

# Scattering theory for the perturbations of periodic Schrödinger operators

By

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## Abstract

In this article, we study the short- and long-range perturbations of periodic Schrödinger operators. The asymptotic completeness is proved in the short-range case by referring to known results on the stationary approach and more explicitly with the time-dependent approach. In the long-range case, one is able to construct modified wave operators. In both cases, the asymptotic observables can be defined as elements of a commutative  $C^*$ -algebra of which the spectrum equals or is contained in the Bloch variety. Especially, the expression of the mean velocity as the gradient of the Bloch eigenvalues is completely justified in this framework, even when the Bloch variety presents singularities.

## 1. Introduction

This paper is devoted to the scattering theory for the perturbations of periodic Schrödinger operators  $H_0 = \frac{1}{2}D^2 + V_\Gamma(x)$ , where  $V_\Gamma$  is a real potential,  $\Gamma$ -periodic for some lattice  $\Gamma$  in  $\mathbf{R}^n$ . The physical phenomenon related to this mathematical problem is called *impurity scattering*. The most basic result in this domain is the proof by Thomas [23] that the spectrum of  $H_0$  is absolutely continuous if the potential  $V_\Gamma$  is not too singular. On the other hand stationary phase arguments using the Floquet-Bloch transformation show that the motion of a particle in a periodic potential should be ballistic. These two facts indicate that the scattering theory for perturbations  $H = H_0 + V$  of  $H_0$  should be quite similar to the scattering theory for the free Laplacian  $\frac{1}{2}D^2$ . However up to now there are only partial results to support this belief. We mention the work of Thomas [23] using the Kato-Birman theory, Simon [21], using the Enss approach, and Bentosela [3] using the Kato-Kuroda stationary approach. All these results either assume a decay of the interaction  $V$  that is too strong or are valid only in a restricted range of energies.

In this paper we reconsider this problem using the Mourre method, which is based on the construction of a conjugate operator. This construction was made in our previous paper [12]. We prove the existence and completeness of the wave operators for the correct class of short-range perturbations. For long-range

perturbations, we construct modified wave operators and characterize their range. The range of the modified wave operators is described using a  $C^*$ -algebra  $\mathcal{U}^+$  of asymptotic observables which correspond to the energy and quasi-momentum for the free Hamiltonian  $H_0$ . Using the algebra  $\mathcal{U}^+$  we can also justify the heuristic fact that the velocity of a particle in a periodic potential is asymptotically given by the gradients of the Bloch functions.

**2. Definitions, assumptions and results**

**2.1. The periodic free Hamiltonian.**

We shall consider the free Hamiltonian

$$H_0 := \frac{1}{2} D^2 + V_\Gamma(x), \quad \text{on } L^2(\mathbf{R}^n),$$

where  $V_\Gamma$  is a real valued potential,  $\Gamma$ -periodic for some lattice  $\Gamma$  in  $\mathbf{R}^n$ :

$$V_\Gamma(x + \gamma) = V_\Gamma(x), \quad \gamma \in \Gamma.$$

We assume that

$$V_\Gamma \text{ is } \Delta \text{ bounded with bound strictly smaller than } 1. \tag{2.1}$$

It follows that  $H_0$  is self-adjoint with domain  $H^2(\mathbf{R}^n)$ . As we mentioned in the Introduction, the first basic question about scattering theory for  $H_0$  is whether the spectrum of  $H_0$  is absolutely continuous. Under the general assumption (2.1) this question is so far unsolved. In [23], Thomas proved the absolute continuity of the spectrum if the Fourier coefficients of  $V_\Gamma$  are in some  $l^p$  space (see [17, Thm. XII.100] for a precise statement). The proof in [23] shows that if we replace (2.1) by the stronger condition:

$$V_\Gamma \text{ is } (-\Delta)^{\frac{1}{2}} \text{ bounded with relative bound } 0, \tag{2.2}$$

then the spectrum of  $H_0$  is absolutely continuous. Our results will have a simpler expression in this case. We next specify our notations about the Floquet-Bloch transformation and refer the reader for details to [17, 22]. With the lattice  $\Gamma$ , we associate the torus  $\mathbf{T}^n = \mathbf{R}^n / \Gamma$ , the fundamental cell

$$F := \{x = \sum_{j=1}^n x_j \gamma_j, \quad 0 \leq x_j < 1\},$$

of which the volume for Lebesgue measure will be denoted by  $\mu_\Gamma$ , the dual lattice

$$\Gamma^* := \{\gamma^* \in \mathbf{R}^n \mid \langle \gamma, \gamma^* \rangle \in 2\pi\mathbf{Z}, \quad \forall \gamma \in \Gamma\}.$$

and symmetrically the sets  $\mathbf{T}^{n*} = \mathbf{R}^n / \Gamma^*$ ,  $F^*$  and the volume  $\mu_{\Gamma^*}$ . For  $x \in \mathbf{R}^n$ , we

define the integer part  $[x]$  of  $x$  as the unique  $\gamma \in \Gamma$  so that  $x - \gamma \in F$ . The Floquet-Bloch transformation:

$$Uu(k, x) := \mu_{\Gamma}^{-\frac{1}{2}} \sum_{\gamma \in \Gamma} e^{-i\langle k, \gamma \rangle} u(x + \gamma), \quad (2.3)$$

first defined for  $u \in S(\mathbf{R}^n)$ , extends as a unitary operator

$$U: L^2(\mathbf{R}^n, dx) \rightarrow L^2(\mathbf{T}^{n*}, dk; L^2(F, dx)).$$

The  $\Gamma^*$ -periodicity w.r.t.  $k$  of  $Uu$  follows from its definition. The distinction between the isomorphic spaces  $L^2(F, dx)$  and  $L^2(\mathbf{T}^n, dx)$  avoids confusion when one works with smooth functions. We shall use the notations

$$M := \mathbf{T}^{n*}, \quad \mathcal{H}' := L^2(F, dx)$$

$$\text{and } \mathcal{H} := L^2(\mathbf{T}^{n*}, dk; L^2(F, dx)) = \int_M^{\oplus} \mathcal{H}' dk \sim L^2(\mathbf{R}^n, dx).$$

The inverse of  $U$  is given by:

$$U^{-1}v(x + \gamma) = \mu_{\Gamma}^{-\frac{1}{2}} \int_M e^{i\langle k, \gamma \rangle} v(k, x) dk, \quad x \in F, \gamma \in \Gamma.$$

One easily deduce from (2.3) the identities

$$UxU^{-1} = x - D_k \quad (2.4)$$

$$U[x]U^{-1} = -D_k. \quad (2.5)$$

Conjugating  $H_0$  with  $U$  yields

$$UH_0U^{-1} = \int_M^{\oplus} H_0(k) dk, \quad (2.6)$$

with

$$H_0(k) = \frac{1}{2} D^2 + V_{\Gamma}(x),$$

$$D(H_0(k)) = \{u = v|_F, v \in H_{\text{loc}}^2(\mathbf{R}^n) v(x + \gamma) = e^{i\langle k, \gamma \rangle} v(x), \forall \gamma \in \Gamma\}.$$

In this representation, the Hamiltonian  $H_0$  satisfies the following properties (see [12]):

- i) the map  $M \ni k \rightarrow (H_0(k) + i)^{-1}$  is analytic with values in  $\mathcal{L}(\mathcal{H}')$ ;
- ii) for all  $k \in M$ , the self-adjoint operator  $H_0(k)$  has purely discrete spectrum;
- iii) the Bloch variety  $\Sigma := \{(\lambda, k) \in \mathbf{R} \times M, \lambda \in \sigma(H_0(k))\}$  is an analytic variety of  $M$  and the projection  $p_{\mathbf{R}}: \Sigma \ni (\lambda, k) \rightarrow \lambda$  is proper.

As a consequence  $H_0$  belongs to the class of analytically fibered operators, introduced

in [12]. We have proved there the

**Theorem 2.1.** *There exists a discrete set  $\tau$  determined by  $H_0$  so that for any interval  $I \subset \mathbb{R} \setminus \tau$  there exists an operator  $A_I$ , essentially self-adjoint on  $D(A_I) = \mathcal{C}_{\text{comp}}^\infty(M; \mathcal{H})$  satisfying the following properties:*

i) *For all  $\chi \in \mathcal{C}_{\text{comp}}^\infty(I)$ , there exists a constant  $c_\chi > 0$  so that*

$$\chi(H_0)[H_0, iA_I]\chi(H_0) \geq c_\chi \chi(H_0)^2.$$

ii) *The multi-commutators  $\text{ad}_{A_I}^k(H_0)$  are bounded for all  $k \in \mathbb{N}$ .*

iii) *The operator  $A_I$  is a first order differential operator in  $k$  with coefficients which belong to  $\mathcal{C}^\infty(M; \mathcal{L}(\mathcal{H}'))$  and there exists  $\chi \in \mathcal{C}_{\text{comp}}^\infty(\mathbb{R} \setminus \tau)$  so that  $A_I = \chi(H_0)A_I = A_I\chi(H_0)$ .*

Here are some other notations related to the free Hamiltonian which be used in our analysis. On the Bloch variety  $\Sigma$  which is locally compact with the topology induced by  $\mathbb{R} \times M$ , we shall consider the open subset

$$\Sigma_{\text{reg}} := \{(\lambda_0, k_0) \in \Sigma, \exists W \in \mathcal{V}_\Sigma(\lambda_0, k_0), \forall (\lambda, k) \in W, \\ \dim 1_{(\lambda)}(H_0(k))\mathcal{H} = \dim 1_{(\lambda_0)}(H_0(k_0))\mathcal{H}\}$$

where  $\mathcal{V}_x(x)$  denotes the set of neighborhoods of  $x$  in the topological space  $X$ . When  $(\lambda_0, k_0)$  belongs to  $\Sigma_{\text{reg}}$ , there exists  $I \in \mathcal{V}_{\mathbb{R}}(\lambda_0)$ ,  $W \in \mathcal{V}_M(k_0)$  and a real analytic function  $\lambda$  on  $W$  so that

$$I \times W \cap \Sigma = \{(\tilde{\lambda}(k), k), k \in W\}.$$

Besides  $1_{\Sigma_{\text{reg}}}$ , there is another useful Borel function defined on the Bloch variety.

**Definition 2.2.** The function  $v$  is defined on  $\Sigma$  by

$$\begin{cases} v(\lambda, k) = \partial_k \tilde{\lambda}(k) & \text{if } (\lambda = \tilde{\lambda}(k), k) \in \Sigma_{\text{reg}} \\ 0 & \text{else.} \end{cases}$$

The function  $v$  will be used in Subsection 2.3 to define the asymptotic velocity observable. We close this review of properties of the free Hamiltonian by some remarks. First if  $p_M: \Sigma \rightarrow M$  denotes the projection on  $M$ , then  $p_M(\Sigma \setminus \Sigma_{\text{reg}})$  has zero Lebesgue measure. Indeed this is a consequence of the stratification argument used in [12], which ensures that  $p_M(\Sigma \setminus \Sigma_{\text{reg}})$  is covered by a countable (finite if one considers  $\Sigma \cap p_{\mathbb{R}}^{-1}(K)$  with  $K \subset \mathbb{R}$  compact) family of real analytic submanifolds with non null codimension. Second, the function  $v$  belongs to  $L_{\text{loc}}^\infty(\Sigma, p_M^* dk)$ . This follows from the local Lipschitz regularity of the eigenvalues of  $H_0(k)$ , which can be proved by a minimax argument.

**2.2. The perturbations.**

We shall consider perturbed Hamiltonians of the form  $H = H_0 + V(x)$  with

$$V(x) = \tilde{V}_s(x) + V_l(x),$$

and where  $\tilde{V}_s$  and  $V_l$  are real-valued functions and satisfy for some  $\mu > 0$  and  $\mu_s > 0$  the

- Hypothesis 2.3.** a) The operator  $\tilde{V}_s \langle x \rangle^{1 + \mu_s} (-\Delta + 1)^{-1}$  is compact on  $L^2(\mathbf{R}^n)$ .  
 b) The function  $V_l$  satisfies:  $|\partial_x^\alpha V_l(x)| \leq C_\alpha \langle x \rangle^{-|\alpha| - \mu}$ .

We set

$$V_s(x) := \tilde{V}_s + V_l(x) - V_l([x]).$$

The reason for decomposing  $V$  as  $V_s + V_l([x])$  is that the functions of the integer part  $[x]$  become after the Floquet-Bloch reduction scalar pseudo-differential operators (see the discussion below). In the sequel we will use the following consequence of assumption a) of Hypotheses 2.3. We denote by  $R$  the operator  $\langle [x] \rangle = (1 + |[x]|^2)^{\frac{1}{2}}$ .

**Lemma 2.4.** *Let  $\chi \in \mathcal{C}_{\text{comp}}^\infty(\mathbf{R})$ . The operator  $R^\alpha V_s \chi(H_0) R^\beta$  is compact on  $L^2(\mathbf{R}^n)$  if  $\alpha + \beta < 1 + \inf(\mu, \mu_s)$  and bounded if  $\alpha + \beta = 1 + \inf(\mu, \mu_s)$ .*

*Proof.* We will use the functional calculus formula:

$$\chi(H) = \frac{1}{2\pi i} \int_{\mathbf{C}} \partial_{\bar{z}} \tilde{\chi}(z) (z - H)^{-1} dz \wedge d\bar{z} \tag{2.7}$$

where  $\tilde{\chi} \in \mathcal{C}_{\text{comp}}^\infty(\mathbf{C})$  is an almost analytic extension of  $\chi$  satisfying:

$$\tilde{\chi}|_{\mathbf{R}} = \chi, \quad \left| \frac{\partial \tilde{\chi}}{\partial \bar{z}}(z) \right| \leq C_N |\text{Im } z|^N, \quad \forall N \in \mathbf{N}. \tag{2.8}$$

Since there exists a constant  $C > 0$  so that

$$C^{-1} \langle x \rangle \leq \langle [x] \rangle \leq C \langle x \rangle,$$

the operator  $R$  can be replaced by  $\langle x \rangle$  in the lemma. By Hypothesis 2.3 b), the function

$$\langle x \rangle^{1 + \mu} (V_l(x) - V_l([x])) = \langle x \rangle^{1 + \mu} \int_0^1 \langle \nabla V_l([x] + s(x - [x])), x - [x] \rangle ds$$

is bounded. Hence the operator  $\langle x \rangle^\alpha V_s (H_0 - z)^{-1}$  is compact if  $\alpha < 1 + \inf(\mu, \mu_s)$  and bounded if  $\alpha = 1 + \inf(\mu, \mu_s)$  with an operator norm  $O(|\text{Im } z|^{-1})$  for  $\text{Im } z \neq 0$ . Commuting inductively powers of  $\langle x \rangle$  with  $(z - H_0)^{-1}$ , we see that for  $\beta \in \mathbf{Z}$ ,  $\beta \leq 0$ ,

$$\|(H_0 + i)\langle x \rangle^{-\beta}(z - H_0)^{-1}\langle x \rangle^\beta\| = O\left(\frac{\langle z \rangle^{N_\beta}}{|\operatorname{Im} z|^{N_\beta}}\right), \quad |\operatorname{Im} z| \neq 0.$$

By interpolation, this estimate extends to any real  $\beta \leq 0$ . Writing

$$\langle x \rangle^\alpha V_s(z - H_0)^{-1}\langle x \rangle^\beta = \langle x \rangle^{\alpha+\beta} V_s(H_0 + i)^{-1}(H_0 + i)\langle x \rangle^{-\beta}(z - H_0)^{-1}\langle x \rangle^\beta$$

and using formula (2.7) and estimate (2.8), we get the result.

Now that the action of conjugating with the Floquet-Bloch transformation  $U$  is specified, an operator  $B$  on  $L^2(\mathbf{R}^n, dx)$  and its image  $UBU^{-1}$  on  $\mathcal{H}$  will both be denoted by  $B$  in the sequel. Formula (2.4) indicates that multiplication operators on  $L^2(\mathbf{R}^n, dx)$  become after conjugation by  $U$  pseudo-differential operators on  $M = T^{n*}$  with operator valued symbols on  $\mathcal{H}'$ . Actually pseudo-differential operators on  $M$  with operator valued symbols of negative order is the natural class of perturbations of  $H_0$  for which a clean scattering theory can be developed. A remarkable fact of the pseudo-differential calculus on  $T^{n*}$  is that complete symbols can be associated with pseudo-differential operators like in  $\mathbf{R}^n$ . We refer to Appendix B for details. Moreover, the right-hand side of the two next identities which are defined by functional calculus, are pseudo-differential operators (see Proposition B.3 iv):

$$URU^{-1} = U\langle [x] \rangle U^{-1} = \langle D_k \rangle. \quad (2.9)$$

$$\text{and } UVU^{-1} = UV_s U^{-1} + V_l(-D_k). \quad (2.10)$$

**Notation.** We denote by  $\operatorname{OpS}^\alpha(M)$  and  $\operatorname{OpS}^\alpha(M; \mathcal{L}(\mathcal{H}'))$  the space of pseudo-differential operators of order  $\alpha \in \mathbf{R}$  on  $M$  with respectively scalar and  $\mathcal{L}(\mathcal{H}')$ -valued symbols. When  $h \in (0, h_0)$  is a small parameter,  $\operatorname{OpS}^{h,\alpha}(M)$  and  $\operatorname{OpS}^{h,\alpha}(M; \mathcal{L}(\mathcal{H}'))$  denote the semiclassical version of these pseudo-differential classes.

The class of pseudo-differential operators that we consider is precisely defined in Definition B.1. Complete symbols are well defined for this class and the operator valued are defined like in [2]. The assertion iv) of Proposition B.3 gives

$$R^\alpha \in \operatorname{OpS}^\alpha(M), \quad (2.11)$$

$$V_l(-D_k) \in \operatorname{OpS}^{-\mu}(M) \quad (2.12)$$

$$\text{and } A_l \in \operatorname{OpS}^1(M; \mathcal{L}(\mathcal{H}')). \quad (2.13)$$

We recall that the estimates of scalar pseudo-differential calculus carry over to the  $\mathcal{L}(\mathcal{H}')$ -valued case except the commutator estimate which holds only when the principal symbols commute. This latter condition is trivially satisfied when one of the symbols is scalar. We refer the reader to [2] for operator valued pseudo-differential operators. The next lemma ensures that  $V$  enters in the class of perturbations considered in [12].

**Lemma 2.5.** *The operator  $V$  is symmetric and satisfies for any compact energy interval  $I$  included in  $\mathbf{R} \setminus \tau$*

- i)  $V(H_0 + i)^{-1}$  is compact;
  - ii)  $[V, iA_I]$  is bounded;
  - iii) the function:  $s \rightarrow e^{isA_I} V e^{-isA} - V$  belongs to  $\mathcal{C}^{1+\varepsilon}(\mathbf{R}; \mathcal{L}(\mathcal{H}))$  with  $0 < \varepsilon < \inf\{1, \mu, \mu_s\}$
- Moreover for  $H = H_0 + V$ , the function  $s \rightarrow e^{isA_I}(H + i)^{-1} e^{-isA_I}$  belongs to  $\mathcal{C}^{1+\varepsilon}(\mathbf{R}; \mathcal{L}(\mathcal{H}))$  with  $0 < \varepsilon < \inf\{1, \mu, \mu_s\}$ .

*Proof.* The compactness of  $V(H_0 + i)^{-1}$  follows at once from Hypothesis 2.3. We next write  $V$  as  $V_s + V_l(-D_k)$ . For  $V_l(-D_k)$ , the pseudo-differential calculus yields

$$\text{ad}_{A_I}^j V_l(-D_k) R^\mu \in \mathcal{L}(\mathcal{H}), \quad \forall j \in \mathbf{N}. \tag{2.14}$$

For  $V_s$ , we recall that  $A_I = \chi(H_0) A_I = A_I \chi(H_0)$ . This gives by expanding the commutator:

$$A_I V_s - V_s A_I = A_I R^{-1} R \chi(H_0) V_s - V_s \chi(H_0) R R^{-1} A_I.$$

Using Lemma 2.4 we see that  $\text{ad}_{A_I} V_s$  is bounded. This implies ii) and also that  $s \rightarrow e^{isA_I} V e^{-isA} - V$  is Lipschitz continuous if  $\inf(\mu, \mu_s) = 0$ . The same method of expanding the commutator shows that  $\text{ad}_{A_I}^2 V_s$  is bounded if  $\inf(\mu, \mu_s) \geq 1$ . The assertion iii) is then derived for general  $(\mu, \mu_s)$  by real interpolation between  $\inf(\mu, \mu_s) = 0$  and  $\inf(\mu, \mu_s) = 1$ . It remains to check the regularity of  $r(s) := e^{isA_I}(H + i)^{-1} e^{-isA_I}$ . We have

$$\begin{aligned} r(s) &= (H + i)^{-1} - i \int_0^s e^{iuA_I} (H + i)^{-1} [A_I, H_0 + V] (H + i)^{-1} e^{-iuA_I} du \\ &= (H + i)^{-1} - i \int_0^s r(u) e^{iuA_I} [A_I, H_0 + V] e^{-iuA_I} r(u) du. \end{aligned} \tag{2.15}$$

Using the first line of (2.15), we first deduce from iii) that  $r(s)$  is Lipschitz continuous, and then using the second line of (2.15) that  $r(s)$  is  $\mathcal{C}^{1+\varepsilon}$ .

*Remark 2.6.* a) About the real interpolation result and the notation  $\mathcal{C}^\alpha$  with  $\alpha \notin \mathbf{N}$  for the Hölder spaces, we refer the reader to [6].

b) The property iii) is indeed stronger than what is needed to develop Mourre theory (see [1] for a sharper version). However, it is convenient while checking the last assertion which is used in our propagation estimates.

By noting that  $\langle x \rangle^s R^{-s}$  and  $R^s (1 + |A_I|)^{-s}$  are bounded for any  $s \in \mathbf{R}$ , standard results for  $H = H_0 + V$  reviewed in [12] can be written in the form

**Theorem 2.7.** *Let  $A_I$  be a conjugate operator for  $H_0$  associated with an arbitrary compact interval  $I \subset \mathbf{R} \setminus \tau$ . Then the following results hold:*

i) *For  $\chi \in \mathcal{C}_{\text{comp}}^\infty(I)$ , there exist a constant  $c_\chi > 0$  and a compact operator  $K_\chi$  so that*

$$\chi(H)[H, iA_I]\chi(H) \geq c_\chi \chi^2(H) + K_\chi.$$

*As a consequence  $\sigma_{\text{pp}}(H)$  is of finite multiplicity in  $\mathbf{R} \setminus \tau$  and has no accumulation points in  $\mathbf{R} \setminus \tau$ .*

ii) *For each  $\lambda \in \Gamma \setminus \sigma_{\text{pp}}(H)$ , there exists  $\epsilon > 0$  and  $c > 0$  so that*

$$1_{[\lambda - \epsilon, \lambda + \epsilon]}(H)[H, iA_I]1_{[\lambda - \epsilon, \lambda + \epsilon]}(H) \geq c 1_{[\lambda - \epsilon, \lambda + \epsilon]}(H).$$

iii) *The limiting absorption principle holds on  $\Gamma \setminus \sigma_{\text{pp}}(H)$ :*

$$\lim_{\epsilon \rightarrow \pm 0} \langle x \rangle^{-s} (H - \lambda + i\epsilon)^{-1} \langle x \rangle^{-s} \text{ exists and is bounded for all } s > \frac{1}{2}.$$

*As a consequence the singular continuous spectrum of  $H$  is empty.*

iv) *When  $V_I = 0$ , the wave operators*

$$\text{s-lim}_{t \rightarrow \pm \infty} e^{itH} e^{-itH_0} 1_c(H_0) =: W^\pm$$

*exist and are asymptotically complete,*

$$1_c(H)\mathcal{H} = W^\pm \mathcal{H}.$$

*Moreover if the condition (2.1) is replaced by (2.2) then we have  $1_c(H_0) = 1$  and  $W^\pm = \text{s-lim}_{t \rightarrow \pm \infty} e^{itH} e^{-itH_0}$ .*

The result iv) for the short-range case will be recovered via the time-dependent approach as a byproduct of the long-range analysis. We close this paragraph with another application of Lemma 2.5 to minimal velocity estimates essentially due to Sigal-Soffer [19]. Its proof is given in Appendix A.1.

**Proposition 2.8.** *Let  $\chi \in \mathcal{C}_{\text{comp}}^\infty(\mathbf{R} \setminus (\tau \cup \sigma_{\text{pp}}(H)))$ . For  $\epsilon_0 > 0$  small enough, we have:*

$$\int_1^\infty \left\| F\left(\frac{R}{t} \leq \epsilon_0\right) \chi(H) e^{-itH} u \right\|_{\frac{2}{t}}^2 dt \leq C \|u\|^2, \quad \forall u \in \mathcal{H}$$

$$\text{and} \quad \text{s-lim}_{t \rightarrow +\infty} F\left(\frac{R}{t} \leq \epsilon_0\right) \chi(H) e^{-itH} = 0.$$

*Moreover the result also holds if  $R$  is replaced by  $\langle x \rangle$ .*

**2.3. Results.**

Part of these results have natural expressions in terms of  $C^*$ -algebras. We first specify this framework. Remind that the energy-momentum space  $\Sigma$  is closed in  $\mathbf{R} \times M$  and is endowed with the induced topology.

**Definition 2.9.** The commutative  $C^*$ -algebra of which the elements are the

$$g(H_0, k) := \int_M^\oplus g(H_0(k), k) dk, \quad \text{with } g \in \mathcal{C}_0^0(\Sigma),$$

is denoted by  $\mathcal{U}_0$ .

The mapping  $g \rightarrow g(H_0, k)$  defines a faithful representation of  $\mathcal{C}_0^0(\Sigma)$ . Therefore  $\mathcal{U}_0$  is a  $C^*$ -algebra with spectrum equal to  $\Sigma$ . Moreover, it is clear that the measure  $(p_M)^*(dk)$  is basic for  $\mathcal{U}_0$ . Hence, the Proposition I.7.1 of [9] ensures that the mapping  $g \rightarrow g(H_0, k)$  weakly or strongly extends as a  $C^*$ -isomorphism from  $L^\infty(\Sigma, (p_M)^*(dk))$  into the Von Neumann algebra  $(\mathcal{U}_0)''$ . The family  $(1_\Omega(H_0, k))$  for  $\Omega$  Borel subset of  $\Sigma$  satisfies

$$1_{\Omega_1}(H_0, k)1_{\Omega_2}(H_0, k) = 1_{\Omega_1 \cap \Omega_2}(H_0, k)$$

so that the next definition makes sense.

**Definition 2.10.** The projection valued measure  $\Omega \rightarrow 1_\Omega(H_0, k)$  will be denoted by  $\mu_0$ . With any Borel function  $g$  on  $\Sigma$ , will be associated the operator

$$g(H_0, k) := \int_\Sigma g(\lambda, k) d\mu_0(\lambda, k), \tag{2.16}$$

$$\text{with } D(g(H_0, k)) = \left\{ \psi \in \mathcal{H}, \int_\Sigma |g(\lambda, k)|^2 d(\psi, \mu_0(\lambda, k)\psi) < \infty \right\}. \tag{2.17}$$

The first result is concerned with the asymptotic observables associated with a class of continuous functions on  $\Sigma$ .

**Theorem 2.11.** For any  $g \in \mathcal{C}_0^0(\Sigma)$ , the strong limit

$$s\text{-lim}_{t \rightarrow +\infty} e^{itH} g(H_0, k) e^{-itH} 1_c(H) = :g(H, k^+)_c \tag{2.18}$$

exist. These limits form a commutative  $C^*$ -algebra  $\mathcal{U}^+$  with spectrum  $\overline{\Sigma \setminus p_{\mathbf{R}}^{-1}(\sigma_{pp}(\overline{H_0}))}$ . Moreover the limit (2.18) equals  $g_{\mathbf{R}}(H)1_c(H)$  if  $g(\lambda, k) = g_{\mathbf{R}}(\lambda)$  depends only on  $\lambda$ .

**Remark 2.12.** The index  $_c$  recalls that our definition of  $g(H, k^+)_c$  includes the projection on the continuous spectrum of  $H$ .

**Corollary 2.13.** *If condition (2.2) holds, then  $\sigma_{\text{pp}}(H_0)$  is empty and the spectrum of  $\mathcal{U}^+$  is equal to  $\Sigma$ .*

The family of projections indexed by open subsets  $\Omega$  of  $\Sigma$  and defined by

$$1_{\Omega}(H, k^+)_{\epsilon} = \sup\{g(H, k^+)_{\epsilon}, g \in \mathcal{C}_0^0(\Sigma), g \leq 1_{\Omega}\},$$

satisfies

$$1_{\Omega_1}(H, k^+)_{\epsilon} 1_{\Omega_2}(H, k^+)_{\epsilon} = 1_{\Omega_1 \cap \Omega_2}(H, k^+)_{\epsilon}.$$

Hence we can introduce the

**Definition 2.14.** The projection valued measure  $\Omega \rightarrow 1_{\Omega}(H, k^+)_{\epsilon}$ , whose definition extends to any Borel set  $\Omega \subset \Sigma$ , will be denoted by  $\mu^+$ . With any Borel function  $g$  on  $\Sigma$ , will be associated the operator

$$g(H, k^+)_{\epsilon} := \int_{\Sigma} g(\lambda, k) d\mu^+(\lambda, k), \quad (2.19)$$

$$\text{with } D(g(H, k^+)_{\epsilon}) = \left\{ \psi \in \mathcal{H}, \int_{\Sigma} |g(\lambda, k)|^2 d(\psi, \mu^+(\lambda, k)\psi) < \infty \right\}. \quad (2.20)$$

*Remark 2.15.* One easily checks that this definition is compatible with the previous result, that  $\mu^+$  is null on  $\Sigma \setminus \overline{\Sigma \setminus \nu_{\mathbf{R}}^{-1}(\sigma_{\text{pp}}(H_0))}$  and that  $g(H, k^+)_{\epsilon}$  is 0 on  $1_{\text{pp}}(H)\mathcal{H}$ .

The asymptotic projection  $1_{\Sigma_{\text{reg}}}(H, k^+)_{\epsilon}$  is of particular importance, especially in the long range case. The states in its range have rather good propagation properties and should be considered as “regular” states. We next introduce the *velocity observable* associated to the function  $v$  given by Definition 2.2.

**Definition 2.16.** The *velocity observable* associated with  $H_0$  is the vector of commuting self-adjoint operators  $v_{H_0} := v(H_0, k)$ . The *asymptotic velocity observable* (for positive times) associated with  $H$  is the vector of commuting self-adjoint operators  $v_H^+ = v(H, k^+)_{\epsilon}$ .

**Theorem 2.17.** a) *For any  $\chi \in \mathcal{C}_{\text{comp}}^{\infty}(\mathbf{R})$ , we have*

$$\chi(H)v_H^+ = \text{s-lim}_{t \rightarrow +\infty} e^{itH}\chi(H_0)v_{H_0}e^{-itH}1_{\Sigma_{\text{reg}}}(H, k^+)_{\epsilon}.$$

b) *For any function  $f \in \mathcal{C}_0^0(\mathbf{R}^n)$ , we have*

$$\text{s-lim}_{t \rightarrow +\infty} e^{itH}f\left(\frac{x}{t}\right)e^{-itH}[1_{\Sigma_{\text{reg}}}(H, k^+)_{\epsilon} + 1_{\text{pp}}(H)] = f(v_H^+).$$

As we shall see in the proof, the first statement in Theorem 2.17 indeed comes at once from the definition of  $v_{H_0}$  while the second one is deeper. For the next two results, we distinguish the short and long-range case. The main difference between these two cases is: in short-range case, one is able to prove  $1_{\Sigma \setminus \Sigma_{\text{reg}}}(H, k^+)_c = 0$ , or in other words that all the states are regular; in the long-range case, this can be checked only in dimension  $n=1$  or with artificial assumptions on the singularities of  $\Sigma$ .

**Theorem 2.18.** *Assume  $V_l=0$ . Then the following properties hold:*

a) *Asymptotic completeness: the wave operator*

$$W^+ = \text{s-lim}_{t \rightarrow \pm \infty} e^{itH} e^{-itH_0} 1_c(H_0)$$

*exists and the system is asymptotically complete:*

$$W^+ \mathcal{H} = 1_c(H) \mathcal{H}.$$

*Moreover we have*

$$(W^+)^* = \text{s-lim}_{t \rightarrow + \infty} e^{itH_0} e^{-itH} 1_c(H)$$

and  $W^+ g(H_0, k) = g(H, k^+)_c W^+, \forall g \in \mathcal{C}_0^0(\Sigma).$

b) *Existence and properties of the asymptotic velocity: for  $f \in \mathcal{C}_0^0(\mathbf{R}^n)$ , we have*

$$\text{s-lim}_{t \rightarrow + \infty} e^{itH} f\left(\frac{x}{t}\right) e^{-itH} = f(v_H^+). \tag{2.21}$$

c) *If moreover the condition (2.2) holds, then the wave operator equals*

$$W^+ = \text{s-lim}_{t \rightarrow + \infty} e^{itH} e^{-itH_0}.$$

Part b) in Theorem 2.18 is the justification of the common idea that the velocity of a particle in a periodic potential is given by the gradient of the eigenvalues of  $H_0(k)$ . Note that this result holds in the presence of perturbations. In the long-range case one has to introduce modifiers  $e^{-iS(t, H_0, k)}$  commuting with  $H_0$  in order to define modified wave operators. Their construction, which will be completely done in Section 4, is local on  $\Sigma$  and involves solutions of Hamilton-Jacobi equations. The asymptotic velocity result is the one given in Theorem 2.17.

**Theorem 2.19.** *The limit*

$$W^+ := \text{s-lim}_{t \rightarrow + \infty} e^{itH} e^{-iS(t, H_0, k)} 1_c(H_0)$$

exists and its range coincides with the range of  $1_{\Sigma_{\text{reg}}}(H, k^+)_c$ . Moreover we have

$$(W^+)^* = \text{s-lim}_{t \rightarrow +\infty} e^{iS(t, H_0, k)} e^{-itH} 1_{\Sigma_{\text{reg}}}(H, k^+)_c,$$

and  $W^+ g(H_0, k) (W^+)^* = g(H, k^+)_c, \quad \forall g \in \mathcal{C}_0^\infty(\overline{\Sigma} \setminus \overline{p_{\mathbf{R}}^{-1}(\sigma_{\text{pp}}(H_0))} \cap \Sigma_{\text{reg}}).$

Finally, if the condition (2.2) holds, then the modified wave operator equals

$$W^+ = \text{s-lim}_{t \rightarrow +\infty} e^{itH} e^{-iS(t, H_0, k)}.$$

In the sequel, we shall prove these results in a more general case where the operator  $V_l(-D_k)$  is replaced by a general self-adjoint element  $V_l(k, D_k) \in \text{OpS}^{-\mu}(M)$ . With this, the reader will be convinced that the important condition is not that the symbol  $V_l(-\eta)$  (the complete symbol is well defined on the torus) does not depend on  $k$  but rather that it is fiberwise scalar. All the proofs and the previous results carry over to the more general framework proposed in [12] with  $M$  equal to a compact real analytic manifold or to  $\mathbf{R}^n$ . In this general situation, the manifold  $M$  has to be endowed with a Riemannian structure, the operator  $R$  is nothing but the square root of  $1 - \Delta_M$ , with  $\Delta_M$  equal to the Laplace-Beltrami operator, and the operator  $D_k$  has to be replaced at some points by  $-i$  times the gradient. Due to the lack of applications of this general framework, we prefer to stick to the case where  $M = \mathbf{T}^{n*}$  and to avoid additional definitions.

### 3. Effective time-dependent dynamic and asymptotic observables

As we said just above, the perturbation  $V$  is the sum of the short-range part  $V_s$  and a self-adjoint scalar pseudo-differential operator  $V_l(k, D_k)$ . The first step of the time-dependent approach consists in introducing an effective dynamic associated with some time-dependent Hamiltonian. We set

$$V_l(t, k, D_k) := F\left(\frac{R}{t} \log t \geq 1\right) V_l(k, D_k) F\left(\frac{R}{t} \log t \geq 1\right), \quad \text{for } t \geq 1.$$

One easily checks that such an operator belongs to  $\text{OpS}^{\frac{1}{t}, -\mu'}(M)$ , for any  $\mu' < \mu$ , so that the estimates below follow at once from pseudo-differential calculus

$$\begin{aligned} \text{ad}_A V_l(t, k, D_k) &= O_{\mu'}(t^{-\mu'}), \\ \text{and } \text{ad}_{(H_0 + i)^{-1}} V_l(t, k, D_k) &= O_{\mu'}(t^{-1-\mu'}), \quad \forall \mu', 0 < \mu' < \mu. \end{aligned}$$

Here and in the sequel, we drop the index  $l$  and the operator  $A$  has to be understood as any  $A_l$ . The effective Hamiltonian is defined by

$$H(t) := H_0 + V_1(t, k, D_k)$$

**Definition 3.1.** The unitary propagator  $U(t, 0)$  associated with  $H(t)$  will be denoted by  $U_1(t)$ .

**Proposition 3.2.** For all  $g \in \mathcal{C}_0^0(\Sigma)$  the norm-limit

$$\lim_{t \rightarrow +\infty} U_1(t)^* g(H_0, k) U_1(t) \tag{3.1}$$

exists. Moreover we have:

- a) There exist a unique densely defined self-adjoint operator  $H_1^+$  on  $\mathcal{H}$  so that the limit (3.1) equals  $g_{\mathbf{R}}(H_1^+)$  for  $g(\lambda, k) = g_{\mathbf{R}}(\lambda) \in \mathcal{C}_0^0(\mathbf{R})$ .
- b) The set of limits (3.1) defines a commutative  $C^*$ -algebra with spectrum  $\Sigma$ , denoted by  $\mathcal{U}_1^+$ .

*Proof.* By density, the function  $g$  can be chosen as the restriction to  $\Sigma$  of some element of  $\mathcal{C}_{\text{comp}}^\infty(\mathbf{R} \times M)$ , still denoted by  $g$ . Then it is clear using (2.7) that  $g(H_0, k)$  belongs to  $\mathcal{C}_{\text{comp}}^\infty(M; \mathcal{L}(\mathcal{H}'))$  and pseudo-differential calculus yields

$$\|[g(H_0, k), V_1(t, k, D_k)]\| = O(t^{-1-\mu}).$$

Hence, the derivative of (3.1) is norm-integrable and the limit exists. The construction of  $H_1^+$  is standard (see for example [8]) and the density of its domain is a consequence of the norm convergence. For b), we note that the representation of  $\mathcal{C}_0^0(\Sigma)$  given by (3.1) is faithful again due to the norm convergence.

From this result, we can construct a projection valued measure by the standard process recalled in Paragraph 2.3 (definition of  $\mu^+$ ).

**Definition 3.3.** The projection valued measure derived from the limits (3.1) will be denoted by  $\mu_1^+$  and we set for any Borel function on  $\Sigma$

$$g(H_1^+, k_1^+) := \int_{\Sigma} g(\lambda, k) d\mu_1^+(\lambda, k), \tag{3.2}$$

with  $D(g(H_1^+, k_1^+)) = \left\{ \psi \in \mathcal{H}, \int_{\Sigma} |g(\lambda, k)|^2 d(\psi, \mu_1^+(\lambda, k)\psi) < \infty \right\}$ . (3.3)

Propagation estimates given in Proposition 2.8 are also valid for  $U_1(t)$  (see Appendix A.1): for any  $\chi \in \mathcal{C}_{\text{comp}}^\infty(\mathbf{R} \setminus \tau)$ , we have

$$\int_1^\infty \left\| F\left(\frac{R}{t} \leq \varepsilon_0\right) \chi(H_0) U_1(t) u \right\|^2 \frac{dt}{t} \leq C \|u\|^2, \quad \forall u \in \mathcal{H} \tag{3.4}$$

and  $s\text{-}\lim_{t \rightarrow +\infty} F\left(\frac{R}{t} \leq \varepsilon_0\right) \chi(H_0) U_1(t) = 0$ . (3.5)

For the next result, we will also need the

**Lemma 3.4.** *For all  $\chi \in \mathcal{C}_{\text{comp}}^\infty(\mathbf{R})$ , the following estimates hold.*

- i)  $\left[ \chi(H), F\left(\frac{R}{t} \geq \varepsilon_0\right) \right] = O(t^{-1}).$
- ii)  $(\chi(H) - \chi(H_0))F\left(\frac{R}{t} \geq \varepsilon_0\right) = O(t^{-\inf\{1, \mu, \mu_s\}}).$

*Proof.* Using formula (2.7), the problem is reduced to getting estimates with  $\chi(H)$  (resp.  $\chi(H_0)$ ) replaced by the resolvent  $(z - H)^{-1}$  (resp.  $(z - H_0)^{-1}$ ). We have

$$\begin{aligned} \left[ (z - H)^{-1}, F\left(\frac{R}{t} \geq \varepsilon_0\right) \right] &= (z - H)^{-1} \left[ H_0, F\left(\frac{R}{t} \geq \varepsilon_0\right) \right] (z - H)^{-1} \\ &\quad + (z - H)^{-1} \left[ V_l, F\left(\frac{R}{t} \geq \varepsilon_0\right) \right] (z - H)^{-1} \\ &\quad + (z - H)^{-1} \left[ V_s, F\left(\frac{R}{t} \geq \varepsilon_0\right) \right] (z - H)^{-1}. \end{aligned}$$

The first term writes

$$-(z - H)^{-1} (H_0 + i) \left[ (H_0 + i)^{-1}, F\left(\frac{R}{t} \geq \varepsilon_0\right) \right] (H_0 + i) (z - H)^{-1}$$

and its norm is estimated via pseudo-differential calculus by  $O(t^{-1}) \frac{\langle z \rangle^2}{|\text{Im}z|^2}$ . If  $F_1$  is a function like  $F$  with  $F_1 \equiv 1$  on  $\text{supp } F$ , then the commutator in the second term equals

$$\left[ V_l, F\left(\frac{R}{t} \geq \varepsilon_0\right) \right] F_1\left(\frac{R}{t} \geq \varepsilon_0\right) + F\left(\frac{R}{t} \geq \varepsilon_0\right) \left[ V_l, F_1\left(\frac{R}{t} \geq \varepsilon_0\right) \right]$$

and pseudo-differential calculus ensures that its norm is  $O(t^{-1-\mu})$ . For the third one, we simply use

$$\left\| F\left(\frac{R}{t} \geq \varepsilon_0\right) V_s (z - H)^{-1} \right\| \leq C t^{-1-\mu} \|R^{1+\mu} V_s (H + i)^{-1}\| \|(H + i)(z - H)^{-1}\|.$$

The statement ii) relies on the same arguments applied to

$$\begin{aligned} [(z - H)^{-1} - (z - H_0)^{-1}] F\left(\frac{R}{t} \geq \varepsilon_0\right) &= \\ &= -(z - H)^{-1} (V_s + V_l) (z - H_0)^{-1} F\left(\frac{R}{t} \geq \varepsilon_0\right). \end{aligned}$$

**Proposition 3.5.** *The limits*

$$\text{s-lim}_{t \rightarrow +\infty} e^{itH} U_1(t) 1_{\mathbf{R} \setminus \tau}(H_1^+) =: W_1^+ \tag{3.6}$$

$$\text{and } \text{s-lim}_{t \rightarrow +\infty} U_1(t)^* e^{-itH} 1_c(H) \tag{3.7}$$

exist. Moreover the limit (3.7) equals  $(W_1^+)^*$ . Finally, the wave operator  $W_1^+$  defines a unitary transformation from  $1_{\mathbf{R} \setminus \tau}(H_1^+) \mathcal{H}$  onto  $1_c(H) \mathcal{H}$  and we have

$$W_1^+ H_1^+ (W_1^+)^* = H 1_c(H). \tag{3.8}$$

*Proof.* The existence of the limits (3.6) and (3.7) rely on the same argument and we shall only consider the existence of (3.7). We choose  $u \in 1_c(H) \mathcal{H}$ . By density, we can assume  $u = \chi^2(H)u$  with  $\chi \in \mathcal{C}_{\text{comp}}^\infty(\mathbf{R} \setminus \sigma_{\text{pp}}(H)) \cup \tau$ . We have

$$U_1(t)^* e^{-itH} u = U_1(t)^* \chi^2(H) e^{-itH} u = U_1(t)^* F\left(\frac{R}{t} \geq \varepsilon_0\right) \chi^2(H) e^{-itH} u + o(1),$$

owing to Proposition 2.8. Lemma 3.4 then implies

$$U_1(t)^* e^{-itH} u = U_1(t)^* \chi(H_0) F\left(\frac{R}{t} \geq \varepsilon_0\right) \chi(H) e^{-itH} u + o(1).$$

We introduce the Heisenberg derivative

$$D_1 B = \frac{\partial}{\partial t} + iH(t)B - iBH$$

and we get

$$\begin{aligned} D_1 \left[ \chi(H_0) F\left(\frac{R}{t} \geq \varepsilon_0\right) \chi(H) \right] = & \\ & - \chi(H_0) \frac{R}{t^2} F'\left(\frac{R}{t} \geq \varepsilon_0\right) \chi(H) + \chi(H_0) \left[ H_0, iF\left(\frac{R}{t} \geq \varepsilon_0\right) \right] \chi(H) \\ & + [\chi(H_0), iV_l(t, k, D_k)] F\left(\frac{R}{t} \geq \varepsilon_0\right) \chi(H) \\ & + \chi(H_0) \left[ V_l(t, k, D_k), iF\left(\frac{R}{t} \geq \varepsilon_0\right) \right] \chi(H) \\ & + \chi(H_0) F\left(\frac{R}{t} \geq \varepsilon_0\right) (iV_l(t, k, D_k) - iV) \chi(H). \end{aligned}$$

By pseudo-differential calculus, the third and fourth terms are  $O(t^{-1-\mu'})$ , with  $0 < \mu' < \mu$ .

The last term equals for large enough  $t$

$$\begin{aligned}
& \chi(H_0) iF\left(\frac{R}{t} \geq \varepsilon_0\right) \left[ V_s + V_l \left( F\left(\frac{R}{t} \log(t) \geq \varepsilon_0\right) - 1 \right) \right] \chi(H) \\
&= \chi(H_0) iF\left(\frac{R}{t} \geq \varepsilon_0\right) V_l F\left(\frac{R}{t} \log(t) \leq \varepsilon_0\right) \chi(H) + O(t^{-1-\mu_s}) \\
&= \chi(H_0) \left[ F\left(\frac{R}{t} \geq \varepsilon_0\right), V_l \right] F\left(\frac{R}{t} \log(t) \leq \varepsilon_0\right) \chi(H) + O(t^{-1-\mu_s}) \\
&= O(t^{-1-\inf(\mu', \mu_s)}).
\end{aligned}$$

For the second term we set  $\tilde{\chi}(u) = (u+i)\chi(u)$  and we choose some cut-off  $F(u=\varepsilon_0) \in \mathcal{C}_{\text{comp}}^\infty((C^{-1}\varepsilon_0, C\varepsilon_0))$  with  $C > 1$  chosen so that  $F(u=\varepsilon_0) \equiv 1$  on  $\text{supp } F'(u \geq \varepsilon_0)$ . We have

$$\begin{aligned}
& \chi(H_0) \left[ H_0, iF\left(\frac{R}{t} \geq \varepsilon_0\right) \right] \chi(H) \\
&= -i\tilde{\chi}(H_0) \left[ (H_0+i)^{-1}, F\left(\frac{R}{t} \geq \varepsilon_0\right) \right] (H_0+i)\chi(H) \\
&= -i\tilde{\chi}(H_0) \left[ (H_0+i)^{-1}, F\left(\frac{R}{t} \geq \varepsilon_0\right) \right] [\tilde{\chi}(H) - V\chi(H)] \\
&= -i\tilde{\chi}(H_0) F\left(\frac{R}{t} = \varepsilon_0\right) \frac{1}{t} \nabla_k [(H_0(k)+i)^{-1}] \frac{D_k}{R} F'\left(\frac{R}{t} \geq \varepsilon_0\right) F\left(\frac{R}{t} = \varepsilon_0\right) \\
&\quad \circ [\tilde{\chi}(H) - V\chi(H)] + O(t^{-2}) \\
&= -i\tilde{\chi}(H_0) F\left(\frac{R}{t} = \varepsilon_0\right) \frac{1}{t} \nabla_k [(H_0(k)+i)^{-1}] \frac{D_k}{R} F'\left(\frac{R}{t} \geq \varepsilon_0\right) F\left(\frac{R}{t} = \varepsilon_0\right) \tilde{\chi}(H) \\
&\quad + O(t^{-1-\inf(\mu', \mu_s)}).
\end{aligned}$$

Hence the complete Heisenberg derivative writes

$$\begin{aligned}
D_1 \left[ \chi(H_0) F\left(\frac{R}{t} \geq \varepsilon_0\right) \chi(H) \right] &= \tilde{\chi}(H_0) F\left(\frac{R}{t} = \varepsilon_0\right) \frac{B(t)}{t} F\left(\frac{R}{t} = \varepsilon_0\right) \tilde{\chi}(H) \\
&\quad + O(t^{-1-\inf(\mu', \mu_s)})
\end{aligned}$$

with  $\|B(t)\| = O(1)$ . By referring to Proposition 2.8, to the propagation estimate (3.4) for  $U_1(t)$  and to the version of the Cook method recalled in Lemma A.2 b), we conclude that the observable  $\chi(H_0) F\left(\frac{R}{t} \geq \varepsilon_0\right) \chi(H)$  is integrable along the evolution. Thus the limit of  $U_1(t) e^{-iHt} u$  as  $t \rightarrow +\infty$  exists. Let  $\tilde{W}_1^+$  denote the limit (3.7). The fact that  $\tilde{W}_1^+ = (W_1^+)^*$  will follow from the properties:

$$W_1^+ \mathcal{H} \subset 1_c(H) \mathcal{H} \quad (3.9)$$

$$\text{and } \tilde{W}_1^+ \mathcal{H} \subset 1_{R \setminus r}(H_1^+) \mathcal{H}. \quad (3.10)$$

For  $E \in \sigma_{\text{pp}}(H)$ ,  $\psi_E \in \mathcal{H}$  so that  $H\psi_E = E\psi_E$  and  $u \in 1_{\mathbf{R} \setminus \tau}(H_1^+) \mathcal{H}$ , we have

$$(\psi_E, W_1^+ u) = \lim_{t \rightarrow +\infty} e^{-itE} (\psi_E, U_1(t)u).$$

As a consequence of the minimal velocity estimate (3.5) for  $U_1(t)$ ,  $U_1(t)u$  weakly converges to 0 and this yields (3.9). Let us consider (3.10). We first check that the convergence

$$\text{s-lim}_{t \rightarrow +\infty} U_1(t)^*(\chi(H_0) - \chi(H))e^{-itH} 1_c(H) = 0, \quad (3.11)$$

holds for any function  $\chi \in \mathcal{C}_{\text{comp}}^\infty(\mathbf{R})$ . Indeed for  $\tilde{\chi} \in \mathcal{C}_{\text{comp}}^\infty(\mathbf{R} \setminus (\tau \cup \sigma_{\text{pp}}(H)))$ , we infer from the minimal velocity bound for  $H$  stated in Proposition 2.8 and from Lemma 3.4 ii) that

$$\begin{aligned} & \text{s-lim}_{t \rightarrow +\infty} U_1(t)^*(\chi(H_0) - \chi(H))e^{-itH} \tilde{\chi}(H) \\ &= \text{s-lim}_{t \rightarrow +\infty} U_1(t)^*(\chi(H_0) - \chi(H))F\left(\frac{R}{t} \geq \varepsilon_0\right)e^{-itH} \tilde{\chi}(H) = 0. \end{aligned}$$

This yields the strong convergence of (3.11). This and the definition of  $H_1^+$  ensure that

$$\tilde{W}_1^+ \chi(H) = \chi(H_1^+) \tilde{W}_1^+, \quad \chi \in \mathcal{C}_{\text{comp}}^\infty(\mathbf{R}). \quad (3.12)$$

Since  $1_c(H) = 1_{\mathbf{R} \setminus \tau}(H)1_c(H)$ , we get that

$$\tilde{W}_1^+ = \tilde{W}_1^+ 1_c(H) = 1_{\mathbf{R} \setminus \tau}(H_1^+) \tilde{W}_1^+,$$

and therefore (3.10). The unitarity of  $\tilde{W}_1^+$  now follows at once: It is one to one as an isometry and the surjectivity is a consequence of (3.6) and (3.7). This also gives  $\tilde{W}_1 = W_1^*$  and the identity (3.8) comes from (3.12).

Next we shall prove Theorems 2.11 and 2.17 about asymptotic observables. Beside the information that they bring about observables, these results are important for the long-range problem. With them, one is able to develop a local analysis on  $\Sigma$ . We begin with a Lemma which in the end allows the identification of the spectrum of  $\mathcal{Q}^+$ .

**Lemma 3.6.** *Let  $E$  be a countable subset of  $\mathbf{R}$ , then the closure in  $\Sigma$  of  $\Sigma \setminus p_{\mathbf{R}}^{-1}(E \cup \tau)$  equals  $\overline{\Sigma \setminus p_{\mathbf{R}}^{-1}(\sigma_{\text{pp}}(H_0))}$ .*

*Proof.* We first note that  $\overline{\Sigma \setminus p_{\mathbf{R}}^{-1}(E \cup \tau)} \subset \overline{\Sigma \setminus p_{\mathbf{R}}^{-1}(\sigma_{\text{pp}}(H_0))}$  because  $\sigma_{\text{pp}}(H_0) \subset \tau$ . If  $(\lambda_0, k_0) \in \Sigma$  does not belong to  $\Sigma \setminus p_{\mathbf{R}}^{-1}(E \cup \tau)$ , then there exist  $I \in \mathcal{V}_{\mathbf{R}}(\lambda_0)$  and  $W \in \mathcal{V}_{\mathbf{M}}(k_0)$  so that  $p_{\mathbf{R}}(I \times W \cap \Sigma)$  is included in  $E \cup \tau$ . Since  $p_{\mathbf{R}}$  is continuous and

$E \cup \tau$  is countable, we have necessarily  $p_{\mathbf{R}}(I \times W \cap \Sigma) = \{\lambda_0\}$ . Hence  $\lambda_0$  belongs to  $\sigma_{\text{pp}}(H_0)$ . We have proved

$$\Sigma \setminus p_{\mathbf{R}}^{-1}(\sigma_{\text{pp}}(H_0)) \subset \overline{\Sigma \setminus p_{\mathbf{R}}^{-1}(E \cup \tau)}$$

and we conclude by taking the closure in  $\Sigma$ .

*Proof of Theorem 2.11.* The existence of (2.18) with  $g \in \mathcal{C}_0^0(\Sigma \setminus p_{\mathbf{R}}^{-1}(\tau \cup \sigma_{\text{pp}}(H)))$  is a direct consequence of Proposition 3.2 and Proposition 3.5. This limit equals

$$W_1^+ g(H_1^+, k_1^+)(W_1^+)^*. \quad (3.13)$$

This result extends to any  $g \in \mathcal{C}_0^0(\Sigma)$  by noticing that

$$\text{s-lim}_{n \rightarrow \infty} \chi_n(H) = 1_c(H),$$

for some sequence of functions  $\chi_n \in \mathcal{C}_0^0(\mathbf{R} \setminus (\sigma_{\text{pp}}(H) \cup \tau))$ ,  $0 \leq \chi_n \leq 1$ , which a.e. converges to 1. Then we have

$$g(H, k^+)_c = \text{s-lim}_{n \rightarrow \infty} g(H, k^+)_c \chi_n(H).$$

Thus, the last statement of the Theorem is a consequence of (3.8). We next verify that the  $C^*$ -morphism

$$\mathcal{C}_0^0(\overline{\Sigma \setminus p_{\mathbf{R}}^{-1}(\sigma_{\text{pp}}(H) \cup \tau)}) \ni g \rightarrow g(H, k^+)_c \in \mathcal{L}(\mathcal{H})$$

defines a faithful representation of  $\mathcal{C}_0^0(\overline{\Sigma \setminus p_{\mathbf{R}}^{-1}(\sigma_{\text{pp}}(H) \cup \tau)})$ . This will imply that the spectrum of  $\mathcal{U}^+$  equals  $\overline{\Sigma \setminus p_{\mathbf{R}}^{-1}(\sigma_{\text{pp}}(H) \cup \tau)} = \overline{\Sigma \setminus p_{\mathbf{R}}^{-1}(\sigma_{\text{pp}}(H_0))}$ , according to Lemma 3.6. Indeed it is enough to check that this morphism is one to one, or

$$\|g(H, k^+)_c\| \geq \frac{\sup}{\overline{\Sigma \setminus p_{\mathbf{R}}^{-1}(\sigma_{\text{pp}}(H) \cup \tau)}} |g|, \quad \forall g \in \mathcal{C}_0^0(\overline{\Sigma \setminus p_{\mathbf{R}}^{-1}(\sigma_{\text{pp}}(H) \cup \tau)}). \quad (3.14)$$

By taking a sequence of functions  $\chi_n$  as above, we get

$$\|g(H, k^+)_c\| \geq \sup_n \|\chi_n(H)g(H, k^+)_c\|.$$

We refer to (3.13) while replacing  $g$  by  $\chi_n g$  and we recall that  $W_1^+$  is unitary from  $1_{\mathbf{R} \setminus \tau}(H_1^+) \mathcal{H}$  onto  $1_c(H) \mathcal{H}$ . We obtain

$$\|\chi_n(H)g(H, k^+)_c\| = \|\chi_n(H_1^+)g(H_1^+, k_1^+)\| = \frac{\sup}{\overline{\Sigma \setminus p_{\mathbf{R}}^{-1}(\sigma_{\text{pp}}(H) \cup \tau)}} |\chi_n g|.$$

By combining the two previous inequalities and by taking the sup-limit as  $n \rightarrow \infty$ ,

we deduce (3.14).

*Proof of Theorem 2.17.* Let us first prove a). Since  $\chi(H_0)v_{H_0}$  is a bounded operator, since we have

$$1_{\Sigma_{\text{reg}}}(H, k^+)_c = 1_{\Sigma_{\text{reg}}}(H, k^+)_c 1_{\mathbf{R} \setminus \tau}(H) 1_c(H)$$

and since  $1_{\Sigma_{\text{reg}} \setminus p_{\mathbf{R}}^{-1}(\sigma_{\text{pp}}(H) \cup \tau)}$  is the pointwise limit of a sequence in  $\mathcal{C}_0^0(\Sigma_{\text{reg}} \setminus p_{\mathbf{R}}^{-1}(\sigma_{\text{pp}}(H) \cup \tau))$ , the quantity  $1_{\Sigma_{\text{reg}}}(H, k^+)_c$  can be replaced by  $g(H, k^+)_c$  with  $g \in \mathcal{C}_0^0(\Sigma_{\text{reg}} \setminus p_{\mathbf{R}}^{-1}(\sigma_{\text{pp}}(H) \cup \tau))$ . With Theorem 2.11, we get

$$\begin{aligned} \text{s-lim}_{t \rightarrow +\infty} e^{itH} \chi(H_0)v_{H_0} e^{-itH} g(H, k^+)_c &= \text{s-lim}_{t \rightarrow +\infty} e^{itH} \chi(H_0)v(H_0, k) g(H_0, k) e^{-itH} \\ &= \chi(H)v(H, k^+)_c g(H, k^+)_c \end{aligned}$$

because  $v$  is smooth on  $\Sigma_{\text{reg}}$ .

Let us now prove b). By the density of  $\mathcal{C}_{\text{comp}}^\infty(\mathbf{R}^n)$  in  $\mathcal{C}_0^0(\mathbf{R}^n)$ , we can assume  $f \in \mathcal{C}_{\text{comp}}^\infty(\mathbf{R}^n)$ . Then we note that we have, for such a function, the estimate

$$\sup_{x \in \mathbf{R}^n} \left| f\left(\frac{x}{t}\right) - f\left(\frac{|x|}{t}\right) \right| = O_f\left(\frac{1}{t}\right).$$

As a consequence, the time-dependent observable  $f(\frac{x}{t})$  can be replaced by  $f(\frac{|x|}{t})$ , which becomes  $f(-\frac{D_k}{t})$  after conjugating with the Floquet-Bloch transformation. One easily checks

$$\text{s-lim}_{t \rightarrow +\infty} e^{itH} f\left(-\frac{D_k}{t}\right) e^{-itH} 1_{\text{pp}}(H) = f(0) 1_{\text{pp}}(H).$$

By its definition,  $v_H^\dagger$  satisfies

$$v_H^\dagger 1_{\text{pp}}(H) = 0,$$

which shows that

$$\text{s-lim}_{t \rightarrow +\infty} e^{itH} f\left(-\frac{D_k}{t}\right) e^{-itH} 1_{\text{pp}}(H) = f(v_H^\dagger) 1_{\text{pp}}(H).$$

It remains to check that

$$\text{s-lim}_{t \rightarrow +\infty} e^{itH} f\left(-\frac{D_k}{t}\right) e^{-itH} 1_{\Sigma_{\text{reg}}}(H, k^+)_c = f(v_H^\dagger) 1_c(H).$$

For the same reason as in the proof of a),  $1_{\Sigma_{\text{reg}}}(H, k^+)_c$  can be replaced by  $g^4(H, k^+)_c$  with  $g \in \mathcal{C}_0^0(\Sigma_{\text{reg}} \setminus p_{\mathbf{R}}^{-1}(\tau \cup \sigma_{\text{pp}}(H)))$ . Since  $p_{\mathbf{R}}(\text{supp } g) \cap \tau = \emptyset$ , we deduce from the construction of the set  $\tau$  given in [12] that  $|v(\lambda, k)|$  is bounded from below by a positive constant on  $\text{supp } g$ . This implies

$$f(v_H^\dagger) = 0, \quad \text{for } f \in \mathcal{C}_{\text{comp}}^\infty(B(0, \epsilon_0)), \quad \epsilon_0 \ll 1.$$

Using the minimal velocity estimate in Proposition 2.8 leads to

$$\text{s-lim}_{t \rightarrow +\infty} e^{itH} f \left( -\frac{D_k}{t} \right) e^{-itH} g(H, k^+)_c = 0, \quad f \in \mathcal{C}_{\text{comp}}^\infty(B(0, \epsilon_0)),$$

for  $\epsilon_0 > 0$  small enough. Thus it suffices to prove b) for  $f \in \mathcal{C}_{\text{comp}}^\infty(\mathbf{R}^n \setminus \{0\})$ . Proposition 3.5 and (3.13) reduce the problem to the existence of

$$\text{s-lim}_{t \rightarrow +\infty} U_1(t) * f \left( -\frac{D_k}{t} \right) U_1(t) g^A(H_1^+, k_1^+). \quad (3.15)$$

By taking a locally finite partition of unity on  $\Sigma_{\text{reg}} \setminus p_{\mathbf{R}}^{-1}(\tau \cup \sigma_{\text{pp}}(H))$ , we can assume that  $g$  is supported in some small enough neighborhood  $I_0 \times V_0$  of  $(\lambda_0, k_0)$  so that  $\pi(k) = 1_{I_0}(H_0(k)) = 1_{\tilde{\lambda}(k)}(H_0(k))$  and  $\tilde{\lambda}(k)$  are real analytic w.r.t.  $k \in V_0$ . We introduce the unitary propagator  $U_2(t)$  generated by the time-dependent Hamiltonian

$$H_2(t) = \chi(k) \tilde{\lambda}(k) \pi(k) + V_1(t, k, D_k), \quad (3.16)$$

with  $\chi \in \mathcal{C}_{\text{comp}}^\infty(V_0)$ ,  $\chi \equiv 1$  on  $\text{supp } g$ . Note that

$$H_0 g(H_0, k) = \chi(k) \tilde{\lambda}(k) \pi(k) g(H_0, k). \quad (3.17)$$

Moreover by pseudo-differential calculus, we have

$$\left\| \left[ g^2(H_0, k), f \left( -\frac{D_k}{t} \right) \right] \right\| = O(t^{-1}) \quad (3.18)$$

$$\text{and} \quad \left\| [g^2(H_0, k), V_1(t, k, D_k)] \right\| = O(t^{-1-\mu'}). \quad (3.19)$$

We next apply Proposition 3.2 and estimate (3.18) so that the existence of the limit (3.15) is equivalent to the one of

$$\text{s-lim}_{t \rightarrow +\infty} U_1(t) * g^2(H_0, k) f \left( -\frac{D_k}{t} \right) g^2(H_0, k) U_1(t).$$

Then we infer from (3.17), (3.19) the existence of

$$\text{s-lim}_{t \rightarrow +\infty} U_1(t) * g(H_0, k) U_2(t) \quad \text{and} \quad \text{s-lim}_{t \rightarrow +\infty} U_2(t) * g(H_0, k) U_1(t).$$

Hence, it suffices to check the existence of

$$\text{s-lim}_{t \rightarrow +\infty} U_2(t) * g(H_0, k) f \left( -\frac{D_k}{t} \right) g(H_0, k) U_2(t).$$

We first check the estimate

$$\| (D_k + t \partial_k (\chi \tilde{\lambda})(k) \pi(k)) U_2(t) R^{-1} \| = O(t^{1-\mu'}). \quad (3.20)$$

Let  $D_2$  denote the derivation  $\frac{\partial}{\partial t} + i[H_2(t), \cdot]$  and let  $\tilde{\chi}$  belong to  $\mathcal{C}_{\text{comp}}^\infty(V_0)$  so that  $\tilde{\chi} \equiv 1$  on  $\text{supp } \chi$ . We have

$$\begin{aligned} & D_2(D_k + t\partial_k(\chi\tilde{\lambda})(k)\pi(k) + \tilde{\chi}[\partial_k\pi(k), i\pi(k)]) \\ &= \partial_k(\chi\tilde{\lambda})(k)\pi(k) - \partial_k(\chi(k)\tilde{\lambda}(k)\pi(k)) - \partial_k V_l(t, k, D_k) \\ & \quad - \chi(k)\tilde{\lambda}(k)[\pi(k), [\partial_k\pi(k), \pi(k)]] \\ & \quad + i[V_l(t, k, D_k), t\partial_k(\chi\tilde{\lambda})(k)\pi(k) + \tilde{\chi}[\partial_k\pi(k), i\pi(k)]]. \end{aligned}$$

By pseudo-differential calculus, the last term and  $\partial_k V_l(t, k, D_k)$  are  $O(t^{-\mu'})$ . The remainder equals

$$-\chi(k)\tilde{\lambda}(k)(\partial_k\pi(k) + [\pi(k), [\partial_k\pi(k), \pi(k)]]) = 0.$$

Indeed the relation  $\pi^2(k) = \pi(k)$  yields

$$\begin{aligned} \partial_k\pi(k) &= \partial_k\pi^2(k) = \partial_k\pi(k)\pi(k) + \pi(k)\partial_k\pi(k) \\ \text{and } \pi(k)\partial_k\pi(k)\pi(k) &= 0. \end{aligned}$$

The estimate (3.20) is then derived by integrating from 0 to  $t$ . The assertion iii) of Proposition B.3 provides the decomposition

$$f\left(-\frac{D_k}{t}\right) - f(\partial_k(\chi\tilde{\lambda})(k)) = R_1(t)\left(\frac{D_k}{t} + \partial_k(\chi\tilde{\lambda})(k)\right) + R_2(t), \quad (3.21)$$

with  $R_1(t) = O(1)$ ,  $R_2(t) = O(t^{-1})$  and therefore  $R_1(t)\frac{D_k}{t} = O(1)$ . Since  $f(0) = 0$  and  $\pi(k)g(H_0, k) = g(H_0, k)$ , we have

$$\begin{aligned} & g(H_0, k)\left[f\left(-\frac{D_k}{t}\right) - f(\partial_k(\chi\tilde{\lambda})(k)\pi(k))\right]g(H_0, k) \\ &= g(H_0, k)\left[f\left(-\frac{D_k}{t}\right) - f(\partial_k(\chi\tilde{\lambda})(k))\pi(k)\right]g(H_0, k) \\ &= g(H_0, k)R_1(t)\left[\frac{D_k}{t} + \partial_k(\chi\tilde{\lambda})(k)\pi(k)\right]g(H_0, k) + O(t^{-1}). \end{aligned}$$

The estimate (3.19) (with  $g^2$  replaced by  $g$ ) provide the existence of

$$s\text{-}\lim_{t \rightarrow +\infty} U_2(t) * g(H_0, k) U_2(t).$$

Moreover we deduce from (3.20)

$$\left\| g(H_0, k)R_1(t)\left(\frac{D_k}{t} + \partial_k(\chi\tilde{\lambda})(k)\pi(k)\right)U_2(t)u \right\| = O(t^{-\mu}), \quad \forall u \in D(R).$$

By using (3.21), we get

$$\text{s-lim}_{t \rightarrow +\infty} g(H_0, k) \left( f \left( -\frac{D_k}{t} \right) - f(\partial_k(\chi \tilde{\lambda})(k)\pi(k)) \right) U_2(t) = 0$$

and, going back to the evolution  $U_1(t)$ ,

$$\begin{aligned} & \text{s-lim}_{t \rightarrow +\infty} U_1(t) * g(H_0, k) \left( f \left( -\frac{D_k}{t} \right) - f(\partial_k(\chi \tilde{\lambda})(k)\pi(k)) \right) g(H_0, k) U_1(t) \\ &= \text{s-lim}_{t \rightarrow +\infty} U_1(t) * \left( f \left( -\frac{D_k}{t} \right) - f(\partial_k(\chi \tilde{\lambda})(k)\pi(k)) \right) g^2(H_0, k) U_1(t) = 0. \end{aligned}$$

Then Proposition 3.2 implies

$$\begin{aligned} & \text{s-lim}_{t \rightarrow +\infty} U_1(t) * g^2(H_0, k) f(\partial_k(\chi \tilde{\lambda})(k)\pi(k)) g^2(H_0, k) U_1(t) \\ &= f(\partial_k(\chi \tilde{\lambda})(k_1^+)\pi(k_1^+)) g^4(H_1^+, k_1^+) \end{aligned}$$

and provides the existence and the expression of (3.15). Finally, this one is nothing but  $f(v(H_1^+, k_1^+)) g^4(H_1^+, k_1^+)$  because  $\chi \equiv 1$  on  $\text{supp } g$ .

We close this section with the proof of the short-range result.

*Proof of Theorem 2.18.* Proposition 3.5 implies part a) of Theorem 2.18 because when  $V_1=0$  we have  $U_1(t) = e^{-itH_0}$  and  $H_1^+ = H_0$ . Moreover it follows from part a) that:

$$g(H, k^+)_c = W^+ g(H_0, k) (W^+)^* \text{ for all Borel functions } g \text{ on } \Sigma.$$

By the remark after Definition 2.2, we have  $1_{\Sigma \setminus \Sigma_{\text{reg}}}(H_0, k) = 0$  and therefore  $1_{\Sigma \setminus \Sigma_{\text{reg}}}(H, k^+)_c = 0$ . Thus, part b) of Theorem 2.18 is a consequence of Theorem 2.17.

#### 4. Existence of modified wave operators in the long-range case

The first step of this analysis is the construction of local (on  $\Sigma$ ) modified wave operators. Let  $(\lambda_0, k_0) \in \Sigma_{\text{reg}}$ . We consider small neighborhoods  $\Omega_0 \in \mathcal{V}_{\Sigma_{\text{reg}}}(\lambda_0, k_0)$ ,  $I_0 \in \mathcal{V}_{\mathbf{R}}(\lambda_0)$ ,  $V_0 \in \mathcal{V}_M(k_0)$  and  $\tilde{V}_0 \in \mathcal{V}_M(k_0)$ , so that  $\Omega_0 \subset \subset I_0 \times V_0$  and  $V_0 \subset \subset \tilde{V}_0$ . Indeed  $I_0$  and  $\tilde{V}_0$  are chosen so that  $\pi(k) = 1_{I_0}(H_0(k)) = 1_{\tilde{\lambda}(k)}(H_0(k))$  and  $\tilde{\lambda}(k)$  are real analytic w.r.t.  $k \in \tilde{V}_0$ . We take  $\chi \in \mathcal{C}_{\text{comp}}^\infty(\tilde{V}_0)$ ,  $\chi \equiv 1$  on  $V_0$ . When  $\tilde{V}_0$  is small enough, it can be identified with some open subset of  $\mathbf{R}^n$  and the construction of Appendix A.2 provides a solution to the Hamilton-Jacobi equation

$$\begin{cases} \partial_t S_0(t, k) = \chi(k) \tilde{\lambda}(k) + \chi(k) [\text{Re } V_J](t, k, -\partial_k S_0(t, k)), & k \in \tilde{V}_0 \\ S_0(T, k) = 0, \end{cases} \quad (4.1)$$

with the estimates for  $\mu' < \mu$

$$\partial_k^\alpha (S_0(t, k) - t\chi(k)\tilde{\lambda}(k)) = O_\alpha(t^{1-\mu'}), \quad \forall k \in \tilde{V}_0, \quad \forall \alpha \in \mathbf{N}^n. \quad (4.2)$$

Note that we introduced the cut-off  $\chi$  in order to have a global definition of  $S_0(t, k)$ : This solution  $S_0(t, \cdot)$  belongs to  $\mathcal{C}_{\text{comp}}^\infty(M; \mathbf{R})$  and is supported in  $\tilde{V}_0$  for all  $t \geq T$ . If the variable  $k$  is restricted to  $V_0$ , then one can drop the cut-off  $\chi$  in the estimates (4.2) in equation (4.1) and all relations locally derived from this equation.

We will need some other propagation estimates. The expression  $U_2(t)$  again denotes the unitary propagator associated with the time-dependent Hamiltonian  $H_2(t)$  given by (3.16). For the sake of simplicity we assume  $T=0$ , which can be done after changing the time origin.

**Lemma 4.1.** *Let  $g$  belong to  $\mathcal{C}_{\text{comp}}^\infty(I_0 \times V_0)$  with  $\text{supp } g|_\Sigma \subset \Omega_0$ . Then we have*

$$\|(D_k + \partial_k S_0(t, k))g(H_0, k)U_2(t)R^{-1}\| = O(1), \quad (4.3)$$

and 
$$\|(D_k + \partial_k S_0(t, k))g(H_0, k)e^{-iS_0(t, k)}R^{-1}\| = O(1). \quad (4.4)$$

*Proof.* The estimate (4.4) is rather easy. Indeed the identity

$$D_k e^{-iS_0(t, k)} = e^{-iS_0(t, k)}(D_k - \partial_k S_0(t, k)),$$

implies

$$\begin{aligned} (D_k + \partial_k S_0(t, k))g(H_0, k)e^{-iS_0(t, k)} &= g(H_0, k)e^{-iS_0(t, k)}D_k \\ &+ [D_k, g(H_0, k)]e^{-iS_0(t, k)}. \end{aligned}$$

But since  $g \in \mathcal{C}_{\text{comp}}^\infty(I_0 \times V_0)$ , the commutator is bounded. This implies (4.4).

The proof of (4.3) is more involved. For  $\tilde{g} \in \mathcal{C}_{\text{comp}}^\infty(I_0 \times V_0)$ , with  $\tilde{g} \equiv 1$  on  $\text{supp } g$ , and for  $p \in \mathbf{N}$  we set

$$G_p := \tilde{g}^{2p}(H_0, k).$$

Pseudo-differential calculus yields

$$(D_k + \partial_k S_0(t, k))g(H_0, k) = g(H_0, k)G_p(D_k + \partial_k S_0(t, k))G_p + O(1).$$

Hence the problem is reduced to checking that

$$F_p(t) = U_2(t)^* G_p(D_k + \partial_k S_0(t, k))G_p U_2(t)R^{-1}$$

is uniformly bounded with respect to  $t \geq 0$  for some  $p \in \mathbf{N}$ . It is clear that  $F_p(0)$  is bounded. Meanwhile its derivative equals

$$F_p'(t) = U_2(t)^* \mathbf{D}_2[G_p(D_k + \partial_k S_0(t, k))G_p]U_2(t)R^{-1},$$

where  $D_2$  is the Heisenberg derivative associated with  $H_2(t)$ . In the next calculation, the expression  $B_r(t)$  will generically denote a bounded operator of which the norm is  $O(t^{-r})$  and  $\mu'$  will be some positive number smaller than  $\mu$ . By noticing that  $G_p \chi(k) \pi(k) = G_p$  because  $\text{supp } \tilde{g} \subset I_0 \times V_0$ , we get

$$\begin{aligned} & D_2(G_p(D_k + \partial_k S_0(t, k))G_p) \\ &= i[V_l(t, k, D_k), G_p](D_k + \partial_k S_0(t, k))G_p + \text{h.c.} \\ & \quad + G_p(-\partial_k \tilde{\lambda}(k) + i[V_l(t, k, D_k), D_k + \partial_k S_0(t, k)] + \partial_{ik}^2 S_0(t, k))G_p \\ &=: I_1(t) + I_2(t). \end{aligned}$$

Pseudo-differential calculus combined with estimate (4.2) leads to

$$I_1(t) = B_{1+\mu'}(t)G_{p-1}(D_k + \partial_k S_0(t, k))G_{p-1} + B_{1+\mu'}(t), \quad \text{for } p \geq 1 \quad (4.5)$$

$$\text{and } I_1(t) = B_{\mu'}(t), \quad \text{for } p = 0. \quad (4.6)$$

For the second term  $I_2(t)$ , we first recall that the principal symbol of  $V_l(t, k, D_k)$  is real so that

$$\begin{aligned} i[V_l(t, k, D_k), D_k + \partial_k S_0(t, k)] &= -\partial_k \mathbf{Re} V_l(t, k, D_k) + \partial_\eta \mathbf{Re} V_l(t, k, D_k) \partial_k^2 S_0(t, k) \\ & \quad + B_{1+\mu'}(t). \end{aligned}$$

By differentiating the Hamilton-Jacobi equation (4.1) with respect to  $k \in V_0$ , we obtain:

$$\partial_{ik}^2 S_0(t, k) = \partial_k \tilde{\lambda}(k) + \partial_k \mathbf{Re} V_l(t, k, -\partial_k S_0(t, k)) - \partial_\eta \mathbf{Re} V_l(t, k, -\partial_k S_0(t, k)) \partial_k^2 S_0(t, k).$$

The two previous identities imply

$$\begin{aligned} I_2(t) &= -G_p[\partial_k \mathbf{Re} V_l(t, k, D_k) - \partial_k \mathbf{Re} V_l(t, k, -\partial_k S_0(t, k))]G_p \\ & \quad + G_p[\partial_\eta \mathbf{Re} V_l(t, k, D_k) - \partial_\eta \mathbf{Re} V_l(t, k, -\partial_k S_0(t, k))] \cdot \partial_k^2 S_0(t, k)G_p + B_{1+\mu'}(t). \end{aligned}$$

By Proposition B.3, we have

$$\begin{aligned} & (\partial_k \mathbf{Re} V_l(t, k, D_k) - \partial_k \mathbf{Re} V_l(t, k, -\partial_k S_0(t, k))) = \\ & B_{1+\mu'}(t)(D_k + \partial_k S_0(t, k, D_k)) + B_{1+\mu'}(t), \\ & (\partial_\eta \mathbf{Re} V_l(t, k, D_k) - \partial_\eta \mathbf{Re} V_l(t, k, -\partial_k S_0(t, k))) = \\ & B_{2+\mu'}(t)(D_k + \partial_k S_0(t, k, D_k)) + B_{2+\mu'}(t), \end{aligned}$$

while (4.2) says that the norm of  $\partial_k^2 S_0(t, k)$  is  $O(t)$ . Hence the term  $I_2(t)$  admits the same decomposition as  $I_1(t)$  in (4.5) (4.6). By going back to the definition of  $F_p(t)$ , we obtain

$$F'_p(t) = B_{1+\mu'}(t)F_{p-1}(t) + B_{1+\mu'}(t) \quad \text{for } p \geq 1$$

$$\text{and } F'_0(t) = B_{\mu'}(t).$$

By integrating and by induction, this yields

$$\|F_p(t)\| \leq C_p t^{-\inf\{0, 1 - (p+1)\mu\}}.$$

We conclude by taking  $p \geq [\mu^{-1}]$ .

**Proposition 4.2.** *The limits*

$$\text{s-lim}_{t \rightarrow +\infty} e^{itH} e^{-iS_0(t,k)} 1_{\Omega_0}(H_0, k) 1_c(H_0) \tag{4.7}$$

$$\text{and } \text{s-lim}_{t \rightarrow +\infty} e^{iS_0(t,k)} e^{-itH} 1_{\Omega_0}(H, k^+)_c \tag{4.8}$$

exist. If  $W_{\Omega_0}^+$  denotes the limit (4.7) then (4.8) equals  $(W_{\Omega_0}^+)^*$ . Moreover, we have:

$$W_{\Omega_0}^+ g(H_0, k) (W_{\Omega_0}^+)^* = g(H, k^+)_c, \quad g \in \mathcal{C}_0^0(\Omega_0).$$

*Proof.* By introducing some locally finite partition of unity on  $(I_0 \setminus (\tau \cup \sigma_{pp}(H))) \times V_0$ ,  $\sum_{j \in \mathbb{N}} g_j^2 = 1$ , with  $g_j \in \mathcal{C}_{\text{comp}}^\infty((I_0 \setminus (\tau \cup \sigma_{pp}(H))) \times V_0)$ , we have

$$\text{s-lim}_{N \rightarrow \infty} \sum_{j \leq N} g_j^2(H_0, k) 1_{\Omega_0}(H_0, k) = 1_{\Omega_0}(H_0, k) 1_c(H_0)$$

$$\text{and } \text{s-lim}_{N \rightarrow \infty} \sum_{j \leq N} g_j^2(H, k^+)_c 1_{\Omega_0}(H, k^+)_c = 1_{\Omega_0}(H, k^+)_c. \tag{4.9}$$

Hence, it suffices to prove the existence of the limits

$$\text{s-lim}_{t \rightarrow +\infty} e^{itH} e^{-iS_0(t,k)} g^2(H_0, k)$$

$$\text{and } \text{s-lim}_{t \rightarrow +\infty} e^{iS_0(t,k)} e^{-itH} g^2(H, k^+)_c = \text{s-lim}_{t \rightarrow +\infty} e^{iS_0(t,k)} g^2(H_0, k) e^{-itH}.$$

By the same method as in the proof of Theorem 2.17, the problem is reduced to the existence of the limits

$$\text{s-lim}_{t \rightarrow +\infty} U_2(t)^* g(H_0, k) e^{-iS_0(t,k)} \tag{4.10}$$

$$\text{and } \text{s-lim}_{t \rightarrow +\infty} e^{iS_0(t,k)} g(H_0, k) U_2(t). \tag{4.11}$$

We calculate

$$\begin{aligned}
& \frac{d}{dt}(e^{iS_0(t,k)}g(H_0, k)U_2(t)u) \\
&= e^{iS_0(t,k)}[i\partial_t S_0(t, k)g(H_0, k) - ig(H_0, k)((\chi\tilde{\lambda})(k)\pi(k) + V_l(t, k, D_k))]U_2(t)u \\
&= ie^{iS_0(t,k)}[\operatorname{Re}V_l(t, k, -\partial_k S_0(t, k)) - \operatorname{Re}V_l(t, k, D_k)]g^2(H_0, k)U_2(t)u + O(t^{-1-\mu'}). \quad (4.12)
\end{aligned}$$

We refer again to Proposition B.3 and write

$$(\operatorname{Re}V_l(t, k, -\partial_k S_0(t, k)) - \operatorname{Re}V_l(t, k, D_k)) = R_1(t)(D_k + \partial_k S_0(t, k)) + R_2(t)$$

with  $R_1(t) = O(t^{-1-\mu'})$  and  $R_2(t) = O(t^{-2-\mu'})$ . By density we can take  $u \in D(R)$  and Lemma 4.1 gives

$$\begin{aligned}
& \left\| \frac{d}{dt} e^{iS_0(t,k)}g(H_0, k)U_2(t)u \right\| \\
& \leq Ct^{-1-\mu'} [\|u\| + \|(D_k + \partial_k S_0(t, k))g(H_0, k)U_2(t)u\|] \\
& \leq Ct^{-1-\mu'}.
\end{aligned}$$

Thus we get the existence of the limit (4.11). We do the same for (4.10). The identification of (4.11) as the adjoint of (4.10) and the last statement rely on the same arguments as the one used for Proposition 3.5. Their proof is even simpler by referring to Theorem 2.11.

In order to construct a global modified dynamic, we take a locally finite covering of  $\Sigma_{\text{reg}} = \cup_j \overline{\Omega}_j$  where the sets  $\Omega_j$  are “smooth enough” open subsets of  $\Sigma_{\text{reg}}$  which satisfy the same properties as  $\Omega_0$  introduced in the beginning of this Section and  $\Omega_j \cap \Omega_{j'} = \emptyset$  for  $j \neq j'$ . The expression “smooth enough” means that the boundary  $\partial\Omega_j$  of  $\Omega_j$  is the finite union of submanifolds of  $\mathbf{R} \times M$  with codimension 2. Such a covering can be done with a triangulation of each stratum of  $\Sigma_{\text{reg}}$  (which is a semi-analytic set of  $\mathbf{R} \times M$  locally diffeomorphic to  $M$  by projection). With every  $\Omega_j$ , we associate the solution  $S_j(t, k)$ ,  $t \geq T_j$ , of the Hamilton-Jacobi equation (4.1) where a suitable cut-off  $\chi_j$  replaces  $\chi$ .

**Definition 4.3.** The modifier  $S(t, H_0, k)$  is the self-adjoint operator defined by

$$S(t, H_0, k) := \sum_j 1_{[T_j, +\infty)}(t) S_j(t, k) 1_{\Omega_j}(H_0, k). \quad (4.13)$$

*Remark 4.4.* We recall that the estimate (4.2) can be made uniform with respect to  $j$  for  $\alpha = 0$ . This combined with  $\sum_j 1_{\Omega_j}(H_0, k) = 1$  ensures that the domain of  $S(t, H_0, k)$  contains  $D(H_0)$  (and equals  $D(H_0)$  if  $T_j = T$  for all  $j$ ).

The Theorem 2.19 is now easily derived from its local form given in Proposition 4.2.

*Proof of Theorem 2.19.* We have

$$e^{-iS(t,H_0,k)} = \sum_j e^{-iS_j(t,k)} 1_{\Omega_j}(H_0, k).$$

The limit which defines the wave operator  $W^+$  exists because  $\sum_j 1_{\Omega_j}(H_0, k) = 1$ . For the converse limit, we first note that for all  $j$ , we have  $1_{\partial\Omega_j}(H_0, k) = 0$ . By applying Proposition 4.2 with finitely many  $\Omega_0$  which cover  $\partial\Omega_j$ , we deduce from this that  $1_{\partial\Omega_j}(H, k^+)_c = 0$ . This implies

$$\sum_j 1_{\Omega_j}(H, k^+)_c = 1_{\Sigma_{\text{reg}}}(H, k^+)_c$$

and the existence of the second limit in Theorem 2.19 becomes a consequence its local form (4.8).

### A. Some topics in scattering theory

In this appendix, we shall prove the minimal velocity estimates required in our analysis. Then, we will detail the construction of the Hamilton-Jacobi equation (4.1).

#### A.1. Minimal velocity estimates.

These abstract propagation estimates are due to Sigal-Soffer. We will follow the presentation given in [8] and [11], and give a sharper version which is needed here.

**Proposition A.1.** *Let  $H$  and  $A$  be two self-adjoint operators on a Hilbert space  $\mathcal{H}$ . Let  $V(t)$  be a bounded time-dependent self-adjoint perturbation so that the unitary propagator  $U(t) = U(t, 0)$ , associated with the Hamiltonian  $H(t) = H + V(t)$ , is well-defined. We suppose that:*

i) *The function  $s \rightarrow e^{isA}(H+i)^{-1}e^{-isA}$  belongs to  $\mathcal{C}^{1+\varepsilon}(\mathbf{R}, \mathcal{L}(\mathcal{H}))$ , for some  $\varepsilon > 0$ .*

ii)  $\|ad_A V(t)\| \in O(t^{-\varepsilon})$ ,  $\|ad_{(H+i)^{-1}} V(t)\| \in O(t^{-1-\varepsilon})$  as  $t \rightarrow \infty$

If  $\Delta$  denotes some interval so that

$$1_{\Delta}(H)[H, iA]1_{\Delta}(H) \geq c_0 E_{\Delta}(H),$$

then we have for any  $g \in \mathcal{C}_{\text{comp}}^{\infty}(\mathbf{R})$ ,  $\text{supp } g \subset (-\infty, c_0)$  and any  $f \in \mathcal{C}_{\text{comp}}^{\infty}(\Delta)$

$$\int_1^{+\infty} \left\| g\left(\frac{A}{t}\right) f(H) U(t) u \right\|^2 \frac{dt}{t} \leq C \|u\|^2, \quad \forall u \in \mathcal{H} \tag{A.1}$$

$$\text{and } s\text{-}\lim_{t \rightarrow +\infty} g\left(\frac{A}{t}\right) f(H) U(t) = 0. \tag{A.2}$$

The Heisenberg derivative  $\frac{d}{dt} + [H(t), \cdot]$  will be denoted by  $D$ . We will use the next

versions of Putnam-Kato inequality and Cook method. The proof can be found in [8].

**Lemma A.2.** *Let  $\Phi$  be a uniformly bounded  $\mathcal{L}(\mathcal{H})$ -valued  $\mathcal{C}^1$ -function on  $\mathbf{R}^+$ .*

a) *If there exist measurable  $\mathcal{L}(\mathcal{H})$ -valued functions  $B(t)$  and  $B_i(t)$ ,  $i=1 \dots n$ , so that*

$$D\Phi(t) = B^*(t)B(t) - \sum_{i=1}^n B_i(t)^*B_i(t)$$

with for all  $i \in \{1, \dots, n\}$

$$\int_1^\infty \|B_i(t)U(t)u\|^2 dt \leq C\|u\|^2, \quad \forall u \in \mathcal{H},$$

then there is a constant  $C_1 > 0$  so that

$$\int_1^\infty \|B(t)U(t)u\|^2 dt \leq C_1\|u\|^2, \quad \forall u \in \mathcal{H}.$$

b) *Let us assume that the function  $\Phi$  satisfies*

$$|(\psi_2, D\Phi(t)\psi_1)| \leq \sum_{i=1}^n \|B_{2i}(t)\psi_2\| \|B_{1i}(t)\psi_1(t)\|,$$

$$\text{with} \quad \int_1^{+\infty} \|B_{2i}(t)U(t)u\|^2 dt \leq C_1\|u\|^2, \quad \forall u \in \mathcal{H}$$

$$\text{and} \quad \int_1^{+\infty} \|B_{1i}(t)U(t)u\|^2 dt \leq C_1\|u\|^2, \quad \forall u \in \mathcal{D},$$

where  $\mathcal{D}$  is a dense subset of  $\mathcal{H}$ . Then, the limit

$$\text{s-lim}_{t \rightarrow +\infty} U(t)^* \Phi(t) U(t)$$

exists.

*Proof of Proposition A.1.* Let  $g \in \mathcal{C}_{\text{comp}}^\infty((-\infty, c_1))$  with  $c_1 < c_0$ . We set

$$F(t) = \int_s^{+\infty} g^2(s_1) ds_1$$

and we consider the observable

$$\Phi(t) = f(H)F\left(\frac{A}{t}\right)f(H).$$

We next calculate  $D\Phi(t)$ . We have

$$\begin{aligned} D\Phi(t) &= f(H) \left( \left[ H, iF\left(\frac{A}{t}\right) \right] - \frac{A}{t^2} g^2\left(\frac{A}{t}\right) \right) f(H) + \left[ V(t), if(H)F\left(\frac{A}{t}\right) f(H) \right] \\ &= f(H) \left( \left[ H, iF\left(\frac{A}{t}\right) \right] + \left[ V(t), iF\left(\frac{A}{t}\right) \right] - \frac{A}{t^2} g^2\left(\frac{A}{t}\right) \right) f(H) \\ &\quad + [V(t), if(H)]F\left(\frac{A}{t}\right) f(H) + \text{h.c.} \end{aligned}$$

In order to estimate the last term, we use Helffer-Sjöstrand functional calculus (2.7) and we reduce the problem to the estimate of commutators of  $V(t)$  with the resolvent  $(H+i)^{-1}$ . Our assumptions on  $V(t)$ , imply that the norm of this commutator is  $O(t^{-1-\epsilon})$ . By using  $\text{supp } g \subset (-\infty, c_1)$ , we get

$$D\Phi(t) \geq f(H) \left[ H, iF\left(\frac{A}{t}\right) \right] f(H) + f(H) [V(t), iF\left(\frac{A}{t}\right)] f(H) - c_1 \frac{1}{t} g^2\left(\frac{A}{t}\right) + O(t^{-1-\epsilon}).$$

For the commutators with  $F\left(\frac{A}{t}\right)$ , it is convenient to introduce the Fourier transform of  $F$ :

$$\begin{aligned} \left[ C, iF\left(\frac{A}{t}\right) \right] &= \frac{1}{2\pi} \int_{\mathbf{R}} \hat{F}(\sigma) [C, ie^{i\sigma \frac{A}{t}}] d\sigma \\ &= \frac{1}{2\pi t} \int_{\mathbf{R}} \hat{F}(\sigma) \sigma e^{i\sigma \frac{A}{t}} \int_0^1 e^{-i\sigma \theta \frac{A}{t}} [C, iA] e^{i\sigma \theta \frac{A}{t}} d\theta d\sigma \\ &= \frac{1}{2\pi t} \iiint_{\mathbf{R}^2 \times [0,1]} [\hat{g}(\sigma - \sigma') \hat{g}(\sigma')] e^{i\sigma(1-\theta)\frac{A}{t}} [C, iA] e^{i\sigma\theta\frac{A}{t}} d\theta d\sigma d\sigma' \\ &= \frac{1}{2\pi t} \iiint_{\mathbf{R}^2 \times [0,1]} [\hat{g}(\sigma) \hat{g}(\sigma')] e^{i(\sigma + \sigma')(1-\theta)\frac{A}{t}} [C, iA] e^{i(\sigma + \sigma')\theta\frac{A}{t}} d\theta d\sigma d\sigma'. \end{aligned} \tag{A.3}$$

By taking  $C = V(t)$ , we get

$$\left[ V(t), iF\left(\frac{A}{t}\right) \right] = O(t^{-1-\epsilon}).$$

For  $C = (H+i)^{-1}$ , our assumptions say that

$$\mathbf{R} \ni s \rightarrow B(s) = e^{isA} [(H+i)^{-1}, iA] e^{-isA} \in \mathcal{L}(\mathcal{H})$$

is Hölder continuous with order  $\epsilon > 0$ . Hence we have the identity

$$\begin{aligned} e^{i(\sigma+\sigma')(1-\theta)\frac{A}{t}}B(0)e^{i(\sigma+\sigma')\theta\frac{A}{t}} &= e^{i\sigma\frac{A}{t}}B\left(\frac{\sigma\theta+(1-\theta)\sigma'}{t}\right)e^{i\sigma'\frac{A}{t}} \\ &= e^{i\sigma\frac{A}{t}}B(0)e^{i\sigma'\frac{A}{t}} + O\left(\left(\frac{\sigma\theta+(1-\theta)\sigma'}{t}\right)^{-\varepsilon}\right) \end{aligned}$$

and we deduce from (A.3)

$$(H+i)^{-1}\left[H, iF\left(\frac{A}{t}\right)\right](H+i)^{-1} = \frac{1}{t}g\left(\frac{A}{t}\right)(H+i)^{-1}[H, iA](H+i)^{-1}g\left(\frac{A}{t}\right) + O(t^{-1-\varepsilon}). \quad (\text{A.4})$$

Further, one easily checks, with Helffer-Sjöstrand formula and the equality (A.3), the estimate

$$\left[g\left(\frac{A}{t}\right), h(H)\right] = O(t^{-1}), \quad \forall h \in \mathcal{C}_{\text{comp}}^{\infty}(\mathbf{R}). \quad (\text{A.5})$$

By left- and right- multiplying (A.4) with  $h(H) = f(H)(H+i)$  the previous estimate (A.5) leads to

$$f(H)\left[H, iF\left(\frac{A}{t}\right)\right]f(H) = \frac{1}{t}f(H)g\left(\frac{A}{t}\right)[H, iA]g\left(\frac{A}{t}\right)f(H) + O(t^{-1-\varepsilon}).$$

We use again (A.5) with  $h = f_1$ ,  $f_1 \in \mathcal{C}_{\text{comp}}^{\infty}(\Delta)$  and  $f_1 f \equiv f$ :

$$\begin{aligned} f(H)\left[H, iF\left(\frac{A}{t}\right)\right]f(H) &= \frac{1}{t}f(H)g\left(\frac{A}{t}\right)f_1(H)[H, iA]f_1(H)g\left(\frac{A}{t}\right)f(H) + O(t^{-1-\varepsilon}) \\ &\geq c_0 \frac{1}{t}f(H)g^2\left(\frac{A}{t}\right)f(H) + O(t^{-1-\varepsilon}). \end{aligned}$$

We have proved

$$D\Phi(t) \geq (c_0 - c_1) \frac{1}{t}f(H)g^2\left(\frac{A}{t}\right)f(H) + O(t^{-1-\varepsilon}).$$

This and Lemma A.2 a) yield (A.1). The existence and the value of the strong limit (A.2) come from the previous result: We calculate the Heisenberg derivative of  $f(H)g^2\left(\frac{A}{t}\right)f(H)$ . With the inequality (A.1) and Lemma A.2 b), we obtain the existence of the strong limit

$$\text{s-lim}_{t \rightarrow +\infty} U(t) * f(H)g^2\left(\frac{A}{t}\right)f(H)U(t).$$

Finally, this one has to be zero because the integral (A.1) is convergent.

Indeed, the estimates (A.1) and (A.2) are not very satisfactory because the conjugate operator is not explicit, by its construction given in [12]. However, it can be estimated by more familiar observables. This point of view is the reason for the next statements.

**Lemma A.3.** *Let  $A$  and  $B$  be two self-adjoint operators on a Hilbert space  $\mathcal{H}$  so that*

$$\begin{aligned} \mathcal{D}(B) &\subset \mathcal{D}(A), \\ A &\leq cB \quad \text{and} \quad 1 \leq B, \\ [A, B]B^{-1} &\in \mathcal{L}(\mathcal{H}). \end{aligned}$$

Then there exist small enough constants  $c_0 > 0$  and  $\varepsilon_0 > 0$  so that

$$\left\| F\left(\frac{B}{t} \leq \varepsilon_0\right) F\left(\frac{A}{t} \geq c_0\right) \right\| = O(t^{-1}).$$

Proposition A.1 and the above Lemma A.3, lead to

**Proposition A.4.** *If  $H$ ,  $A$  and  $B$  are three self-adjoint operators on  $\mathcal{H}$  which satisfy the assumptions of Proposition A.1 and Lemma A.3, then we have for any  $f \in \mathcal{C}_{\text{comp}}^\infty(\Delta)$  and for  $\varepsilon_0 > 0$  small enough,*

$$\int_1^{+\infty} \left\| F\left(\frac{B}{t} \leq \varepsilon_0\right) f(H) U(t) u \right\|^2 \frac{dt}{t} \leq C \|u\|^2, \quad \forall u \in \mathcal{H} \tag{A.6}$$

and  $\text{s-lim}_{t \rightarrow +\infty} F\left(\frac{B}{t} \leq \varepsilon_0\right) f(H) U(t) = 0.$  (A.7)

*Proof of Lemma A.3.* Let us first verify

$$\left[ G\left(\frac{B}{t}\right), A \right] = O(1) \tag{A.8}$$

for  $G \in \mathcal{C}_{\text{comp}}^\infty(\mathbf{R})$ . We use again Helffer-Sjöstrand formula (2.7) which gives

$$\begin{aligned} \left[ G\left(\frac{B}{t}\right), A \right] &= \frac{1}{2\pi i} \int_{\mathbf{C}} \partial_{\bar{z}} \tilde{G}(z) \left[ \left(z - \frac{B}{t}\right)^{-1}, A \right] dz \wedge d\bar{z} \\ &= \frac{1}{2\pi i} \int_{\mathbf{C}} \partial_{\bar{z}} \tilde{G}(z) \left(z - \frac{B}{t}\right)^{-1} \left[ \frac{B}{t}, A \right] B^{-1} B \left(z - \frac{B}{t}\right)^{-1} dz \wedge d\bar{z} \end{aligned}$$

where  $\tilde{G}$  is an almost analytic extension of  $G$  which satisfies

$$|\partial_{\bar{z}, z}^\alpha \partial_z \tilde{G}(z)| \leq C_{N, \alpha} |\text{Im } z|^N \langle z \rangle^{-N}, \quad \forall N \in \mathbf{N}, \alpha \in \mathbf{N}^2.$$

We have  $\|(z - \frac{B}{t})^{-1}\| = O(|\text{Im } z|^{-1})$  while

$$\left\| B \left( z - \frac{B}{t} \right)^{-1} \right\| = O \left( \frac{t \langle z \rangle}{|\text{Im } z|} \right).$$

The estimate (A.8) now comes at once. Let  $R(t)$  and  $R_1(t)$  respectively denote  $F\left(\frac{B}{t} \leq \varepsilon_0\right)$  and  $F\left(\frac{B}{t} \leq 2\varepsilon_0\right)$ . We have  $R(t)R_1(t) = R(t)$ . Let  $A_1(t) = R_1(t)AR_1(t)^*$ . For  $\varepsilon_0$  small enough,

$$A_1(t) \leq cR_1(t)BR_1(t) \leq \frac{1}{2}c_0t$$

which yields  $F\left(\frac{A_1(t)}{t} \geq c_0\right) = 0$ . It remains to check that

$$R(t) \left[ F\left(\frac{A}{t} \geq c_0\right) - F\left(\frac{A_1(t)}{t} \geq c_0\right) \right] \in O(t^{-1}).$$

We write  $F(s \geq c_0) = (s + i)F_{-1}(s)$  where  $F_{-1}$  satisfies  $|\partial_s^\alpha F_{-1}(s)| \leq C_\alpha \langle s \rangle^{-1-\alpha}$ . We take some almost analytic extension  $\tilde{F}_{-1}(z)$  of  $F_{-1}$  satisfying

$$|\partial_{z,\bar{z}}^\alpha \tilde{F}_{-1}(z)| \leq C_{\alpha,N} |\text{Im } z|^N \langle z \rangle^{-2-\alpha-N} \quad N \in \mathbb{N}, \alpha \in \mathbb{N}^2,$$

and we write

$$\begin{aligned} R(t) \left[ F\left(\frac{A}{t} \geq c_0\right) - F\left(\frac{A_1(t)}{t} \geq c_0\right) \right] &= R(t) \left( \frac{A}{t} - \frac{A_1(t)}{t} \right) F_{-1} \left( \frac{A}{t} \right) \\ &\quad + R(t) \left( \frac{A_1(t)}{t} + i \right) \left[ F_{-1} \left( \frac{A}{t} \right) - F_{-1} \left( \frac{A_1(t)}{t} \right) \right]. \end{aligned}$$

By (A.8) with  $G(\frac{B}{t}) = F_1(\frac{B}{t} \leq \varepsilon_0)$ , we estimate the first term by

$$R(t) \left( \frac{A}{t} - \frac{A_1(t)}{t} \right) = R(t)R_1(t) \frac{A}{t} - R(t)R_1(t) \frac{A}{t} R_1(t) = R(t) \left[ R_1(t), \frac{A}{t} \right] \in O(t^{-1}). \tag{A.9}$$

For the second term, we combine the above estimate with (A.8) and we get

$$\begin{aligned} &R(t) \left( \frac{A_1(t)}{t} + i \right) \left[ F_{-1} \left( \frac{A}{t} \right) - F_{-1} \left( \frac{A_1(t)}{t} \right) \right] \\ &= \left( \frac{A_1(t)}{t} + i \right) R(t) \left[ F_{-1} \left( \frac{A}{t} \right) - F_{-1} \left( \frac{A_1(t)}{t} \right) \right] + O(t^{-1}). \end{aligned} \tag{A.10}$$

By recalling that  $\frac{A_1(t)}{t}$  is uniformly bounded by  $\frac{1}{2}c_0$ , we are led to consider

$$\begin{aligned} & R(t) \left[ F_{-1} \left( \frac{A}{t} \right) - F_{-1} \left( \frac{A_1(t)}{t} \right) \right] \\ &= \frac{1}{2\pi i} \int_{\mathcal{C}} \partial_{\bar{z}} \tilde{F}_{-1}(z) R(t) \left[ \left( z - \frac{A}{t} \right)^{-1} - \left( z - \frac{A_1(t)}{t} \right)^{-1} \right] dz \wedge d\bar{z} \\ &= \frac{1}{2\pi i} \int_{\mathcal{C}} \partial_{\bar{z}} \tilde{F}_{-1}(z) R(t) \left( z - \frac{A}{t} \right)^{-1} \left( \frac{A}{t} - \frac{A_1(t)}{t} \right) \left( z - \frac{A_1(t)}{t} \right)^{-1} dz \wedge d\bar{z}. \end{aligned}$$

We commute  $R(t)$  and the resolvent  $(z - \frac{A}{t})^{-1}$ :

$$R(t) \left( z - \frac{A}{t} \right)^{-1} = \left( z - \frac{A}{t} \right)^{-1} R(t) - \left( z - \frac{A}{t} \right)^{-1} \left[ R(t), \frac{A}{t} \right] \left( z - \frac{A}{t} \right)^{-1}$$

and we conclude with (A.8) and (A.9).

### A.2 About the Hamilton-Jacobi equation.

In order to construct modified wave operators in the long-range case, we need solutions of Hamilton-Jacobi equations with Hamiltonians having the form

$$h(t, x, \xi) = E(\xi) + V(t, x, \xi)$$

where  $E$  belongs to  $\mathcal{C}_{\text{comp}}^{\infty}(\mathbf{R}^n)$  and  $V \in \mathcal{C}^{\infty}(\mathbf{R} \times T^*\mathbf{R}^n)$  satisfies

$$|\partial_t^{\alpha} \partial_x^{\beta} \partial_{\xi}^{\gamma} V(t, x, \xi)| \leq C_{\alpha\beta\gamma} \langle |\xi| + |t| \rangle^{-\mu + \varepsilon - |\alpha| - |\beta|}.$$

**Theorem A.5.** *There exists  $T > 0$  large enough so that the equation*

$$\begin{cases} \partial_t S(t, \xi) = E(\xi) + V(t, \partial_{\xi} S(t, \xi), \xi) \\ S(T, \xi) = 0 \end{cases} \tag{A.11}$$

*admits a unique solution under the condition  $\partial_{\xi}^2 S(t, \xi) \in L_{\text{loc}}^{\infty}(\mathbf{R}^n)$ . This solution is then infinitely differentiable with respect to  $\xi \in \mathbf{R}^n$  and satisfies*

$$\partial_{\xi}^{\alpha} [S(t, \xi) - tE(\xi)] = O(t^{1-\mu+\varepsilon}), \quad \text{for } |\alpha| \geq 0. \tag{A.12}$$

In order to prove this result, we shall use the Theorem A.3.1 of [8] which says that the solution is given by

$$S(t, \xi) = Q(t, \eta(t, \xi)) \tag{A.13}$$

$$\text{with } Q(t, \eta) = \int_T^t h(u, x(u, \eta), \xi(u, \eta)) + \langle x(u, \eta), \partial_u \xi(u, \eta) \rangle du, \tag{A.14}$$

where  $(x(t, \eta), \xi(t, \eta))$  is the solution to the Hamilton equations with the initial data  $(x(T, \eta), \xi(T, \eta)) = (0, \eta)$ . In order to define  $\xi \rightarrow \eta(t, \xi)$ , we have to study the Hamilton equation with prescribed initial position and final momentum.

**Proposition A.6.** *There exists  $T > 0$  large enough so that there is a unique trajectory in  $T^*\mathbf{R}^n$  which solves*

$$\begin{cases} \partial_t y(t) = \partial_{\xi} h(t, y(t), \eta(t)) \\ \partial_t \eta(t) = -\partial_x h(t, y(t), \eta(t)) \\ y(t_1) = x_1, \quad \eta(t_2) = \xi_2, \end{cases} \quad (\text{A.15})$$

when  $T \leq t_1 \leq t_2 \leq +\infty$  and  $(x_1, \xi_2) \in T^*\mathbf{R}^n$ . This solution denoted by

$$(y(t; t_1, t_2, x_1, \xi_2), \eta(t; t_1, t_2, x_1, \xi_2))$$

is indeed infinitely differentiable with respect to  $\xi_2 \in \mathbf{R}^n$  and satisfies

$$|\partial_{\xi_2}^{\alpha} (y(t; t_1, t_2, x_1, \xi_2) - x_1 - (t - t_1) \partial_{\xi} E(\xi_2))| \leq O(t_1^{-\mu + \varepsilon}) |t - t_1| \quad (\text{A.16})$$

$$\text{and} \quad |\partial_{\xi_2}^{\alpha} (\eta(t; t_1, t_2, x_1, \xi_2) - \partial_{\xi} E(\xi_2))| \leq O(t_1^{-\mu + \varepsilon}), \quad \text{for } \alpha \geq 0. \quad (\text{A.17})$$

*Proof.* The local existence and uniqueness of a solution to the initial value problem for the considered Hamilton equations makes no problem. For such a solution, we get by differentiation

$$\begin{cases} \partial_t^2 y(t) = \Phi(t, y(t), \eta(t)) \\ \partial_t \eta(t) = \Psi(t, y(t), \eta(t)) \end{cases}$$

$$\text{with} \quad \Phi = \partial_{t\xi}^2 V + \partial_{\xi x} V \partial_{\xi} E + \partial_{\xi x} V \partial_{\xi} V - \partial_{\xi}^2 E \partial_x V - \partial_{\xi}^2 V \partial_x V$$

$$\text{and} \quad \Psi = -\partial_x V.$$

These functions actually satisfy

$$|\partial_t^{\alpha} \partial_x^{\beta} \partial_{\xi}^{\gamma} \Phi(t, x, \xi)| \leq C_{\alpha\beta\gamma} \langle |\xi| + |t| \rangle^{-1 - \mu + \varepsilon - |\alpha| - |\beta|}$$

$$|\partial_t^{\alpha} \partial_x^{\beta} \partial_{\xi}^{\gamma} \Psi(t, x, \xi)| \leq C_{\alpha\beta\gamma} \langle |\xi| + |t| \rangle^{-1 - \mu + \varepsilon - |\alpha| - |\beta|}.$$

We set

$$Y(t) = y(t) - x_1 - (t - t_1) \partial_{\xi} E(\xi_2)$$

$$\text{and} \quad \Theta(t) = \eta(t) - \partial_{\xi} E(\xi_2).$$

The system (A.15) is then equivalent to the fixed point problem

$$\begin{pmatrix} Y \\ \Theta \end{pmatrix} = \mathcal{P} \begin{pmatrix} Y \\ \Theta \end{pmatrix}, \quad (\text{A.18})$$

where the mapping  $\mathcal{P}$  is given by

$$\mathcal{P} \begin{pmatrix} Y \\ \Theta \end{pmatrix} (t) = \begin{pmatrix} -\int_{t_1}^t (s-t_1)\Phi(s, y(s), \eta(s))ds - (t-t_1)\int_{t_1}^{t_2}\Phi(s, y(s), \eta(s))ds \\ -\int_{t_1}^{t_2}\Psi(s, y(s), \eta(s))ds \end{pmatrix}.$$

We introduce the functions  $\zeta_{t_1, t_2}^0$  and  $\zeta_{t_1, t_1}^1$ , defined by

$$\zeta_{t_1, t_2}^0(s) = \begin{cases} 0 & \text{if } s \leq t \\ 1 & \text{if } t < s \leq t_2 \\ 0 & \text{if } t_2 < s \end{cases} \quad \text{and} \quad \zeta_{t_1, t_1}^1(s) = \begin{cases} 0 & \text{if } s \leq t_1 \\ (s-t_1) & \text{if } t_1 < s \leq t \\ (t-t_1) & \text{if } t < s \end{cases}.$$

The mapping  $\mathcal{P}$  then writes

$$\mathcal{P} \begin{pmatrix} Y \\ \Theta \end{pmatrix} (t) = \begin{pmatrix} -\int_{t_1}^{+\infty} \zeta_{t_1, t_1}^1(s)\Phi(s, x_1 + (s-t_1)\partial_\xi E(\xi_2) + Y(s), \partial_\xi E(\xi_2) + \Theta(s))ds \\ -\int_{t_1}^{+\infty} \zeta_{t_1, t_2}^0(s)\Psi(s, x_1 + (s-t_1)\partial_\xi E(\xi_2) + Y(s), \partial_\xi E(\xi_2) + \Theta(s))ds \end{pmatrix}.$$

We shall solve the fixed point problem in the vector space  $Z_{t_1}^1 \times Z_{t_1}^0$  where

$$Z_{t_1}^i := \left\{ f \in \mathcal{C}^0([t_1, +\infty), \mathbb{R}^n), \sup_{t \in [T, \infty[} \frac{|f(t)|}{|t-t_1|^i} < \infty \right\}, \quad i=0, 1,$$

is endowed with its natural norm. The functions  $\zeta_{t_1, t_2}^0(s)$  and  $\zeta_{t_1, t_1}^1(s)$  satisfy

$$0 \leq \zeta_{t_1, t_2}^0 \leq 1 \quad \text{and} \quad 0 \leq \frac{\zeta_{t_1, t_1}^1}{|t-t_1|} \leq 1,$$

so that  $\mathcal{P}$  is an endomorphism of  $Z_{t_1}^1 \times Z_{t_1}^0$ . Moreover the estimates on  $\Phi$  and  $\Psi$  ensure that  $\mathcal{P}$  is infinitely Fréchet-differentiable with a derivative estimated by

$$\|\partial_{Y, \Theta} \mathcal{P}(Y, \Theta)\|_{\mathcal{L}(Z_{t_1}^1 \times Z_{t_1}^0)} \leq Ct_1^{-\mu+\varepsilon}.$$

By taking  $t_1$  large enough, the mapping  $\mathcal{P}$  is a contraction on  $Z_{t_1}^1 \times Z_{t_1}^0$  and the fixed point problem (A.18) admits a unique solution. Indeed,  $\mathcal{P}$  is parametrized by  $(x_1, \xi_2)$  and the derivative of the solution  $(\tilde{Y}(x_1, \xi_2), \tilde{\Theta}(x_1, \xi_2))$  of (A.18) with respect to  $\xi_2 \in \mathbb{R}^n$  equals

$$[-(1 - \partial_{Y, \Theta} \mathcal{P})^{-1} \partial_{\xi_2} \mathcal{P}](\tilde{Y}(x_1, \xi_2), \tilde{\Theta}(x_1, \xi_2)).$$

By referring again to the estimates for  $\Phi$  and  $\Psi$  we deduce that  $\partial_{\xi_2} \mathcal{P}$  is of order  $O(t_1^{-\mu+\varepsilon})$  and the estimates (A.16)(A.17) come at once for  $|\alpha| \leq 1$ . The estimates for any  $\alpha$  follow by differentiating with respect to  $\xi_2 \in \mathbb{R}^n$  the above relation.

*Proof of Theorem A.5.* The function  $\eta(t, \xi)$  involved in (A.13) is constructed by considering the solution to (A.15) with  $t_1 = T$  large enough,  $t_2 = t$ ,  $x_1 = 0$  and  $\xi_2 = \xi$ . We then take  $\eta(t, \xi) = \eta(t; T, t, 0, \xi)$ , where the estimate (A.17) ensures that

$\eta(t, \xi)$  is Lipschitz continuous with respect to  $\xi \in \mathbf{R}^n$ . The Theorem A.3.1 of [8] states that the function  $S(t, \xi)$  given by (A.13) and (A.14) is the unique solution to (A.11) with  $\partial_\xi^2 S(t, \xi) \in L_{\text{loc}}^\infty(\mathbf{R}^n)$ . Moreover this result provides the identity

$$\partial_\xi S(t, \xi) = x(t, \eta(t, \xi)) = y(t; T, t, 0, \xi).$$

The estimate (A.12) is then easily derived by integration

$$\partial_t \partial_\xi^2 [S(t, \xi) - tE(\xi)] = \partial_\xi^2 [V(t, \partial_\xi S(t, \xi), \xi)]$$

from  $t$  to  $+\infty$ , by using the estimates on  $V$  and (A.16).

### B. Pseudo-differential calculus on the torus

There are several ways of considering pseudo-differential calculus on the torus. The one which we point out consists in going back to  $\mathbf{R}^n$  and using Weyl-Hörmander calculus. This method presents two advantages: 1) this procedure associates a complete symbol with any pseudo-differential operator; 2) the precise estimates of Weyl-Hörmander calculus provide estimates for parameter dependent pseudo-differential operators (semi-classical calculus). The final remark reviews other approaches and relationships between them. Let  $\Gamma$  denote the lattice  $\mathbf{Z}^n$  in  $\mathbf{R}^n$  and  $\Gamma^* = (2\pi\mathbf{Z}^n)$  its dual lattice. The distributions on  $T^n = \mathbf{R}^n/\Gamma$  will be identified with the  $\Gamma$ -periodic elements  $u(k)$  of  $\mathcal{S}'(\mathbf{R}^n)$ ,

$$u(k + \gamma) = u(k), \quad \forall \gamma \in \Gamma.$$

Then we have

$$H^s(T^n) := \{u(k) \in H_{\text{loc}}^s(\mathbf{R}^n), u(k + \gamma) = u(k), \quad \forall \gamma \in \Gamma\},$$

and the scalar product on  $L^2(T^n, dk)$  is given by

$$(u, v)_{L^2(T^n)} = \int_F \bar{u}(k)v(k)dk,$$

where  $F$  is any fixed fundamental cell of  $\Gamma$ .

The pseudo-differential operators are defined by

$$a(k, D_k)u(k) = \iint_{\mathbf{R}^{2n}} e^{-i(k-k')\eta} a(k, \eta) u(k') d\eta dk'$$

with  $a \in S\left(\langle \eta \rangle^m, g_\eta = dk^2 + \frac{d\eta^2}{\langle \eta \rangle^2}\right)$  and

$$[\tau_\gamma, a(k, D_k)] = 0, \quad \forall \gamma \in \Gamma.$$

Note that the last condition is equivalent to  $a(k + \gamma, \eta) = a(k, \eta)$ ,  $\forall \gamma \in \Gamma$ . These

operators send  $\mathcal{S}'(\mathbf{R}^n)$  into itself and preserve periodicity. Thus they can be considered as continuous operators on  $\mathcal{D}'(\mathbf{T}^n)$ .

**Definition B.1.** i) The expression  $\text{OpS}^m(\mathbf{T}^n)$  denotes the space of operators  $a(k, D_k)$  where the symbol  $a$  belongs to  $\mathcal{C}^\infty(T^*\mathbf{T}^n)$  and satisfies

$$|\partial_x^\alpha \partial_\xi^\beta a(x, \xi)| \leq C_{\alpha, \beta} \langle \xi \rangle^{m - |\beta|}, \quad \forall (x, \xi) \in T^*\mathbf{T}^n, \quad \forall (\alpha, \beta) \in \mathbf{N}^{2n}.$$

ii) The expression  $\text{OpS}^{h,m}(\mathbf{T}^n)$  denotes the space of families  $(a(k, D_k; h))_{h \in (0,1)}$  where the symbols  $a(h)$  satisfy the estimates

$$|\partial_x^\alpha \partial_\xi^\beta a(x, \xi)| \leq C_{\alpha, \beta} h^{|\beta| - m} \langle \xi \rangle^{m - |\beta|}, \quad \forall (x, \xi) \in T^*\mathbf{T}^n, \quad \forall (\alpha, \beta) \in \mathbf{N}^{2n},$$

uniformly with respect to  $h \in (0, 1)$ .

The symbols of these operators are defined on  $T^*\mathbf{R}^n$  as  $\Gamma$  periodic elements of  $S\left(\langle \eta \rangle^m, g_\eta = dk^2 + \frac{d\eta^2}{\langle \eta \rangle^2}\right)$  and the  $\#$  operation defined by  $(a\#b)(k, D_k) = a(k, D_k)b(k, D_k)$  inherits all the properties of the same operation defined for general symbols on  $T^*\mathbf{R}^n$  (see [14]).

We next check the  $L^2$  continuity on  $\mathbf{T}^n$ .

**Lemma B.2.** *If  $a \in S(\langle \eta \rangle^m, g_\eta)$ , then the operator  $a(k, D_k)$  is continuous from  $H^s(\mathbf{T}^n)$  into  $H^{s-m}(\mathbf{T}^n)$  for any  $s \in \mathbf{R}$ . Moreover its norm is estimated by some fixed semi-norm of the symbol  $a$ .*

*Proof.* It suffices to consider the case  $m = s = 0$ . A fixed fundamental cell of  $\Gamma$  is still denoted by  $F$  and we choose  $\chi \in \mathcal{C}_{\text{comp}}^\infty(\mathbf{R}^n)$  a cut-off function so that  $\chi \equiv 1$  on  $F$ .

Then we have the norm equivalence

$$C^{-1} \|u\|_{L^2(\mathbf{T}^n)} \leq \|\chi u\|_{L^2(\mathbf{R}^n)} \leq C \|u\|_{L^2(\mathbf{T}^n)}$$

and it remains to find an estimate for  $\|\chi a(k, D_k)u\|_{L^2(\mathbf{R}^n)}$ . We take  $\chi_0 \in \mathcal{C}_{\text{comp}}^\infty(\mathbf{R}^n)$  so that  $\sum_{\gamma \in \Gamma} \chi_0(k - \gamma) = 1$  and  $\tilde{\chi}_0 \in \mathcal{C}_{\text{comp}}^\infty(\mathbf{R}^n)$  so that  $\tilde{\chi}_0 \equiv 1$  on  $\text{supp } \chi_0$ . By using the periodicity of  $u$ , we get

$$\begin{aligned} [\chi a(k, D_k)u](k) &= \sum_{|\gamma| \leq \gamma_0} [\chi(k)a(k, D_k)\chi_0(k - \gamma)u](k) \\ &+ \sum_{|\gamma| > \gamma_0} \iint_{\mathbf{R}^{2n}} e^{i(k - k' + \gamma)\eta} \chi(k)a(k, \eta)\chi_0(k')\tilde{\chi}_0(k')u(k')d\eta dk'. \end{aligned} \tag{B.1}$$

For  $|\gamma| \leq \gamma_0$ , we refer to the continuity of  $a(k, D_k)$  on  $L^2(\mathbf{R}^n)$ . For  $|\gamma| > \gamma_0$  integration by parts applied to

$$K_\gamma(k, k') = \int_{\mathbf{R}^n} e^{i(k-k'+\gamma)\eta} \chi(k) a(k, \eta) \chi_0(k') d\eta$$

shows that  $K_\gamma$  is bounded, with some fixed compact support and the estimate

$$\|K_\gamma\|_{L^\infty(\mathbf{R}^{2n})} \leq C_N \|a\|_N \langle \gamma \rangle^{-N}$$

where  $\|\cdot\|_N$  is some seminorm on  $S(1, g_\eta)$  depending on  $N$ . Schur's Lemma then provides the estimate for the second term of (B.1),

$$C_N \|a\|_N \sum_{|\gamma| > \gamma_0} \langle \gamma \rangle^{-N} \leq C_N \|a\|_N$$

by taking  $N$  large enough.

From the definition that we took, we already know that the pseudo-differential operators form an algebra of continuous operators on  $\mathcal{D}'(\mathbf{T}^n)$ . The above Lemma B.2 also ensures that pseudo-differential operators are continuous on  $\mathcal{C}^\infty(\mathbf{T}^n)$ . Moreover this yields that the operator  $A = a(k, D_k)$  defined on  $L^2(\mathbf{T}^n)$  with domain  $\{u \in L^2(\mathbf{T}^n), Au \in L^2(\mathbf{T}^n)\}$  is closed and that  $\mathcal{C}^\infty(\mathbf{T}^n)$  is a core for  $A$ .

**Proposition B.3.** i) If  $A_i$  belongs to  $\text{OpS}^{h, m_1}(\mathbf{T}^n)$ ,  $i = 1, 2$ , with  $m_1 + m_2 \leq 1$ , then we have

$$\|[A_1, A_2]\|_{\mathcal{L}(L^2(\mathbf{T}^n))} = O(h^{1-m_1-m_2}).$$

ii) If  $A = (a(k, D_k; h))_{h \in (0, 1)}$  belongs to  $\text{OpS}^{h, m}(\mathbf{T}^n)$ , then the family of adjoint operators  $A^*$  belongs to  $\text{OpS}^{h, m}(\mathbf{T}^n)$  and

$$\frac{A + A^*}{2} - (\text{Re} a(k, D_k; h))_{h \in (0, 1)} \in \text{OpS}^{h, m-1}(\mathbf{T}^n).$$

iii) If  $A = (a(k, D_k; h))_{h \in (0, 1)}$  belongs to  $\text{OpS}^{h, m}(\mathbf{T}^n)$  and if  $(h\varphi(k; h))_{h \in (0, h_0)}$  is a bounded family in  $\mathcal{C}^\infty(\mathbf{T}^n)$ , then we have

$$a(k, D_k; h) - a(k, \varphi(k; h); h) = R_1(h) (D_k - \varphi(k; h)) + R_2(h) \quad (\text{B.2})$$

with  $\|R_1(h)\|_{\mathcal{L}(L^2(\mathbf{T}^n))} = O(h^{1-m})$  and  $\|R_2(h)\|_{\mathcal{L}(L^2(\mathbf{T}^n))} = O(h^{1-m})$ .

iv) The operator  $V(D_k)$  defined as the closure on  $L^2(\mathbf{R}^n)$  of an element of  $\text{OpS}^m(\mathbf{T}^n)$ , is the same as the operator defined by functional calculus.

*Proof.* If  $u$  and  $v$  taken in  $\mathcal{C}^\infty(\mathbf{T}^n)$  are considered as  $\Gamma$ -periodic elements of  $\mathcal{C}^\infty(\mathbf{R}^n)$  and  $A = (a(k, D_k))$  as an element of  $\text{OpS}^m(\mathbf{R}^n)$ , the periodicity condition ensures that

$$\int_F \bar{u}(k)[Av](k)dk = \int_F \overline{[A^\dagger u]}(k)v(k)dk,$$

where  $A^\dagger$  is the formal adjoint of  $A$  on  $L^2(\mathbf{R}^n)$ . Hence, the assertions i) and ii) are byproducts of pseudo-differential calculus on  $\mathbf{R}^n$  combined with Lemma B.2.

The assertion iii) is also derived from a result on  $\mathbf{R}^n$  which may be found in [8] (use a Taylor expansion).

Let us now consider iv). We first by  $V_{pd}(D_k)$  the closure of the pseudo-differential operator and  $V(D_k)$  the function of the vector of commuting self-adjoint operators  $D_k$ . For  $u \in \mathcal{C}^\infty(\mathbf{T}^n)$  considered as a  $\Gamma$ -periodic element of  $\mathcal{C}^\infty(\mathbf{R}^n)$ , the Fourier transform equals

$$\hat{u}(\eta)(\eta) = (2\pi)^n \sum_{\gamma^* \in \Gamma^*} \hat{u}_{\gamma^*} \delta(\eta - \gamma^*),$$

where  $\hat{u}_{\gamma^*}$ ,  $\gamma^* \in \Gamma^*$ , are the Fourier coefficients of  $u$ . Hence, we have

$$[V_{pd}(D_k)u](k) = \int_{\mathbf{R}^n} e^{ik\eta} V(\eta) \hat{u}(\eta) d\eta = \sum_{\gamma^* \in \Gamma^*} e^{ik\gamma^*} V(\gamma^*) \hat{u}_{\gamma^*} = [V(D_k)u](k).$$

We conclude by recalling that  $\mathcal{C}^\infty(\mathbf{T}^n)$  is a core for  $\overline{V_{pd}(D_k)}$  and  $V(D_k)$ .

We close this appendix by recalling two other approaches to pseudo-differential calculus on the torus.

*Remark B.4.* i) The standard pseudo-differential calculus on compact manifolds applies to the torus. Indeed, it is rather easy to check that the pseudo-differential operators defined in this appendix are classical pseudo-differential operators and by using charts that classical pseudo-differential operators are of this form up to negligible remainders.

ii) Another approach to pseudo-differential calculus on the torus, consists in replacing Fourier transform by Fourier series and derivatives with respect to  $\eta$  by discrete derivatives with respect to  $\gamma^*$ . Here again, by introducing the right interpolation, one can show that this pseudo-differential calculus coincides with the two previous ones modulo negligible remainders.

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### References

- [ 1 ] W. Amrein, A. Boutet de Monvel and V. Georgescu,  $C_0$ -Groups, Commutator Methods and Spectral Theory of  $N$ -Body Hamiltonians, Progress in Mathematics 135, Birkhäuser, Basel-Boston-Berlin, 1996.
- [ 2 ] A. Balazard-Konlein, Calcul fonctionnel pour des opérateurs  $h$ -admissibles à symboles opérateur

- et applications, thèse, Univ. Nantes, 1985.
- [ 3 ] F. Bentosela, Scattering for Impurities in a Crystal, *Comm. Math. Phys.*, **46** (1976), 153–166.
  - [ 4 ] E. Bierstone and P.D. Milman, Semi-analytic and Subanalytic Sets, *Inst. Hautes Études Scient. Publ. Math.*, **67** (1988), 5–42.
  - [ 5 ] A. Boutet de Monvel, V. Georgescu and M. Mantoïu, Locally Smooth Operators and the Limiting Absorption Principle for  $N$ -Body Hamiltonians, *Rev. Math. Phys.*, **5-1** (1993), 105–189.
  - [ 6 ] J.-Y. Chemin, Fluides parfaits incompressibles, *Astérisque* **230**, Société Mathématique de France, 1995.
  - [ 7 ] J. M. Delort, F.B.I. Transformation, *Lecture Notes in Math.* 1522, Springer-Verlag, 1992.
  - [ 8 ] J. Dereziński and C. Gérard, Scattering theory of clonical and quantum  $N$ -particle systems, *Texts and Monographs in Physics*, Springer-Verlag 1997.
  - [ 9 ] J. Dixmier, *Les algèbres d'opérateurs dans l'espace hilbertien*, Gauthier-Villars, 1957.
  - [ 10 ] R. Froese and I. Herbst, A New Proof of the Mourre Estimate, *Duke Math. J.*, **49** (1982), 1075–1085.
  - [ 11 ] C. Gérard and I. Laba,  $N$ -particle Systems in Constant 2D Magnetic Fields, in preparation.
  - [ 12 ] C. Gérard and F. Nier, The Mourre Theory for analytically fibered operators, *J. of Funct. Anal.* **152** (1) 1998, 202–219.
  - [ 13 ] H. Hironaka, Stratification and Flatness, in P. Holm, editor, *Real and Complex Singularities*, pages 199–265. Proceedings of the Nordic summer school/NAVF, Sijthoff and Noordhoff, August 1976.
  - [ 14 ] L. Hörmander, *The Analysis of Linear Partial Differential Operators* 3, Springer-Verlag, 1985.
  - [ 15 ] A. Jensen, E. Mourre and P. Perry, Multiple Commutator Estimates and Resolvent Smoothness in Quantum Scattering Theory, *Ann. I.H.P.*, **41** (1984), 207–225.
  - [ 16 ] P. Perry, I.M. Sigal and B. Simon, Spectral Analysis of  $N$ -body Schrödinger Operators, *Ann. Math.*, **114** (1981) 519–567.
  - [ 17 ] M. Reed and B. Simon, *Methods of Modern Mathematical Physics*, volume 4, Acad. Press, 1975.
  - [ 18 ] I.M. Sigal and A. Soffer, Long-Range Many-Body Scattering: Asymptotic Completeness for Short-Range Quantum Systems, *Ann. of Math.*, **125** (1987), 35–108.
  - [ 19 ] I.M. Sigal and A. Soffer, Local Decay and Propagation estimates for Time-Dependent and Time-Independent Hamiltonians, preprint, Princeton University, 1988.
  - [ 20 ] I.M. Sigal and A. Soffer, Long-Range Many-Body Scattering: Asymptotic Clustering for Coulomb-Type Potentials, *Invent. Math.*, **99** (1990), 115–143.
  - [ 21 ] B. Simon, Phase Space Analysis of Simple Scattering Systems: Extension of some Work of Enss, *Duke Math. J.*, **46** (1979), 119–168.
  - [ 22 ] M.M. Skriganov, Geometric and Arithmetic Methods in the Spectral Theory of Multi-Dimensional Periodic Operators, *Proceedings of the Steklov Institute of Mathematics*, **2** 1987.
  - [ 23 ] L.E. Thomas, Time-Dependent Approach to Scattering from Impurities in a Crystal, *Comm. Math. Phys.*, **33** (1973), 335–343.