is also of class $C^{1,1}(A)$. Furthermore, the product of a finite number of bounded potentials of class $C^{1,1}(A)$ belongs to the same class (this is easily proved by using Lemma 6.2.1 and Proposition 5.2.3 of [ABG]). Finally, both requirements of definition 2.4.3 are satisfied by the potential V , which is therefore cartesian. Note that the example given in the Introduction is of this type.

2.6 The asymptotic velocity

In this section, we prove the existence of the asymptotic velocity and state some of its properties. This velocity is going to play an essential role in the definition of the wave operators. Most of the results of this section are inspired or adapted from Section 6.6 of [DG]. However, since cartesian potentials and N-body potentials differ substantially, none of the results of this reference can be directly quoted. We refer to that book for further comments on the asymptotic velocity and other applications.

Proposition 2.6.1. *Let V be a cartesian potential such that $H = -\Delta + V$ is of class $C_u^1(A)$. Assume also that for each $j \in \{1, \dots, n\}$ and for some asymptotic localization function ξ ,*

$$\int_0^\infty \left\| \xi \left(\pm \frac{Q_j}{r} \right) \nabla_j V(Q) \right\|_{\mathcal{H}^2 \rightarrow \mathcal{H}^{-2}} dr < \infty. \quad (2.6)$$

Then,

i) *there exists a n -tuple \mathcal{P} of commuting self-adjoint operators such that for all $f \in C_0(\mathbb{R}^n)$:*

$$s - \lim_{t \rightarrow +\infty} e^{iHt} f \left(\frac{Q}{2t} \right) e^{-iHt} = f(\mathcal{P}),$$

ii) *for each $\eta \in C_0(\mathbb{R})$ and each $f \in C_0(\mathbb{R}^n)$, $[\eta(H), f(\mathcal{P})] = 0$, i.e. the asymptotic velocity \mathcal{P} commutes with the Hamiltonian H ,*

iii) *the subspace of the states with zero asymptotic velocity is equal to the subspace spanned by the eigenvectors of H .*

Since the limit $t \rightarrow -\infty$ could be handled similarly, we simply do not consider it. The entire section is devoted to the proof of this proposition and therefore, unless

otherwise stated, it is always assumed that the potential V satisfies its hypotheses. The proofs involve a considerable number of commutator computations, which will of course not be presented in full details. We start with some considerations on the notations and with a technical lemma that will be used freely subsequently.

Let us consider an operator-valued mapping $\Phi : [1, \infty) \ni t \mapsto \Phi(t) \in \mathcal{B}(\mathcal{H})$. If there exists some constant $c < \infty$ such that $\|\Phi(t)\| \leq c$ for all $t \geq 1$, then Φ is said to be a *bounded* operator-valued mapping. We write $\Phi \in BC^1([1, \infty), \mathcal{B}(\mathcal{H}))$ if the mapping is bounded and differentiable in norm with bounded derivative. Let m be any positive integer and $t \in [1, \infty)$. Then Φ (or by a slight abuse of notation $\Phi(t)$) belongs to $L^m((1, \infty), dt)$ if $\|\Phi(\cdot)\| \in L^m((1, \infty), dt)$, to $o(t^{-m})$ if $\lim_{t \rightarrow \infty} t^m \|\Phi(t)\| = 0$, or to $O(t^{-m})$ if $t^m \|\Phi(t)\| \leq c < \infty$ for all $t \geq 1$. We say that Φ is *integrable along the evolution* (with respect to H) if there exists a constant $c < \infty$ such that $\int_1^\infty |\langle e^{-iHt}\varphi, \Phi(t)e^{-iHt}\varphi \rangle| dt \leq c\|\varphi\|^2$ for all $\varphi \in \mathcal{H}$.

For each $\alpha \in \mathcal{L}$ we define the open subset of \mathbb{R}^n :

$$Y_\alpha := \{x \in \mathbb{R}^n \mid \alpha_j x_j > 0 \text{ for all } j \text{ with } \alpha_j \neq 0\}.$$

If $\alpha < o$ we also use the more familiar notation $Y_j^\pm := \{x \in \mathbb{R}^n \mid \pm x_j > 0\}$ with j and the sign \pm given by the only $\alpha_j \neq 0$. Let us make an obvious but very useful observation. For each $\alpha \in \mathcal{L}$ and each $f \in C_c(\mathbb{R}^n)$ with support in Y_α there exists $\delta > 0$ such that $\prod_{\{j \mid \alpha_j \neq 0\}} \xi(\alpha_j \frac{x_j}{\delta}) f(x) = f(x)$ for any asymptotic localization function ξ and all $x \in \mathbb{R}^n$.

In the sequel, unless explicitly mentioned, all functions η, f, \dots are assumed to be real.

Lemma 2.6.2. *For each $\eta \in C_c^\infty(\mathbb{R})$, each $j \in \{1, \dots, n\}$, each $\alpha \in \mathcal{L}$ and all $t \geq 1$, the following statements are true:*

- i) if f is a twice differentiable function on \mathbb{R}^n with bounded derivatives of order 0, 1 and 2, then $\left[\eta(H), f\left(\frac{Q}{2t}\right) \right] (H + i) \in O(t^{-1})$,*
- ii) if $f \in C_c^2(\mathbb{R}^n)$ with support in Y_j^\pm , then $\eta(H) f\left(\frac{Q}{2t}\right) \nabla_j V(Q) \eta(H)$ belongs to $L^1((1, \infty), dt)$,*
- iii) if $f \in C_c(\mathbb{R}^n)$ with support in Y_j^\pm , then $[P_j, \eta(H)] f\left(\frac{Q}{2t}\right)$ belongs to $o(t^0)$ and to $L^1((1, \infty), dt)$,*
- iv) if $f \in C_c(\mathbb{R}^n)$ with support in Y_α , then $f\left(\frac{Q}{2t}\right) (\eta(H) - \eta(H_\alpha)) \in o(t^0)$,*
- v) the operator $(P_j + i)Q_j \eta(H)(1 + Q^2)^{-1/2}$ belongs to $\mathcal{B}(\mathcal{H})$.*

The proof of this lemma is given in the Appendix. Let us however mention that the statement *i)* requires only the hypothesis that V be Δ -bounded with relative bound less than one. In line with *iv)*, one could also prove some anisotropic non-propagation estimates at suitable energies. More general results of this type can be found in [AMP].

For each operator-valued mapping $\Phi \in BC^1([1, \infty), \mathcal{B}(\mathcal{H}))$ we define its *Heisenberg derivative* $\mathbf{D}\Phi$: let φ, ψ in \mathcal{H}^2 (the domain of H) and $t \geq 1$, then

$$\langle \psi, \mathbf{D}\Phi(t)\varphi \rangle := i\langle H\psi, \Phi(t)\varphi \rangle - i\langle \psi, \Phi(t)H\varphi \rangle + \langle \psi, \frac{d}{dt}\Phi(t)\varphi \rangle. \quad (2.7)$$

One notices that $\langle \psi, e^{iHt}\mathbf{D}\Phi(t)e^{-iHt}\varphi \rangle$ is equal to $\frac{d}{dt}\langle \psi, e^{iHt}\Phi(t)e^{-iHt}\varphi \rangle$ for each $\varphi, \psi \in \mathcal{H}^2$. If, for each $t \geq 1$, $\mathbf{D}\Phi(t)$ extends continuously to a bounded operator (we keep the same notation for this extension), and if there exists some constant $c < \infty$ such that $\|\mathbf{D}\Phi(t)\| \leq c$ for all $t \geq 1$, then we write $\Phi \in BC_H^1([1, \infty), \mathcal{B}(\mathcal{H}))$. In our applications $\Phi(t)$ will often be equal $\eta(H)f\left(\frac{Q}{2t}\right)\eta(H)$ with $\eta \in C_c^\infty(\mathbb{R})$ and f a bounded function defined on \mathbb{R}^n . Then a sufficient condition such that $\Phi \in BC_H^1([1, \infty), \mathcal{B}(\mathcal{H}))$ is that $f \in C^2(\mathbb{R}^n)$ and that all first order partial derivatives of f have a bounded support.

As mentioned in the Introduction, we shall prove various propagation estimates. For this purpose, we review two standard results that will be constantly used (proofs can be found in the Appendix).

Lemma 2.6.3. *Let $\Phi \in BC^1([1, \infty), \mathcal{B}(\mathcal{H}))$ be a self-adjoint operator-valued mapping. Assume that there exist some bounded operator-valued mappings B, L, F , with $L \in L^1((1, \infty), dt)$ and F integrable along the evolution, such that one of the following two inequalities is satisfied for all $t \geq 1$ and each $\varphi \in \mathcal{H}^2$:*

$$\pm\langle \varphi, \mathbf{D}\Phi(t)\varphi \rangle \geq \langle \varphi, B^*(t)B(t)\varphi \rangle + \langle \varphi, F(t)\varphi \rangle + \langle \varphi, L(t)\varphi \rangle.$$

Then there exists $c < \infty$ such that $\int_1^\infty \|B(t)e^{-iHt}\varphi\|^2 dt \leq c\|\varphi\|^2$ for all $\varphi \in \mathcal{H}^2$.

Lemma 2.6.4. *Let $\Phi \in BC^1([1, \infty), \mathcal{B}(\mathcal{H}))$ be an operator-valued mapping, and let H_1 and H_2 be two self-adjoint operators in \mathcal{H} of domain \mathcal{D}_1 and \mathcal{D}_2 respectively. Assume that there exist a finite integer N and some bounded operator-valued mappings E_k, F_k and L such that for all $\varphi \in \mathcal{D}_1$, $\psi \in \mathcal{D}_2$ and all $t \geq 1$:*

$$\begin{aligned} & |i\langle H_2\psi, \Phi(t)\varphi \rangle - i\langle \psi, \Phi(t)H_1\varphi \rangle + \langle \psi, \frac{d}{dt}\Phi(t)\varphi \rangle| \\ & \leq \sum_{k=1}^N \|E_k(t)\psi\| \|F_k(t)\varphi\| + \|L(t)\| \|\psi\| \|\varphi\|. \end{aligned} \quad (2.8)$$

Assume furthermore that L belongs to $L^1((1, \infty), dt)$ and that there is a constant $c < \infty$ such that for each $k \in \{1, \dots, N\}$, $\int_1^\infty \|E_k(\tau)e^{-iH_2\tau}\psi\|^2 d\tau \leq c^2\|\psi\|^2$ for all $\psi \in \mathcal{D}_2$ and $\int_1^\infty \|F_k(\tau)e^{-iH_1\tau}\varphi\|^2 d\tau \leq c^2\|\varphi\|^2$ for all $\varphi \in \mathcal{D}_1$. Then $s\text{-}\lim_{t \rightarrow \infty} e^{iH_2t}\Phi(t)e^{-iH_1t}$ exists.

In most of our applications H_1 and H_2 are equal to H , and therefore (2.8) is nothing but $|\langle \psi, \mathbf{D}\Phi(t)\varphi \rangle|$.

The next lemma contains two statements usually called *maximal velocity estimates*. Both are proved under the single assumption that the potential V be Δ -bounded with relative bound less than one. It slightly extends the validity of similar results obtained in [DG].

To shorten some equations below and when the context leaves no doubt, the arguments of certain functions are not repeated all along the proofs.

Lemma 2.6.5. *For each $\eta \in C_c^\infty(\mathbb{R})$, there exists a constant $c_\eta > 0$ with the property that*

i) for each $f \in C_c^\infty(\mathbb{R})$ with support in (c_η, ∞) , there exists $c < \infty$ such that for all $\varphi \in \mathcal{H}$,

$$\int_1^\infty \left\| f \left(\frac{|Q|}{2t} \right) \eta(H) e^{-iHt} \varphi \right\|^2 \frac{dt}{t} \leq c \|\varphi\|^2,$$

ii) if f is a C^∞ -function on \mathbb{R} with support in (c_η, ∞) and such that $f = 1$ in a neighbourhood of ∞ , then

$$s - \lim_{t \rightarrow \infty} e^{iHt} \eta(H) f \left(\frac{|Q|}{2t} \right) \eta(H) e^{-iHt} = 0. \quad (2.9)$$

Proof. We fix a number $c'_\eta \in \mathbb{R}$ such that $\text{supp } \eta \subset (-\infty, c'_\eta)$ and a function $\tilde{\eta} \in C_c^\infty((-\infty, c'_\eta))$ satisfying $\tilde{\eta}\eta = \eta$ and $0 \leq \tilde{\eta} \leq 1$. We let c''_η be a positive constant such that $\sup_j \|\chi_{(-\infty, c'_\eta]}(H) P_j\| \leq c''_\eta/n$, where χ_I is the characteristic function of the interval I . We now fix the constant c_η such that $c_\eta > c''_\eta$.

a) For the proof of *i)*, choose $\tilde{f} \in C_c^\infty(\mathbb{R})$ with support in (c_η, ∞) and such that $\tilde{f}f = f$ and $0 \leq \tilde{f} \leq 1$. For $t \geq 1$, set $\Phi(t) := \eta(H) F \left(\frac{|Q|}{2t} \right) \eta(H)$ with $F(s) = \int_{-\infty}^s f^2(\tau) d\tau$. Then $\Phi \in BC_H^1([1, \infty), \mathcal{B}(\mathcal{H}))$ and one has

$$-\mathbf{D}\Phi(t) = \frac{1}{t} \eta \left\{ \frac{|Q|}{2t} f^2 \left(\frac{|Q|}{2t} \right) - \frac{1}{2} P \cdot \frac{Q}{|Q|} f^2 \left(\frac{|Q|}{2t} \right) - \frac{1}{2} f^2 \left(\frac{|Q|}{2t} \right) \frac{Q}{|Q|} \cdot P \right\} \eta.$$

By using *i)* of Lemma 2.6.2, one can check that

$$\tilde{\eta}(H) P \cdot \frac{Q}{|Q|} f^2 + f^2 \frac{Q}{|Q|} \cdot P \tilde{\eta}(H) = f \left\{ \tilde{\eta} P \cdot \frac{Q}{|Q|} \tilde{f} + \tilde{f} \frac{Q}{|Q|} \cdot P \tilde{\eta} \right\} f + O(t^{-1}).$$

Our choice of c''_η implies that $-c''_\eta \leq \frac{1}{2} \left\{ \tilde{\eta} P \cdot \frac{Q}{|Q|} \tilde{f} + \tilde{f} \frac{Q}{|Q|} \cdot P \tilde{\eta} \right\} \leq c''_\eta$. Furthermore one has $\frac{|Q|}{2t} f^2 \left(\frac{|Q|}{2t} \right) \geq c_\eta f^2 \left(\frac{|Q|}{2t} \right)$, and hence $-\mathbf{D}\Phi(t) \geq \frac{1}{t} \eta f \{c_\eta - c''_\eta\} f \eta + O(t^{-2})$. Since $c_\eta - c''_\eta > 0$ and by observing that for any $\varphi \in \mathcal{H}$, $\tilde{\eta}(H)\varphi$ belongs to \mathcal{H}^2 , the statement *i)* is seen to be a consequence of Lemma 2.6.3.

b) For f as in *i)* or *ii)*, let $\tilde{f} \in C_c^\infty(\mathbb{R})$ with support in (c_η, ∞) be such that $\tilde{f}f' = f'$ and $0 \leq \tilde{f} \leq 1$. For $r \geq 1$ set $\Phi_r(t) := \eta(H) f \left(\frac{|Q|}{2rt} \right) \eta(H)$ and observe that Φ_r is an operator-valued mapping belonging to $BC_H^1([1, \infty), \mathcal{B}(\mathcal{H}))$. As in a) above, one finds that

$$\mathbf{D}\Phi_r(t) = \frac{1}{t} \eta \tilde{f} \left\{ \frac{1}{2r} \tilde{\eta} P \cdot \frac{Q}{|Q|} f' + \frac{1}{2r} f' \frac{Q}{|Q|} \cdot P \tilde{\eta} - \frac{|Q|}{2rt} f' \right\} \tilde{f} \eta + O(t^{-2}).$$

All terms between brackets are norm bounded independently of t for $t \geq 1$. So by applying Lemma 2.6.4 and by using *i)* one gets the existence of $s - \lim_{t \rightarrow \infty} e^{iHt} \Phi_r(t) e^{-iHt}$.

c) Let us show that this limit is zero if f satisfies the hypothesis of *i*). Indeed, one may then choose $\tilde{f} \in C_c^\infty(\mathbb{R})$ with support in (c_η, ∞) and such that $\tilde{f}f = f$. Then by *i*) there exists $c < \infty$ such that for all $\varphi \in \mathcal{H}$,

$$\begin{aligned} \int_1^\infty |\langle \varphi, e^{iHt} \Phi_r(t) e^{-iHt} \varphi \rangle| \frac{dt}{t} &\leq \|f\|_{L^\infty} \int_1^\infty \left\| \tilde{f} \left(\frac{|Q|}{2rt} \right) \eta(H) e^{-iHt} \varphi \right\|^2 \frac{dt}{t} \\ &\leq c \|\varphi\|^2. \end{aligned}$$

This implies that $\lim_{t \rightarrow \infty} \langle \varphi, e^{iHt} \Phi_r(t) e^{-iHt} \varphi \rangle$ must be zero for each $\varphi \in \mathcal{H}$, and hence $w - \lim_{t \rightarrow \infty} e^{iHt} \Phi_r(t) e^{-iHt} = 0$ by polarization.

d) Let f satisfy the hypothesis *ii*) and assume in addition that $f' = g^2$ for some $g \in C_c^\infty(\mathbb{R})$. Let $\tilde{f} \in C_c^\infty(\mathbb{R})$ with support in (c_η, ∞) be such that $\tilde{f}f' = f'$ and $0 \leq \tilde{f} \leq 1$. As in a), one finds that

$$\begin{aligned} \mathbf{D}\Phi_r(t) &= \frac{1}{t} \eta g \left\{ \frac{1}{2r} \tilde{\eta} P \cdot \frac{Q}{|Q|} \tilde{f} + \frac{1}{2r} \tilde{f} \frac{Q}{|Q|} \cdot P \tilde{\eta} - \frac{|Q|}{2rt} \right\} g \eta + O(t^{-2} r^{-2}) \\ &\leq - \left(c_\eta - \frac{c_\eta''}{r} \right) \frac{1}{t} \eta f' \eta + O(t^{-2} r^{-2}) \leq O(t^{-2} r^{-2}). \end{aligned}$$

Inserting this inequality in the formal identity

$$e^{iHt} \Phi_r(t) e^{-iHt} = e^{iHt_0} \Phi_r(t_0) e^{-iHt_0} + \int_{t_0}^t e^{iH\tau} \mathbf{D}\Phi_r(\tau) e^{-iH\tau} d\tau$$

with $t \geq t_0 \geq 1$, one obtains the existence of some $c < \infty$ such that for all $\varphi \in \mathcal{H}^2$,

$$0 \leq \langle \varphi, e^{iHt} \Phi_r(t) e^{-iHt} \varphi \rangle \leq \langle \varphi, e^{iHt_0} \Phi_r(t_0) e^{-iHt_0} \varphi \rangle + c \|\varphi\|^2 t_0^{-1} r^{-2}. \quad (2.10)$$

Both terms on the r.h.s. of (2.10) are independent of t and tend to zero as r increases. Since the existence of $s - \lim_{t \rightarrow \infty} e^{iHt} \Phi_r(t) e^{-iHt}$ was shown in b), the inequalities in (2.10) imply that

$$s - \lim_{r \rightarrow \infty} \left(s - \lim_{t \rightarrow \infty} e^{iHt} \Phi_r(t) e^{-iHt} \right) = 0. \quad (2.11)$$

Now set $\Phi_1(t) = \Phi_r(t) + \tilde{\Phi}_r(t)$ with $\tilde{\Phi}_r(t) := \eta \left\{ f \left(\frac{|Q|}{2t} \right) - f \left(\frac{|Q|}{2rt} \right) \right\} \eta$. Since the function $\left\{ f \left(\frac{\cdot}{r} \right) - f \left(\frac{\cdot}{r} \right) \right\}$ has compact support in (c_η, ∞) for any $r \geq 1$, the equation (2.9) is obtained by choosing r large enough and by using (2.11) and the result of c).

e) To prove *ii*) without assuming an additional condition for f , choose any real function $g \in C_c^\infty(\mathbb{R})$ such that $\text{supp } g \subset (c_\eta, \infty)$ and $\int_{-\infty}^\infty g^2(y) dy = 1$, and set $F(x) = \int_{-\infty}^x g^2(y) dy$. If f satisfies the hypothesis of *ii*), then $f - F$ satisfies that of *i*), and (2.9) follows by combining the results of c) and d). \square

In the next lemma, a certain distortion of the mapping $\mathbb{R}^n \ni x \mapsto \frac{1}{2}x^2 \in \mathbb{R}$ will play a crucial technical role. We refer to [Gr] and especially to [DG] for similar constructions used in the N-body problem. For $\delta > 0$, let $m_\delta \in C^\infty(\mathbb{R})$ be a real convex function such that $m_\delta(y) = \frac{1}{2}\delta^2$ if $|y| \leq \delta$ and $m_\delta(y) = \frac{1}{2}y^2$ if $|y| \geq 2\delta$. We set $r_\delta(x) := \sum_{j=1}^n m_\delta(x_j)$ for $x \in \mathbb{R}^n$. Observe that r_δ is a C^∞ -function on \mathbb{R}^n with $\partial_{jk}^2 r_\delta(x) := \frac{\partial^2 r_\delta}{\partial x_j \partial x_k}(x) = 0$ if $j \neq k$ and $\partial_{jj}^2 r_\delta(x) \geq \xi^2 \left(-\frac{x_j}{2\delta} \right) + \xi^2 \left(\frac{x_j}{2\delta} \right)$ for any asymptotic localization function ξ and all $x \in \mathbb{R}^n$.

Lemma 2.6.6. *For each $\eta \in C_c^\infty(\mathbb{R})$, each $j \in \{1, \dots, n\}$ and each $f \in C_c^\infty(\mathbb{R}^n)$ with support in Y_j^\pm , there exists a constant $c < \infty$ such that for all $\varphi \in \mathcal{H}$,*

$$\int_1^\infty \left\| f\left(\frac{Q}{2t}\right) \left(P_j - \frac{Q_j}{2t}\right) \eta(H) e^{-iHt} \varphi \right\|^2 \frac{dt}{t} \leq c \|\varphi\|^2. \quad (2.12)$$

Furthermore,

$$s - \lim_{t \rightarrow \infty} f\left(\frac{Q}{2t}\right) \left(P_j - \frac{Q_j}{2t}\right) \eta(H) e^{-iHt} = 0.$$

Proof. Let us fix a number $c'_\eta \in \mathbb{R}$ such that $\text{supp} \eta \subset (-\infty, c'_\eta)$ and a function $\tilde{\eta} \in C_c^\infty((-\infty, c'_\eta))$ satisfying $\tilde{\eta} \eta = \eta$ and $0 \leq \tilde{\eta} \leq 1$. Let c_η be the positive constant depending on η given by the previous lemma.

a) Consider $h \in C_c^\infty(\mathbb{R})$ such that $h(|x|)f(x) = f(x)$ for all $x \in \mathbb{R}^n$ and $h(y) = 1$ if $y \in [0, c_\eta + 1)$. For $\delta > 0$ and $t \geq 1$, set

$$L(t) := \frac{1}{2} \left(P - \frac{Q}{2t}\right) \cdot \nabla r_\delta \left(\frac{Q}{2t}\right) + \frac{1}{2} \nabla r_\delta \left(\frac{Q}{2t}\right) \cdot \left(P - \frac{Q}{2t}\right) + r_\delta \left(\frac{Q}{2t}\right),$$

and $\Phi(t) := \eta(H) h \left(\frac{|Q|}{2t}\right) L(t) h \left(\frac{|Q|}{2t}\right) \eta(H)$. One can check that Φ is a self-adjoint element of $BC_H^1([1, \infty), \mathcal{B}(\mathcal{H}))$ and that

$$\begin{aligned} \mathbf{D}\Phi(t) &= \eta\{\mathbf{D}h\}Lh\eta + \eta h L\{\mathbf{D}h\}\eta - \eta h \nabla V(Q) \cdot \nabla r_\delta h \eta \\ &\quad + \frac{1}{t} \eta h \left[P - \frac{Q}{2t}\right]^T \partial^2 r_\delta \left[P - \frac{Q}{2t}\right] h \eta + O(t^{-3}), \end{aligned} \quad (2.13)$$

where $\partial^2 r_\delta$ is the matrix of second derivatives of r_δ . In order to be able to use Lemma 2.6.3, we obtain now some estimates for each term of (2.13).

Some commutator calculations, using repeatedly *i)* of Lemma 2.6.2, show that $\eta\{\mathbf{D}h\}Lh\eta + \eta h L\{\mathbf{D}h\}\eta$ can be rewritten as

$$\frac{1}{t} \eta g \left(\frac{|Q|}{2t}\right) \Psi(t) g \left(\frac{|Q|}{2t}\right) \eta + O(t^{-2}),$$

where Ψ is a bounded operator-valued mapping and g belongs to $C_c^\infty(\mathbb{R})$ and satisfies the conditions $\text{supp} g \subset (c_\eta, \infty)$ and $g(y)h'(y) = h'(y)$ for all $y \geq 0$. The statement *i)* of the previous lemma implies that the term $\frac{1}{t} \eta g \Psi g \eta$ is integrable along the evolution. We also observe that $h^2 \nabla_j r_\delta$ belongs to $C_c^\infty(\mathbb{R}^n)$ and has its support in $Y_j^- \cup Y_j^+$. Therefore, using *ii)* of Lemma 2.6.2, the term $\eta h \nabla V \cdot \nabla r_\delta h \eta$ belongs to $L^1((1, \infty), dt)$. Finally, the properties of r_δ mentioned before this lemma imply that

$$\eta h \left[P - \frac{Q}{2t}\right]^T \partial^2 r_\delta \left[P - \frac{Q}{2t}\right] h \eta \geq \eta h \left(P_j - \frac{Q_j}{2t}\right) \xi^2 \left(\pm \frac{Q_j}{4\delta t}\right) \left(P_j - \frac{Q_j}{2t}\right) h \eta$$

for any asymptotic localization function ξ and each $j \in \{1, \dots, n\}$. Thus, by applying Lemma 2.6.3 with $B^*(t)B(t) = \frac{1}{t} \eta h \left(P_j - \frac{Q_j}{2t}\right) \xi^2 \left(\pm \frac{Q_j}{4\delta t}\right) \left(P_j - \frac{Q_j}{2t}\right) h \eta$, one obtains that there exists $c < \infty$ such that for each $j \in \{1, \dots, n\}$ and all $\varphi \in \mathcal{H}$:

$$\int_1^\infty \left\| \xi \left(\pm \frac{Q_j}{4\delta t}\right) \left(P_j - \frac{Q_j}{2t}\right) h \left(\frac{|Q|}{2t}\right) \eta(H) e^{-iHt} \varphi \right\|^2 \frac{dt}{t} \leq c \|\varphi\|^2. \quad (2.14)$$

Since f has a compact support in Y_j^\pm , we may fix j and δ such that $\xi\left(\pm\frac{x_j}{2\delta}\right)f(x) = f(x)$ for all $x \in \mathbb{R}^n$. Then the first assertion of the lemma is a simple consequence of (2.14) and of the estimate $\left[P_j, h\left(\frac{|\mathcal{Q}|}{2t}\right)\right] \in O(t^{-1})$.

b) For $t \geq 1$, set

$$\Phi(t) := \eta(H) \left\{ P_j - \frac{Q_j}{2t} \right\} f\left(\frac{Q}{2t}\right) \tilde{\eta}^2(H) f\left(\frac{Q}{2t}\right) \left\{ P_j - \frac{Q_j}{2t} \right\} \eta(H),$$

and notice that Φ belongs to $BC_H^1([1, \infty), \mathcal{B}(\mathcal{H}))$. One can check that

$$\begin{aligned} \mathbf{D}\Phi(t) &= -\frac{2}{t}\Phi(t) - \eta\nabla_j V f \tilde{\eta}^2 f \left\{ P_j - \frac{Q_j}{2t} \right\} \eta - \eta \left\{ P_j - \frac{Q_j}{2t} \right\} f \tilde{\eta}^2 f \nabla_j V \eta \\ &+ \frac{1}{2t} \eta \left\{ P_j - \frac{Q_j}{2t} \right\} \left\{ \left(P - \frac{Q}{2t} \right) \cdot \nabla f + \nabla f \cdot \left(P - \frac{Q}{2t} \right) \right\} \tilde{\eta}^2 f \left\{ P_j - \frac{Q_j}{2t} \right\} \eta \\ &+ \frac{1}{2t} \eta \left\{ P_j - \frac{Q_j}{2t} \right\} f \tilde{\eta}^2 \left\{ \left(P - \frac{Q}{2t} \right) \cdot \nabla f + \nabla f \cdot \left(P - \frac{Q}{2t} \right) \right\} \left\{ P_j - \frac{Q_j}{2t} \right\} \eta. \end{aligned}$$

Having in mind the use of Lemma 2.6.4, we collect some estimates for each of these terms.

The second and the third terms on the r.h.s. belong to $L^1((1, \infty), dt)$ because $\eta\nabla_j V f \tilde{\eta}$ and $\tilde{\eta} f \nabla_j V \eta$ are integrable in norm and the remaining factors are norm bounded independently of t for $t \geq 1$. Some further commutator calculations based on Lemma 2.6.2 show that the last two terms of the r.h.s. can be rewritten as

$$\frac{1}{2t} \eta \left\{ P_j - \frac{Q_j}{2t} \right\} g\left(\frac{Q}{2t}\right) \Psi(t) g\left(\frac{Q}{2t}\right) \left\{ P_j - \frac{Q_j}{2t} \right\} \eta + O(t^{-2}),$$

where Ψ is a well defined bounded operator-valued mapping and g is a $C_c^\infty(\mathbb{R}^n)$ -function with support in Y_j^\pm and satisfying $gf = f$. One has now the estimate

$$\begin{aligned} & \frac{1}{2t} \left| \langle \psi, \eta \left\{ P_j - \frac{Q_j}{2t} \right\} g \Psi g \left\{ P_j - \frac{Q_j}{2t} \right\} \eta \varphi \rangle \right| \\ & \leq \frac{c}{t} \left\| g \left\{ P_j - \frac{Q_j}{2t} \right\} \eta \psi \right\| \left\| g \left\{ P_j - \frac{Q_j}{2t} \right\} \eta \varphi \right\| \end{aligned}$$

for some positive constant $c < \infty$ and all $\psi, \varphi \in \mathcal{H}$.

Since the term $-\frac{2}{t}\Phi(t)$ satisfies a similar estimate, we can apply Lemma 2.6.4 with $E_k = F_k = \sqrt{\frac{c}{t}} g \left\{ P_j - \frac{Q_j}{2t} \right\} \eta$. By taking into account the first statement of the present lemma we obtain the existence of $s - \lim_{t \rightarrow \infty} e^{iHt} \Phi(t) e^{-iHt}$. It follows that the limit $\lim_{t \rightarrow \infty} \left\| \tilde{\eta}(H) f\left(\frac{Q}{2t}\right) \left(P_j - \frac{Q_j}{2t} \right) \eta(H) e^{-iHt} \varphi \right\|$ exists for each $\varphi \in \mathcal{H}$. By commuting $\tilde{\eta}(H)$ to the right with the help of *i*) and *iii*) of Lemma 2.6.2, we get that $\lim_{t \rightarrow \infty} \left\| f\left(\frac{Q}{2t}\right) \left(P_j - \frac{Q_j}{2t} \right) \eta(H) e^{-iHt} \varphi \right\|$ exists for each $\varphi \in \mathcal{H}$. But this limit has to be equal to zero because of (2.12). \square

We now prove the existence of the asymptotic velocity. One major ingredient is a class of functions with some special property. Let \mathfrak{F} be the set of all functions

$f \in C_c^\infty(\mathbb{R}^n)$ such that, for each $j \in \{1, \dots, n\}$, there exists a neighbourhood of the hypersurface $x_j = 0$ in which f does not depend on x_j . One can check that \mathfrak{F} is dense in $C_0(\mathbb{R}^n)$.

Lemma 2.6.7. *For each $f \in C_0(\mathbb{R}^n)$, the following limit exists:*

$$s - \lim_{t \rightarrow \infty} e^{iHt} f \left(\frac{Q}{2t} \right) e^{-iHt}.$$

Proof. By density in \mathcal{H} of the set of vectors of the form $\eta^2(H)\varphi$ with $\eta \in C_c^\infty(\mathbb{R})$ and $\varphi \in \mathcal{H}$, it is enough to prove that $s - \lim_{t \rightarrow \infty} e^{iHt} f \left(\frac{Q}{2t} \right) e^{-iHt} \eta^2(H)$ exists, which is equivalent by *i*) of Lemma 2.6.2 with the existence of

$$s - \lim_{t \rightarrow \infty} \eta(H) e^{iHt} f \left(\frac{Q}{2t} \right) e^{-iHt} \eta(H). \quad (2.15)$$

Since \mathfrak{F} is dense in $C_0(\mathbb{R}^n)$, there is also no loss of generality in assuming that $f \in \mathfrak{F}$. For $t \geq 1$, set

$$\Phi(t) := \eta \left\{ \frac{1}{2} \left(P - \frac{Q}{2t} \right) \cdot \nabla f \left(\frac{Q}{2t} \right) + \frac{1}{2} \nabla f \left(\frac{Q}{2t} \right) \cdot \left(P - \frac{Q}{2t} \right) + f \left(\frac{Q}{2t} \right) \right\} \eta.$$

One observes that $\Phi \in BC_H^1([1, \infty), \mathcal{B}(\mathcal{H}))$ and that, similarly to (2.13),

$$\mathbf{D}\Phi(t) = -\eta \nabla f \cdot \nabla V(Q) \eta + \frac{1}{t} \eta \left[P - \frac{Q}{2t} \right]^T \partial^2 f \left[P - \frac{Q}{2t} \right] \eta + O(t^{-3}). \quad (2.16)$$

For each $j \in \{1, \dots, n\}$, $\nabla_j f$ belongs to $C_c^\infty(\mathbb{R}^n)$ and has its support in $Y_j^- \cup Y_j^+$. Thus by *ii*) of Lemma 2.6.2 the first term on the r.h.s. of (2.16) belongs to $L^1((1, \infty), dt)$. The second term is equal to

$$\sum_{j,k=1}^n \frac{1}{t} \eta \left(P_j - \frac{Q_j}{2t} \right) g_j \left(\frac{Q}{2t} \right) \{ \partial_{jk}^2 f \} g_k \left(\frac{Q}{2t} \right) \left(P_k - \frac{Q_k}{2t} \right) \eta,$$

where each g_j belongs to $C_c^\infty(\mathbb{R}^n)$, has support in $Y_j^- \cup Y_j^+$ and satisfies $g_j \nabla_j f = \nabla_j f$. By applying Lemma 2.6.4 and by using the first statement of Lemma 2.6.6, one obtains the existence of $s - \lim_{t \rightarrow \infty} e^{iHt} \Phi(t) e^{-iHt}$. But the second assertion of Lemma 2.6.6 implies that this limit is equal to (2.15), which therefore exists. \square

Assume for a while that f is a complex function belonging to $C_0(\mathbb{R}^n)$. By writing $f = f_1 + if_2$ with f_1, f_2 two real $C_0(\mathbb{R}^n)$ -functions, one gets from the previous lemma the existence of $s - \lim_{t \rightarrow \infty} e^{iHt} f \left(\frac{Q}{2t} \right) e^{-iHt}$, which we denote by $\mathfrak{P}(f)$. Since $\mathfrak{P}(fg) = \mathfrak{P}(f)\mathfrak{P}(g)$ and $\mathfrak{P}(\bar{f}) = \mathfrak{P}(f)^*$ for two complex functions $f, g \in C_0(\mathbb{R}^n)$, the mapping $\mathfrak{P} : C_0(\mathbb{R}^n) \rightarrow \mathcal{B}(\mathcal{H})$ is a morphism between two C*-algebras. Let $BO(\mathbb{R}^n)$ be the unital C*-algebra of bounded Borel functions on \mathbb{R}^n . We say that a sequence $\{f_k\}_{k \in \mathbb{N}}$ in $C_0(\mathbb{R}^n)$ is *boundedly convergent* if the limit $\lim_{k \rightarrow \infty} f_k(x) \equiv f(x)$ exists for each $x \in \mathbb{R}^n$ and $|f_k(x)| \leq c$ for some constant $c < \infty$ independent of k and x (f belongs

then to $BO(\mathbb{R}^n)$, cf. [ABG], Section 8.1.1). It is also proved in this reference that the morphism \mathfrak{P} has a unique extension to a morphism $\tilde{\mathfrak{P}} : BO(\mathbb{R}^n) \rightarrow \mathcal{B}(\mathcal{H})$ such that $s - \lim_{k \rightarrow \infty} \tilde{\mathfrak{P}}(f_k) = \tilde{\mathfrak{P}}(f)$ if $\{f_k\}_{k \in \mathbb{N}}$ converges boundedly to f .

Let χ_{Ξ} denote the characteristic function of the Borel set $\Xi \subset \mathbb{R}^n$ and $\mathbb{I}_{\Xi} := \tilde{\mathfrak{P}}(\chi_{\Xi})$. Then $\mathbb{I} : \mathbb{R}^n \supset \Xi \mapsto \mathbb{I}_{\Xi} \in \mathcal{B}(\mathcal{H})$ determines a projection-valued measure on \mathbb{R}^n . In the next lemma we shall prove that $\mathbb{I}_{\mathbb{R}^n}$ is the identity operator in $\mathcal{B}(\mathcal{H})$, and therefore \mathbb{I} becomes a spectral measure on \mathbb{R}^n . So, if $\mathcal{P} := \int_{\mathbb{R}^n} x \mathbb{I}(dx)$ is the n -tuple of commuting self-adjoint operators in \mathcal{H} determined by \mathbb{I} , then clearly $\mathfrak{P}(f) = f(\mathcal{P})$. The n -tuple \mathcal{P} is commonly called the asymptotic velocity.

Lemma 2.6.8. *i) The projection-valued measure \mathbb{I} satisfies the relation $\mathbb{I}_{\mathbb{R}^n} = I$.*

ii) For each $\eta \in C_0(\mathbb{R})$ and each $f \in C_0(\mathbb{R}^n)$ one has $[\eta(H), f(\mathcal{P})] = 0$, i.e. the asymptotic velocity \mathcal{P} commutes with the Hamiltonian H .

Proof. a) Let $f \in C_c^\infty(\mathbb{R})$ be such that $f = 1$ in a neighbourhood of 0. Then, since $\left\{f\left(\frac{|\cdot|}{r}\right)\right\}_{r \geq 1}$ converges boundedly to the function $\mathbb{R}^n \ni x \mapsto 1$, the relation $\mathbb{I}_{\mathbb{R}^n} = I$ is satisfied if $s - \lim_{r \rightarrow \infty} s - \lim_{t \rightarrow \infty} e^{iHt} f\left(\frac{|Q|}{2rt}\right) e^{-iHt} = I$.

Let $\eta \in C_c^\infty(\mathbb{R})$ and $r \geq 1$. Using *i)* of Lemma 2.6.2, one observes that

$$s - \lim_{t \rightarrow \infty} \left\{ I - e^{iHt} f\left(\frac{|Q|}{2rt}\right) e^{-iHt} \right\} \eta^2 = s - \lim_{t \rightarrow \infty} e^{iHt} \eta \left\{ I - f\left(\frac{|Q|}{2rt}\right) \right\} \eta e^{-iHt}.$$

The r.h.s. is zero for r large enough (depending on η) by the second assertion of Lemma 2.6.5. Hence $s - \lim_{r \rightarrow \infty} s - \lim_{t \rightarrow \infty} \left\{ I - e^{iHt} f\left(\frac{|Q|}{2rt}\right) e^{-iHt} \right\} \eta^2(H) = 0$. Since the set of vectors of the form $\eta^2(H)\varphi$ with $\eta \in C_c^\infty(\mathbb{R})$ and $\varphi \in \mathcal{H}$ is dense in \mathcal{H} , this finishes the proof of *i)*.

b) The proof that $[\eta(H), f(\mathcal{P})] = 0$ for each $\eta \in C_c^\infty(\mathbb{R})$ and each $f \in C_c^\infty(\mathbb{R}^n)$ is easily obtained with the help of the statement *i)* of Lemma 2.6.2. The assertion *ii)* follows then by density of $C_c^\infty(\mathbb{R}^n)$ in $C_0(\mathbb{R}^n)$ and density of $C_c^\infty(\mathbb{R})$ in $C_0(\mathbb{R})$. \square

The next statement is usually called *minimal velocity estimate*. It is a non-trivial consequence of the Mourre estimate obtained in Section 2.5. We point out that the $C_u^1(A)$ -condition of Proposition 2.6.1 is required in order to fulfil the hypotheses of Proposition 2.5.4. Let us recall that $\kappa(H)$ is a closed countable set which contains the thresholds and the eigenvalues of H .

Lemma 2.6.9. *For each $\eta \in C_c^\infty(\mathbb{R} \setminus \kappa(H))$, there exists $\varepsilon_\eta > 0$ such that for some $c < \infty$ and all $\varphi \in \mathcal{H}$,*

$$\int_1^\infty \left\| \chi_{[0, \varepsilon_\eta]} \left(\frac{|Q|}{2t} \right) \eta(H) e^{-iHt} \varphi \right\|^2 \frac{dt}{t} \leq c \|\varphi\|^2.$$

Proof. Let $\tilde{\eta} \in C_c^\infty(\mathbb{R} \setminus \kappa(H))$ be such that $\tilde{\eta}\eta = \eta$ and $0 \leq \tilde{\eta} \leq 1$. Let $\theta := \min_\lambda \varrho_H^A(\lambda)$ for $\lambda \in \text{supp } \tilde{\eta}$. It follows from Propositions 2.5.3 and 2.5.4 that θ is strictly positive and that $\tilde{\eta}(H)[iH, A]\tilde{\eta}(H) \geq \theta \tilde{\eta}^2(H)$.

We now fix ε_η and ε'_η such that $0 < \varepsilon_\eta < \varepsilon'_\eta < \frac{\theta}{2n} (\sup_j \|\tilde{\eta}(H)P_j\|)^{-1}$. The case $\tilde{\eta}(H) = 0$ is excluded because the statement is then trivial. If $B(0, \delta)$ denotes the open ball in \mathbb{R}^n of center 0 and radius $\delta > 0$, let $f \in \mathfrak{F}$ be such that $\text{supp} f \subset B(0, \varepsilon'_\eta)$ and $f = 1$ on $B(0, \varepsilon_\eta)$. Let also $\tilde{f} \in C_c^\infty(\mathbb{R}^n)$ with support in $B(0, \varepsilon'_\eta)$ be such that $\tilde{f}f = f$ and $0 \leq \tilde{f} \leq 1$. For $t \geq 1$, set

$$M(t) := \left(P - \frac{Q}{2t}\right) \cdot \nabla f \left(\frac{Q}{2t}\right) + f \left(\frac{Q}{2t}\right) \quad \text{and} \quad \Phi(t) := \eta(H)M\tilde{\eta}(H)\frac{A}{t}\tilde{\eta}(H)M^*\eta(H).$$

The statement *v)* of Lemma 2.6.2 assures that Φ is a bounded operator-valued mapping. Moreover, one can easily check that Φ is differentiable in norm with bounded derivative. It follows then that $\Phi \in BC_H^1([1, \infty), \mathcal{B}(\mathcal{H}))$. So, let us calculate the Heisenberg derivative of Φ :

$$\begin{aligned} \mathbf{D}\Phi(t) = & -\eta\nabla f \cdot \nabla V \tilde{\eta} \frac{A}{t} \tilde{\eta} M^* \eta - \eta M \tilde{\eta} \frac{A}{t} \tilde{\eta} \nabla f \cdot \nabla V \eta \\ & + \frac{1}{t} \eta \left[P - \frac{Q}{2t} \right]^x \partial^2 f \left[P - \frac{Q}{2t} \right] \tilde{\eta} \frac{A}{t} \tilde{\eta} M^* \eta + \text{hc} \\ & + \eta M \tilde{\eta} \left\{ \left[iH, \frac{A}{t} \right] - \frac{A}{t^2} \right\} \tilde{\eta} M^* \eta + O(t^{-2}). \end{aligned} \quad (2.17)$$

In order to be able to use Lemma 2.6.3 we obtain now some estimates for each of these terms.

Since $f \in \mathfrak{F}$, the statement *ii)* of Lemma 2.6.2 implies that the first two terms on the r.h.s. of (2.17) belong to $L^1((1, \infty), dt)$. Some further commutator calculations (based on Lemma 2.6.2) show that the third and the fourth terms on the r.h.s. of (2.17) can be rewritten as

$$\begin{aligned} & \sum_{j,k=1}^n \frac{1}{t} \eta \left(P_j - \frac{Q_j}{2t} \right) g_j \left(\frac{Q}{2t} \right) \Psi_{jk}(t) g_k \left(\frac{Q}{2t} \right) \left(P_k - \frac{Q_k}{2t} \right) \eta \\ & + O(t^{-2}) + \frac{1}{t} L^1((1, \infty), dt), \end{aligned} \quad (2.18)$$

where $\Psi_{jk} = (\partial_{jk}^2 f) \tilde{\eta} \frac{A}{t} \tilde{\eta} M^* \tilde{\eta} + \tilde{\eta} M \tilde{\eta} \frac{A}{t} \tilde{\eta} (\partial_{jk}^2 f)$ is a bounded operator-valued mapping and each g_j belongs to $C_c^\infty(\mathbb{R}^n)$, has its support in $Y_j^- \cup Y_j^+$ and satisfies $g_j \nabla_j f = \nabla_j f$. By taking Lemma 2.6.6 into account, one finds that the first term of (2.18) is integrable along the evolution.

For the fifth term on the r.h.s. of (2.17) one can check that

$$\eta M \tilde{\eta} \left[iH, \frac{A}{t} \right] \tilde{\eta} M^* \eta \geq \frac{\theta}{t} \eta M \tilde{\eta}^2 M^* \eta = \frac{\theta}{t} \eta M M^* \eta + O(t^{-2}) + \frac{1}{t} L^1((1, \infty), dt), \quad (2.19)$$

where the equality has been obtained with the help of *i)* and *iii)* of Lemma 2.6.2. Furthermore, since $A = \frac{1}{4}(P \cdot Q + Q \cdot P)$, one finds that (by commuting the first \tilde{f} to the right for the second inequality)

$$\begin{aligned} \left\| \tilde{f} \tilde{\eta} \frac{A}{t} \tilde{\eta} \tilde{f} \right\| & \leq \left\| \tilde{f} \tilde{\eta} P \cdot \frac{Q}{2t} \tilde{\eta} \tilde{f} \right\| + O(t^{-1}) \leq n \sup_j \left\{ \|\tilde{\eta} P_j\| \left\| \tilde{f} \frac{Q_j}{2t} \right\| \right\} + O(t^{-1}) \\ & \leq n \varepsilon'_\eta \sup_j \|\tilde{\eta} P_j\| + O(t^{-1}), \end{aligned}$$

which is less than $\frac{\theta}{2} + O(t^{-1})$. It follows that

$$-\frac{1}{t}\eta M \tilde{f} \tilde{\eta} \frac{A}{t} \tilde{\eta} \tilde{f} M^* \eta \geq -\frac{\theta}{2t} \eta M M^* \eta + O(t^{-2})$$

and hence one gets that:

$$\eta M \tilde{\eta} \left\{ \left[iH, \frac{A}{t} \right] - \frac{A}{t^2} \right\} \tilde{\eta} M^* \eta \geq \frac{\theta}{2t} \eta M M^* \eta + O(t^{-2}) + \frac{1}{t} L^1((1, \infty), dt). \quad (2.20)$$

From the inequality $(a+b)(a+b)^* \geq (1-\nu)aa^* + (1-\frac{1}{\nu})bb^*$, valid for any ν with $0 < \nu < 1$ one deduces that (take $\nu = \frac{1}{2}$)

$$\eta M M^* \eta \geq \frac{1}{2} \eta f^2 \eta - \eta \left\{ P - \frac{Q}{2t} \right\} \cdot \nabla f \nabla f \cdot \left\{ P - \frac{Q}{2t} \right\} \eta. \quad (2.21)$$

One can check with Lemma 2.6.6 that the term $\frac{1}{t} \eta \left\{ P - \frac{Q}{2t} \right\} \cdot \nabla f \nabla f \cdot \left\{ P - \frac{Q}{2t} \right\} \eta$ is integrable along the evolution. Thus by inserting (2.21) into (2.20), by applying then Lemma 2.6.3 with the term $B^*(t)B(t)$ equal to $\frac{\theta}{4t} \eta f^2 \eta$ and by taking into account all previous estimates, one obtains the expected result. \square

In the next lemma, we prove that the subspace of \mathcal{H} of the states with zero asymptotic velocity is equal to the subspace spanned by the eigenvectors of H .

Lemma 2.6.10. *The range of $E_{\{0\}}(\mathcal{P})$ is equal to the range of $E_p(H)$.*

Proof. First, let $\varphi \in \mathcal{H}$ such that $H\varphi = \lambda\varphi$. For each $f \in C_0(\mathbb{R}^n)$ and $t \geq 1$, one has

$$\begin{aligned} \left\| e^{iHt} f \left(\frac{Q}{2t} \right) e^{-iHt} \varphi - f(0)\varphi \right\| &= \left\| e^{i(H-\lambda)t} f \left(\frac{Q}{2t} \right) \varphi - f(0)\varphi \right\| \\ &= \left\| \left(f \left(\frac{Q}{2t} \right) - f(0) \right) \varphi \right\|. \end{aligned}$$

The r.h.s. tends to zero as t increases, and therefore $f(\mathcal{P})\varphi = f(0)\varphi$, or equivalently $\varphi \in E_{\{0\}}(\mathcal{P})\mathcal{H}$. Since $E_p(H)$ and $E_{\{0\}}(\mathcal{P})$ are closed subspaces, it follows that any $\varphi \in E_p(H)\mathcal{H}$ belongs to $E_{\{0\}}(\mathcal{P})\mathcal{H}$.

Let us now show that $E_{\{0\}}(\mathcal{P})\mathcal{H}$ is orthogonal to the continuous subspace of \mathcal{H} with respect to H . So let $\varphi \in E_{\{0\}}(\mathcal{P})\mathcal{H}$, i.e. $f(\mathcal{P})\varphi = f(0)\varphi$ for each $f \in C_0(\mathbb{R}^n)$. It is enough to prove that $\langle \psi, \varphi \rangle = 0$ for any ψ satisfying $\eta(H)\psi = \psi$ with $\eta \in C_c^\infty(\mathbb{R} \setminus \kappa(H))$. Let ε_η be given by the previous lemma, and let $f \in C_c^\infty(\mathbb{R}^n)$ with support in $B(0, \varepsilon_\eta)$ be such that $f(0) \neq 0$. We observe that $\lim_{t \rightarrow \infty} \eta e^{iHt} f^2 \left(\frac{Q}{2t} \right) e^{-iHt} \eta = 0$ since the limit exists and since there exists $c < \infty$ such that $\int_1^\infty \left\| f \left(\frac{Q}{2t} \right) \eta(H) e^{-iHt} v \right\|^2 \frac{dt}{t} \leq c \|v\|^2$ for all $v \in \mathcal{H}$. We finally have

$$\langle \psi, \varphi \rangle = \frac{1}{f^2(0)} \langle \eta \psi, f^2(\mathcal{P}) \eta \varphi \rangle = \frac{1}{f^2(0)} \lim_{t \rightarrow \infty} \langle \eta e^{iHt} f^2 \left(\frac{Q}{2t} \right) e^{-iHt} \eta \psi, \varphi \rangle = 0.$$

\square

2.7 Asymptotic completeness

In this last section, we prove the existence of some suitably defined wave operators and, as a by-product, obtain the asymptotic completeness. For this purpose, we assume firstly that V is a cartesian potential such that $H = -\Delta + V$ is of class $C_u^1(A)$, and secondly that V satisfies the requirement

$$\int_0^\infty \left\| \xi \left((\beta - \alpha) \cdot \frac{Q}{r} \right) (V^\alpha(Q) - V^\beta(Q)) \right\|_{\mathcal{H}_\alpha^2 \rightarrow \mathcal{H}_\alpha} dr < \infty \quad (2.22)$$

for each $\alpha \in \mathcal{L}$, each $\beta \prec \alpha$ and some asymptotic localization function ξ . This last assumption means that each function V^α tends to its asymptotic limits in a short-range way.

Let us show that the above hypotheses are sufficient for the existence of the asymptotic velocity for each operator H^α . Indeed, let $\alpha, \beta \in \mathcal{L}$ and $j \in \{1, \dots, n\}$ be such that $\beta \prec \alpha$, $\alpha_j = 0$ and $\beta_j = \pm 1$. In such a situation V^β does not depend on x_j , and thus $\nabla_j V^\alpha(Q)$ is formally equal to $iP_j(V^\alpha(Q) - V^\beta(Q)) - i(V^\alpha(Q) - V^\beta(Q))P_j$. Then some simple calculations, using this observation and the assumption (2.22), show that for each j such that $\alpha_j = 0$:

$$\int_0^\infty \left\| \xi \left(\pm \frac{Q_j}{r} \right) \nabla_j V^\alpha(Q) \right\|_{\mathcal{H}_\alpha^2 \rightarrow \mathcal{H}_\alpha^{-2}} dr < \infty. \quad (2.23)$$

Let us notice that in the special case $\alpha = o$, (2.23) is nothing but (2.6). So, for each $\alpha \in \mathcal{L}$, V^α is a cartesian potential relative to \mathcal{L}^α which satisfies (2.23) and such that $H^\alpha = -\Delta^\alpha + V^\alpha$ is of class $C_u^1(A^\alpha)$ (cf. Lemma 2.5.2). A proposition similar to Proposition 2.6.1 can therefore be stated for H^α , with the only difference that the corresponding asymptotic velocity \mathcal{P}^α is a $|\alpha|$ -tuple instead of a n -tuple. For the case $\alpha = o$, we keep the notation \mathcal{P} instead of \mathcal{P}^o .

Moreover, a direct consequence of Lemma 9.4.8 of [ABG] is that if the requirement (2.22) is assumed, then this condition is also satisfied with the norm $\|\cdot\|_{\mathcal{H}^2 \rightarrow \mathcal{H}}$ instead of the norm $\|\cdot\|_{\mathcal{H}_\alpha^2 \rightarrow \mathcal{H}_\alpha}$. It follows that (2.23) is fulfilled with the norm $\|\cdot\|_{\mathcal{H}^2 \rightarrow \mathcal{H}^{-2}}$ instead of the norm $\|\cdot\|_{\mathcal{H}_\alpha^2 \rightarrow \mathcal{H}_\alpha^{-2}}$. We notice furthermore that (2.23) is trivially satisfied for k such that $\alpha_k \neq 0$ (since V^α does not depend on the variable x_k) and that V^α is a cartesian potential relative to \mathcal{L} . Hence, since $H_\alpha = -\Delta + V^\alpha$ is of class $C_u^1(A)$, the hypotheses of Proposition 2.6.1 are fulfilled with H_α instead of H , and all developments of the previous section can be rewritten in terms of H_α . Let \mathcal{P}_α denote the asymptotic velocity obtained for the operator H_α . The relation between \mathcal{P}_α and \mathcal{P}^α will be given later on.

Let us mention that there exist situations for which the condition (2.22) can easily be checked.

Example 2.7.1. If V is the sum of a Mourre potential V_m constructed in Example 2.5.5 and of a short-range potential V_{SR} satisfying $\lim_{r \rightarrow \infty} \left\| \xi \left(\frac{|Q|}{r} \right) V_{\text{SR}}(Q) \right\|_{\mathcal{H}^2 \rightarrow \mathcal{H}} = 0$ for some asymptotic localization function ξ , then (2.22) is automatically satisfied. A similar conclusion is obtained if in Example 2.5.6 each V_j reaches its limits in a short-range way. In both situations all hypotheses of Theorems 2.1.1 and 2.1.2 are fulfilled.

Proposition 2.7.2. *Let V be a cartesian potential such that $H = -\Delta + V$ is of class $C_u^1(A)$. Assume moreover that the condition (2.22) is satisfied. Then for each $\alpha \in \mathcal{L}$, the following wave operators exist:*

$$W_{\alpha o}^+ := s - \lim_{t \rightarrow +\infty} e^{iH_\alpha t} e^{-iHt} E_{Y_\alpha}(\mathcal{P}),$$

$$W_{o\alpha}^+ := s - \lim_{t \rightarrow +\infty} e^{iHt} e^{-iH_\alpha t} E_{Y_\alpha}(\mathcal{P}_\alpha).$$

These operators satisfy the relations

$$W_{o\alpha}^+ E_\Xi(\mathcal{P}_\alpha) = E_\Xi(\mathcal{P}) W_{\alpha o}^+ \quad \text{and} \quad W_{\alpha o}^+ E_\Xi(\mathcal{P}) = E_\Xi(\mathcal{P}_\alpha) W_{o\alpha}^+ \quad (2.24)$$

for any Borel subset Ξ of Y_α .

Proof. In order to prove the existence of $W_{\alpha o}^+$, it is enough to show that for each $\eta \in C_c^\infty(\mathbb{R})$ and each f in a dense subset of all $C_0(\mathbb{R}^n)$ -functions with support in Y_α , the limit $s - \lim_{t \rightarrow \infty} e^{iH_\alpha t} e^{-iHt} f(\mathcal{P}) \eta^2(H)$ exists.

a) Let $f \in \mathfrak{F}$ be such that $\text{supp } f \subset Y_\alpha$. For $t \geq 1$, set

$$M(t) := f\left(\frac{Q}{2t}\right) + \nabla f\left(\frac{Q}{2t}\right) \cdot \left(P - \frac{Q}{2t}\right) \quad \text{and} \quad \Phi(t) := \eta(H_\alpha) M(t) \eta(H).$$

One can check that Φ belongs to $BC^1([1, \infty), \mathcal{B}(\mathcal{H}))$. Let us assume for a while that the limit $s - \lim_{t \rightarrow \infty} e^{iH_\alpha t} \Phi(t) e^{-iHt}$ exists. Then one observes that (in the strong topology)

$$\begin{aligned} \lim_{t \rightarrow \infty} e^{iH_\alpha t} \eta(H_\alpha) M(t) \eta(H) e^{-iHt} &= \lim_{t \rightarrow \infty} e^{iH_\alpha t} \eta(H) M(t) \eta(H) e^{-iHt} \\ &= \lim_{t \rightarrow \infty} e^{iH_\alpha t} \eta(H) f\left(\frac{Q}{2t}\right) \eta(H) e^{-iHt} = \lim_{t \rightarrow \infty} e^{iH_\alpha t} e^{-iHt} f(\mathcal{P}) \eta^2(H), \end{aligned}$$

where we have used successively *iv)* of Lemma 2.6.2, the second assertion of Lemma 2.6.6 and the hypothesis $f \in \mathfrak{F}$, and finally the existence of the asymptotic velocity \mathcal{P} . Thus the existence of $s - \lim_{t \rightarrow \infty} e^{iH_\alpha t} e^{-iHt} f(\mathcal{P}) \eta^2(H)$ follows from the existence of $s - \lim_{t \rightarrow \infty} e^{iH_\alpha t} \Phi(t) e^{-iHt}$, and the latter will be established below with the help of Lemma 2.6.4.

b) One can check that

$$\begin{aligned} iH_\alpha \Phi(t) - i\Phi(t)H + \frac{d}{dt} \Phi(t) &= -i\eta(H_\alpha)(V(Q) - V^\alpha(Q))M\eta(H) \\ + \eta(H_\alpha) \left\{ -\nabla f \cdot \nabla V + \frac{1}{t} \left[P - \frac{Q}{2t} \right]^T \partial^2 f \left[P - \frac{Q}{2t} \right] \right\} \eta(H) &+ O(t^{-2}). \end{aligned} \quad (2.25)$$

Since $\nabla_j f$ has support in $Y_j^- \cup Y_j^+$, the term $\eta(H_\alpha) \nabla f \cdot \nabla V \eta(H)$ belongs to $L^1((1, \infty), dt)$ (the proof of this fact is similar to that of the statement *ii)* of Lemma 2.6.2). One observes that the term $\frac{1}{t} \eta(H_\alpha) \left[P - \frac{Q}{2t} \right]^T \partial^2 f \left[P - \frac{Q}{2t} \right] \eta(H)$ in (2.25) is equal to

$$\sum_{j,k=1}^n \frac{1}{t} \eta(H_\alpha) \left(P_j - \frac{Q_j}{2t} \right) g_j \left(\frac{Q}{2t} \right) \{ \partial_{jk}^2 f \} g_k \left(\frac{Q}{2t} \right) \left(P_k - \frac{Q_k}{2t} \right) \eta(H), \quad (2.26)$$

where each g_j belongs to $C_c^\infty(\mathbb{R}^n)$, has support in $Y_j^- \cup Y_j^+$ and satisfies $g_j \nabla_j f = \nabla_j f$. In relation with (2.26), it is useful to recall (from Lemma 2.6.6) that for each $k \in \{1, \dots, n\}$, there exists $c < \infty$ such that

$$\int_1^\infty \left\| g_k \left(\frac{Q}{2t} \right) \left(P_k - \frac{Q_k}{2t} \right) \eta(H) e^{-iHt} \varphi \right\|^2 \frac{dt}{t} \leq c \|\varphi\|^2$$

for all $\varphi \in \mathcal{H}$, and that a similar result can be obtained with H_α instead of H (see the discussion before Example 2.7.1).

We finally notice that $\int_1^\infty \left\| \prod_{\{j|\alpha_j \neq 0\}} \xi \left(\alpha_j \frac{Q_j}{\delta r} \right) (V - V^\alpha) \right\|_{\mathcal{H}^2 \rightarrow \mathcal{H}} dr < \infty$ for each $\delta > 0$. This follows directly from (2.22) and Lemma 9.4.8 of [ABG] by inserting and removing suitable terms between V and V^α . Then by choosing δ such that $\prod_{\{j|\alpha_j \neq 0\}} \xi \left(\alpha_j \frac{x_j}{\delta} \right) f(x) = f(x)$ for all $x \in \mathbb{R}^n$, one can easily show that $\eta(H_\alpha)(V - V^\alpha)M\eta(H)$ belongs to $L^1((1, \infty), dt)$.

In view of the preceding estimates, the existence of

$$s - \lim_{t \rightarrow \infty} e^{iH_\alpha t} \Phi(t) e^{-iHt}$$

is seen to be a direct consequence of Lemma 2.6.4.

c) By similar arguments, we can show the existence of $W_{\alpha\alpha}^+$. For the last assertion of the proposition, one easily observes that $W_{\alpha\alpha}^+ f(\mathcal{P}_\alpha) = f(\mathcal{P})W_{\alpha\alpha}^+$ and that $W_{\alpha\alpha}^+ f(\mathcal{P}) = f(\mathcal{P}_\alpha)W_{\alpha\alpha}^+$ for each $f \in C_0(\mathbb{R}^n)$ with support in Y_α . The conclusion follows then by taking a sequence $\{f_k\}_{k \in \mathbb{N}}$ of functions in $C_0(\mathbb{R}^n)$ with $\text{supp} f_k \subset Y_\alpha$ such that this sequence converges boundedly to χ_Ξ . \square

Proof of Theorem 2.1.2. Since Z_α is a subset of Y_α , the existence of Ω_α^+ follows from Proposition 2.7.2. One gets from the relations (2.24) that

$$\text{Ran}(W_{\alpha\alpha}^+ E_{Z_\alpha}(\mathcal{P}_\alpha)) \subset E_{Z_\alpha}(\mathcal{P})\mathcal{H} \quad \text{and} \quad \text{Ran}(W_{\alpha\alpha}^+ E_{Z_\alpha}(\mathcal{P})) \subset E_{Z_\alpha}(\mathcal{P}_\alpha)\mathcal{H}.$$

The Lemma B.5.1 of [DG] implies then the second part of the assertion *i*).

Clearly $I = \sum_{\alpha \in \mathcal{L}} E_{Z_\alpha}(\mathcal{P})$ and by using Lemma 2.6.10 and the absence of singularly continuous spectrum, one obtains the equalities:

$$\mathcal{H}_{\text{ac}}(H) = \bigoplus_{\alpha \neq 0} E_{Z_\alpha}(\mathcal{P})\mathcal{H} = \bigoplus_{\alpha \neq 0} \text{Ran } \Omega_\alpha^+.$$

The statement *iii*) is due to the relation between \mathcal{P}^α and \mathcal{P}_α . Since $H_\alpha = -\Delta^{\alpha^+} \otimes I + I \otimes H^\alpha$, and since the asymptotic velocity for the operator $-\Delta_j$ is P_j , one has $(\mathcal{P}_\alpha)_j = P_j$ if $\alpha_j \neq 0$ and $(\mathcal{P}_\alpha)_j = (\mathcal{P}^\alpha)_j$ if $\alpha_j = 0$. Then $E_{Z_\alpha}(\mathcal{P}_\alpha)$ is obtained from the fact that Z_α is a cartesian product and from the relation $E_{\{0\}}(\mathcal{P}^\alpha) = E_{\mathcal{P}}(H^\alpha)$. \square

2.8 Appendix

Proof of Lemma 2.6.2. If $z \in \mathbb{C} \setminus \sigma(H)$, let us write $R(z)$ for $(H - z)^{-1}$. In order to express $\eta(H)$ in terms of the resolvent of H we shall make use of the formula (6.1.26)

of [ABG] for $m \geq 2$:

$$\begin{aligned} \eta(H) &= \frac{1}{\pi} \Im \int_{\mathbb{R}} \left[\sum_{k=0}^{m-1} \frac{i^k}{k!} \eta^{(k)}(\lambda) \right] R(\lambda + i) d\lambda \\ &\quad + \frac{1}{\pi} \Im \int_{\mathbb{R}} \int_0^1 \frac{i^m}{(m-1)!} \mu^{m-1} \eta^{(m)}(\lambda) R(\lambda + i\mu) d\lambda d\mu. \end{aligned} \quad (2.27)$$

We shall also use the first resolvent equation

$$R(\lambda + i\mu) = \left[I + (\lambda + i(\mu - 1))R(\lambda + i\mu) \right] R(i), \quad (2.28)$$

and the fact that if p, k, m are positive integers, with $m \geq p + 1$, then the integrals

$$\begin{aligned} &\int_{\mathbb{R}} |\eta^{(k)}(\lambda)| [1 + |\lambda|]^p d\lambda \quad \text{and} \\ &\int_{\mathbb{R}} \int_0^1 |\eta^{(m)}(\lambda)| \left[1 + (|\lambda| + |\mu - 1|) \frac{1}{|\mu|} \right]^p \mu^{m-1} d\lambda d\mu \end{aligned} \quad (2.29)$$

are finite.

a) Let us replace $\eta(H)$ by (2.27) in the statement *i*) and observe that

$$\left[R(z), f \left(\frac{Q}{2t} \right) \right] = \frac{1}{t} R(z) \left\{ iP \cdot \nabla f \left(\frac{Q}{2t} \right) - \frac{1}{4t} \Delta f \left(\frac{Q}{2t} \right) \right\} R(z). \quad (2.30)$$

By taking $z = \lambda + i\mu$ and using (2.28) for the resolvents on the r.h.s. of (2.30), one obtains that the norm of $\left[R(z), f \left(\frac{Q}{2t} \right) \right] (H + i)$ is less than

$$\frac{1}{t} \left(1 + (|\lambda| + |\mu - 1|) \frac{1}{|\mu|} \right)^2 \left\| R(i) \left\{ iP \cdot \nabla f - \frac{1}{4t} \Delta f \right\} \right\| \|R(i)(H + i)\|.$$

Since the two norms are bounded uniformly in t for $t \geq 1$, the statement *i*) is now easily proved by taking into account (2.29) with $m = 3$.

b) For the proof of the first statement of *iii*), let ξ be an asymptotic localization function and $\delta > 0$ such that $\xi(\pm \frac{x_j}{\delta}) f(x) = f(x)$ for all $x \in \mathbb{R}^n$. We start by replacing $\eta(H)$ by (2.27) in the statement *iii*). By using that $\xi(2y)\xi'(y) = \xi'(y)$ for all $y \in \mathbb{R}$, some commutator calculations show that

$$\begin{aligned} [P_j, R(z)] \xi \left(\pm \frac{Q_j}{2\delta t} \right) &= iR(z) \xi \left(\pm \frac{Q_j}{2\delta t} \right) \nabla_j V(Q) R(z) \\ &\mp \frac{1}{\delta t} \xi' \left(\pm \frac{Q_j}{2\delta t} \right) R(z) \xi \left(\pm \frac{Q_j}{\delta t} \right) \nabla_j V(Q) R(z) P_j R(z) + \left(\frac{1}{2\delta t} \right)^2 \mathcal{R} \end{aligned} \quad (2.31)$$

where \mathcal{R} is equal to

$$\begin{aligned} &iR \nabla_j V(Q) R \xi'' \left(\pm \frac{Q_j}{2\delta t} \right) R \\ &+ R \left\{ -4iP_j \xi'' \left(\pm \frac{Q_j}{2\delta t} \right) \pm \frac{1}{\delta t} \xi''' \left(\pm \frac{Q_j}{2\delta t} \right) \right\} R \xi \left(\pm \frac{Q_j}{\delta t} \right) \nabla_j V(Q) R P_j R \\ &+ R \nabla_j V(Q) R \left\{ -4i\xi'' \left(\pm \frac{Q_j}{2\delta t} \right) P_j \mp \frac{1}{\delta t} \xi''' \left(\pm \frac{Q_j}{2\delta t} \right) \right\} R P_j R. \end{aligned}$$

(we have written R for $R(z)$). Again, by taking $z = \lambda + i\mu$ and using (2.28) for the resolvents of the first two terms on the r.h.s. of (2.31), one obtains that their norm is less than

$$\begin{aligned} & \left(1 + (|\lambda| + |\mu - 1|) \frac{1}{|\mu|}\right)^2 \left\| R(i)\xi \left(\pm \frac{Q_j}{2\delta t}\right) \nabla_j V(Q) R(i) \right\| \\ & + c \left(1 + (|\lambda| + |\mu - 1|) \frac{1}{|\mu|}\right)^3 \left\| R(i)\xi \left(\pm \frac{Q_j}{\delta t}\right) \nabla_j V(Q) R(i) \right\| \|P_j R(i)\|, \end{aligned} \quad (2.32)$$

where $c = \frac{1}{\delta} \|\xi'\|_{L^\infty}$ is independent of t, η and μ (one has used that $\frac{1}{t} \leq 1$ for all $t \geq 1$). Similarly, one can check that the norm of \mathcal{R} is less than a polynomial in $\left(1 + (|\lambda| + |\mu - 1|) \frac{1}{|\mu|}\right)$ of order 4 with coefficients independent of t, λ and μ . One finishes the proof by taking into account (2.29) with $m = 5$ and by observing that the two norms in (2.32) and the factor $\left(\frac{1}{2\delta t}\right)^2$ in (2.31) belong to $L^1((1, \infty), dt)$.

c) For the second statement of *iii*) let us denote by α the only element of \mathcal{L} such that $\alpha \leq o$ and $\alpha_j = \pm 1$. One observes that $[P_j, V(Q)] = [P_j, V(Q) - V^\alpha(Q)]$ since V^α does not depend on x_j . Hence, one has

$$[P_j, R(z)] = \{R(z)(V(Q) - V^\alpha(Q))\} P_j R(z) - R(z) P_j \{(V(Q) - V^\alpha(Q)) R(z)\}.$$

Then, the same method and the same arguments already used in a) and b) may be applied. Since $\xi \left(\pm \frac{Q_j}{2\delta t}\right) (V(Q) - V^\alpha(Q)) R(i) \in o(t^0)$ by definition of the cartesian potential V , one obtains that $[P_j, \eta(H)] f \left(\frac{Q}{2t}\right) \in o(t^0)$.

d) For the statement *v*), let us observe that

$$\begin{aligned} & (P_j + i) Q_j R(z) (1 + Q^2)^{-1/2} \\ & = (P_j + i) R(z) Q_j (1 + Q^2)^{-1/2} - 2i (P_j + i) R(z) P_j R(z) (1 + Q^2)^{-1/2}. \end{aligned}$$

In order to make the calculation of the commutator $[Q_j, R(z)]$ properly, one has invoked the invariance of \mathcal{H}^2 under the group $\{e^{iyQ_j}\}_{y \in \mathbb{R}}$ and the statement (a) of Theorem 6.3.4 of [ABG]. Then the end of the proof follows the scheme of the previous points.

e) For the statement *ii*), let $\delta > 0$ and ξ be an asymptotic localization function such that $\xi \left(\pm \frac{x_j}{\delta}\right) f(x) = f(x)$ for all $x \in \mathbb{R}^n$. One has

$$\begin{aligned} & \eta(H) f \left(\frac{Q}{2t}\right) \nabla_j V(Q) \eta(H) = f \left(\frac{Q}{2t}\right) \eta(H) \xi \left(\pm \frac{Q_j}{2\delta t}\right) \nabla_j V(Q) \eta(H) \\ & + \left[\eta(H), f \left(\frac{Q}{2t}\right) \right] (\Delta + i) (\Delta + i)^{-1} \xi \left(\pm \frac{Q_j}{2\delta t}\right) \nabla_j V(Q) \eta(H). \end{aligned}$$

One observes that $f \left(\frac{Q}{2t}\right)$ and $\left[\eta(H), f \left(\frac{Q}{2t}\right) \right] (\Delta + i)$ are norm bounded independently of t for $t \geq 1$ (use *i*) for the second term). By taking (2.6) into account, one gets the expected result.

f) The proof of *iv*) is similar to the one given in the paragraph b) of Lemma 2.4.1. If $\delta > 0$ and ξ is an asymptotic localization function, one observes that

$\left\{1 - \prod_{\{j|\alpha_j \neq 0\}} \xi\left(\alpha_j \frac{x_j}{2\delta t}\right)\right\}_{t \geq 1}$ is an approximate unit for the ideal $\langle J_\alpha \cdot C_0(\mathbb{R}^{n^*}) \rangle$. Since $\eta(H) - \eta(H_\alpha)$ belongs to this ideal, it follows that

$$\lim_{t \rightarrow \infty} \left\| \prod_{\{j|\alpha_j \neq 0\}} \xi\left(\alpha_j \frac{Q_j}{2\delta t}\right) (\eta(H) - \eta(H_\alpha)) \right\| = 0.$$

□

Proof of Lemma 2.6.3. Since the following inequality is satisfied for all $t \geq 1$ and all $\varphi \in \mathcal{H}^2$:

$$\langle \varphi, B^*(t)B(t)\varphi \rangle \leq \pm \langle \varphi, \mathbf{D}\Phi(t)\varphi \rangle - \langle \varphi, F(t)\varphi \rangle - \langle \varphi, L(t)\varphi \rangle,$$

one obtains that

$$\begin{aligned} \int_1^\infty \|B(t)e^{-iHt}\varphi\|^2 dt &\leq \left| \int_1^\infty \langle e^{-iHt}\varphi, \mathbf{D}\Phi(t)e^{-iHt}\varphi \rangle dt \right| \\ &\quad + \int_1^\infty |\langle e^{-iHt}\varphi, F(t)e^{-iHt}\varphi \rangle| dt + \|\varphi\|^2 \int_1^\infty \|L(t)\| dt. \end{aligned}$$

But one has noticed that $\langle e^{-iHt}\varphi, \mathbf{D}\Phi(t)e^{-iHt}\varphi \rangle = \frac{d}{dt} \langle e^{-iHt}\varphi, \Phi(t)e^{-iHt}\varphi \rangle$, and hence $\left| \int_1^\infty \langle e^{-iHt}\varphi, \mathbf{D}\Phi(t)e^{-iHt}\varphi \rangle dt \right| \leq 2\|\Phi\|_{L^\infty} \|\varphi\|^2$. The conclusion is now straightforward. □

Proof of Lemma 2.6.4. Let $\psi \in \mathcal{D}_2$, $\varphi \in \mathcal{D}_1$ and $1 \leq s < t$. One has

$$\begin{aligned} &\left| \langle \psi, \{e^{iH_2 t} \Phi(t) e^{-iH_1 t} - e^{iH_2 s} \Phi(s) e^{-iH_1 s}\} \varphi \rangle \right| \\ &\leq \int_s^t \left| \left\langle \psi, e^{iH_2 \tau} \left(iH_2 \Phi(\tau) - i\Phi(\tau)H_1 + \frac{d}{d\tau} \Phi(\tau) \right) e^{-iH_1 \tau} \varphi \right\rangle \right| d\tau \\ &\leq \sum_{k=1}^N \left(\int_s^t \|E_k(\tau) e^{-iH_2 \tau} \psi\|^2 d\tau \right)^{\frac{1}{2}} \left(\int_s^t \|F_k(\tau) e^{-iH_1 \tau} \varphi\|^2 d\tau \right)^{\frac{1}{2}} \\ &\quad + \left(\int_s^t \|L(\tau)\| d\tau \right) \|\psi\| \|\varphi\|. \end{aligned}$$

Thus, one gets that

$$\begin{aligned} &\|e^{iH_2 t} \Phi(t) e^{-iH_1 t} \varphi - e^{iH_2 s} \Phi(s) e^{-iH_1 s} \varphi\| \\ &= \sup_{\psi \in \mathcal{D}_2, \|\psi\|=1} \left| \langle \psi, \{e^{iH_2 t} \Phi(t) e^{-iH_1 t} - e^{iH_2 s} \Phi(s) e^{-iH_1 s}\} \varphi \rangle \right| \\ &\leq c \sum_{k=1}^N \left(\int_s^t \|F_k(\tau) e^{-iH_1 \tau} \varphi\|^2 d\tau \right)^{\frac{1}{2}} + \left(\int_s^t \|L(\tau)\| d\tau \right) \|\varphi\|. \end{aligned} \quad (2.33)$$

Since (2.33) can be made arbitrarily small by choosing s large enough, one gets the existence of $s - \lim_{t \rightarrow \infty} e^{iH_2 t} \Phi(t) e^{-iH_1 t} \varphi$ for all $\varphi \in \mathcal{D}_1$, which implies the result of this lemma. □

Chapitre 3

Minimal escape velocities for unitary evolution groups

3.1 Introduction

This paper is a natural sequel of [HSS] on the minimal escape velocity for the evolution group generated by a self-adjoint operator in a Hilbert space. By improving part of the mentioned work (as suggested in [Geo]) and by applying these new results to some Schrödinger operators in $L^2(\mathbb{R}^n)$, we deduce some sharp propagation estimates. The minimal escape velocity is one variant of the generically called minimal velocity estimates, which are a key ingredient in the proof of asymptotic completeness for various models in quantum mechanics. We refer for example to [SS2], [Sk], [Ger] and [DG] for their importance in the N-body problem, and to [GN] and [Ri] for their use in some other anisotropic situations.

Let us first concentrate on Schrödinger operators and explain the interest of our estimates. We consider the Hilbert space $\mathcal{H} := L^2(\mathbb{R}^n)$, the usual Sobolev space \mathcal{H}^2 of order two on \mathbb{R}^n and the generator A of the dilation group in \mathcal{H} . Let $V(Q)$ be a Δ -bounded operator with relative bound less than one, and let $H := -\Delta + V$ be the corresponding Schrödinger operator in \mathcal{H} with domain \mathcal{H}^2 . Assume that H is of class $C_u^1(A)$. The conditions of regularity of H with respect to A are explained in Section 3.2, but let us already mention that this requirement is very weak in the setting of the conjugate operator theory. Assume moreover that there exists an open interval J of \mathbb{R} such that A is strictly conjugate to H on J . We show then that there exist a strictly positive constant v_{\min} and a dense set of vectors φ in the spectral subspace $E_H(J)\mathcal{H}$ of \mathcal{H} such that for each $v < v_{\min}$,

$$\|\chi(|Q| \leq vt)e^{-iHt}\varphi\| \rightarrow 0 \quad \text{as } t \rightarrow \infty, \quad (3.1)$$

where $\chi(|Q| \leq vt)$ is the characteristic function of the ball in \mathbb{R}^n centered at the origin and of radius equal to vt .

The physical interpretation of this result is that the probability of finding the state $e^{-iHt}\varphi$ in the growing ball goes to zero as the time t goes to infinity. In other

words, the state $e^{-iHt}\varphi$ propagates to infinity or “flees the origin” [Do] with a velocity at least equal to v_{\min} . Let us point out that the hypotheses of the previous estimate are easily fulfilled by Schrödinger operators with very general N-body potentials or cartesian potentials [Ri]. In the case where V is a two-body potential, the relation (3.1) is similar to some results obtained in [En2].

The natural question which arises is about the nature of the spectrum of H on J . Do such propagation estimates imply the absence of singularly continuous spectrum on J ? We do not know the answer but two related works could corroborate a positive one. We mention first the paper [Si] in which a connection is drawn between the time of sojourn of the state $e^{-iHt}\varphi$ in any finite region of the space and the absolutely continuous subspace of \mathcal{H} with respect to H . Secondly, let us assume for a while that V is a bounded function on \mathbb{R}^n satisfying $\lim_{|x|\rightarrow\infty}|x|V(x) = 0$. In that case, one shows that the relation (3.1) holds for the corresponding Schrödinger operator on any open interval J of \mathbb{R}_+ with 0 not in the closure of J (cf. Remark 3.5.2). But then, it has been proved in [Re] that any Schrödinger operator $-\Delta + V$ in $L^2([0, \infty))$, with a bounded function V satisfying $\lim_{x\rightarrow\infty}xV(x) = 0$, has purely absolutely continuous spectrum on $(0, \infty)$. Anyway, any proof (based on the method of the conjugate operator) of the absolute continuity of the spectrum of H on J requires a stronger condition than the $C_u^1(A)$ -condition needed above. We refer to Chapter 7 of [ABG] for the most refined version of such results.

Let us now develop the abstract side of the minimal escape velocity. We consider two self-adjoint operators H and A in a Hilbert space \mathcal{H} (with norm $\|\cdot\|$ and scalar product $\langle\cdot,\cdot\rangle$). The starting point is a strict Mourre inequality, *i.e.* the existence of an open interval J of \mathbb{R} and of a strictly positive constant θ such that $\eta(H)[iH, A]\eta(H) \geq \theta\eta^2(H)$ for all smooth real functions η with support in J . In order to give an unambiguous meaning to that expression, a regularity condition on H with respect to A must be imposed : H has to be of class $C^1(A)$. But if H is only slightly more regular we are able to state our first main result. Let us denote by $C_c^\infty(J)$ the set of all smooth complex functions defined on J which have a compact support in J . We use the notations $\chi(A \leq c)$ and $\chi(A \geq c)$ for the spectral projections of the operator A on the intervals $(-\infty, c]$ and $[c, \infty)$ respectively.

Theorem 3.1.1. *Let H and A be self-adjoint operators in \mathcal{H} with H of class $C_u^1(A)$. Assume that there exist an open interval J of \mathbb{R} and $\theta > 0$ such that the inequality $\eta(H)[iH, A]\eta(H) \geq \theta\eta^2(H)$ holds for all real $\eta \in C_c^\infty(J)$. Let a and t be real numbers. Then for each real $\eta \in C_c^\infty(J)$ and for each $v < \theta$ one has*

$$\|\chi(A \leq a + vt)e^{-iHt}\eta(H)\chi(A \geq a)\| \rightarrow 0 \quad \text{as } t \rightarrow \infty \quad (3.2)$$

uniformly in a .

The localization of the evolution in the spectrum of a conjugate operator has already a long history. We refer for example to [En1], [Mo2], [Je] or more recently to [BGS] or [Sa] for different but related results. It is worth mentioning that in all those references, the operator H has to be more regular with respect to A than in Theorem 3.1.1. However, by requiring more regularity of H one may obtain a better control

on the decrease of the norm in (3.2), cf. [HSS] for this kind of results. We point out that in this reference, H is at least of class $C^2(A)$.

Let us finally describe the content of this paper. In Section 3.2 we introduce some notations and definitions. The proof of Theorem 3.1.1 is given in Section 3.3. In certain situations, one has some interest in localizing the evolution in the spectrum of another self-adjoint operator B rather than in the spectrum of A . Section 3.4 is devoted to that question and Proposition 3.4.4 contains some sufficient conditions between A and B to that purpose. The last section is the application to Schrödinger operators. Our second main statement, Theorem 3.5.1, is exposed and proved. The relation (3.1) previously discussed is then a straightforward corollary of this theorem.

3.2 Some notations

Almost all the notations and definitions are borrowed from [ABG], to which we refer for details. For any positive integer k let $C^k(\mathbb{R})$ be the algebra of complex functions on \mathbb{R} that are k times continuously differentiable. We also consider various subalgebras of $C^\infty(\mathbb{R}) := \bigcap C^k(\mathbb{R})$, namely : $C_{\text{pol}}^\infty(\mathbb{R})$, the functions whose derivatives have at most polynomial growth at infinity, $\mathcal{S}^\mu(\mathbb{R})$ with $\mu \leq 0$, the symbols of degree μ , and $C_c^\infty(\mathbb{R})$, the functions with compact support. Let us recall that $f \in C^\infty(\mathbb{R})$ is a symbol of degree μ if for each k there exists a constant c_k such that $|f^{(k)}(x)| \leq c_k(1+x^2)^{\frac{\mu-k}{2}}$ for all $x \in \mathbb{R}$.

We collect some definitions related to the conjugate operator theory. \mathcal{H} is a Hilbert space, $\mathcal{B}(\mathcal{H})$ denotes the set of bounded operators in \mathcal{H} and $\{W_t\}_{t \in \mathbb{R}}$ is the unitary group in \mathcal{H} generated by a self-adjoint operator A . For any $T \in \mathcal{B}(\mathcal{H})$, we write $T \in C_u(A)$, $T \in C^k(A)$ or $T \in C_u^k(A)$ if the mapping $\mathbb{R} \ni t \mapsto W_{-t}TW_t \in \mathcal{B}(\mathcal{H})$ is continuous in norm, strongly C^k or C^k in norm respectively. By assuming that $T \in C^1(A)$, the commutator $[iT, A]$, defined in form sense on the domain $D(A)$ of A , extends continuously to a bounded operator in \mathcal{H} . Let us mention that $T \in C_u^1(A)$ if and only if $T \in C^1(A)$ and $[iT, A]$ belongs to $C_u(A)$. A self-adjoint operator H in \mathcal{H} is of class $C^k(A)$, resp. $C_u^k(A)$, if $(H-z)^{-1} \in C^k(A)$, resp. $(H-z)^{-1} \in C_u^k(A)$, for some, and then for all, $z \in \mathbb{C} \setminus \sigma(H)$. We have used the notation $\sigma(H)$ for the spectrum of H .

Let $\Phi : [1, \infty) \ni t \mapsto \Phi(t) \in \mathcal{B}(\mathcal{H})$ be an operator-valued mapping. We say that Φ (or by a slight abuse of notation $\Phi(t)$) belongs to $o(t^{-k})$ if $\|\Phi(t)\| \in o(t^{-k})$ or to $O(t^{-k})$ if $\|\Phi(t)\| \in O(t^{-k})$, i.e. if $\lim_{t \rightarrow \infty} t^k \|\Phi(t)\| = 0$ or if $t^k \|\Phi(t)\| \leq c < \infty$ for all $t \geq 1$.

We shall use on \mathbb{R} the *Fourier measure* $\underline{dx} := (2\pi)^{-1/2} dx$, where dx is the usual Lebesgue measure. Then a function $f : \mathbb{R} \rightarrow \mathbb{C}$ belongs to $L^1(\mathbb{R})$ if $\|f\|_{L^1} := \int_{\mathbb{R}} |f(x)| \underline{dx} < \infty$. For such a function, its Fourier transform $\mathcal{F}f \equiv \hat{f}$ is defined by $\hat{f}(x) := \int_{\mathbb{R}} e^{-ixy} f(y) \underline{dy}$. We recall that \mathcal{F} extends canonically to an isomorphism of the space of tempered distributions $\mathcal{S}^*(\mathbb{R})$ onto itself.

For any complex Radon measure on \mathbb{R} (simply called *measure*), we use the notation $\nu(x) \underline{dx}$ for $\nu(dx)$. With such a measure ν we associate its variation $|\nu|$, i.e. the smallest

positive measure such that $|\nu(\Omega)| \leq |\nu|(\Omega)$ for each bounded and closed subset Ω of \mathbb{R} . The measure ν is *integrable on* \mathbb{R} if $|\nu|(\mathbb{R}) < \infty$. The space of all integrable measures on \mathbb{R} is identified with a subspace of $\mathcal{S}^*(\mathbb{R})$ by the formula $\langle f, \nu \rangle := \int_{\mathbb{R}} \overline{f(x)} \nu(x) \underline{d}x$, where f is any element of the space $\mathcal{S}(\mathbb{R})$ of tempered test functions on \mathbb{R} and $\langle \cdot, \cdot \rangle$ is the duality between $\mathcal{S}(\mathbb{R})$ and $\mathcal{S}^*(\mathbb{R})$.

We are finally in position to recall a functional calculus. Let A be a self-adjoint operator in \mathcal{H} and $f \in \mathcal{S}^*(\mathbb{R})$ such that \hat{f} is an integrable measure on \mathbb{R} . Then for any $\varphi, \psi \in \mathcal{H}$, one has (cf. Definition 3.2.7 of [ABG]) :

$$\langle \varphi, f(A)\psi \rangle := \int_{\mathbb{R}} \langle \varphi, e^{iAx}\psi \rangle \hat{f}(x) \underline{d}x. \quad (3.3)$$

3.3 The abstract theory

We first consider a self-adjoint operator A in \mathcal{H} and prove estimates for operators which have a certain regularity with respect to A . In the sequel, it is assumed that a and s are real numbers with $s \geq 1$ and that f, h, η, \dots are real functions.

Lemma 3.3.1. *Consider a bounded operator $T \in C^1(A)$ and let h be a bounded $C_{\text{pol}}^\infty(\mathbb{R})$ -function such that \hat{h}' is an integrable measure on \mathbb{R} . The norm of the commutator $[T, h(\frac{A-a}{s})]$ is then less or equal to $\frac{1}{s} \|[T, A]\| \|\hat{h}'\|_{L^1}$.*

In the following proofs, we write A_s for the operator $\frac{A-a}{s}$.

Proof. By using the commutator expansions given in Theorem 5.5.3 of [ABG], one has the following equality in form sense on any core for A :

$$[T, h(A_s)] = \frac{1}{s} \int_0^1 d\tau \int_{\mathbb{R}} e^{iA_s\tau x} [T, A] e^{iA_s(1-\tau)x} \hat{h}'(x) \underline{d}x.$$

Since $T \in C^1(A)$ the commutator $[T, A]$ extends continuously to a bounded operator in \mathcal{H} , and the estimate on the norm follows straightforwardly. \square

Corollary 3.3.2. *Assume that T and h satisfy the hypotheses of Lemma 3.3.1 and that h has support in $(-\infty, 0]$. Then the norm of the operator $\chi(A-a \geq 0)Th(\frac{A-a}{s})$ is less or equal to $\frac{1}{s} \|[T, A]\| \|\hat{h}'\|_{L^1}$.*

Proof. Since $\chi(x \geq 0)h(\frac{x}{s}) = 0$ for any $s \geq 1$ and all $x \in \mathbb{R}$, one has the equality:

$$\chi(A-a \geq 0)Th(A_s) = \chi(A-a \geq 0)[T, h(A_s)].$$

The conclusion is then implied by Lemma 3.3.1. \square

Lemma 3.3.3. *Consider a bounded operator $B \in C_u(A)$ and let $h \in L^\infty(\mathbb{R})$ be such that \hat{h} is an integrable measure on \mathbb{R} . Then the commutator $[B, h(\frac{A-a}{s})]$ belongs to $o(s^0)$, uniformly in a .*

Proof. By using the functional calculus introduced in equation (3.3), one has :

$$\begin{aligned} \|[B, h(A_s)]\| &\leq \int_{\mathbb{R}} \left\| e^{\frac{i}{s}Ax} B e^{-\frac{i}{s}Ax} - B \right\| |\widehat{h}(x)| dx \\ &\leq 2\|B\| \int_{|x| \geq s^{1/2}} |\widehat{h}(x)| dx + \int_{|x| < s^{1/2}} \left\| e^{\frac{i}{s}Ax} B e^{-\frac{i}{s}Ax} - B \right\| |\widehat{h}(x)| dx. \end{aligned} \quad (3.4)$$

The first term of (3.4) goes to 0 as s increases, and the second term is less or equal to $\sup_{|y| < s^{-1/2}} \|e^{iAy} B e^{-iAy} - B\| \|\widehat{h}\|_{L^1}$. By the regularity of B with respect to A , this belongs to $\mathfrak{o}(s^0)$. \square

The next proposition imposes some apparently strong conditions on a certain function. But we shall show in a subsequent remark the existence of a class of functions satisfying all those requirements.

Proposition 3.3.4. *Let H be a self-adjoint operator in \mathcal{H} of class $C_u^1(A)$. Assume that there exist an open interval J of \mathbb{R} and $\theta > 0$ such that $\eta(H)[iH, A]\eta(H) \geq \theta\eta^2(H)$ for all $\eta \in C_c^\infty(J)$. Let f be a bounded $C_{\text{pol}}^\infty(\mathbb{R})$ -function such that $f' = -g^2$ for some bounded $C_{\text{pol}}^\infty(\mathbb{R})$ -function g . Moreover assume that \widehat{f}' , \widehat{g} and \widehat{g}' are integrable measures on \mathbb{R} . Then for each $\eta \in C_c^\infty(J)$ the operator $\eta(H) \left[iH, f\left(\frac{A-a}{s}\right) \right] \eta(H)$ satisfies the estimate*

$$\eta(H) \left[iH, f\left(\frac{A-a}{s}\right) \right] \eta(H) \leq \frac{\theta}{s} \eta(H) f' \left(\frac{A-a}{s} \right) \eta(H) + o(s^{-1}), \quad (3.5)$$

where $o(s^{-1})$ is uniform in a .

Proof. a) Let $\tilde{\eta} \in C_c^\infty(J)$ be such that $\tilde{\eta}\eta = \eta$. We set $T := H\tilde{\eta}(H)$ (which belongs to $C_u^1(A)$ by Corollary 6.2.6 (b) of [ABG]) and denote by B the continuous extension of the operator formally given by $[iT, A]$ (B belongs to $C_u(A)$). One observes that

$$\eta(H)[iH, f(A_s)]\eta(H) = \eta(H)[iT, f(A_s)]\eta(H)$$

and that the strict Mourre inequality can be rewritten as

$$\eta(H)B\eta(H) \geq \theta\eta^2(H) \quad \text{for all } \eta \in C_c^\infty(J).$$

Through the use of the commutator expansions of Theorem 5.5.3 of [ABG], one obtains the following equality:

$$[iT, f(A_s)] = \frac{1}{s}R_s + \frac{1}{s}Bf'(A_s) \quad (3.6)$$

with $R_s = \int_0^1 d\tau \int_{\mathbb{R}} \left(e^{\frac{i}{s}A\tau x} B e^{-\frac{i}{s}A\tau x} - B \right) e^{iA_s x} \widehat{f}'(x) dx$. Since the terms on the r.h.s. of (3.6) are bounded, the l.h.s. term of (3.5) extends continuously to

$$\eta(H) \left\{ \frac{1}{s}R_s + \frac{1}{s}Bf'(A_s) \right\} \eta(H).$$

b) Let us now observe that $\frac{1}{s}Bf'(A_s) = -\frac{1}{s}g(A_s)Bg(A_s) + o(s^{-1})$, where $o(s^{-1})$ is independent of a (we have used Lemma 3.3.3). Moreover, since $\eta(H) \in C^1(A)$, some commutator calculations based on Lemma 3.3.1 show that

$$\begin{aligned} -\frac{1}{s}\eta(H)g(A_s)Bg(A_s)\eta(H) &= -\frac{1}{s}g(A_s)\eta(H)B\eta(H)g(A_s) + O(s^{-2}) \\ &\leq -\frac{\theta}{s}g(A_s)\eta^2(H)g(A_s) + O(s^{-2}) = \frac{\theta}{s}\eta(H)f'(A_s)\eta(H) + O(s^{-2}), \end{aligned}$$

where $O(s^{-2})$ is independent of a .

c) It only remains to show that R_s belongs to $o(s^0)$ uniformly in a . One has that its norm is less or equal to

$$2\|B\| \int_{|x| \geq s^{1/2}} |\widehat{f}'(x)| \underline{d}x + \int_0^1 d\tau \int_{|x| < s^{1/2}} \left\| e^{\frac{i}{s}A\tau x} B e^{-\frac{i}{s}A\tau x} - B \right\| |\widehat{f}'(x)| \underline{d}x. \quad (3.7)$$

The first term of (3.7) goes to 0 as s increases. The second term of (3.7) is less or equal to $\sup_{|y| < s^{-1/2}} \|e^{iAy} B e^{-iAy} - B\| \|\widehat{f}'\|_{L^1}$, which belongs to $o(s^0)$ by the regularity of B with respect to A . One observes that both convergences are uniform in a . \square

Remark 3.3.5. Consider $g \in \mathcal{S}^\mu(\mathbb{R})$ for some $\mu < -1$. Since $g^2 \in \mathcal{S}^{2\mu}(\mathbb{R})$ and $g' \in \mathcal{S}^{\mu-1}(\mathbb{R})$, then $\widehat{g}, \widehat{g}^2$ and \widehat{g}' are integrable measures on \mathbb{R} (Proposition 5.4.5 of [ABG]). Moreover if $f(x) := -\int_0^x g^2(y)dy$, then f belongs to $C_{\text{pol}}^\infty(\mathbb{R})$ and satisfies all the assumptions of Proposition 3.3.4.

Proposition 3.3.6. *Let H be a self-adjoint operator in \mathcal{H} of class $C_u^1(A)$. Assume that there exist an open interval J of \mathbb{R} and $\theta > 0$ such that $\eta(H)[iH, A]\eta(H) \geq \theta\eta^2(H)$ for all $\eta \in C_c^\infty(J)$. Let t be a real number with $t \geq 1$. Then for each $\eta \in C_c^\infty(J)$, for each $f \in L^\infty(\mathbb{R})$ with support in $(-\infty, 0]$ and for each $v < \theta$, one has*

$$f\left(\frac{A-a}{t} - v\right) \eta(H) e^{-iHt} \chi_{(A-a \geq 0)} \in o(t^0)$$

uniformly in a .

The following proof is inspired from that of Theorem 1.1 of [HSS], but is considerably simpler in our situation.

Proof. a) Let $g \in C_c^\infty(\mathbb{R})$ with support in $(v-\theta, 0)$ and such that $\int_{-\infty}^\infty g^2(y)dy = 1$. We set $h(x) = -\int_0^x g^2(y)dy$ and observe that h satisfies all conditions imposed on f in Proposition 3.3.4. Furthermore, since $h^{1/2}(x-\theta)f(x-v) = f(x-v)$ for all $x \in \mathbb{R}$, it is enough to prove that

$$h^{1/2}\left(\frac{A-a}{t} - \theta\right) \eta(H) e^{-iHt} \chi_{(A-a \geq 0)} \in o(t^0) \quad (3.8)$$

uniformly in a .

b) Let us set $\Phi_s(t) := \eta(H)h(A_{t,s})\eta(H)$, with $A_{t,s}$ equal to $\frac{A-a-\theta t}{s}$. For each $\psi \in \mathcal{H}$, we define $\psi_t := e^{-iHt}\chi(A-a \geq 0)\psi$. Then (3.8) is equivalent to the statement that for all $\psi \in \mathcal{H}$,

$$\langle \psi_t, \Phi_t(t)\psi_t \rangle \leq \mathfrak{o}(t^0)\|\psi\|^2, \quad (3.9)$$

with $\mathfrak{o}(t^0)$ independent of ψ and a . One observes that

$$\begin{aligned} \langle \psi_t, \Phi_s(t)\psi_t \rangle &= \langle \psi_0, \Phi_s(0)\psi_0 \rangle + \int_0^t \frac{d}{d\tau} \langle \psi_\tau, \Phi_s(\tau)\psi_\tau \rangle d\tau \\ &= \langle \psi_0, \Phi_s(0)\psi_0 \rangle - \frac{\theta}{s} \int_0^t \langle \psi_\tau, \eta(H)h'(A_{\tau,s})\eta(H)\psi_\tau \rangle d\tau \\ &\quad + \int_0^t \langle \psi_\tau, \eta(H)[iH, h(A_{\tau,s})]\eta(H)\psi_\tau \rangle d\tau. \end{aligned} \quad (3.10)$$

By inserting (3.5) into (3.10) with a replaced by $a + \theta\tau$, we find that

$$\langle \psi_t, \Phi_s(t)\psi_t \rangle \leq \langle \psi_0, \Phi_s(0)\psi_0 \rangle + \int_0^t \mathfrak{o}(s^{-1})\|\psi\|^2 d\tau$$

with $\mathfrak{o}(s^{-1})$ independent of a , τ and ψ . Moreover, with the help of Corollary 3.3.2, one gets that

$$\langle \psi_0, \Phi_s(0)\psi_0 \rangle \leq \frac{1}{s}\|\eta\|_{L^\infty}\|\eta(H), A\| \|\widehat{h}'\|_{L^1}\|\psi\|^2.$$

Hence, one has obtained that

$$\langle \psi_t, \Phi_s(t)\psi_t \rangle \leq \frac{c}{s}\|\psi\|^2 + t\mathfrak{o}(s^{-1})\|\psi\|^2$$

with $\mathfrak{o}(s^{-1})$ and c independent of a , t and ψ . By setting $s = t$, this implies (3.9). \square

Proof of Theorem 3.1.1. Since $\chi(\frac{1}{t}x - v \leq 0) = \chi(x \leq vt)$ for any $t \geq 1$ and all $x \in \mathbb{R}$, the statement of the theorem is a special case of Proposition 3.3.6 with $f(\cdot) = \chi(\cdot \leq 0)$. \square

3.4 From one localization to another

The content of this section is inspired from Section 4.4.1 of [GL]. The main difference is that the parameter a is not considered in that monograph.

Let us recall from Lemma 7.2.15 of [ABG] that if T is a bounded operator belonging to $C^1(A)$, the closure of the symmetric, densely defined operator T^*AT ($D(T^*AT) \supset D(A)$) is a self-adjoint operator which we still denote by T^*AT . Moreover, $D(A)$ is a core for this operator. Therefore, if H is of class $C^1(A)$ and $\tilde{\eta} \in C_c^\infty(\mathbb{R})$, the operator $\tilde{\eta}(H)A\tilde{\eta}(H)$, defined on $D(A)$, admits a unique self-adjoint extension (cf. Theorem 6.2.5 of [ABG] for the proof that $\tilde{\eta}(H)$ belongs to $C^1(A)$). We also mention (Proposition 7.2.16 of the same reference) that if $\eta \in C_c^\infty(\mathbb{R})$, then $\eta(H)$ belongs to $C^1(\tilde{\eta}(H)A\tilde{\eta}(H))$.

Lemma 3.4.1. *Let H and A be self-adjoint operators in \mathcal{H} with H of class $C^1(A)$. Let $\eta, \tilde{\eta}$ be $C_c^\infty(\mathbb{R})$ -functions such that $\tilde{\eta}\eta = \eta$, and let f be a $C^\infty(\mathbb{R})$ -function such that $f = 0$ in a neighbourhood of $-\infty$ and $f = 1$ in a neighbourhood of $+\infty$. Then one has*

$$\left\{ f\left(\frac{A-a}{s}\right) - f\left(\frac{\tilde{\eta}(H)A\tilde{\eta}(H)-a}{s}\right) \right\} \eta(H) \in O(s^{-1})$$

uniformly in a .

Proof. Let us set $A_s := \frac{A-a}{s}$, $\tilde{A}_s := \frac{\tilde{\eta}(H)A\tilde{\eta}(H)-a}{s}$, $R(z) := (A_s - z)^{-1}$ and $\tilde{R}(z) := (\tilde{A}_s - z)^{-1}$ for $z \in \mathbb{C} \setminus \mathbb{R}$. For space reasons, we write η for $\eta(H)$ and $\tilde{\eta}$ for $\tilde{\eta}(H)$. Let φ, ψ be elements of \mathcal{H} . By using Theorem 6.1.4 (b) of [ABG] for any integer $r \geq 1$, one has that $\langle \varphi, \{f(A_s) - f(\tilde{A}_s)\}\eta\psi \rangle$ is equal to

$$\begin{aligned} & \sum_{k=0}^{r-1} \frac{1}{\pi k!} \int_{\mathbb{R}} f^{(k)}(\lambda) \Im \langle \varphi, i^k \{R(\lambda+i) - \tilde{R}(\lambda+i)\} \eta\psi \rangle d\lambda \\ & + \frac{1}{\pi(r-1)!} \int_0^1 d\mu \int_{\mathbb{R}} \mu^{r-1} f^{(r)}(\lambda) \Im \langle \varphi, i^r \{R(\lambda+i\mu) - \tilde{R}(\lambda+i\mu)\} \eta\psi \rangle d\lambda. \end{aligned}$$

Moreover, one observes that there exist two constants c_1 and c_2 , independent of a and s , such that for any $z \in \mathbb{C} \setminus \mathbb{R}$:

$$\begin{aligned} & |\langle \varphi, \{R(z) - \tilde{R}(z)\}\eta\psi \rangle| = |\langle \{\tilde{A}_s - A_s\}R(\bar{z})\varphi, \tilde{R}(z)\eta\psi \rangle| \\ & = |\langle \eta\{\tilde{A}_s - A_s\}R(\bar{z})\varphi, \tilde{R}(z)\psi \rangle + \frac{1}{s} \langle \{R(\bar{z}) - \tilde{R}(\bar{z})\}\varphi, [\eta, \tilde{\eta}A\tilde{\eta}]\tilde{R}(z)\psi \rangle| \\ & \leq \frac{1}{s} |\langle \eta[A, \tilde{\eta}]R(\bar{z})\varphi, \tilde{R}(z)\psi \rangle| + \frac{c_1}{s} \{\|R(\bar{z})\varphi\| + \|\tilde{R}(\bar{z})\varphi\|\} \|\tilde{R}(z)\psi\| \\ & \leq \frac{c_2}{s} \|R(\bar{z})\varphi\| \|\tilde{R}(z)\psi\| + \frac{c_1}{s} \|\tilde{R}(\bar{z})\varphi\| \|\tilde{R}(z)\psi\|, \end{aligned}$$

where we have used that $[\tilde{R}(z), \eta] = \frac{1}{s} \tilde{R}(z)[\eta, \tilde{\eta}A\tilde{\eta}]\tilde{R}(z)$. By using then the Hölder inequality and the identity (cf. Chap. XIII.7, Example 2 of [RS]) valid for any self-adjoint operator K :

$$\int_{\mathbb{R}} \|(K - \lambda - i\mu)^{-1}\varphi\|^2 d\lambda = \frac{\pi}{|\mu|} \|\varphi\|^2,$$

we find that for $\mu \neq 0$,

$$\left| \int_{\mathbb{R}} f^{(k)}(\lambda) \Im \langle \varphi, i^k \{R(\lambda+i\mu) - \tilde{R}(\lambda+i\mu)\} \eta\psi \rangle d\lambda \right| \leq \frac{d}{s|\mu|} \|\varphi\| \|\psi\|.$$

with $d = \pi(c_1 + c_2) \|f^{(k)}\|_{L^\infty}$. By choosing $r \geq 2$, one has $\int_0^1 \mu^{r-1} \frac{1}{|\mu|} d\mu < \infty$, and we have therefore obtained that

$$|\langle \varphi, \{f(A_s) - f(\tilde{A}_s)\}\eta(H)\psi \rangle| \leq \frac{c}{s} \|\varphi\| \|\psi\|$$

for some c independent of a and s . □

Let us recall from Theorem 6.2.10 of [ABG] that if A and B are self-adjoint operators in \mathcal{H} with B of class $C^1(A)$, then $D(A) \cap D(B)$ is a core for B .

Lemma 3.4.2. *Let A and B be self-adjoint operators in \mathcal{H} . Assume that*

- i) B is of class $C^1(A)$ and $A \leq B$ on $D(A) \cap D(B)$,*
- ii) $[h\left(\frac{B}{s}\right), A] \in O(s^0)$ for each $h \in C_c^\infty(\mathbb{R})$.*

Let f and g be $C^\infty(\mathbb{R})$ -functions such that $\max(\text{supp } g) < \min(\text{supp } f)$. Moreover assume that $f = 1$ in a neighbourhood of $+\infty$ and that g has compact support. Then there exists $c < \infty$ independent of a and s such that

$$\left\| g\left(\frac{B}{s}\right) f\left(\frac{A-a}{s}\right) \right\| \leq \frac{c}{s}(1+|a|). \quad (3.11)$$

Proof. Let \tilde{g} be in $C_c^\infty(\mathbb{R})$ such that $\max(\text{supp } \tilde{g}) < \min(\text{supp } f)$, $\tilde{g}g = g$ and $0 \leq \tilde{g} \leq 1$. Then the operator $\tilde{g}\left(\frac{B}{s}\right)$ belongs to $C^1(A)$ and the operator $\tilde{g}\left(\frac{B}{s}\right)\frac{A}{s}\tilde{g}\left(\frac{B}{s}\right)$, defined on $D(A)$, admits a unique self-adjoint extension which we denote by \tilde{A}_s (cf. the observations made before Lemma 3.4.1).

It follows from hypothesis *i)* that $\tilde{A}_s \leq \tilde{g}\left(\frac{B}{s}\right)\frac{B}{s}\tilde{g}\left(\frac{B}{s}\right) < \min(\text{supp } f)$ on $D(A)$, and therefore that $f(\tilde{A}_s) = 0$ for any $s \geq 1$. In order to obtain (3.11), it is hence enough to show that there exists $c < \infty$ independent of a and s such that

$$\left\| g\left(\frac{B}{s}\right) \{f(A_s) - f(\tilde{A}_s)\} \right\| \leq \frac{c}{s}(1+|a|).$$

The rest of the proof is now analogous to that given in Lemma 3.4.1 and we shall only point out the minor difference. Let us set $R(z) := (A_s - z)^{-1}$ and $\tilde{R}(z) := (\tilde{A}_s - z)^{-1}$ for $z \in \mathbb{C} \setminus \mathbb{R}$. One has, in form sense on \mathcal{H} , that

$$\begin{aligned} g\left(\frac{B}{s}\right) \{R(z) - \tilde{R}(z)\} &= \tilde{R}(z)g\left(\frac{B}{s}\right) (\tilde{A}_s - A_s)R(z) \\ &+ \frac{1}{s}\tilde{R}(z) \left[\tilde{g}\left(\frac{B}{s}\right) A\tilde{g}\left(\frac{B}{s}\right), g\left(\frac{B}{s}\right) \right] \{R(z) - \tilde{R}(z)\}, \end{aligned}$$

and that

$$\tilde{R}(z)g\left(\frac{B}{s}\right) (\tilde{A}_s - A_s)R(z) = \frac{1}{s}\tilde{R}(z)g\left(\frac{B}{s}\right) \left\{ \left[A, \tilde{g}\left(\frac{B}{s}\right) \right] + a \right\} R(z).$$

Hypothesis *ii)* is now used in order to obtain a uniform bound for the commutators. \square

We now refine Lemma 3.4.2 to the case where B dominates only a localized version of A .

Lemma 3.4.3. *Let H , A and B be self-adjoint operators in \mathcal{H} and let $\eta, \tilde{\eta}$ be $C_c^\infty(\mathbb{R})$ -functions such that $\tilde{\eta}\eta = \eta$. Assume that*

- i)* H is of class $C^1(A)$ and of class $C^1(B)$, B is of class $C^1(A)$,
- ii)* the operators $(B \pm i)^{-1}A\tilde{\eta}(H)$ defined on $D(A)$ extend continuously to bounded operators in \mathcal{H} ,
- iii)* $\tilde{\eta}(H)A\tilde{\eta}(H) \leq B$ on $D(\tilde{\eta}(H)A\tilde{\eta}(H)) \cap D(B)$,
- iv)* $[h(\frac{B}{s}), A] \in O(s^0)$ for each $h \in C_c^\infty(\mathbb{R})$.

Let f and g be $C^\infty(\mathbb{R})$ -functions such that $\max(\text{supp } g) < \min(\text{supp } f)$. Moreover assume that $f = 1$ in a neighbourhood of $+\infty$ and that g has a compact support. Then there exists $c < \infty$ independent of a and s such that

$$\left\| g\left(\frac{B}{s}\right) f\left(\frac{A-a}{s}\right) \eta(H) \right\| \leq \frac{c}{s}(1 + |a|).$$

Proof. For space reasons, we write $\tilde{\eta}$ for $\tilde{\eta}(H)$. One has

$$\begin{aligned} & \left\| g\left(\frac{B}{s}\right) \left\{ f\left(\frac{A-a}{s}\right) - f\left(\frac{\tilde{\eta}A\tilde{\eta}-a}{s}\right) + f\left(\frac{\tilde{\eta}A\tilde{\eta}-a}{s}\right) \right\} \eta(H) \right\| \\ & \leq \|\eta\|_{L^\infty} \left\| g\left(\frac{B}{s}\right) f\left(\frac{\tilde{\eta}A\tilde{\eta}-a}{s}\right) \right\| + O(s^{-1}), \end{aligned} \quad (3.12)$$

where we have used Lemma 3.4.1 and thus obtained that $O(s^{-1})$ is independent of a .

In order to deal with the first term of (3.12) we shall use Lemma 3.4.2 with $\tilde{\eta}A\tilde{\eta}$ instead of A . It follows from hypotheses *i)* and *ii)* that B is of class $C^1(\tilde{\eta}A\tilde{\eta})$ (the proof is similar to that of Lemma 4.4.7 of [GL]). Thus we only have to prove that $[h(\frac{B}{s}), \tilde{\eta}A\tilde{\eta}]$ belongs to $O(s^0)$ for each $h \in C_c^\infty(\mathbb{R})$. This commutator is equal to (in form sense on $D(A)$) :

$$\left[h\left(\frac{B}{s}\right), \tilde{\eta} \right] A\tilde{\eta} + \tilde{\eta} \left[h\left(\frac{B}{s}\right), A \right] \tilde{\eta} + \tilde{\eta}A \left[h\left(\frac{B}{s}\right), \tilde{\eta} \right]. \quad (3.13)$$

By hypothesis *iv)* the second term of (3.13) is bounded uniformly in s . So let us concentrate on the first term (the third one being similar). Let φ, ψ belong to $D(A)$ and let r be a strictly positive integer. By using Theorem 6.1.4 (b) of [ABG], the term $\langle \varphi, [h(\frac{B}{s}), \tilde{\eta}] A\tilde{\eta}\psi \rangle$ is equal to

$$\begin{aligned} & \sum_{k=0}^{r-1} \frac{1}{\pi k!} \int_{\mathbb{R}} h^{(k)}(\lambda) \mathfrak{S}\langle \varphi, i^k \left[\left(\frac{B}{s} - \lambda - i\right)^{-1}, \tilde{\eta} \right] A\tilde{\eta}\psi \rangle d\lambda \\ & + \frac{1}{\pi(r-1)!} \int_0^1 d\mu \int_{\mathbb{R}} \mu^{r-1} h^{(r)}(\lambda) \mathfrak{S}\langle \varphi, i^r \left[\left(\frac{B}{s} - \lambda - i\mu\right)^{-1}, \tilde{\eta} \right] A\tilde{\eta}\psi \rangle d\lambda. \end{aligned} \quad (3.14)$$

Let us observe that for $z \in \mathbb{C} \setminus \mathbb{R}$,

$$\left[\left(\frac{B}{s} - z\right)^{-1}, \tilde{\eta} \right] = \left(\frac{B}{s} - z\right)^{-1} [\tilde{\eta}, B](B - sz)^{-1},$$

where $[\tilde{\eta}, B]$ extends continuously to a bounded operator. By inserting the first resolvent equation

$$(B - s\lambda - is\mu)^{-1} = \{I + (s\lambda + is\mu + i)(B - s\lambda - is\mu)^{-1}\} (B + i)^{-1}$$

and by taking into account hypothesis *ii*), one obtains that for any $s \geq 1$,

$$\left| \left\langle \varphi, \left[\left(\frac{B}{s} - \lambda - i\mu \right)^{-1}, \tilde{\eta} \right] A\tilde{\eta}\psi \right\rangle \right| \leq \frac{c}{|\mu|^2} \{|\lambda| + |\mu| + 1\} \|\varphi\| \|\psi\|$$

where c is independent of s . Finally, by using this estimate in (3.14) with $r \geq 3$ one finds that

$$\left| \left\langle \varphi, \left[h \left(\frac{B}{s} \right), \tilde{\eta} \right] A\tilde{\eta}\psi \right\rangle \right| \leq c' \|\varphi\| \|\psi\|$$

for some constant c' independent of s . \square

Proposition 3.4.4. *Let H , A and B be self-adjoint operators in \mathcal{H} such that H is of class $C_u^1(A)$ and of class $C^1(B)$, B of class $C^1(A)$ and $B \geq 0$. Assume that there exist an open interval J of \mathbb{R} and $\theta > 0$ such that $\eta(H)[iH, A]\eta(H) \geq \theta\eta^2(H)$ for all $\eta \in C_c^\infty(J)$. Let t be a real number with $t \geq 1$ and let $\eta, \tilde{\eta}$ be $C_c^\infty(J)$ -functions such that $\tilde{\eta}\eta = \eta$. Assume moreover that*

- i) the operators $(B \pm i)^{-1}A\tilde{\eta}(H)$ defined on $D(A)$ extend continuously to bounded operators in \mathcal{H} ,*
- ii) $\tilde{\eta}(H)A\tilde{\eta}(H) \leq B$ on $D(\tilde{\eta}(H)A\tilde{\eta}(H)) \cap D(B)$,*
- iii) $[h \left(\frac{B}{t} \right), A] \in O(t^0)$ for each $h \in C_c^\infty(\mathbb{R})$.*

Then for each positive $v < \theta$, there exists $c < \infty$ independent of a and t such that

$$\|\chi(B \leq vt)e^{-iHt}\eta(H)\chi(A \geq a)\| \leq \mathfrak{o}(t^0) + \frac{c}{t}|a|,$$

where $\mathfrak{o}(t^0)$ is uniform in a .

Proof. Let $v' \in (v, \theta)$ and let $g \in C_c^\infty(\mathbb{R}, [0, 1])$ such that $\text{supp } g \subset (-\infty, v')$ and $g = 1$ on $[0, v]$. Let f be a $C^\infty(\mathbb{R}, [0, 1])$ -function such that $\max(\text{supp } g) < \min(\text{supp } f)$ and $f(x) = 1$ for all $x \geq v'$. Since $\chi(B \leq vt) = \chi\left(\frac{B}{t} \leq v\right) = \chi\left(\frac{B}{t} \leq v\right)g\left(\frac{B}{t}\right)$, one has

$$\begin{aligned} \|\chi(B \leq vt)e^{-iHt}\eta(H)\chi(A \geq a)\| &\leq \left\| g\left(\frac{B}{t}\right) f\left(\frac{A-a}{t}\right) \eta(H) \right\| \\ &+ \left\| \left\{ 1 - f\left(\frac{A-a}{t}\right) \right\} e^{-iHt}\eta(H)\chi(A \geq a) \right\|. \end{aligned}$$

By Lemma 3.4.3, there exists a constant $c < \infty$ independent of a and t such that the first term on the r.h.s. is less or equal to $\frac{c}{t}(1 + |a|)$. Since $\{1 - f(\cdot + v')\}$ has support in $(-\infty, 0]$, one obtains from Proposition 3.3.6 that the second term on the r.h.s belongs to $\mathfrak{o}(t^0)$ uniformly in a . \square

Remark 3.4.5. Since $\chi(A \geq a)\chi(A \geq 0) = \chi(A \geq a)$ for any $a \geq 0$, the statement of Proposition 3.4.4 can be rewritten in such a situation : for each $a \geq 0$ and each $v < \theta$, one has

$$\chi(B \leq vt)e^{-iHt}\eta(H)\chi(A \geq a) \in o(t^0),$$

where $o(t^0)$ is uniform in a .

3.5 Application to Schrödinger operators

We consider the Hilbert space $L^2(\mathbb{R}^n)$ and the Sobolev spaces of order s on \mathbb{R}^n denoted by \mathcal{H}^s . We recall that for $j \in \{1, \dots, n\}$, Q_j is the operator of multiplication by the variable x_j , $P_j := -i\nabla_j$ is a component of the momentum operator and $-\Delta$ is equal to P^2 . For any real number a , let us define a_- which is equal to $\max\{-a, 0\}$.

Theorem 3.5.1. *Let $V(Q)$ be a Δ -bounded operator with relative bound less than one, and let $H := -\Delta + V$ be the corresponding Schrödinger operator in $L^2(\mathbb{R}^n)$ with domain \mathcal{H}^2 . Assume that H is of class $C_u^1(A)$, with $A := \frac{1}{2}(P \cdot Q + Q \cdot P)$ the generator of dilation, and that there exist an open interval J of \mathbb{R} and $\theta > 0$ such that $\eta(H)[iH, A]\eta(H) \geq \theta\eta^2(H)$ for all real $\eta \in C_c^\infty(J)$. Let a and t be real numbers with $t \geq 1$. Then there exists $v_{\min} > 0$ such that for each real $\eta \in C_c^\infty(J)$ and each $v < v_{\min}$ one has*

$$\|\chi(|Q| \leq vt)e^{-iHt}\eta(H)\chi(A \geq a)\| \leq o(t^0) + \frac{c}{t}a_-,$$

where $o(t^0)$ is uniform in a , and where c is a positive constant independent of a and t .

Remark 3.5.2. Theorem 9.4.10 of [ABG] contains some sufficient conditions on the potential V such that $-\Delta + V$ is a N -body Hamiltonian of class $C_u^1(A)$. In particular, if $V(Q)$, $[iV(Q), A]$ are compact operators from \mathcal{H}^2 to \mathcal{H} , from \mathcal{H}^2 to \mathcal{H}^{-2} respectively, then H is a two-body Hamiltonian of class $C_u^1(A)$. For example if V is a bounded real function on \mathbb{R}^n satisfying $\lim_{|x| \rightarrow \infty} |x|V(x) = 0$, then the corresponding two-body Hamiltonian H is of class $C_u^1(A)$. Its essential spectrum is equal to $[0, \infty)$ and all its eigenvalues are negative and can accumulate only on 0; moreover, the operator A is strictly conjugate to H on any open interval J of \mathbb{R}_+ with 0 not in the closure of J (cf. Corollary 1.4 of [FH2] and Theorem 7.2.9 and Corollary 7.2.11 of [ABG]). Hence Theorem 3.5.1 applies and H has very good propagation properties on J .

Remark 3.5.3. We also mention that if the operator $V(Q) : \mathcal{H}^2 \rightarrow \mathcal{H}$ is compact and of the usual short-range or long-range type (cf. for example Definition 9.4.15 of [ABG]), then the corresponding two-body Hamiltonian H is of class $C_u^1(A)$. In fact, in that situation H satisfies even a slightly stronger regularity condition, the one required in order to prove a limiting absorption principle.

Proof of Theorem 3.5.1. This theorem is an application of Proposition 3.4.4. Let b be any strictly positive number and let $\tilde{\eta}$ be a $C_c^\infty(J)$ -function such that $\tilde{\eta}\eta = \eta$. The first step consists in verifying that the positive operator $B := b\langle Q \rangle \equiv b(1 + Q^2)^{1/2}$ is of

class $C^1(A)$, and that H is of class $C^1(B)$. This can be easily obtained with the help of Theorem 6.3.4 (a) of [ABG]. Secondly, let us observe that hypothesis *ii*) of Proposition 3.4.4 is fulfilled if the operator $\langle Q \rangle^{-1/2} \tilde{\eta}(H) A \tilde{\eta}(H) \langle Q \rangle^{-1/2}$ is bounded and if the value of b is chosen equal to its norm. But this new condition is quite standard and can be easily proved with some commutators calculations (statement *i*) of Lemma 6.2 of [Ri] may help). The other requirements of Proposition 3.4.4 are then also easily checked. One finishes the proof by setting $v_{\min} := \frac{\theta}{b}$ and by taking into account Remark 3.4.5 and the fact that if $v < \frac{v'}{b}$ then $\chi(b\langle Q \rangle \leq v't) \chi(|Q| \leq vt) = \chi(|Q| \leq vt)$ for t large enough. \square

One obtains the estimate (3.1) by observing that the set of vectors of the form $\eta(H) \chi(A \geq a) \psi$ with $\eta \in C_c^\infty(J)$, $a \in \mathbb{R}$ and $\psi \in \mathcal{H}$ is dense in the subspace $E_H(J) \mathcal{H}$ of \mathcal{H} .

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