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PROPAGATION ESTIMATES FOR DIRAC OPERATORS AND APPLICATION TO SCATTERING THEORY

by **Thierry DAUDÉ**

1. Introduction.

Time-dependent methods in scattering theory were introduced by Enss twenty five years ago in [10] and [11]. They were originally developed to solve the N-body problem in nonrelativistic quantum mechanics. This was achieved thanks to subsequent improvements due, among others, to Sigal and Soffer [30], Graf [18] and Dereziński [7] (in chronological order). A detailed and complete presentation of these methods can be found in the book by Dereziński and Gérard [8]. In the framework of relativistic quantum mechanics, such techniques provide an intuitive description of scattering, based on the essential structure of relativity: the light cone. In this work, we use such an approach to give a complete scattering theory for massive Dirac operators with long-range potentials in flat spacetime.

Similar results have been obtained first by Enss and Thaller [12] and Mutharamaligam and Sinha [26] using the Enss method and the RAGE theorem. Recently, Gâtel and Yafaev [13] improved these results for a large class of potentials by means of a stationary approach based on a limiting absorption principle and radiation estimates for time-independent observables. The novelty in our proof is the systematic use of time-dependent observables as proposed in [8]. In particular, this leads to

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propagation estimates for the Dirac fields which, in turn, will greatly simplify the construction of wave operators. The Mourre theory and commutator methods will be the basic tools in our study. Let us point out that these results can be used to develop scattering theories in General Relativity. For instance, we have in mind the works by Häfner and Nicolas [20], Melnyk [24] and Nicolas [27], on the scattering for Dirac fields on black hole spacetimes. In the case of Kerr black holes, it has been shown in [20] that a Mourre theory and time-dependent techniques are necessary.

We consider a massive Dirac hamiltonian denoted by H acting on the Hilbert space of physical states $\mathcal{H} = [L^2(\mathbb{R}^3)]^4$. The hamiltonian H is the sum of the usual free Dirac operator $H_0 = \Gamma \cdot p + m\Gamma^0$, $m > 0$, $p = -i\nabla$ where $\Gamma^0, \Gamma = (\Gamma^1, \Gamma^2, \Gamma^3)$ are Dirac matrices and a potential $V(x)$ of Coulombian type at infinity which is the sum of a scalar and a matrix-valued multiplication operator. According to the Heisenberg description of quantum mechanics, we shall focus our attention on the unitary evolution e^{-itH} and on the behaviour of (time-dependent) observables along this evolution; that is to say, if A_t denotes a time-dependent function with values in selfadjoint operators on \mathcal{H} then we are interested in studying the behaviour of operators of the following type

$$A_t(t) := e^{itH} A_t e^{-itH}.$$

Note that for $\psi \in \mathcal{H}$ such that the expectation value $(\psi, A_t(t)\psi)$ is well-defined, this quantity corresponds to the mean value of the results of many measurements which are all performed on systems identically prepared to be in the state ψ . Actually, our main objects of study will be *asymptotic observables* defined by

$$s - \lim_{t \rightarrow \pm\infty} e^{itH} A_t e^{-itH},$$

when the limit exists. It was the essential idea of Enss [10], [11] to describe the evolution of asymptotic observables such as position and momentum and to use this information to obtain results in scattering theory. More precisely, in the case of Dirac operators, Enss and Thaller [12] proved the vanishing of the following limit

$$(1.1) \quad \lim_{t \rightarrow \pm\infty} e^{itH} \left(f\left(\frac{x}{t}\right) - f(\mathcal{V}) \right) e^{-itH} \psi, \quad \forall \psi \in \mathcal{H}^c(H),$$

where $\mathcal{H}^c(H)$ denotes the continuous spectral subspace of H and $f \in C_\infty(\mathbb{R}^3)$, the space of smooth functions tending to 0 at infinity. Here x is the *standard position operator* and $\mathcal{V} = pH_0^{-1}$ is the *classical velocity operator*. This result can be interpreted as follows: there exists a correlation between

the localization of a scattering state at late times in a narrow cone (linearly increasing with time t) and its velocity, that is to say this result describes “propagation in phase space”. One consequence of this is that “scattering states have been incoming in the remote past and will be outgoing in the far future, moving away from the region of significant interactions” (quoted from [12]) which is already a weak version of scattering.

More recently, many authors turned their attention to the construction of such observables and their application to scattering. In particular, Sigal and Soffer [30], [31], Graf [18] and Dereziński and Gérard [8] improved the methods of Enss by using the method of *positive commutator* also called method of *positive Heisenberg derivative* due mainly to Mourre in [25] and refined, among others, by Amrein, Boutet-de-Monvel Berthier, Georgescu in [1]. A motivation of their work was related to one of the main problems in scattering theory: how to define wave operators when the interaction V is long-range (that is to say when the potential falls off no faster than $|x|^{-1}$ when $|x|$ tends to infinity). In such a case, the classical wave operators

$$\Omega^\pm = s - \lim_{t \rightarrow \pm\infty} e^{itH} e^{-itH_0} \mathbf{1}^{ac}(H_0),$$

are no longer available. Instead it is necessary to replace the comparison dynamics e^{-itH_0} by a more complicated one, usually in the form $e^{-iS(t,\mathcal{V})}$ where the function S has to be well chosen. Unfortunately, this choice has no reason to be unique and thus it would be interesting to find some natural and uniquely defined objects that, in turn, entail a natural and unambiguous definition of the wave operators.

One example of uniquely defined construction associated to the dynamics e^{-itH} is the selfadjoint operator called *asymptotic velocity* denoted by P^\pm and defined by

$$(1.2) \quad P^\pm := s - C_\infty - \lim_{t \rightarrow \pm\infty} e^{itH} \frac{x}{t} e^{-itH},$$

The notion of strong- C_∞ -limit is explained at the beginning of Section 5. The asymptotic velocity admits the other characterization in terms of the classical velocity operator \mathcal{V}

$$(1.3) \quad P^\pm := s - C_\infty - \lim_{t \rightarrow \pm\infty} e^{itH} \mathcal{V} e^{-itH},$$

and we see that (1.2) together with (1.3) imply (1.1). For instance, Dereziński and Gérard succeeded in constructing wave operators of the form $\Omega^\pm = e^{itH} e^{-iS(t,\mathcal{V})}$ satisfying in particular the intertwining relations

$$\begin{aligned} \Omega^\pm H_0 (\Omega^\pm)^* &= H \mathbf{1}^c(H), \\ \Omega^\pm \mathcal{V} (\Omega^\pm)^* &= P^\pm. \end{aligned}$$

Let us emphasize that it is the essence of wave operators to make the link between the physical quantities associated to the system (here the energy H and the asymptotic velocity P^\pm) and simpler physical quantities which allow us to make some computations (here the energy of the free system H_0 and the classical velocity operator \mathcal{V}).

Although it is not obligatory to introduce such an observable in the case of Dirac operators, the asymptotic velocity turns out to be a relevant construction at least for two reasons. First it exists under rather weak conditions. It can be shown (see [8], Section 4.10) that for certain 2-body hamiltonians for which the asymptotic velocity exists, the wave operators fail to be complete. Thus, in this sense, it could serve to define a “weak” notion of scattering theory. Secondly the asymptotic velocity can be used as a very convenient tool to prove the existence and asymptotic completeness of wave operators. For instance, an important feature of P^\pm is

$$(1.4) \quad \mathbf{1}_{\{0\}}(P^\pm) = \mathbf{1}^{pp}(H),$$

that is to say the states of zero asymptotic velocity coincide with the bound states of H . This property not only gives a first classification between the states in \mathcal{H} , which is the initial purpose of scattering, but will allow us to use the standard Cook method in the proof of asymptotic completeness.

Let us now briefly describe the content of each sections.

In Section 2, we give an abstract framework for massive Dirac Hamiltonians and analyse some basic properties concerning their spectrum and problems of domain invariance. Next we study in details the Zitterbewegung phenomenon for the free Dirac operator H_0 which arises when one tries to define the velocity operator \mathcal{V} . Recall that, in the case of Schrödinger operators, the velocity operator is defined as the time derivative of the position operator and it turns out that it is independent of time. However, for Dirac operators, the time derivative of the position operator is time-dependent and oscillates around a mean value which is the classical velocity operator \mathcal{V} . This phenomenon will be the source of technical problems in the derivation of weak propagation estimates in Section 4. To overcome these future difficulties, we must introduce a new position observable, called the Newton-Wigner operator, whose time derivative is exactly \mathcal{V} .

Section 3 is devoted to a short overview of Mourre theory as presented in the initial work of Mourre [25] but also revisited by Amrein, Boutet de Monvel Berthier, Georgescu in [2] and Georgescu and Gérard in [14]. In particular we define a new locally conjugate operator for Dirac Hamiltonians which turns out to be convenient for our purpose.

Section 4 establishes the weak propagation estimates. *Large* and *minimal velocity estimates* give an important information on the probability to find the particle in certain cones in spacetime at late times. For instance, the minimal velocity estimates asserts that a particle having an energy strictly larger than its mass m has to escape from a narrow cone $|x| \leq c_m t$ asymptotically in time. On the other hand, *microlocal velocity estimates* are a slightly stronger version of (1.1) and indicate that we can approach the position operator x by $t\mathcal{V}$ at late times. All these estimates rely entirely on positive commutator methods and Mourre theory. In particular, we state a result ([17] and [22]) which shows how the minimal velocity estimates are intimately related to the existence of a locally conjugate operator. At last we state two results due to Cook and Kato which allow to make the link between weak propagation estimates and the existence of asymptotic observables.

In Section 5, we prove that the asymptotic velocity P^\pm defined by (1.2) exists and can also be characterized by (1.3). Then we study its spectrum which, physically, corresponds to the asymptotic propagation velocity of the fields and we prove that

$$\sigma(P^\pm) = \overline{B}(0, 1),$$

$\overline{B}(0, 1)$ being the closed ball in \mathbb{R}^3 of center 0 and radius 1. Eventually, using only the minimal velocity estimates, we also prove property (1.4).

Section 6 is devoted to the construction of wave operators Ω^\pm . In our case where potentials of coulombian types are considered, a Dollard modification is enough for the definition of these operators when combined with an idea due to Thaller [12], that allows us to define properly this modification and avoid problems caused by the matrix-valued potential. We will then make a crucial use of the asymptotic velocity operator P^\pm and property (1.4) to transform the problem into a time-dependent one for which Cook's method can be applied. It could seem strange to introduce such a time dependence in the proof but, in fact, one obtains an agreeable way of proving the existence and asymptotic completeness of the wave operators by handling only time-dependent quantities which are integrable along the evolution.

In Appendix A, we recall two well-known techniques used for the manipulation of functions of selfadjoint operators: for integrable functions, the Fourier transform can be used, but in the case of smooth and not necessarily integrable functions, the correct tool is the Helffer-Sjöstrand formula [21]. In each case, we state a commutator expansion of $[T, f(A)]$

in terms of the multiple commutators $ad_A^k(T)$ for two selfadjoint operators A, T . In particular, the required assumptions on the operators A and T are carefully detailed.

Eventually, in Appendix B, we establish weak propagation estimates for time-dependent Dirac Hamiltonians and we construct the associated asymptotic velocity used in Section 6 for the construction of the wave operators.

2. Properties of Dirac operators.

2.1. Abstract framework.

In this paper, we shall denote by H_0 the free massive Dirac Hamiltonian on flat spacetime acting on $\mathcal{H} = [L^2(\mathbb{R}^3)]^4$ the Hilbert space of four component square integrable functions. Precisely, we consider the differential operator

$$H_0 = \Gamma \cdot p + m\Gamma^0 = \Gamma^1 p_1 + \Gamma^2 p_2 + \Gamma^3 p_3 + m\Gamma^0, \quad p_j = -i\partial_j,$$

m being the mass of the field. We shall assume that the mass m is strictly positive. H_0 is a selfadjoint operator on $D(H_0) = [H^1(\mathbb{R}^3)]^4$ where $H^1(\mathbb{R}^3)$ denotes the usual Sobolev space of order one in \mathbb{R}^3 . Here Γ^μ correspond to the Dirac matrices satisfying the anti-commutation relations $\{\Gamma^\mu, \Gamma^\nu\} = 2\delta^{\mu\nu}$ for every $\mu, \nu = 0, \dots, 3$ ($\delta^{\mu\nu}$ stands for the Kronecker symbol). We shall use the following usual representation for the Dirac matrices.

$$\Gamma^0 = \begin{pmatrix} \sigma^0 & 0 \\ 0 & -\sigma^0 \end{pmatrix}, \quad \Gamma^k = \begin{pmatrix} 0 & \sigma^k \\ \sigma^k & 0 \end{pmatrix},$$

where the Pauli matrices σ^i are given by

$$\begin{aligned} \sigma^0 &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, & \sigma^1 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\ \sigma^2 &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, & \sigma^3 &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned}$$

The free Hamiltonian H_0 will be perturbed by some external field. Let us consider two functions V_1 and V_2 belonging to the space

$$S^{-1}(\mathbb{R}^3) = \left\{ f \in C^\infty(\mathbb{R}^3) / \forall \alpha \in \mathbb{N}^3, |\partial_x^\alpha f(x)| \leq C \langle x \rangle^{-1-|\alpha|} \right\},$$

where $\langle x \rangle$ denotes the multiplication operator by $(1 + |x|^2)^{\frac{1}{2}}$ acting on each component of \mathcal{H} . The perturbation will be given by the matrix-valued multiplication operator $V(x) = V_1(x) + V_2(x)\Gamma^0$ acting on \mathcal{H} . The potential V_1 (resp. $V_2\Gamma^0$) is understood as an *electric potential* (resp. *scalar potential*) i.e. $V_2\Gamma^0$ corresponds to an x -dependent rest mass). We refer to [32], chapter 4, for a presentation of the usual external fields for Dirac equation. Thus the interacting Dirac operator given by the sum of H_0 and V ,

$$(2.1) \quad H = H_0 + V(x),$$

is a self-adjoint operator on the domain $D(H) = D(H_0)$ by the Kato-Rellich theorem.

It is well known (see [32], chapter 1) that the spectrum of H_0 has the following structure

$$\sigma(H_0) = \sigma_{ac}(H_0) = (-\infty, -m] \cup [+m, +\infty).$$

Moreover, the assumptions imposed on the interaction V imply that the difference of the resolvents $(H - z)^{-1} - (H_0 - z)^{-1} = -(H - z)^{-1}V(x)(H_0 - z)^{-1}$ is a compact operator in \mathcal{H} . Therefore by the Weyl theorem, the essential spectrum of H is the same as the essential spectrum of H_0 .

$$\sigma_{ess}(H) = \sigma_{ess}(H_0) = (-\infty, -m] \cup [+m, +\infty).$$

However the operator H may have non-empty pure point spectrum. It will be crucial for the later analysis that the operator H be invertible. But assuming that $0 \in \sigma(H)$, it is then possible to find a smooth positive function e.g. $f \in \mathcal{S}(\mathbb{R}^3)$ the space of Schwartz functions such that the operator $H + f(x)$ be invertible. Thus, up to a smooth function, we can always consider that $0 \notin \sigma(H)$. For more details we refer to [4].

2.2. Domain invariance.

In this section, we are interested in studying the invariance of the domain $D(\langle x \rangle^n)$, $n \in \mathbb{N}$ under the action of the unitary one-parameter group $\{e^{-itH}\}_{t \in \mathbb{R}}$. As a consequence, we shall also obtain some information on the invariance of $D(\langle x \rangle^n)$, $n \in \mathbb{N}$ under the action of the resolvent $(H - z)^{-1}$, $z \notin \sigma(H)$ and of any operator $\chi(H)$ with $\chi \in C_0^\infty(\mathbb{R})$. We state now the main result.

THEOREM 2.1. — Let H be the Dirac operator (2.1). Let x be the standard position observable. Then for any $n \in \mathbb{N}$,

$$(2.2) \quad e^{-itH} D(\langle x \rangle^n) \subset D(\langle x \rangle^n),$$

and there exists a constant C_n such that

$$(2.3) \quad \|\langle x \rangle^n e^{-itH} \psi\| \leq C_n (1 + |t|)^n \|\langle x \rangle^n \psi\|.$$

Proof. — We proceed by induction on n . The result is trivial for $n = 0$ and given $n > 0$ assume that (2.2) is satisfied for $n - 1$. The key of the proof is to approach $\langle x \rangle^n$ by a bounded operator X_λ for which estimate (2.2) is true uniformly in λ . We define

$$X_\lambda = \frac{\langle x \rangle^n}{1 + \lambda \langle x \rangle^n}.$$

Clearly we have

$$\lim_{\lambda \rightarrow 0} X_\lambda \psi = \langle x \rangle^n \psi, \quad \forall \psi \in D(\langle x \rangle^n),$$

and this operator is bounded as well as its derivative

$$[\partial_x, X_\lambda] = \frac{nx \langle x \rangle^{n-2}}{(1 + \lambda \langle x \rangle^n)^2}.$$

Let us compute the Heisenberg derivative of X_λ .

$$(2.4) \quad \begin{aligned} \frac{d}{dt} X_\lambda(t) &= e^{itH} i[H, X_\lambda] e^{-itH}, \\ &= e^{itH} \Gamma i[p, X_\lambda] e^{-itH}, \\ &= e^{itH} \Gamma \frac{n \frac{x}{\langle x \rangle} \langle x \rangle^{n-1}}{(1 + \lambda \langle x \rangle^n)^2} e^{-itH}. \end{aligned}$$

Integrating (2.4) between 0 and t , we obtain $\forall \psi \in D(\langle x \rangle^n)$

$$(2.5) \quad \begin{aligned} \|X_\lambda e^{-itH} \psi\| &\leq \|X_\lambda \psi\| + \int_0^{|t|} \left\| \Gamma \frac{n \frac{x}{\langle x \rangle} \langle x \rangle^{n-1}}{(1 + \lambda \langle x \rangle^n)^2} e^{-isH} \psi \right\| ds, \\ &\leq \|X_\lambda \psi\| + n \int_0^{|t|} \left\| \frac{\langle x \rangle^{n-1}}{(1 + \lambda \langle x \rangle^n)^2} e^{-isH} \psi \right\| ds, \end{aligned}$$

$$(2.6) \quad \leq \|X_\lambda \psi\| + n \int_0^{|t|} \|\langle x \rangle^{n-1} e^{-isH} \psi\| ds.$$

As $D(\langle x \rangle^n) \subset D(\langle x \rangle^{n-1})$, the induction hypothesis implies

$$(2.7) \quad \|X_\lambda e^{-itH} \psi\| \leq \|X_\lambda \psi\| + n C_{n-1} \|\langle x \rangle^{n-1} \psi\| \int_0^{|t|} (1 + |s|)^{n-1} ds.$$

The right-hand side of (2.7) is uniformly bounded in λ , as $\lambda \rightarrow 0$. Therefore, computing the last integral, we obtain

$$(2.8) \quad \begin{aligned} \|\langle x \rangle^n e^{-itH} \psi\| &\leq \|\langle x \rangle^n \psi\| + n C_{n-1} \|\langle x \rangle^{n-1} \psi\| (1 + |t|)^n, \\ &\leq C_n (1 + |t|)^n \|\langle x \rangle^n \psi\|, \end{aligned}$$

which concludes the proof. \square

Theorem 2.1 has the following corollary, essential to derive the weak propagation estimates in Section 4.

COROLLARY 2.1. — *Let H a self-adjoint operator satisfying the conclusions of Theorem 2.1. Let $z \in \mathbb{C}$ such that $\text{Im } z \neq 0$ and $n \in \mathbb{N}$. Then*

$$(2.9) \quad (H - z)^{-1} D(\langle x \rangle^n) \subset D(\langle x \rangle^n).$$

Proof. — It is an easy consequence of (2.2) and the resolvent formula

$$(2.10) \quad (H - z)^{-1} \psi = i\epsilon \int_0^\infty e^{i\epsilon z t} e^{-itH} \psi dt, \quad \forall \psi \in \mathcal{H},$$

where $\epsilon = \text{sgn}(\text{Im } z)$ and the integral converges in norm. As $\langle x \rangle^n$ is closed, we have $\forall \psi \in D(\langle x \rangle^n)$,

$$(2.11) \quad \begin{aligned} \|\langle x \rangle^n (H - z)^{-1} \psi\| &= \left\| \int_0^\infty e^{i\epsilon z t} \langle x \rangle^n e^{-itH} \psi dt \right\|, \\ &\leq C_n \|\langle x \rangle^n \psi\| \int_0^\infty (1 + t)^n e^{-\epsilon(\text{Im } z)t} dt. \end{aligned}$$

Let us denote I_n this last integral. An integration by part yields

$$(2.12) \quad I_n = \frac{1}{\epsilon \text{Im } z} (1 + n I_{n-1}).$$

We deduce by induction from (2.12) that

$$(2.13) \quad I_n \leq C_n \frac{\langle z \rangle^n}{|\text{Im } z|^{n+1}},$$

which is bounded for z fixed. This proves the corollary. \square

2.3. Zitterbewegung and velocity operator.

In this section, we give a short presentation of the *Zitterbewegung* phenomenon which naturally arises when one tries to define the “velocity” operator for the free Dirac operator H_0 . For more details, we refer to [32].

The velocity operator is usually defined as the time derivative of the position operator. The most natural choice is to consider the operator of multiplication by x acting on \mathcal{H} . Then we define

$$x(t) = e^{itH_0} x e^{-itH_0},$$

the time translated position operator. Formally we have

$$\begin{aligned} \frac{dx(t)}{dt} &= e^{itH_0} i[H_0, x] e^{-itH_0}, \\ (2.14) \quad &= e^{itH_0} \Gamma e^{-itH_0} =: \Gamma(t). \end{aligned}$$

According to classical relativistic kinematics, we would have expected to obtain $\mathcal{V} = p H_0^{-1}$ i.e. the classical velocity operator instead of $\Gamma(t)$. Let us analyse the time dependence of $\Gamma(t)$.

$$\begin{aligned} \frac{d\Gamma(t)}{dt} &= e^{itH_0} i[H_0, \Gamma] e^{-itH_0}, \\ &= e^{itH_0} i H_0 [\Gamma - H_0^{-1} \Gamma H_0] e^{-itH_0}. \end{aligned}$$

An explicit short calculation shows that $\Gamma - H_0^{-1} \Gamma H_0 = 2(\Gamma - \mathcal{V})$. Thus

$$(2.15) \quad \frac{dx(t)}{dt} = 2i H_0 F(t),$$

where $F = \Gamma - \mathcal{V}$. The operator F is one aspect of the Zitterbewegung phenomenon. One of its main features is that it anticommutes with H_0

$$(2.16) \quad F H_0 = -H_0 F.$$

We conclude from (2.16) that $F(t) = e^{2itH_0} F$ and integrating (2.15) between 0 and t , we see that

$$\Gamma(t) = \mathcal{V} + e^{2itH_0} F.$$

Thus we see that the standard velocity oscillates without damping around the classical velocity operator \mathcal{V} and this oscillation is called Zitterbewegung. Integrating again, we obtain

$$x(t) = x + p H_0^{-1} t + \frac{1}{2i H_0} (e^{2itH_0} - 1) F.$$

All these formal results can be made rigorous and we have the following theorem (Thaller [32], Theorem 1.3, p. 20):

THEOREM 2.2. — *The domain $D(x)$ of the multiplication operator x is left invariant by the free evolution*

$$D(x(t)) \subset D(x),$$

and on this domain, we have

$$(2.17) \quad x(t) = x + pH_0^{-1}t + \frac{1}{2iH_0}(e^{2itH_0} - 1)F.$$

The problem arising from the Dirac equation is that certain observables such as the position operator $x(t)$, mix positive and negative energies. To overcome this difficulty we can choose some other operators to be the position observables of the theory. In particular we are interested in the so-called *Newton-Wigner* observable. Let us first define the Foldy-Wouthuysen transformation U_{FW} . This transformation diagonalizes the Dirac operator H_0 in \mathcal{H} . Denoting \mathcal{F} the Fourier transform on \mathcal{H} we have

$$(2.18) \quad (\mathcal{F}H_0\mathcal{F}^{-1})(k) = \Gamma \cdot k + m\Gamma^0,$$

and for each $k \in \mathbb{R}^3$, the right-hand side of (2.18) is a Hermitian 4×4 matrix which has the two eigenvalues $\{-\lambda(k), \lambda(k)\}$ where $\lambda(k) = \sqrt{k^2 + m^2}$ and both eigenvalues have multiplicity 2. Let us call $P(k)$ the unitary matrix such that

$$P(k)(\Gamma \cdot k + m\Gamma^0)P(k)^{-1} = \begin{pmatrix} \lambda(k) & 0 & 0 & 0 \\ 0 & \lambda(k) & 0 & 0 \\ 0 & 0 & -\lambda(k) & 0 \\ 0 & 0 & 0 & -\lambda(k) \end{pmatrix},$$

where

$$(2.19) \quad P(k) = \frac{(m + \lambda(k))\mathbf{1} + \Gamma^0\Gamma \cdot k}{\sqrt{2\lambda(k)(m + \lambda(k))}} = a_+(k)\mathbf{1} + a_-(k)\Gamma^0\frac{\Gamma \cdot k}{|k|},$$

and

$$(2.20) \quad a_{\pm}(k) = \frac{1}{\sqrt{2}}\sqrt{1 \pm \frac{m}{\lambda(k)}}.$$

We also have

$$(2.21) \quad P^{-1}(k) = \frac{(m + \lambda(k))\mathbf{1} - \Gamma^0\Gamma \cdot k}{\sqrt{2\lambda(k)(m + \lambda(k))}} = a_+(k)\mathbf{1} - a_-(k)\Gamma^0\frac{\Gamma \cdot k}{|k|},$$

We define the Foldy-Wouthuysen transformation $U_{FW} = P(p) = \mathcal{F}^{-1}P(k)\mathcal{F}$ acting from \mathcal{H} to \mathcal{H} . This transformation is clearly unitary on \mathcal{H} and H_0 conjugated by U_{FW} can be written as

$$U_{FW}H_0U_{FW}^{-1} = \begin{pmatrix} \sqrt{p^2 + m^2} & 0 \\ 0 & -\sqrt{p^2 + m^2} \end{pmatrix}.$$

Whence H_0 is unitarily equivalent to a pair of square root of Klein-Gordon hamiltonians.

Now we turn to the definition of the Newton-Wigner operator denoted x_{nw} . We set

$$x_{nw} = U_{FW}^{-1} x U_{FW}.$$

This operator has the following properties (see [32])

- It leaves invariant positive and negative energy subspaces of H_0 i.e. $[x_{nw}, \mathbf{1}_{\mathbb{R}^\pm}(H_0)] = 0$.

- On $D(x_{nw})$, the following equality holds

$$(2.22) \quad x_{nw}(t) = e^{itH_0} x_{nw} e^{-itH_0} = x_{nw} + \mathcal{V}t,$$

or equivalently

$$(2.23) \quad i[H_0, x_{nw}] = \mathcal{V}.$$

It is worth pointing out that the Zitterbewegung does not appear in the formula (2.22). This important feature of the Newton-Wigner operator will be helpful for the construction of the asymptotic velocity in the next sections. However the results we need to prove involve the standard position operator and so, we have to make the link between x and x_{nw} . Unfortunately we have the following complicated formula, see [32]

$$(2.24) \quad x_{nw} = x - \frac{\Gamma^0}{2i\lambda} \left(\Gamma - \frac{1}{\lambda(\lambda+m)} (\Gamma \cdot p)p \right) - \frac{1}{\lambda(\lambda+m)} S \wedge p,$$

where S denotes the spin angular momentum and is defined by $S = -\frac{i}{4} \Gamma \wedge \Gamma$ and $\lambda = \sqrt{p^2 + m^2}$. The symbol $\Gamma \wedge \Gamma$ denotes the three matrices $\sum_{k,l} \epsilon_{jkl} \Gamma^k \Gamma^l$ where ϵ is the totally antisymmetric tensor. Observe that the spin angular momentum S is bounded, everywhere defined and self-adjoint. Concisely, we shall denote by Z the bounded operator on \mathcal{H} such that $x_{nw} = x + Z$. As the expression of Z is difficult to handle, the Newton-Wigner operator has not been used in previous works [5], [12] or [13] on Dirac's equation. However we shall need this operator for deriving the microlocal velocity estimates in Section 4 especially the formula (2.23) will be of great help to us. Eventually the only information on Z we shall need is given by the following lemma.

LEMMA 2.1. — *The commutator $[x, Z]$ between x and Z is a bounded operator in \mathcal{H} .*

Proof. — This result follows from the definition (2.24) of Z . According to this definition, we can view the operator Z as a matrix-valued function of p . Moreover we have

$$Z = (Z_{ij}(p))_{ij}, \text{ where } Z_{ij} \in S^{-1}(\mathbb{R}^3), \forall i, j = 1, 2, 3.$$

Therefore using the Helffer-Sjöstrand formula (A.29), we get for any $m = 1, 2, 3$

$$\begin{aligned}
 [x_m, Z] &= \frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{Z}(z) \sum_{l=1}^3 \left(\prod_{k_1=1}^l R_{k_1} \right) [x_m, p_l] \left(\prod_{k_2=l}^3 R_{k_2} \right) dz \wedge d\bar{z}, \\
 &= \frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{Z}(z) \sum_{l=1}^3 \left(\prod_{k_1=1}^l R_{k_1} \right) i\delta_{lm} \left(\prod_{k_2=l}^3 R_{k_2} \right) dz \wedge d\bar{z},
 \end{aligned}$$

where $R_k = (z_k - p_k)^{-1}$. Thus $[x_m, Z]$ is bounded by (A.22). □

3. Locally conjugate operator.

The main idea of Mourre theory is to find an operator, usually denoted by A , which increases along the evolution e^{-itH} in a suitable sense. If we denote $A(t) = e^{itH} A e^{-itH}$, this means that the time derivative of $A(t)$ must be essentially positive or equivalently, the commutator between H and A has to be essentially positive. Precisely, can we find an open interval Δ of \mathbb{R} , a strictly positive constant ϵ and a compact operator K on \mathcal{H} such that

$$(3.1) \quad \mathbf{1}_\Delta(H) i[H, A] \mathbf{1}_\Delta(H) \geq \epsilon \mathbf{1}_\Delta^2(H) + \mathbf{1}_\Delta(H) K \mathbf{1}_\Delta(H).$$

In the case of the Schrödinger operator, the usual generator of dilation $D = \frac{1}{2} \{x.p + p.x\}$ is a good candidate for a conjugate operator. It turns out that the same operator also satisfies (3.1), when H is the Dirac operator previously defined, for a suitable open interval Δ in \mathbb{R} . However, there exist many other possible choices for A which may be more adapted to the Dirac equation and make the verification of the assumptions easier. For instance, see [5], [15] and [23]. We shall use a locally conjugate operator which is close to the choice made in [23].

Let us define the operator

$$A_0 = \frac{1}{2} \{x.pH_0^{-1} + H_0^{-1}p.x\}.$$

Concisely, we write $A_0 = \frac{1}{2} \{x.\mathcal{V} + \mathcal{V}.x\}$ and commuting x and \mathcal{V} , it is easy to see that $A_0 = \mathcal{V}.x + B_0$ where $B_0 = \frac{i}{2} H_0^{-1} \Gamma.F$ is a bounded operator in \mathcal{H} . It is defined and essentially self-adjoint on $D(x)$ (see [23], Lemma 3.1). This operator has the important property

$$(3.2) \quad i[H_0, A_0] = \mathcal{V}^2,$$

where the commutator is computed on a suitable domain e.g. $C_0^\infty(\mathbb{R}^3)$. Therefore the commutator between A_0 and H_0 is positive which seems to indicate that it could be another good candidate for being the operator A . Unfortunately, the addition of a matrix-valued potential V to H_0 prevents us from proving the Mourre estimate (3.1) for (H, A_0) .

Actually, it is better to consider the following operator

$$(3.3) \quad A = \frac{1}{2} \left\{ x \cdot p H^{-1} + H^{-1} p \cdot x \right\},$$

which is also defined and essentially self-adjoint on $D(x)$ (see below). It is easy to see that this operator is related to A_0 by a bounded operator. Precisely, using the resolvent identity, we have

$$A = A_0 - \frac{1}{2} x \cdot p H^{-1} V(x) H_0^{-1} - \frac{1}{2} H_0^{-1} V(x) H^{-1} p \cdot x = A_0 + B,$$

and B is bounded. Thus the Heisenberg derivative of A will be essentially \mathcal{V}^2 plus or minus some compact terms. Indeed,

$$(3.4) \quad \begin{aligned} i[H, A] &= \frac{i}{2} \left[H, x \cdot p H^{-1} + H^{-1} p \cdot x \right], \\ &= \frac{1}{2} \left(\Gamma \cdot p H^{-1} + H^{-1} p \cdot \Gamma \right) - \frac{1}{2} \left(x \cdot \nabla V(x) H^{-1} + H^{-1} \nabla V(x) \cdot x \right). \end{aligned}$$

The second term in the right-hand side of (3.4) is clearly compact in \mathcal{H} since $x \cdot \nabla V(x)$ belongs to $S^{-1}(\mathbb{R}^3)$ and thus the standard compactness criterion applies.

To see that the first term in the right-hand side of (3.4) is essentially equal to \mathcal{V}^2 , observe that

$$\Gamma \cdot p H_0^{-1} - \Gamma \cdot p H^{-1} = \Gamma \cdot p H_0^{-1} V(x) H^{-1} = L,$$

where the operator L is compact in \mathcal{H} by the standard compactness criterion. Thus this term is equal to

$$\frac{1}{2} \left(\Gamma \cdot p H^{-1} + H^{-1} p \cdot \Gamma \right) = \frac{1}{2} \left(\Gamma \cdot \mathcal{V} + \mathcal{V} \cdot \Gamma \right) - \frac{1}{2} \left(L + L^* \right).$$

Now we write $\Gamma = \mathcal{V} + F$ and noting that $\frac{1}{2}(\mathcal{V} \cdot F + F \cdot \mathcal{V}) = 0$, we eventually obtain

$$(3.5) \quad i[H, A] = \mathcal{V}^2 - \frac{1}{2} \left(L + L^* \right) - \frac{1}{2} \left(x \cdot \nabla V(x) H^{-1} + H^{-1} \nabla V(x) \cdot x \right),$$

or concisely, $i[H, A] = \mathcal{V}^2 + K$ where K is compact. We use this result to prove the following lemma:

LEMMA 3.1. — *Let Δ be an open interval of \mathbb{R} such that $\Delta \cap [-m, +m] = \emptyset$. Then there exists a strictly positive constant ϵ depending on Δ and a compact operator K such that (3.1) holds.*

Proof. — Let $\chi \in C_0^\infty(\mathbb{R})$ a function such that $\text{supp } \chi \subset (-\infty, -m) \cup (+m, +\infty)$ and $\chi = 1$ on Δ . Let us compute the commutator

$$\begin{aligned} \chi(H)i[H, A]\chi(H) &= \chi(H)\mathcal{V}^2\chi(H) + K, \\ &= \chi(H_0)\mathcal{V}^2\chi(H_0) + K, \end{aligned}$$

because $\chi(H) - \chi(H_0)$ is compact. But if we diagonalize H_0 via the Foldy-Wouthuysen transformation, the first term can be written as

$$\begin{aligned} \chi(H_0)\mathcal{V}^2\chi(H_0) &= U_{FW}^{-1}\chi(\Gamma^0\lambda(p))U_{FW}\mathcal{V}^2U_{FW}^{-1}\chi(\Gamma^0\lambda(p))U_{FW}, \\ &= U_{FW}^{-1}\Gamma^0\chi(\lambda(p))\frac{p^2}{p^2 + m^2}\Gamma^0\chi(\lambda(p))U_{FW}. \end{aligned}$$

Now provided the support of χ strictly avoids $[-m, +m]$, there exists a strictly positive constant $\tilde{\epsilon}$ such that $\chi(\lambda(p)) = 0$ for $p^2 < \tilde{\epsilon}$. Hence we get

$$\begin{aligned} U_{FW}^{-1}\Gamma^0\chi(\lambda(p))\frac{p^2}{p^2 + m^2}\Gamma^0\chi(\lambda(p))U_{FW} \\ \geq \frac{\tilde{\epsilon}}{\tilde{\epsilon} + m^2} U_{FW}^{-1}\Gamma^0\chi(\lambda(p))\Gamma^0\chi(\lambda(p))U_{FW}, \end{aligned}$$

or, if we set $\epsilon = \frac{\tilde{\epsilon}}{\tilde{\epsilon} + m^2}$,

$$\chi(H_0)\mathcal{V}^2\chi(H_0) \geq \epsilon\chi^2(H_0),$$

which concludes the proof of the lemma. □

Even though the Mourre estimate (3.1) is the crucial property of the a locally conjugate operator, some extra assumptions are needed to obtain a complete scattering theory. There exist several versions in the litterature depending on the degree of refinement required by the problem. A very complete account of the theory can be found in [1]. We shall use for the definition of a locally conjugate operator a certain notion of regularity between two self-adjoint operators introduced by Amrein, Boutet de Monvel-Berthier, Georgescu [1]. Precisely,

DEFINITION 3.1. — *For a selfadjoint operator A , we say that another selfadjoint operator H belongs to $C^k(A)$, $k \in \mathbb{N}$, if and only if*

$$\text{(ABG)} \quad \exists z \in \mathbb{C} \setminus \sigma(H), s \longrightarrow e^{isA}(H - z)^{-1}e^{-isA} \in C^k(\mathbb{R}_s; \mathcal{B}(\mathcal{H})),$$

for the strong topology of $\mathcal{B}(\mathcal{H})$.

We give now the definition of a locally conjugate operator A and the main theorem we shall use.

DEFINITION 3.2. — *Let H, A two self-adjoint operators on \mathcal{H} . Let $\Delta \subset \mathbb{R}$ an open interval. We shall say that A is a locally conjugate operator of H on Δ if it satisfies the following assumptions:*

(i) $H \in C^1(A)$.

(ii) $i[H, A]$ defined as a quadratic form on $D(H) \cap D(A)$ extends to an element of $\mathcal{B}(D(H), \mathcal{H})$.

(iii) $[A, [A, H]]$ well defined as a quadratic form on $D(H) \cap D(A)$ by (ii), extends to an element of $\mathcal{B}(D(H), D(H)^*)$.

(iv) There exists a strictly positive constant ϵ and a compact operator K such that the Mourre estimate (3.1) holds.

THEOREM 3.1. — *Let H, A two selfadjoint operators on \mathcal{H} . Assume that A is a locally conjugate operator of H on the interval Δ . Then H has no singular continuous spectrum in Δ and the number of eigenvalues of H in Δ is finite (counting multiplicity).*

The assumptions on the commutators are rather straightforward to check by a direct computation on a suitable dense domain e.g. $C_0^\infty(\mathbb{R}^3)$. On the other hand, the first assumption is somewhat more subtle. We have the following equivalent definitions for $C^1(A)$.

$$\exists z \in \mathbb{C} \setminus \sigma(H), |((H - z)^{-1}u, Au) - (Au, (H - z)^{-1}u)| \leq C\|u\|^2, \quad \forall u \in D(A) \cap D(H).$$

(**ABG'**)

(**ABG''**)

- (i) $\exists z \in \mathbb{C} \setminus \sigma(H), (H - z)^{-1}D(A) \subset D(A), (H - \bar{z})^{-1}D(A) \subset D(A),$
- (ii) $|(Hu, Au) - (Au, Hu)| \leq C(\|Hu\|^2 + \|u\|^2), \forall u \in D(H) \cap D(A).$

Unfortunately, it is not easy to check $(H - z)^{-1}D(A) \subset D(A)$ in general without a better knowledge of $D(A)$. Therefore it is useful to consider another operator N called a *comparison operator* whose domain has to be well-known and that will allow to make the link between H and A . We shall use the following lemmata [16].

LEMMA 3.2 (Nelson). — *Let $N \geq 1$ a self-adjoint operator on \mathcal{H} . Let A a symmetric operator on \mathcal{H} such that $D(N) \subset D(A)$. Assume that*

$$(3.6) \quad \begin{aligned} (i) \quad & \|Au\| \leq C\|Nu\|, \quad \forall u \in D(N), \\ (ii) \quad & |(Au, Nu) - (Nu, Au)| \leq C\|N^{\frac{1}{2}}u\|^2, \quad \forall u \in D(N). \end{aligned}$$

Then A is essentially self-adjoint on $D(N)$. Furthermore every core of N is also a core for A .

LEMMA 3.3 (Gérard, Laba). — *Let H, H_0 and N three self-adjoint operators on \mathcal{H} satisfying $N \geq 1, D(H) = D(H_0)$ and $(H - z)^{-1}D(N) \subset$*

$D(N)$. Let A a symmetric operator on $D(N)$. Assume that H_0 and A satisfy the assumptions of Lemma 3.2 and

$$(3.7) \quad |(Au, Hu) - (Hu, Au)| \leq C(\|Hu\|^2 + \|u\|^2), \quad \forall u \in D(N).$$

Then we have

- $D(N)$ is dense in $D(A) \cap D(H)$ with the norm $\|Hu\| + \|Au\| + \|u\|$,
- the quadratic form $i[H, A]$ defined on $D(A) \cap D(H)$ is the unique extension of $i[H, A]$ on $D(N)$,
- $H \in C^1(A)$.

We now prove the assumptions of Theorem 3.1 with H the Dirac operator and A the operator defined above. Let us define $N = p^2 + x^2 + 1 = p^2 + \langle x \rangle^2$ as the comparison operator. This operator is essentially selfadjoint on $[C_0^\infty(\mathbb{R}^3)]^4$ by Theorem X.28 in [28], Vol 3. We also denote by N its closure which is a selfadjoint operator on \mathcal{H} with domain $D(N) = \{u \in \mathcal{H}, Nu \in \mathcal{H}\}$. Moreover, it is easy to see that

$$\begin{aligned} \|x^2u\|^2 &\leq \|Nu\|^2 + \|u\|^2, \\ \|p^2u\|^2 &\leq \|Nu\|^2 + \|u\|^2, \end{aligned}$$

from which it follows that the domain $D(N)$ is characterized by ([28], chapter X, problem 23)

$$D(N) = [H^2(\mathbb{R}^3)]^4 \cap [D(x^2)]^4.$$

Now, we check the assumptions of Nelson’s Lemma for H_0 and A .

- $D(N) \subset D(H_0)$, $D(N) \subset D(A)$ are obvious.
- For any $u \in D(N)$, we have

$$\begin{aligned} \|H_0u\|^2 &= (u, p^2u) + m^2\|u\|^2, \\ &\leq C\|u\|(\|Nu\| + \|u\|), \\ &\leq C\|Nu\|^2. \end{aligned}$$

$$\begin{aligned} \|Au\| &= \frac{1}{2} \sum_j \left\| \left(x^j p_j H^{-1} + H^{-1} p_j x^j \right) u \right\|, \\ &= \frac{1}{2} \sum_j \left\{ \|p_j H^{-1} x^j u\| + \|H^{-1} p_j x^j u\| + \|[x^j, p_j H^{-1}]u\| \right\}, \\ &\leq \frac{1}{2} \sum_j \left\{ C\|x^j u\| + \|(iH^{-1} - ip_j H^{-1} \Gamma^j H^{-1})u\| \right\}, \\ &\leq C \sum_j \left\{ \|\langle x \rangle u\| + \|u\| \right\} \leq C\|Nu\|. \end{aligned}$$

where we used the fact that $H^{-1}p_j$ and p_jH^{-1} are bounded on \mathcal{H} for any $j = 1, 2, 3$.

- It remains to see that for any $u \in C_0^\infty(\mathbb{R}^3)$,

$$\begin{aligned} |(u, i[H_0, N]u)| &= |(u, i[H_0, \langle x \rangle^2]u)|, \\ &= |(u, 2\Gamma.xu)|, \\ &\leq C\|u\| \| |x|u \|, \\ &\leq C\|\langle x \rangle u\|^2, \\ &\leq C\|N^{\frac{1}{2}}u\|^2. \end{aligned}$$

We also have

$$|(u, [A, N]u)| = \frac{1}{2}|(u, [x.pH^{-1} + H^{-1}p.x, p^2 + x^2 + 1]u)|.$$

A straightforward calculation leads to

$$\begin{aligned} [x.pH^{-1}, p^2 + x^2] &= 2ip^2H^{-1} - ix.pH^{-1}(\nabla V(x).p + p.\nabla V(x))H^{-1} \\ &\quad + 2ix.pH^{-1}\Gamma.H^{-1}x - 2ix.H^{-1}x - 2x.H^{-1}\Gamma H^{-1} \\ &\quad + 2x.pH^{-1}\Gamma.H^{-1}\Gamma H^{-1}. \end{aligned}$$

Whence

$$\begin{aligned} |(u, [x.pH^{-1}, p^2 + x^2]u)| &\leq C\{\|\langle p \rangle u\| \|u\| + \|\langle x \rangle u\|^2 + \|\langle x \rangle u\| \|u\|\}, \\ &\leq C\|N^{\frac{1}{2}}u\|. \end{aligned}$$

The same estimate is true for the term $(u, [H^{-1}p.x, p^2 + x^2]u)$. Thus the assumptions of Nelson’s lemma are proved.

Moreover, the assumptions of the G erard - Laba Lemma are entirely fulfilled since $(H - z)^{-1}D(\langle x \rangle^2) \subset D(\langle x \rangle^2)$ by domain invariance properties of Section 2 and since the commutator between H and A is bounded in \mathcal{H} by (3.5). Therefore, we have proved that $H \in C^1(A)$ as well as the second assumption of theorem 3.1.

The hypothesis on the double commutator can easily be checked and it turns out that it is a bounded operator in \mathcal{H} . Recall that

$$[A, i[H, A]] = \left[A, \mathcal{V}^2 - \frac{1}{2}(L + L^*) - \frac{1}{2}(x.\nabla V(x)H^{-1} + H^{-1}\nabla V(x).x) \right].$$

As the operator A is equal to $\mathcal{V}.x + B$ where \mathcal{V}, B are bounded and as $i[H, A]$ is also bounded, we actually just need show that the commutator between $x.\mathcal{V}$ and $i[H, A]$ remains bounded. We decompose the problem. First, $[x.\mathcal{V}, \mathcal{V}^2] = [x, \mathcal{V}^2].\mathcal{V}$ is clearly bounded. According to the definition of $L = \Gamma.pH_0^{-1}V(x)H^{-1}$, we see after some commutations that both terms in the following commutator

$$[x.\mathcal{V}, L] = x.\mathcal{V}L - Lx.\mathcal{V},$$

are bounded since $x.V(x) \in L^\infty(\mathbb{R}^3)$. The fact that the remaining term is bounded follows immediately by the same procedure since $x.(x.\nabla V(x))$ also belongs to $L^\infty(\mathbb{R}^3)$.

We have thus proven the theorem:

THEOREM 3.2. — *Let H be the dirac operator defined above. Then the spectrum of H has no singular continuous spectrum. Moreover, $\sigma_{ac}(H) = (-\infty, -m) \cup (+m, +\infty)$ and in any compact interval contained in $(-\infty, -m) \cup (+m, +\infty)$, the number of eigenvalues is finite.*

We deduce from this theorem and $\sigma_{ess}(H) = (-\infty, -m] \cup [+m, +\infty)$ that $\sigma_{pp}(H) \subset [-m, +m]$.

Before we turn to the minimal velocity estimates, we make the following remark. The assumptions required in Theorem 3.1 actually imply that the operator H belongs to the class $C^2(A)$. From [1] (Theorem 6.3.1), we know that if we assume the invariance of $D(H)$ under the action of the unitary one-parameter group e^{isA} , then the conditions $i[H, A]$ and $[A, [A, H]]$ bounded on \mathcal{H} entail that $H \in C^2(A)$. But the condition on the invariance follows from the following Lemma quoted in [14].

LEMMA 3.4. — *Let H and A two self-adjoint operators such that $H \in C^1(A)$ and $i[H, A] \in \mathcal{B}(D(H), \mathcal{H})$ then $e^{isA}D(H) \subset D(H)$ for all $s \in \mathbb{R}$.*

4. Weak propagation estimates.

The following weak propagation estimates denoted **WPE** are the main ingredients for constructing the asymptotic velocity. They take the general form

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

where $B(t)$ is a time-dependent self-adjoint operator on \mathcal{H} . These estimates give a very weak fall-off with respect to t of the function under the integral. We are mainly interested in the *maximal* and *minimal velocity estimates* which, roughly speaking, assert that given a state ψ in \mathcal{H} with bounded energy, there exist two constants c_m and c_M such that the “particle” can neither escape faster than c_M nor slower than c_m . The last type of estimates

called *microlocal estimates* will help us to give another definition for the asymptotic velocity in terms of the classical velocity operator that will allow us to study its spectrum.

For the proof of the **WPE**, we shall use the following proposition given in [8], (p. 384). We recall that $\mathbf{D} = \frac{d}{dt} + i[H, \cdot]$ is the Heisenberg derivative and satisfies

$$\frac{d}{dt} [e^{itH} B(t) e^{-itH}] = e^{itH} \mathbf{D}B(t) e^{-itH}.$$

PROPOSITION 4.1. — *Let $\Phi(t)$ be a family of self-adjoint operators belonging to $W_{\text{loc}}^{1,1}(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ i.e. there exists $B(t) \in L^1_{\text{loc}}(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ such that*

$$\Phi(t_1) - \Phi(t_2) = \int_{t_1}^{t_2} B(s) ds.$$

(i) *Assume $\mathbf{D}\Phi(t) \in L^1_{\text{loc}}(\mathbb{R}^+, \mathcal{B}(\mathcal{H}))$. Then*

$$\|\Phi(t)e^{-itH}\Psi\| \leq \|\Phi(0)\Psi\| + \int_0^t \|\mathbf{D}\Phi(s)e^{-isH}\Psi\| ds.$$

(ii) *Assume that $\Phi(t)$ is uniformly bounded and that there exists $C_0 > 0$ and some operator valued functions $B(t)$ and $B_i(t)$, $i = 1, \dots, n$ such that*

$$\mathbf{D}\Phi(t) \geq C_0 B^*(t)B(t) - \sum_{i=1}^n B_i^*(t)B_i(t),$$

with

$$\int_1^\infty \|B_i(t)e^{-itH}\psi\|^2 dt \leq C\|\psi\|^2, \quad \forall \psi \in \mathcal{H}, \quad i = 1, \dots, n.$$

Then there exists a constant C such that

$$(4.1) \quad \int_1^\infty \|B(t)e^{-itH}\psi\|^2 dt \leq C\|\psi\|^2, \quad \forall \psi \in \mathcal{H}.$$

We stress the fact that the ideas of the proof are very simple, the essential step being to find an observable $\Phi(t)$ called *propagation observable* such that its Heisenberg derivative is essentially positive. Before we turn to the proof of the estimates, we briefly indicate how to make the link with the existence of asymptotic observables i.e. with observables taking the form

$$s - \lim_{t \rightarrow \infty} e^{itH} \Phi(t) e^{-itH},$$

where $\Phi(t)$ is a self-adjoint operator valued function. For this we shall use the following lemma given in [8] but which contains results initially due to Cook and Kato.

LEMMA 4.1 (Cook, Kato). — *Let $\Phi(t)$ be a uniformly bounded function with values in self-adjoint operators, belonging to $W^{1,1}(\mathbb{R}, \mathcal{B}(\mathcal{H}))$. Let \mathcal{D} a dense subspace of \mathcal{H} .*

(i) (Cook) *Assume that $\forall \psi \in \mathcal{D}$,*

$$\int_1^\infty \|\mathbf{D}\Phi(t)e^{-itH}\psi\| dt < \infty,$$

then there exists

$$(4.2) \quad s - \lim_{t \rightarrow \infty} e^{itH}\Phi(t)e^{-itH}.$$

(ii) (Kato) *Assume that*

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

with

$$\int_1^\infty \|B_{2i}(t)e^{-itH}\psi\|^2 dt \leq C\|\psi\|^2, \quad \psi \in \mathcal{H}, i = 1, \dots, n,$$

$$\int_1^\infty \|B_{1i}(t)e^{-itH}\psi\|^2 dt \leq C\|\psi\|^2, \quad \psi \in \mathcal{D}, i = 1, \dots, n,$$

then the limit (4.2) exists.

4.1. Minimal velocity estimates.

It has been well-known since Ruelle’s theorem [29] that the states ψ belonging to the continuous subspace \mathcal{H}^c of H tend to escape for large time t in a mean ergodic sense, that is to say

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \int_{|x| \leq R} \|e^{-itH}\psi\|^2 dx = 0,$$

for any finite R . Nevertheless this decay is not sufficient to prove precise results of scattering theory. We need more subtle estimates on how fast the states move away from the centre of the interaction. The following minimal velocity estimates improve the previous result in a very weak sense but which is enough for applications. These estimates ensure that the probability to find the “particle” in a narrow cone $|x| < \theta t$ goes to zero when $t \rightarrow \infty$ for θ small enough. The “particle” here simply refers to the wave function $\psi(t, x)$, i.e. the field. There is no second quantization involved. Exactly, we shall prove the following proposition

PROPOSITION 4.2. — *Let $\chi \in C_0^\infty(\mathbb{R})$ such that $\text{supp } \chi \cap \{-m, +m, \sigma_{pp}(H)\} = \emptyset$. Then there exists a constant $\epsilon_0(\chi) > 0$ depending on χ such that*

$$(4.3) \quad \int_1^\infty \left\| \mathbf{1}_{[0, \epsilon_0]} \left(\frac{|x|}{t} \right) \chi(H) e^{-itH} \psi \right\|^2 \frac{dt}{t} \leq C \|\psi\|^2, \quad \forall \psi \in \mathcal{H}.$$

Furthermore,

$$(4.4) \quad s - \lim_{t \rightarrow +\infty} \mathbf{1}_{[0, \epsilon_0]} \left(\frac{|x|}{t} \right) \chi(H) e^{-itH} = 0.$$

Before we give the proof, we mention that these estimates first appeared in the paper [31] by Sigal and Soffer and have been intensively used to organize the proofs of asymptotic completeness for N -body problems in quantum mechanics. It appears that there exists a strong link between the notion of locally conjugate operator and minimal velocity estimates as stated in the next proposition (our proof will follow the result obtained by C. Gérard and F. Nier in [17]).

PROPOSITION 4.3 (Gérard, Nier). — *Let H, A two self-adjoint operators on \mathcal{H} . Assume that for $\epsilon > 0$, $H \in C^{1+\epsilon}(A)$, and the Mourre estimate*

$$(4.5) \quad \mathbf{1}_\Delta(H) i[H, A] \mathbf{1}_\Delta(H) \geq c_0 \mathbf{1}_\Delta^2(H),$$

holds on an open interval Δ . Then

(i) $\forall g \in C_0^\infty(\mathbb{R})$, $\forall \chi \in C_0^\infty(\mathbb{R})$ such that $\text{supp } g \subset (-\infty, c_0)$ and $\text{supp } \chi \subset \Delta$,

$$(4.6) \quad \int_1^\infty \left\| g \left(\frac{A}{t} \right) \chi(H) e^{-itH} \psi \right\|^2 \frac{dt}{t} \leq C \|\psi\|^2, \quad \forall \psi \in \mathcal{H},$$

and

$$(4.7) \quad s - \lim_{t \rightarrow \infty} g \left(\frac{A}{t} \right) \chi(H) e^{-itH} = 0.$$

(ii) Furthermore assume that there exists another self-adjoint operator A_1 which satisfies

$$\begin{aligned} D(A_1) &\subset D(A), \\ \pm A &\leq C A_1, \quad A_1 \geq 1, \\ [A, A_1] A_1^{-1} &\in \mathcal{B}(\mathcal{H}), \end{aligned}$$

then, $\forall \chi \in C_0^\infty(\mathbb{R})$, $\text{supp } \chi \subset \Delta$, there exists ϵ_0 small enough such that

$$(4.8) \quad \int_1^\infty \left\| \mathbf{1} \left(\frac{A_1}{t} \leq \epsilon_0 \right) \chi(H) e^{-itH} \psi \right\|^2 \frac{dt}{t} \leq C \|\psi\|^2, \quad \forall \psi \in \mathcal{H},$$

and

$$(4.9) \quad s - \lim_{t \rightarrow +\infty} \mathbf{1}_{[0, \epsilon_0)} \left(\frac{A_1}{t} \right) \chi(H) e^{-itH} = 0.$$

Proof of Proposition 4.2. — We already know from the previous section that the Dirac operator H belongs to the class $C^2(A)$. Since $\sigma(H) \cap (-m, +m) \subset \sigma_{pp}(H)$, we can assume that $\text{supp } \chi \subset (-\infty, -m) \cup (+m, +\infty)$. Let $\lambda \in (-\infty, -m) \cup (+m, +\infty)$. We can find a closed interval I containing λ on which Mourre estimate (3.1) holds

$$\mathbf{1}_I(H) i[H, A] \mathbf{1}_I(H) \geq \epsilon \mathbf{1}_I(H) + \mathbf{1}_I(H) K \mathbf{1}_I(H).$$

Since $\lambda \notin \sigma_{pp}(H)$, we have

$$s - \lim_{|I| \rightarrow 0} \mathbf{1}_I(H) = \mathbf{1}_{\{\lambda\}}(H) = 0.$$

Now, the fact that K is compact implies that $K \mathbf{1}_I(H)$ tends to 0 in norm when $|I|$ tends to 0. Thus, if we consider I with $\lambda \in I$ with $|I|$ small enough, there exists c_0 a strictly positive constant such that

$$\mathbf{1}_I(H) i[H, A] \mathbf{1}_I(H) \geq c_0 \mathbf{1}_I(H).$$

Therefore, for any χ such that $\text{supp } \chi \subset I$, minimal velocity estimates hold for the operator A according to (i) of Proposition 4.3. Now we apply the second part of this proposition with $A_1 = \langle x \rangle$. We have to check the following assumptions.

- $D(\langle x \rangle) \subset D(A)$ has been seen in the previous section.
- For all u in $D(A)$, we have

$$(4.10) \quad |(u, Au)| \leq \frac{1}{2} \sum_j \left(|(u, x^j p_j H^{-1} u)| + |(u, H^{-1} p_j x^j u)| \right).$$

But the first term in (4.10) can be estimated as follows

$$\begin{aligned} |(u, x^j p_j H^{-1} u)| &\leq \left| \left(\frac{x^j}{\langle x^j \rangle^{\frac{1}{2}}} u, p_j H^{-1} \langle x^j \rangle^{\frac{1}{2}} u \right) \right| \\ &\quad + \left| \left(\frac{x^j}{\langle x^j \rangle^{\frac{1}{2}}} u, [\langle x^j \rangle^{\frac{1}{2}}, p_j H^{-1}] u \right) \right|, \\ &\leq C \left(\|\langle x^j \rangle^{\frac{1}{2}} u\|^2 + \left| \left(\frac{x^j}{\langle x^j \rangle^{\frac{1}{2}}} u, \frac{x^j}{\langle x^j \rangle^{\frac{3}{2}}} H^{-1} u \right) \right| \right) \\ &\quad + \left| \left(\frac{x^j}{\langle x^j \rangle^{\frac{1}{2}}} u, p_j H^{-1} \Gamma^j \frac{\langle x^j \rangle}{\langle x^j \rangle^{\frac{3}{2}}} H^{-1} u \right) \right|, \\ &\leq C \left(\|\langle x^j \rangle^{\frac{1}{2}} u\|^2 + \|u\|^2 \right) \leq C \|\langle x \rangle^{\frac{1}{2}} u\|^2. \end{aligned}$$

We can prove the same estimate for the second term in (4.10) and we obtain

$$|(u, Au)| \leq C(u, \langle x \rangle u).$$

- Eventually $[A, \langle x \rangle] \langle x \rangle^{-1}$ is clearly bounded. Indeed it suffices to expand the commutator and use the fact that $[p, \langle x \rangle]$ and $[H^{-1}, \langle x \rangle]$ are bounded in \mathcal{H} .

To conclude the proof, observe that for t large enough, $\mathbf{1}_{[0, \frac{\epsilon_0}{2}]}(\frac{|x|}{t}) \leq \mathbf{1}_{[0, \epsilon_0]}(\frac{\langle x \rangle}{t})$ therefore we can replace $\langle x \rangle$ by $|x|$ in the estimate. Thus proposition 4.2 is proved for any χ with sufficiently small support. Let us prove the general case. Let χ be any function in $C_0^\infty(\mathbb{R})$ which satisfies the assumptions of proposition 4.2. We can write, by a compactness argument,

$$\chi = \sum_{j=1}^N \chi_j,$$

where χ_j are $C_0^\infty(\mathbb{R})$ functions with sufficiently small supports, such that

$$\int_1^\infty \left\| \mathbf{1}_{[0, \epsilon_0]} \left(\frac{|x|}{t} \right) \chi_j(H) e^{-itH} \psi \right\|^2 \frac{dt}{t} \leq C \|\psi\|^2, \quad \forall \psi \in \mathcal{H}, \quad j = 1, \dots, N.$$

By the Schwarz inequality, we have

$$\begin{aligned} & \int_1^\infty \left(\mathbf{1}_{[0, \epsilon_0]} \left(\frac{|x|}{t} \right) \chi_i(H) e^{-itH} \psi, \mathbf{1}_{[0, \epsilon_0]} \left(\frac{|x|}{t} \right) \chi_j(H) e^{-itH} \psi \right) \frac{dt}{t} \\ & \leq \left(\int_1^\infty \left\| \mathbf{1}_{[0, \epsilon_0]} \left(\frac{|x|}{t} \right) \chi_i(H) e^{-itH} \psi \right\|^2 \frac{dt}{t} \right)^{\frac{1}{2}} \\ & \quad \left(\int_1^\infty \left\| \mathbf{1}_{[0, \epsilon_0]} \left(\frac{|x|}{t} \right) \chi_j(H) e^{-itH} \psi \right\|^2 \frac{dt}{t} \right)^{\frac{1}{2}}, \\ & \leq C \|\psi\|^2. \end{aligned}$$

Hence,

$$\int_1^\infty \left\| \mathbf{1}_{[0, \epsilon_0]} \left(\frac{|x|}{t} \right) \chi(H) e^{-itH} \psi \right\|^2 \frac{dt}{t} \leq N^2 C \|\psi\|^2, \quad \forall \psi \in \mathcal{H},$$

which concludes the proof of the Proposition. □

4.2. Large velocity estimates.

This estimate says that the energy of the field in the region $|x| \geq t$ tends to zero as t becomes large. Recall that the light velocity c is here

taken to be 1, so this means that the particle does not travel faster than light. Precisely, we prove

PROPOSITION 4.4. — Let $1 < \theta_1 < \theta_2$. Let $\chi \in C_0^\infty(\mathbb{R})$. There exists a constant C such that

$$(4.11) \quad (i) \quad \int_1^\infty \left\| \mathbf{1}_{[\theta_1, \theta_2]} \left(\frac{|x|}{t} \right) \chi(H) e^{-itH} \psi \right\|^2 \frac{dt}{t} \leq C \|\psi\|^2, \quad \forall \psi \in \mathcal{H}.$$

Given any $g \in C^\infty(\mathbb{R})$ with $g' \in C_0^\infty(\mathbb{R})$ and $\text{supp } g \subset (1, +\infty)$, we have

$$(4.12) \quad (ii) \quad s - \lim_{t \rightarrow +\infty} g\left(\frac{|x|}{t}\right) \chi(H) e^{-itH} = 0.$$

Remark 4.1. — We stress the fact that the cut-off function χ could be avoided in the previous proposition without any change, that is to say that the constant C does not depend on the support of χ if $\|\chi\|_{L^\infty} \leq 1$. Therefore, whatever the energy of a state ψ , it cannot escape to infinity faster than the light velocity.

Proof. — Let $1 < \theta_0 < \theta_1 < \theta_2$ and let $f \in C_0^\infty([\theta_0, +\infty))$ such that $f = 1$ on $[\theta_1, \theta_2]$ and $f \geq 0$. We define

$$F(s) = \int_{-\infty}^s f^2(u) du,$$

which is clearly bounded and continuous on \mathbb{R} . Let us define the propagation observable

$$\phi(t) = \chi(H) F\left(\frac{|x|}{t}\right) \chi(H).$$

$\phi(t)$ is a self-adjoint operator valued function uniformly bounded in t . We compute the Heisenberg derivative.

$$-\mathbf{D}\phi(t) = \frac{1}{t} \chi(H) f^2\left(\frac{|x|}{t}\right) \frac{|x|}{t} \chi(H) - \chi(H) i \left[H, F\left(\frac{|x|}{t}\right) \right] \chi(H).$$

Now

$$\begin{aligned} i \left[H, F\left(\frac{|x|}{t}\right) \right] &= i \left[\Gamma \cdot p, F\left(\frac{|x|}{t}\right) \right], \\ &= \frac{1}{t} \sum_j \Gamma^j \cdot \frac{x_j}{|x|} f^2\left(\frac{|x|}{t}\right) = \frac{1}{t} \Gamma \cdot \frac{x}{|x|} f^2\left(\frac{|x|}{t}\right). \end{aligned}$$

Thus

$$-\mathbf{D}\phi(t) = \frac{1}{t} \chi(H) \left\{ f^2\left(\frac{|x|}{t}\right) \frac{|x|}{t} - \Gamma \cdot \frac{x}{|x|} f^2\left(\frac{|x|}{t}\right) \right\} \chi(H).$$

Now using the facts that $\Gamma \cdot \frac{x}{|x|} \leq 1_{4 \times 4}$ and $f \geq 0$, we have

$$-\mathbf{D}\phi(t) \geq \frac{1}{t}(\theta_0 - 1)\chi(H)\mathbf{1}_{[\theta_1, \theta_2]} \left(\frac{|x|}{t} \right) \chi(H).$$

As $(\theta_0 - 1) > 0$ by assumption, the assertion (i) follows from Proposition 4.1.

Let us prove (ii). It is enough to assume $g \geq 0$ and $g = 1$ for $x \geq R_0$. Let $\tilde{g} \in C_0^\infty(\mathbb{R})$ chosen such that $\text{supp } \tilde{g} \subset (1, +\infty)$ and $\tilde{g} = 1$ on $\text{supp } g'$. We define

$$\phi(t) = \chi(H)g\left(\frac{|x|}{t}\right)\chi(H),$$

and

$$\mathbf{D}\phi(t) = -\frac{1}{t}\chi(H)g'\left(\frac{|x|}{t}\right)\frac{|x|}{t}\chi(H) + \frac{1}{t}\chi(H)\Gamma \cdot \frac{x}{|x|}g'\left(\frac{|x|}{t}\right)\chi(H).$$

Using $\tilde{g}g' = g'$ we get

$$(4.13) \quad \mathbf{D}\phi(t) = \frac{1}{t}\chi(H)\tilde{g}\left(\frac{|x|}{t}\right)B(t)\tilde{g}\left(\frac{|x|}{t}\right)\chi(H),$$

where $B(t) = -g'\left(\frac{|x|}{t}\right)\frac{|x|}{t} + \Gamma \cdot \frac{x}{|x|}g'\left(\frac{|x|}{t}\right)$ is uniformly bounded with respect to t . Now with (4.11) and (4.13), the existence of the limit

$$(4.14) \quad s - \lim_{t \rightarrow +\infty} e^{itH}\phi(t)e^{-itH},$$

follows from Lemma 4.1. Assume first that g has a compact support contained in $(1, +\infty)$ then (4.11) implies that

$$0 \leq \int_1^\infty (\psi, e^{itH}\phi(t)e^{-itH}\psi) \frac{dt}{t} \leq C\|\psi\|^2.$$

Hence the limit in (4.14) must be zero. Finally, to prove the general case, let us consider $g_1 \in C^\infty(\mathbb{R})$ and $g \in C_0^\infty(\mathbb{R})$ such that $\text{supp } g_1 \subset (\theta_0, +\infty)$ with $\theta_0 > 1$, $g_1 \geq 0$, $g_1 = 1$ for $|x| \geq R_0$ and $g'_1 = g^2$. We define the propagation observables by

$$\phi(t) = \chi(H)g_1\left(\frac{|x|}{t}\right)\chi(H),$$

and

$$\phi_R(t) = \chi(H)g_1\left(\frac{|x|}{Rt}\right)\chi(H),$$

where R is a positive real number. By the previous lemma, we know that $s - \lim_{t \rightarrow +\infty} e^{itH}\phi_R(t)e^{-itH}$ exists. Let us compute the Heisenberg derivative.

$$(4.15) \quad \begin{aligned} -\mathbf{D}\phi_R(t) &= \frac{1}{t}\chi(H)g^2\left(\frac{|x|}{Rt}\right)\frac{|x|}{Rt}\chi(H) - \frac{1}{Rt}\chi(H)\Gamma \cdot \frac{x}{|x|}g^2\left(\frac{|x|}{Rt}\right)\chi(H), \\ &\geq \frac{1}{t}\left(\theta_0 - \frac{1}{R}\right)\chi(H)g^2\left(\frac{x}{Rt}\right)\chi(H). \end{aligned}$$

For $\theta_0 > 1$ and $R \geq 1$, we see that $(\theta_0 - \frac{1}{R})$ is strictly positive and thus $-\mathbf{D}\phi_R(t)$ is a positive operator. Now given some $t_0 \in \mathbb{R}$ fixed, we can write

$$s - \lim_{t \rightarrow +\infty} e^{itH} \phi_R(t) e^{-itH} = e^{it_0H} \phi_R(t_0) e^{-it_0H} + \int_{t_0}^{\infty} e^{isH} \mathbf{D}\phi_R(s) e^{-isH} ds.$$

From the positivity of $-\mathbf{D}\phi_R(t)$, we deduce

$$(4.16) \quad 0 \leq s - \lim_{t \rightarrow +\infty} e^{itH} \phi_R(t) e^{-itH} \leq e^{it_0H} \phi_R(t_0) e^{-it_0H}, \quad \forall R \geq 1.$$

Now according to the definition of $\phi_R(t)$, observe that for t_0 fixed

$$s - \lim_{R \rightarrow +\infty} (e^{it_0H} \phi_R(t_0) e^{-it_0H}) = 0.$$

Hence we obtain from (4.16) that

$$(4.17) \quad s - \lim_{R \rightarrow +\infty} (s - \lim_{t \rightarrow +\infty} e^{itH} \phi_R(t) e^{-itH}) = 0.$$

We conclude observing that $g_1(\frac{|x|}{t}) - g_1(\frac{|x|}{Rt})$ has a compact support. Thus by the previous result (4.14), we get

$$s - \lim_{t \rightarrow +\infty} e^{itH} [\phi(t) - \phi_R(t)] e^{-itH} = 0.$$

Then if R tends to $+\infty$, we prove (ii) by (4.17). □

4.3. Microlocal velocity estimates.

In this section, we shall prove the following proposition:

PROPOSITION 4.5. — *Let $0 < \theta_1 < \theta_2$ and let $\chi \in C_0^\infty(\mathbb{R})$ such that $\text{supp } \chi \cap \{-m, +m, \sigma_{pp}(H)\} = \emptyset$. Then*

$$(4.18) \quad (i) \quad \int_1^\infty \left\| \mathbf{1}_{[\theta_1, \theta_2]} \left(\frac{|x|}{t} \right) \left(\nu - \frac{x}{t} \right) \chi(H) e^{-itH} \psi \right\|^2 \frac{dt}{t} \leq C \|\psi\|^2, \quad \forall \psi \in \mathcal{H}.$$

$$(4.19) \quad (ii) \quad s - \lim_{t \rightarrow +\infty} \mathbf{1}_{[\theta_1, \theta_2]} \left(\frac{|x|}{t} \right) \left(\nu - \frac{x}{t} \right) \chi(H) e^{-itH} = 0.$$

Proof. — Let $0 < \theta_0 < \theta_1 < \theta_2 < \theta_3$. Given two real numbers r_1, r_2 such that $0 < r_1 < r_2$, we denote by $C(r_1, r_2)$ the annulus $C(r_1, r_2) = \{x \in \mathbb{R}^3 : r_1 < |x| < r_2\}$. Let $J \in C_0^\infty(\mathbb{R}^3)$ such that $\text{supp } J \subset C(\frac{\theta_0}{2}, 2\theta_3)$ and $J = 1$ on $C(\theta_1, \theta_2)$. Let $\chi \in C_0^\infty(\mathbb{R})$ satisfying the above condition. We choose θ_0 and θ_3 such that $\theta_0 < \epsilon_\chi$ where ϵ_χ is defined according to the minimal velocity estimates and $\theta_3 > 1$.

We consider the following propagation observable

$$\phi(t) = \chi(H)J\left(\frac{x}{t}\right)\left\{\frac{x_{nw}^2}{t^2} - 2\frac{A}{t}\right\}J\left(\frac{x}{t}\right)\chi(H),$$

which is uniformly bounded for $t \geq 1$. Indeed $J\left(\frac{x}{t}\right)\frac{x_{nw}^2}{t^2}J\left(\frac{x}{t}\right) = J\left(\frac{x}{t}\right)\left\{\frac{x^2}{t^2} + \frac{x}{t}\cdot\frac{Z}{t} + \frac{Z}{t}\cdot\frac{x}{t} + \frac{Z^2}{t^2}\right\}J\left(\frac{x}{t}\right)$. This term is uniformly bounded since Z and $J\left(\frac{x}{t}\right)\frac{x}{t}$ are bounded. Furthermore $J\left(\frac{x}{t}\right)\frac{A}{t}J\left(\frac{x}{t}\right) = \frac{1}{2}J\left(\frac{x}{t}\right)\left\{\frac{x}{t}\cdot pH^{-1} + H^{-1}p\cdot\frac{x}{t}\right\}J\left(\frac{x}{t}\right)$ is also uniformly bounded since pH^{-1} and $H^{-1}p$ are bounded. Let us compute its Heisenberg derivative.

$$\begin{aligned} -\mathbf{D}\phi(t) &= -\frac{1}{t}\chi(H)\left(\Gamma - \frac{x}{t}\right)\cdot\nabla J\left(\frac{x}{t}\right)\left\{\frac{x_{nw}^2}{t^2} - 2\frac{A}{t}\right\}J\left(\frac{x}{t}\right)\chi(H) + hc, \\ &\quad + \frac{2}{t}\chi(H)J\left(\frac{x}{t}\right)\left\{\frac{x_{nw}^2}{t^2} - \frac{A}{t}\right\}J\left(\frac{x}{t}\right)\chi(H), \\ &\quad - \frac{1}{t^2}\chi(H)J\left(\frac{x}{t}\right)i[H, x_{nw}^2]J\left(\frac{x}{t}\right)\chi(H), \\ &\quad + \frac{2}{t}\chi(H)J\left(\frac{x}{t}\right)i[H, A]J\left(\frac{x}{t}\right)\chi(H). \end{aligned}$$

Now we compute $i[H, x_{nw}^2]$ using $x_{nw} = x + Z$ and (2.23)

$$\begin{aligned} i[H, x_{nw}^2] &= i[H_0, x_{nw}^2] + i[V(x), x_{nw}^2], \\ &= (x_{nw}\mathcal{V} + \mathcal{V}x_{nw}) + (i[V(x), Z]x_{nw} + x_{nw}i[V(x), Z]). \end{aligned}$$

But the first term is equal to $2A_0$ plus a bounded operator in \mathcal{H} . And the second term is also a bounded operator in \mathcal{H} by Lemma 2.1 and the fact that V belongs to $S^{-1}(\mathbb{R}^3)$. Furthermore, we have already seen that $i[H, A] = \mathcal{V}^2 + K$ and from the exact expression of K , it is easy to show that $J\left(\frac{x}{t}\right)KJ\left(\frac{x}{t}\right) \in O(t^{-1})$. Thus, we obtain

$$\begin{aligned} -\mathbf{D}\phi(t) &= -\frac{1}{t}\chi(H)\left(\Gamma - \frac{x}{t}\right)\cdot\nabla J\left(\frac{x}{t}\right)\left\{\frac{x_{nw}^2}{t^2} - 2\frac{A}{t}\right\}J\left(\frac{x}{t}\right)\chi(H) + hc, \\ &\quad + \frac{2}{t}\chi(H)J\left(\frac{x}{t}\right)\left\{\frac{x_{nw}^2}{t^2} - \frac{A}{t} - \frac{A_0}{t} + \mathcal{V}^2\right\}J\left(\frac{x}{t}\right)\chi(H), \\ &\quad + O(t^{-2}). \end{aligned}$$

Using that $A = A_0 + B$ and $x_{nw} = x + Z$ again, we can replace the second term by $\frac{2}{t}\chi(H)J\left(\frac{x}{t}\right)\left\{\frac{x^2}{t^2} - 2\frac{A_0}{t} + \mathcal{V}^2\right\}J\left(\frac{x}{t}\right)\chi(H) + O(t^{-2})$. Moreover, we have the following equality $\left\{\frac{x^2}{t^2} - 2\frac{A_0}{t} + \mathcal{V}^2\right\} = (\mathcal{V} - \frac{x}{t})^2$. Therefore the second term is equal to

$$\frac{2}{t}\chi(H)J\left(\frac{x}{t}\right)\left(\mathcal{V} - \frac{x}{t}\right)^2J\left(\frac{x}{t}\right)\chi(H) + O(t^{-2}).$$

Finally, if we introduce $\tilde{J} \in C_0^\infty(\mathbb{R})$ such that $\text{supp } \tilde{J} \subset [\frac{\theta_0}{2}, 2\theta_3]$ and $\tilde{J}(|x|)\nabla J(x) = \nabla J(x)$, then after some commutations the first term can be written as

$$\frac{1}{t}\chi(H)\tilde{J}\left(\frac{|x|}{t}\right)B(t)\tilde{J}\left(\frac{|x|}{t}\right)\chi(H) + O(t^{-2}),$$

where $B(t)$ is a uniformly bounded operator in t . Hence this term is integrable along the evolution by Propositions 4.2 and 4.4. Eventually, we obtain

$$-\mathbf{D}\phi(t) \geq \frac{2}{t}\chi(H)J\left(\frac{x}{t}\right)\left(\mathcal{V} - \frac{x}{t}\right)^2J\left(\frac{x}{t}\right)\chi(H) + L^1(dt).$$

Commuting $J\left(\frac{x}{t}\right)$ and $\left(\mathcal{V} - \frac{x}{t}\right)$ and provided $J^2\left(\frac{x}{t}\right) - \mathbf{1}_{[\theta_1, \theta_2]}(\frac{|x|}{t}) \geq 0$, we get

$$-\mathbf{D}\phi(t) \geq \frac{2}{t}\chi(H)\left(\mathcal{V} - \frac{x}{t}\right)\mathbf{1}_{[\theta_1, \theta_2]}\left(\frac{x}{t}\right)\left(\mathcal{V} - \frac{x}{t}\right)\chi(H) + L^1(dt).$$

We conclude the proof of (i) by Proposition 4.1.

To prove (ii), let us consider the following propagation observable

$$\phi_0(t) = \chi(H)J\left(\frac{x}{t}\right)\left\{\frac{x^2}{t^2} - 2\frac{A_0}{t} + \mathcal{V}^2\right\}J\left(\frac{x}{t}\right)\chi(H),$$

and observe that it is equal to $\chi(H)J\left(\frac{x}{t}\right)\left(\mathcal{V} - \frac{x}{t}\right)^2J\left(\frac{x}{t}\right)\chi(H)$. In particular it is a positive operator for any t . For technical reasons we shall approach $\phi_0(t)$ by another observable denoted $\phi(t)$ and given by

$$\phi(t) = \chi(H)J\left(\frac{x}{t}\right)\left\{\frac{x_{nw}^2}{t^2} - 2\frac{A}{t} + \mathcal{V}^2\right\}J\left(\frac{x}{t}\right)\chi(H).$$

It is easy to see that $\phi(t) = \phi_0(t) + O(t^{-1})$. Let us compute the Heisenberg derivative of $\phi(t)$. As shown in the previous calculation, we obtain

$$\begin{aligned} -\mathbf{D}\phi(t) &= \frac{2}{t}\chi(H)J\left(\frac{x}{t}\right)\left(\mathcal{V} - \frac{x}{t}\right)^2J\left(\frac{x}{t}\right)\chi(H), \\ &\quad - \chi(H)J\left(\frac{x}{t}\right)i[H, \mathcal{V}^2]J\left(\frac{x}{t}\right)\chi(H), \\ &\quad + O(t^{-2}) + L^1(dt). \end{aligned}$$

But $i[H, \mathcal{V}^2] = i[V(x), \mathcal{V}^2]$ and from the exact expression of $\mathcal{V}^2 = \frac{p^2}{p^2+m^2}$, this last term leads to

$$\begin{aligned} [V(x), \mathcal{V}^2] &= [V(x), p^2]H_0^{-2} + p^2H_0^{-2}[H_0^2, V(x)]H_0^{-2}, \\ &= i\nabla V(x).pH_0^{-2} + ip.\nabla V(x)H_0^{-2} - ip^2H_0^{-2}\nabla V(x).pH_0^{-2} \\ &\quad - ip^2H_0^{-2}p.\nabla V(x)H_0^{-2}. \end{aligned}$$

Therefore, after some commutations and since $\nabla V(x)$ belongs to $S^{-2}(\mathbb{R}^3)$, the second term in the Heisenberg derivative belongs to $O(t^{-2})$. Now applying Lemma 4.1, we have proved that the following limit exists

$$(4.20) \quad s - \lim_{t \rightarrow +\infty} e^{itH}\phi(t)e^{-itH}.$$

Clearly, we can replace $\phi(t)$ by $\phi_0(t)$ in (4.20). But we also know by (i) that

$$0 \leq \int_1^{+\infty} (e^{-itH}\psi, \phi_0(t)e^{-itH}\psi) \frac{dt}{t} < +\infty,$$

Hence the limit (4.20) must vanish which concludes the proof. □

5. Asymptotic velocity P^\pm .

5.1. Construction of P^\pm .

In this section, we shall focus our attention on the construction of the asymptotic velocity P^\pm defined by

$$P^\pm := s - C_\infty - \lim_{t \rightarrow \pm\infty} e^{itH} \frac{x}{t} e^{-itH}.$$

Here the convergence means that for any $\psi \in \mathcal{H}$ and any $J \in C_\infty(\mathbb{R}^3)$, the limit

$$(5.1) \quad J(P^\pm)\psi := \lim_{t \rightarrow \pm\infty} e^{itH} J\left(\frac{x}{t}\right) e^{-itH}\psi,$$

exists. If (5.1) holds then the operators P^\pm are uniquely defined as vectors of (possibly non-densely defined) commuting self-adjoint operators. P^\pm are densely defined if, for some $g \in C_\infty(\mathbb{R}^3)$ such that $g(0) = 1$ we have $s - \lim_{R \rightarrow +\infty} (s - \lim_{t \rightarrow \pm\infty} e^{itH} g(\frac{x}{Rt}) e^{-itH}) = 1$ (see [8], Appendix B.2). The main tools will be Lemma 4.1 and the *weak propagation estimates* defined in the previous section. We only treat the case $t \rightarrow +\infty$ and we construct P^+ , the construction is identical for P^- with $t \rightarrow -\infty$. Let us prove the theorem.

THEOREM 5.1. — *Let H be the Dirac operator (2.1). Let $J \in C_\infty(\mathbb{R}^3)$. Then there exists the limit*

$$(5.2) \quad s - \lim_{t \rightarrow +\infty} e^{itH} J\left(\frac{x}{t}\right) e^{-itH}.$$

Moreover, if $J = 1$ on a neighbourhood of 0, then

$$(5.3) \quad s - \lim_{R \rightarrow +\infty} \left(s - \lim_{t \rightarrow +\infty} e^{itH} J\left(\frac{x}{Rt}\right) e^{-itH} \right) = 1.$$

If we define P^+ by (5.1) then P^+ is a vector of commuting self-adjoint operators on \mathcal{H} defined on a dense subspace of \mathcal{H} and P^\pm commutes with H .

Proof. — First, consider the case where ψ is an eigenvector of H . Then, there exists $E \in \mathbb{R}$ such that $H\psi = E\psi$. Let $J \in C_\infty(\mathbb{R}^3)$. We have

$$e^{itH} J\left(\frac{x}{t}\right) e^{-itH} \psi = J(0)\psi + e^{it(H-E)} \left\{ J\left(\frac{x}{t}\right) - J(0) \right\} \psi.$$

By Lebesgue's Theorem, it is immediate that $\lim_{t \rightarrow \infty} e^{it(H-E)} \left\{ J\left(\frac{x}{t}\right) - J(0) \right\} \psi = 0$. Therefore

$$(5.4) \quad \lim_{t \rightarrow +\infty} e^{itH} J\left(\frac{x}{t}\right) e^{-itH} \psi = J(0)\psi,$$

and we conclude that limit (5.2) exists on \mathcal{H}^{pp} the pure point subspace of H .

Now, let us assume that $\psi \in \mathcal{H}^c$ the continuous subspace of H . Our first task is to find a good propagation observable $\phi(t)$ in order to apply Lemma 4.1. Since $\psi \in \mathcal{H}^c$, remark that by a density argument, the existence of (5.2) is equivalent to the existence of

$$s - \lim_{t \rightarrow +\infty} e^{itH} \chi(H) J\left(\frac{x}{t}\right) \chi(H) e^{-itH},$$

for any $\chi \in C_0^\infty(\mathbb{R})$ satisfying $\text{supp } \chi \cap \{-m, +m, \sigma_{pp}(H)\} = \emptyset$ and any $J \in C_0^\infty(\mathbb{R}^3)$ such that J is constant on a neighbourhood of 0. Let us define $\phi(t) = \chi(H) \{J(\frac{x}{t}) + (\mathcal{V} - \frac{x}{t}) \nabla J(\frac{x}{t})\} \chi(H)$. By Proposition 4.5, it is enough to prove the existence of

$$s - \lim_{t \rightarrow +\infty} e^{itH} \phi(t) e^{-itH}.$$

Unfortunately, this propagation observable is not easy to work with. In order to avoid problems due to the Zitterbewegung phenomenon and the matrix-valued potential $V_2(x)\Gamma^0$, we need to approach $\phi(t)$ by another propagation observable which we denote by $\phi_a(t)$ and define as follows

$$\phi_a(t) = \chi(H) \left\{ J\left(\frac{x_{nw}}{t}\right) + (\mathcal{V}_a - \frac{x_{nw}}{t}) \cdot \nabla J\left(\frac{x_{nw}}{t}\right) \right\} \chi(H),$$

where $\mathcal{V}_a = \frac{1}{2}(pH^{-1} + H^{-1}p)$ is a bounded selfadjoint operator on \mathcal{H} . Clearly we have $\mathcal{V}_a = \mathcal{V} + B$ where B is bounded on \mathcal{H} . The next lemma will enable us to make the link between the operators $f(\frac{x}{t})$ and $f(\frac{x_{nw}}{t})$ and as a consequence give an estimate of $(\phi(t) - \phi_a(t))$.

LEMMA 5.1. — *Let $f \in C_0^\infty(\mathbb{R}^3)$. Then*

$$(i) \quad f\left(\frac{x}{t}\right) - f\left(\frac{x_{nw}}{t}\right) \in O(t^{-1}).$$

Assume moreover that $f = 0$ on a neighbourhood of 0 and let $g \in S^{-\rho}(\mathbb{R}^3)$ where $\rho > 0$ is a real number. Then

$$(ii) \quad g(x) f\left(\frac{x_{nw}}{t}\right) \in O(t^{-\rho}),$$

$$(iii) \quad (\mathcal{V} - \mathcal{V}_a) f\left(\frac{x_{nw}}{t}\right) \in O(t^{-1}).$$

Then it follows that $\phi_a(t) - \phi(t) \in O(t^{-1})$ and thus it is enough to prove the existence of

$$(5.5) \quad s - \lim_{t \rightarrow +\infty} e^{itH} \phi_a(t) e^{-itH}.$$

Let us compute its Heisenberg derivative.

$$\begin{aligned} \mathbf{D}\phi_a(t) &= \frac{1}{t}\chi(H)\left(\mathcal{V}_a - \frac{x_{nw}}{t}\right)\nabla^2 J\left(\frac{x_{nw}}{t}\right)\left(-\frac{x_{nw}}{t}\right)\chi(H) \\ &\quad + \chi(H)i\left[H, J\left(\frac{x_{nw}}{t}\right) + \left(\mathcal{V}_a - \frac{x_{nw}}{t}\right)\cdot\nabla J\left(\frac{x_{nw}}{t}\right)\right]\chi(H). \end{aligned}$$

To compute the remaining commutator, we use the following lemma which we prove later

LEMMA 5.2. — *Let $f \in C_0^\infty(\mathbb{R}^3)$ such that f is constant on a neighbourhood of 0. Then*

$$(5.6) \quad i\left[H, f\left(\frac{x_{nw}}{t}\right)\right] = \frac{1}{t}\nabla f\left(\frac{x_{nw}}{t}\right)\cdot\mathcal{V} + O(t^{-2}).$$

Therefore, we get

$$\begin{aligned} \mathbf{D}\phi_a(t) &= \frac{1}{t}\chi(H)\left(\mathcal{V}_a - \frac{x_{nw}}{t}\right)\nabla^2 J\left(\frac{x_{nw}}{t}\right)\left(\mathcal{V} - \frac{x_{nw}}{t}\right)\chi(H) \\ &\quad + \chi(H)i[H, \mathcal{V}_a]\cdot\nabla J\left(\frac{x_{nw}}{t}\right)\chi(H) \\ &\quad + O(t^{-2}). \end{aligned}$$

But $i[H, \mathcal{V}_a]\nabla J\left(\frac{x_{nw}}{t}\right) = -\frac{1}{2}(\nabla V(x)H^{-1} + hc)\nabla J\left(\frac{x_{nw}}{t}\right) \in O(t^{-2})$ by Lemma 5.2 and the fact that $\nabla V(x)\nabla J\left(\frac{x_{nw}}{t}\right) \in O(t^{-2})$. Moreover, we can replace \mathcal{V}_a by \mathcal{V} as well as $\frac{x_{nw}}{t}$ by $\frac{x}{t}$ and we eventually obtain (using Lemma 5.1)

$$\mathbf{D}\phi_a(t) = \frac{1}{t}\chi(H)\left(\mathcal{V} - \frac{x}{t}\right)\nabla^2 J\left(\frac{x}{t}\right)\left(\mathcal{V} - \frac{x}{t}\right)\chi(H) + O(t^{-2}).$$

Then by Proposition 4.5 and by Lemma 4.1, (5.5) exists.

The proof of (5.3) is a direct consequence of Proposition 4.4, part (ii). Indeed, (5.3) is equivalent to $s\text{-}\lim_{R \rightarrow +\infty} (s\text{-}\lim_{t \rightarrow \pm\infty} e^{itH} J\left(\frac{x}{Rt}\right) e^{-itH}) = 0$, for $J \in C^\infty(\mathbb{R}^3)$ such that $\text{supp } J \cap \overline{B}(0, 1) = \emptyset$ and $\nabla J \in C_0^\infty(\mathbb{R}^3)$.

The fact that H commutes with P^+ follows from $[H, f\left(\frac{x}{t}\right)] \in O(t^{-1})$. \square

Proof (of Lemma 5.1). — The first assertion follows readily from the Fourier transform. Indeed

$$\begin{aligned} f\left(\frac{x}{t}\right) - f\left(\frac{x_{nw}}{t}\right) &= \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\mathbb{R}^3} \hat{f}(\xi) \left\{ e^{i\xi\frac{x}{t}} - e^{i\xi\frac{x_{nw}}{t}} \right\} d\xi, \\ &= -\frac{1}{(2\pi)^{\frac{3}{2}}t} \int_{\mathbb{R}^3} \widehat{\nabla} f(\xi) \int_0^1 e^{i\xi\sigma\frac{x}{t}} Z e^{i\xi(1-\sigma)\frac{x_{nw}}{t}} d\sigma d\xi, \\ &\in O(t^{-1}), \end{aligned}$$

since Z is bounded in \mathcal{H} .

By the definition of the Newton-Wigner observable, we have

$$\begin{aligned}
 g(x)f\left(\frac{x_{nw}}{t}\right) &= g(x)U_{FW}^{-1}f\left(\frac{x}{t}\right)U_{FW}, \\
 (5.7) \qquad \qquad \qquad &= g(x)f\left(\frac{x}{t}\right) + g(x)\left[U_{FW}, f\left(\frac{x}{t}\right)\right]U_{FW}.
 \end{aligned}$$

Clearly the first term in (5.7) belongs to $O(t^{-\rho})$. Now recall that $U_{FW}^{-1} = P^{-1}(p)$ with P^{-1} given by (2.21). Thus each component of the matrix-valued function P^{-1} is in $S^0(\mathbb{R}^3)$ and we can use the Helffer-Sjöstrand formula (A.28) to estimate the commutator in the second term of (5.7). Hence

$$(5.8) \qquad \left[P^{-1}(p), f\left(\frac{x}{t}\right)\right] = \sum_{k=1}^N \frac{\nabla^k f\left(\frac{x}{t}\right)}{t^k k!} ad_x^k(P^{-1}(p)) + O(t^{-(N+1)}),$$

since $ad_x^k(P^{-1}(p))$ bounded for any $k \in \mathbb{N}$. To see this, we use once again the Helffer-Sjöstrand formula and we have for any $m = 1, 2, 3$

$$[P^{-1}(p), x_m] = \frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{P}^{-1}(z) \left(\sum_{l=1}^3 \left(\prod_{k_1=1}^l R_{k_1} \right) (-i\delta_{lm}) \left(\prod_{k_2=l}^3 R_{k_2} \right) \right) dz \wedge d\bar{z},$$

where $R_k = (z_k - p_k)^{-1}$. Therefore the first commutator is bounded. Noting that $[R_k, x_n] = R_k(-i\delta_{kn})R_k$, the multiple commutators are also bounded by induction. Finally, if we take $N \geq \rho$, then the assertion (ii) follows immediately from (5.7) and (5.8).

Now, using (i), we can write $(\mathcal{V} - \mathcal{V}_a)f\left(\frac{x_{nw}}{t}\right)$ as $(\mathcal{V} - \mathcal{V}_a)f\left(\frac{x}{t}\right) + O(t^{-1})$. Moreover,

$$\begin{aligned}
 (\mathcal{V} - \mathcal{V}_a)f\left(\frac{x}{t}\right) &= \left(\frac{1}{2}pH^{-1}V(x)H_0^{-1} + hc\right)f\left(\frac{x}{t}\right), \\
 &= \frac{1}{2}pH^{-1}V(x)f\left(\frac{x}{t}\right)H_0^{-1} \\
 &\quad - \frac{1}{2}pH^{-1}V(x)H_0^{-1}\left[H_0, f\left(\frac{x}{t}\right)\right]H_0^{-1} + hc, \\
 &\in O(t^{-1}),
 \end{aligned}$$

since $V(x)f\left(\frac{x}{t}\right) \in O(t^{-1})$ and $[H_0, f\left(\frac{x}{t}\right)] = -\frac{i}{t}\Gamma \cdot \nabla f\left(\frac{x}{t}\right) \in O(t^{-1})$ which concludes the proof of the lemma. \square

Proof (of Lemma 5.2). — Using the Fourier transform, we have the following formula (A.9).

$$\begin{aligned}
 i\left[H, f\left(\frac{x_{nw}}{t}\right)\right] &= \frac{1}{(2\pi)^{\frac{3}{2}}t} \int_{\mathbb{R}^3} \widehat{\nabla} f(\xi) \int_0^1 e^{i(1-s)\xi \cdot \frac{x_{nw}}{t}} \{\mathcal{V} + i[V(x), Z]\} e^{is\xi \cdot \frac{x_{nw}}{t}} ds d\xi.
 \end{aligned}$$

Since the term $\mathcal{V} + i[V(x), Z]$ is bounded, the integral converges in the norm of \mathcal{H} . We then commute $\mathcal{V} + iV(x)Z$ with $e^{is\xi \frac{x_{nw}}{t}}$ and $-iZV(x)$ with $e^{-i(1-s)\xi \frac{x_{nw}}{t}}$. We obtain

$$\begin{aligned} & i\left[H, f\left(\frac{x_{nw}}{t}\right)\right] \\ &= \frac{1}{(2\pi)^{\frac{3}{2}}t} \int_{\mathbb{R}^3} \widehat{\nabla}f(\xi) \left(e^{i\xi \cdot \frac{x_{nw}}{t}} \{\mathcal{V} + iV(x)Z\} - iZV(x)e^{i\xi \cdot \frac{x_{nw}}{t}} \right) d\xi \\ & \quad + \frac{1}{(2\pi)^{\frac{3}{2}}t} \int_{\mathbb{R}^3} \widehat{\nabla}f(\xi) \int_0^1 e^{i(1-s)\xi \cdot \frac{x_{nw}}{t}} [\mathcal{V} + iV(x)Z, e^{is\xi \cdot \frac{x_{nw}}{t}}] ds d\xi \\ & \quad - \frac{i}{(2\pi)^{\frac{3}{2}}t} \int_{\mathbb{R}^3} \widehat{\nabla}f(\xi) \int_0^1 [e^{i(1-s)\xi \cdot \frac{x_{nw}}{t}}, ZV(x)] e^{is\xi \cdot \frac{x_{nw}}{t}} ds d\xi. \end{aligned}$$

Now we use the formula (A.1) to estimate these last commutators. We have

$$[\mathcal{V}, e^{is\xi \cdot \frac{x_{nw}}{t}}] = \frac{is\xi}{t} \int_0^1 e^{i(1-\sigma)s\xi \cdot \frac{x_{nw}}{t}} [\mathcal{V}, x_{nw}] e^{i\sigma s\xi \cdot \frac{x_{nw}}{t}} d\sigma,$$

which clearly belongs to $O(\xi t^{-1})$ since $[\mathcal{V}, x_{nw}]$ is bounded in \mathcal{H} . We also have

$$[V(x)Z, e^{is\xi \cdot \frac{x_{nw}}{t}}] = \frac{is\xi}{t} \int_0^1 e^{i(1-\sigma)s\xi \cdot \frac{x_{nw}}{t}} [V(x)Z, x_{nw}] e^{i\sigma s\xi \cdot \frac{x_{nw}}{t}} d\sigma,$$

where $[V(x)Z, x_{nw}] = [V(x)Z, x] + [V(x)Z, Z] = V(x)[Z, x] + [V(x)Z, Z]$ is bounded by Lemma (2.1). Therefore, this term also belongs to $O(\xi t^{-1})$.

We thus obtain

$$\begin{aligned} i\left[H, f\left(\frac{x_{nw}}{t}\right)\right] &= \left(\frac{1}{(2\pi)^{\frac{3}{2}}t} \int_{\mathbb{R}^3} e^{i\xi \cdot \frac{x_{nw}}{t}} \widehat{\nabla}f(\xi) d\xi \right) \left\{ \mathcal{V} + iV(x)Z \right\} \\ & \quad - iZV(x) \left(\frac{1}{(2\pi)^{\frac{3}{2}}t} \int_{\mathbb{R}^3} e^{i\xi \cdot \frac{x_{nw}}{t}} \widehat{\nabla}f(\xi) d\xi \right) + O(t^{-2}), \\ &= \frac{1}{t} \nabla f\left(\frac{x_{nw}}{t}\right) \mathcal{V} + \frac{i}{t} \nabla f\left(\frac{x_{nw}}{t}\right) V(x)Z \\ & \quad - \frac{i}{t} ZV(x) \nabla f\left(\frac{x_{nw}}{t}\right) + O(t^{-2}). \end{aligned}$$

Now using Lemma 5.1, it is easy to see that $V(x)\nabla f(\frac{x_{nw}}{t}) \in O(t^{-1})$ which concludes the proof of Lemma 5.2. □

In order to analyse the spectrum of P^\pm , we now give another characterization of the asymptotic velocity. Precisely, we make the link between P^\pm and the standard velocity operator \mathcal{V} .

PROPOSITION 5.1. — *Let $J \in C_\infty(\mathbb{R}^3)$. Then*

$$(5.9) \quad \mathbf{1}_{\{0\}}(P^\pm) = \mathbf{1}^{pp}(H),$$

and consequently,

$$(5.10) \quad \mathbf{1}_{\mathbb{R}^3 \setminus \{0\}}(P^\pm) = \mathbf{1}^c(H),$$

where $\mathbf{1}^{pp}(H)$ and $\mathbf{1}^c(H)$ denote respectively the projection onto the pure point subspace of H and onto the continuous subspace of \mathcal{H} . Furthermore, we have

$$(5.11) \quad s - \lim_{t \rightarrow \pm\infty} e^{itH} J(\mathcal{V}) e^{-itH} \mathbf{1}_{\mathbb{R}^3 \setminus \{0\}}(P^\pm) = J(P^\pm) \mathbf{1}_{\mathbb{R}^3 \setminus \{0\}}(P^\pm).$$

Proof. — The proof of (5.9) entirely relies on the minimal velocity estimates. We successively show that $\mathbf{1}_{\{0\}}(P^+) \geq \mathbf{1}^{pp}(H)$ and $\mathbf{1}_{\{0\}}(P^+) \leq \mathbf{1}^{pp}(H)$. Let $\psi \in \mathcal{H}$ such that $H\psi = E\psi$ and $J \in C_\infty(\mathbb{R}^3)$. We already saw in (5.4) that

$$\lim_{t \rightarrow +\infty} e^{itH} J\left(\frac{x}{t}\right) e^{-itH} \psi = J(0)\psi.$$

This shows that $P^+\psi = 0$ and proves $\mathbf{1}_{\{0\}}(P^+) \geq \mathbf{1}^{pp}(H)$. Conversely, let us consider a function $\chi \in C_0^\infty(\mathbb{R})$ such that $\text{supp } \chi \cap \{-m, +m, \sigma_{pp}(H)\} = \emptyset$. Let $J \in C_0^\infty(\mathbb{R}^3)$ such that $J(0) = 1$ and $\text{supp } J \subset \overline{B}(0, \epsilon_\chi)$ where $\epsilon_\chi > 0$ is defined by the minimal velocity estimates.

Then Theorem 5.1 implies

$$(5.12) \quad \begin{aligned} s - \lim_{t \rightarrow +\infty} e^{itH} \chi(H) J^2\left(\frac{x}{t}\right) \chi(H) e^{-itH} &= \chi^2(H) J^2(P^+), \\ &\geq \chi^2(H) \mathbf{1}_{\{0\}}(P^+). \end{aligned}$$

But by Proposition 4.2, the strong limit in (5.12) vanishes. Thus we have proved that

$$\mathbf{1}_{\{0\}}(P^+) \leq \mathbf{1}_{\overline{\{-m, +m, \sigma_{pp}(H)\}}}(H).$$

As the eigenvalues of H can only accumulate in $\{-m, +m\}$, we have $\mathbf{1}_{\overline{\{-m, +m, \sigma_{pp}(H)\}}}(H) = \mathbf{1}^{pp}(H)$ and the result holds.

Now, let us prove (5.11). We only treat the case $t \rightarrow +\infty$ and characterize P^+ . Using (5.10), by a density argument, it is enough to show

$$s - \lim_{t \rightarrow +\infty} e^{itH} \left(J(\mathcal{V}) - J\left(\frac{x}{t}\right) \right) f\left(\frac{x}{t}\right) \chi(H) e^{-itH} = 0,$$

for any $J, f \in C_0^\infty(\mathbb{R}^3)$ such that $f = 0$ in a neighbourhood of 0 and $\chi \in C_0^\infty(\mathbb{R})$ satisfying $\text{supp } \chi \cap \{-m, +m, \sigma_{pp}(H)\} = \emptyset$. By the Helffer-Sjöstrand formula (A.32), we have

$$J(\mathcal{V}) - J\left(\frac{x}{t}\right) = B_1\left(\mathcal{V} - \frac{x}{t}\right) + B_2(t),$$

where B_1 bounded and $B_2(t) \in O(t^{-1})$ since $[\mathcal{V}^j, x_k]$ bounded for any j, k . Then we have to prove that the following limit vanishes

$$s - \lim_{t \rightarrow +\infty} e^{itH} B_1 \left(\mathcal{V} - \frac{x}{t} \right) f \left(\frac{x}{t} \right) \chi(H) e^{-itH}.$$

But this follows from Proposition 4.5. □

5.2. Spectrum of P^\pm .

This section is devoted to the analysis of the spectrum of P^\pm which corresponds to the physically relevant information given by the asymptotic velocity. We have already seen that

$$\mathbf{1}_{\{0\}}(P^\pm) = \mathbf{1}^{pp}(H),$$

which means that the states of zero asymptotic velocity coincide with the bound states of H . Now we are interested in the *scattering states* that is to say the states in $\mathcal{H}^c = \mathbf{1}^c(H)\mathcal{H}$ and we would like to classify them according to their asymptotic behaviours. We prove the proposition

PROPOSITION 5.2. — *Let P^\pm be the asymptotic velocity defined in Theorem 5.1. Then*

$$\sigma(P^\pm) = \overline{B}(0, 1).$$

Proof. — As usual, we only give the proof for P^+ . Let us first prove that

$$\sigma(P^+) \subset \overline{B}(0, 1).$$

Let $\xi_0 \in \mathbb{R}^3 \setminus \overline{B}(0, 1)$ and let $\chi \in C_0^\infty(\mathbb{R}^3)$ such that $\chi = 1$ in a neighbourhood of ξ_0 and $\text{supp } \chi \cap \overline{B}(0, 1) = \emptyset$. We have to show that

$$\chi(P^+) = 0.$$

But by Proposition 5.1, we have

$$\chi(P^+) = s - \lim_{t \rightarrow +\infty} e^{itH} \chi(\mathcal{V}) e^{-itH}.$$

Now it is easy to see that the spectrum of \mathcal{V} is equal to $\overline{B}(0, 1)$. Hence, $\chi(\mathcal{V}) = 0$ and $\chi(P^+) = 0$ which concludes the first part of the proof. Let us prove the reverse inclusion.

Let $\xi_0 \in \overline{B}(0, 1)$, $\xi_0 \neq 0$ and $|\xi_0| = r_2 > r_1 > r_0 > 0$. Let $g \in C_0^\infty(B(\xi_0, r_0))$ such that $g(\xi_0) \neq 0$. Here $B(\xi_0, r_0)$ denotes the ball

centered at ξ_0 with radius r_0 . We want to show here that $g(P^+) \neq 0$. Let $J \in C^\infty(\mathbb{R})$ such that $J = 1$ on $(-\infty, r_1]$, $J = 0$ on $[r_2 - \frac{r_2 - r_1}{2}, +\infty)$ and $j = -J' \geq 0$. Clearly J and g satisfy the following relations

$$(5.13) \quad \bullet \quad J(|\xi - \xi_0|)g(\xi) = g(\xi).$$

$$(5.14) \quad \bullet \quad j(|\xi - \xi_0|)|\xi - \xi_0| \geq r_1 j(|\xi - \xi_0|).$$

$$(5.15) \quad \bullet \quad g(\xi)|\xi - \xi_0| \leq r_0 g(\xi).$$

We define the propagation observable

$$\phi_a(t) = J\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right)g^2(\mathcal{V}_a)J\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right),$$

where $\mathcal{V}_a = \frac{1}{2}(pH^{-1} + H^{-1}p)$ and by Proposition 5.1 and Lemma 5.1, we have

$$(5.16) \quad g^2(P^+) = s - \lim_{t \rightarrow +\infty} e^{itH} \phi_a(t) e^{-itH}.$$

Let us compute its Heisenberg derivative.

$$\begin{aligned} \mathbf{D}\phi_a(t) &= \frac{1}{t}j\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right)\frac{\frac{x_{nw}}{t} - \xi_0}{\left|\frac{x_{nw}}{t} - \xi_0\right|} \cdot (\xi_0 - \mathcal{V})g^2(\mathcal{V}_a)J\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right) + hc \\ &\quad + \frac{1}{t}j\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right)\left|\frac{x_{nw}}{t} - \xi_0\right|g^2(\mathcal{V}_a)J\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right) + hc \\ &\quad + J\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right)i[H, g^2(\mathcal{V}_a)]J\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right) + O(t^{-2}). \end{aligned}$$

Now we commute the different terms in the last expression using the following result we shall prove later

$$(5.17) \quad \left[g(\mathcal{V}_a), f\left(\frac{x_{nw}}{t}\right) \right] \in O(t^{-1}).$$

We obtain

$$\begin{aligned} \mathbf{D}\phi_a(t) &= \frac{1}{t}(Jj)^{\frac{1}{2}}\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right)\frac{\frac{x_{nw}}{t} - \xi_0}{\left|\frac{x_{nw}}{t} - \xi_0\right|} \cdot (\xi_0 - \mathcal{V})g^2(\mathcal{V}_a)(Jj)^{\frac{1}{2}}\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right) + hc \\ &\quad + \frac{1}{t}g(\mathcal{V}_a)j\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right)\left|\frac{x_{nw}}{t} - \xi_0\right|J\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right)g(\mathcal{V}_a) + hc \\ &\quad + J\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right)i[H, g^2(\mathcal{V}_a)]J\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right) + O(t^{-2}). \end{aligned}$$

In the first two terms, we can replace \mathcal{V}_a by \mathcal{V} by Lemma 5.1 again. Then by (5.14) and (5.15), we get

$$\begin{aligned} \mathbf{D}\phi_a(t) &\geq \frac{1}{t}(r_1 - r_0)g(\mathcal{V})(Jj)\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right)g(\mathcal{V}) \\ &\quad + J\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right)i[H, g^2(\mathcal{V}_a)]J\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right) + O(t^{-2}). \end{aligned}$$

Moreover we claim and prove later that

$$(5.18) \quad J\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right) i[H, g^2(\mathcal{V}_a)] J\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right) \in O(t^{-2}).$$

This implies

$$\mathbf{D}\phi_a(t) \geq \frac{1}{t}(r_1 - r_0)g(\mathcal{V})(Jj)\left(\left|\frac{x_{nw}}{t} - \xi_0\right|\right)g(\mathcal{V}) + R(t),$$

where $R(t) \in L^1(dt)$. As $g, J, j \geq 0$ and $r_1 - r_0 > 0$, we get

$$(5.19) \quad \mathbf{D}\phi(t) \geq R(t).$$

We now conclude the proof. By (5.16) and (5.19), we have

$$(5.20) \quad \begin{aligned} g^2(P^+) &= e^{it_0H} \phi(t_0) e^{-it_0H} + \int_{t_0}^{+\infty} e^{itH} \mathbf{D}\phi(t) e^{-itH} dt, \\ &\geq e^{it_0H} \phi(t_0) e^{-it_0H} - \int_{t_0}^{+\infty} \|R(t)\| dt, \end{aligned}$$

and allowing t_0 to tend to infinity, we can make the integral in (5.20) as small as we want. We claim that

$$\lim_{t_0 \rightarrow +\infty} \|e^{it_0H} \phi_a(t_0) e^{-it_0H}\|,$$

exists and is non-zero. Indeed first observe that using Lemma 5.1, we have

$$\lim_{t_0 \rightarrow +\infty} \|e^{it_0H} \phi_a(t_0) e^{-it_0H}\| = \lim_{t_0 \rightarrow +\infty} \|e^{it_0H} \phi(t_0) e^{-it_0H}\|,$$

where $\phi(t) = J(|\frac{x}{t} - \xi_0|)g^2(\mathcal{V})J(|\frac{x}{t} - \xi_0|)$. Then we have

$$\begin{aligned} \|e^{it_0H} \phi(t_0) e^{-it_0H}\| &= \|e^{it_0\xi_0 \cdot p} \phi(t_0) e^{-it_0\xi_0 \cdot p}\|, \\ &= \|J\left(\frac{|x|}{t_0}\right)g^2(\mathcal{V})J\left(\frac{|x|}{t_0}\right)\|. \end{aligned}$$

Thus, $\lim_{t_0 \rightarrow +\infty} \|e^{it_0H} \phi(t_0) e^{-it_0H}\| = \|g^2(\mathcal{V})\| \neq 0$ and the result holds.

It remains to prove (5.17) and (5.18). First observe that we can replace $f(\frac{x_{nw}}{t})$ by $f(\frac{x}{t})$ in (5.17) using Lemma 5.1. Now using the formula (A.2), we have

$$(5.21) \quad \left[g(\mathcal{V}_a), f\left(\frac{x}{t}\right)\right] = \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\mathbb{R}^3} \widehat{\nabla}g(\xi) \int_0^1 e^{i(1-s)\xi\mathcal{V}_a} \left[\mathcal{V}_a, f\left(\frac{x}{t}\right)\right] e^{is\xi\mathcal{V}_a} ds d\xi,$$

and the commutator in the right-hand-side of (5.21) is equal to $\frac{1}{2t}\{pH^{-1}i\Gamma \cdot \nabla f(\frac{x}{t})H^{-1} - i\nabla f(\frac{x}{t})H^{-1} + hc\}$ which clearly belongs to $O(t^{-1})$.

Let us show (5.18). Since $[H, \mathcal{V}_a]$ is bounded and \mathcal{V}_a bounded, we can use the Helffer-Sjöstrand formula (A.29) to estimate $i[H, g^2(\mathcal{V}_a)]$. If we

denote $J(|\frac{x_{nw}}{t} - \xi_0|)$ by $J_{\xi_0}(\frac{x_{nw}}{t})$ we obtain

$$\begin{aligned}
 (5.22) \quad & J_{\xi_0}\left(\frac{x_{nw}}{t}\right) i[H, g^2(\mathcal{V}_a)] J_{\xi_0}\left(\frac{x_{nw}}{t}\right) \\
 &= \frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{g}^2(z) \left(\sum_{l=1}^3 J_{\xi_0}\left(\frac{x_{nw}}{t}\right) \left(\prod_{k_1=1}^l R_{k_1} \right) \frac{-1}{2} (\partial_l V(x) H^{-1} + hc) \right. \\
 & \quad \left. \left(\prod_{k_2=l}^3 R_{k_2} \right) J_{\xi_0}\left(\frac{x_{nw}}{t}\right) \right) dz \wedge d\bar{z},
 \end{aligned}$$

where $R_k = (z_k - \mathcal{V}_a^k)^{-1}$. Next we commute the operators $J_{\xi_0}(\frac{x_{nw}}{t})$ with $\prod_{k_1=1}^l R_{k_1}$ and $\prod_{k_2=l}^3 R_{k_2}$ under the integral (5.22). Furthermore note that, since $[R_k, x_{nw}]$ and $[[R_k, x_{nw}], x_{nw}]$ are bounded for any k , the Helffer-Sjöstrand formula (A.31) gives

$$\left[J_{\xi_0}\left(\frac{x_{nw}}{t}\right), \prod_{k_1=1}^l R_{k_1} \right] = \frac{1}{t} \left[x_{nw}, \prod_{k_1=1}^l R_{k_1} \right] \nabla J_{\xi_0}\left(\frac{x_{nw}}{t}\right) + O(t^{-2}),$$

and

$$\left[\prod_{k_2=1}^l R_{k_2}, J_{\xi_0}\left(\frac{x_{nw}}{t}\right) \right] = \frac{1}{t} \nabla J_{\xi_0}\left(\frac{x_{nw}}{t}\right) \left[x_{nw}, \prod_{k_2=1}^l R_{k_2} \right] + O(t^{-2}).$$

Now using that $J_{\xi_0}(\frac{x_{nw}}{t}) \nabla V(x)$ and $\nabla J_{\xi_0}(\frac{x_{nw}}{t}) \cdot \nabla V(x)$ belong to $O(t^{-2})$ by Lemma 5.1, we conclude that (5.22) also belongs to $O(t^{-2})$ which ends the proof of the proposition. □

6. Wave operators.

We turn now to the construction of wave operators for the massive Dirac operator H in order to describe precisely the asymptotic behaviour of the field when t goes to infinity. As is well known, the presence of a long-range potential $V(x)$ prevents us from taking e^{-itH_0} for the comparison dynamics. In our case $V \in S^{-1}(\mathbb{R}^3)$, we can use the ideas of Dollard and Velo [9] and define the following comparison dynamics denoted by $U_0(t)$

$$(6.1) \quad U_0(t) = e^{-itH_0} T \left(e^{-i \int_0^t (V_1(s\mathcal{V}) + mH_0^{-1} V_2(s\mathcal{V})) ds} \right),$$

where T denotes time ordering. In this definition of the Dollard modification, we add a phase (formally) denoted $e^{-iX(t)}$ to e^{-itH_0} . This phase must be chosen in such a way that the standard Cook method applies

(see Lemma 4.1). Thus it must satisfy two rules. First, it must commute with e^{-itH_0} . Second, the operator $H - H_0 - X'(t)$ must be “short-range”. We see from this last assumption that a good candidate for X would be $X'(t) = V(x)$ but it does not fulfill the first assumption. As it is suggested by the microlocal velocity estimates, we can approach (asymptotically) the position operator x by $t\mathcal{V}$ which commutes with e^{-itH_0} and define

$$X'(t) = V_1(t\mathcal{V}) + \Gamma^0 V_2(t\mathcal{V}).$$

Unfortunately, the matrix Γ^0 which appears in the potential also does not commute with e^{-itH_0} and this is why we replaced it in the definition of $U_0(t)$ by the operator mH_0^{-1} using ideas of Thaller [32]. Precisely, we use the following lemma

LEMMA 6.1. — *Let H_0 be the free Dirac operator. Let us denote $G = \Gamma^0 - mH_0^{-1}$ and*

$$E(t) = \int_0^t e^{isH_0} G e^{-isH_0} ds.$$

Then $E(t)$ is a bounded operator uniformly in t . As a consequence, we have $\lim_{t \rightarrow \infty} \frac{1}{t} \|E(t)\| = 0$.

Proof. — First, remark that G anticommutes with H_0 . Therefore, we have

$$e^{isH_0} G e^{-isH_0} = e^{i2sH_0} G, \quad \forall s \in \mathbb{R},$$

and we obtain by integration the following explicit form for $E(t)$

$$E(t) = (e^{i2tH_0} - 1)(2iH_0)^{-1}G.$$

Thus, $E(t)$ is uniformly bounded, in operator norm, with respect to t . \square

Then we define $X'(t) = V_1(t\mathcal{V}) + mH_0^{-1}V_2(t\mathcal{V})$ which leads to the definition (6.1) of the Dollard modification. The main result of this part is given by the theorem.

THEOREM 6.1. — *The wave operators defined by*

$$(6.2) \quad \Omega^\pm := s - \lim_{t \rightarrow \pm\infty} e^{itH} U_0(t),$$

$$(6.3) \quad \tilde{\Omega}^\pm := s - \lim_{t \rightarrow \pm\infty} U_0^*(t) e^{-itH} \mathbf{1}_{\mathbb{R}^3 \setminus \{0\}}(P^\pm),$$

exist in \mathcal{H} . Furthermore, we have $\tilde{\Omega}^\pm \Omega^\pm = \mathbf{1}_{\mathcal{H}}$, $\Omega^\pm \tilde{\Omega}^\pm = \mathbf{1}^c(H)$, $(\Omega^\pm)^ = \tilde{\Omega}^\pm$ and \mathcal{V} and P^\pm satisfy the intertwining relation*

$$(6.4) \quad (\Omega^\pm) \mathcal{V} (\Omega^\pm)^* = P^\pm.$$

At last, we have

$$(6.5) \quad (\Omega^\pm)H_0(\Omega^\pm)^* = H\mathbf{1}^c(H).$$

Note that in the definition of the wave operator (6.3), we make a crucial use of the characterization (5.10) of the projection onto the continuous spectrum of H i.e.

$$\mathbf{1}^c(H) = \mathbf{1}_{\mathbb{R}^3 \setminus \{0\}}(P^\pm).$$

Proof. — For the proof of this theorem, we shall follow the strategy used in [8] and appeal to some results for time-dependent Dirac hamiltonians given in Appendix B. This fully time-dependent approach avoids the use of a *limiting absorption principle* as well as a detailed study of the resolvent $(H - z)^{-1}$ and related estimates. Here, the central objects are time-dependent observables such as $J(\frac{x}{t})$ where J has a compact support, and propagation estimates obtained in Section 4. Let us now explain this strategy for the proof of (6.2). First, remark that by a density argument it is enough to prove the existence of

$$(6.6) \quad s - \lim_{t \rightarrow \pm\infty} e^{itH}U_0(t)\chi(H_0)\mathbf{1}_\Theta(\mathcal{V}),$$

where $\chi \in C_0^\infty(\mathbb{R})$ such that $\text{supp } \chi \cap \{-m, +m, \sigma_{pp}(H)\} = \emptyset$ and Θ denotes a compact subset of $\mathbb{R}^3 \setminus \{0\}$ such that the annulus $C(\frac{\epsilon_0(\chi)}{2}, 1)$ is a subset of Θ (remember that $\epsilon_0(\chi)$ is defined by the minimal velocity estimates, see Proposition 4.2). Now consider a function $J \in C_0^\infty(\mathbb{R}^3 \setminus \{0\})$ such that $J = 1$ on a neighbourhood of Θ . Let us associate to any function $f \in S^{-1}(\mathbb{R}^3)$ the time-dependent function

$$f_J(t, x) = f(x)J\left(\frac{x}{t}\right),$$

defined for $t \geq 1$. Such a function obviously satisfies the properties

- For any y in a neighbourhood of Θ ,

$$(6.7) \quad f(ty) = f_J(t, ty)$$

- For any $t \geq 1$ fixed, $x \rightarrow f_J(t, x) \in C_0^\infty(\mathbb{R}^3)$ and there is a constant M such that

$$\text{supp } f_J(t, \cdot) \subset B(0, Mt).$$

- The following estimates hold

$$(6.8) \quad \left| \partial_x^\alpha f_J(t, x) \right| \leq C \langle t \rangle^{-1-|\alpha|}, \quad \forall \alpha \in \mathbb{N}^3,$$

$$(6.9) \quad \left| \partial_t^k f_J(t, x) \right| \leq C \langle t \rangle^{-1-k}, \quad \forall k \in \mathbb{N}.$$

We introduce now some notations. We call *effective time-dependent potential* the potential $V_J(t, x) = V_{1,J}(t, x) + V_{2,J}(t, x)\Gamma^0$. We denote by $H_J(t)$ the time-dependent hamiltonian $H_0 + V_J(t, x)$ and by $U_J(t, s)$ the associated dynamics (see [8], Appendix B.3, Proposition B.3.6). We also denote by $U_{0,J}(t)$ the following time-dependent Dollard modification

$$U_{0,J}(t) = e^{-itH_0}T\left(e^{-i\int_0^t(V_{1,J}(s,s\mathcal{V})+mH_0^{-1}V_{2,J}(s,s\mathcal{V}))ds}\right),$$

We rewrite (6.6) as follows

$$s - \lim_{t \rightarrow \pm\infty} e^{itH}U_0(t)\chi(H_0)\mathbf{1}_\Theta(\mathcal{V}) = s - \lim_{t \rightarrow \pm\infty} e^{itH}\chi(H_0)U_J(t, 0)U_J(0, t)\mathbf{1}_\Theta(\mathcal{V})U_J(t, 0)U_J(0, t)U_{0,J}(t).$$

where we used the facts that $U_0(t)\mathbf{1}_\Theta(\mathcal{V}) = U_{0,J}(t)\mathbf{1}_\Theta(\mathcal{V}) = \mathbf{1}_\Theta(\mathcal{V})U_{0,J}(t)$ by (6.7) and that H_0 commutes with $U_0(t)$. Now assume the existence of the limits

$$\begin{aligned} & s - \lim_{t \rightarrow \pm\infty} U_J(0, t)U_{0,J}(t), \\ & s - \lim_{t \rightarrow \pm\infty} U_J(0, t)\mathbf{1}_\Theta(\mathcal{V})U_J(t, 0) =: \mathbf{1}_\Theta(\mathcal{V}_J^\pm), \\ & s - \lim_{t \rightarrow \pm\infty} e^{itH}\chi(H_0)U_J(t, 0)\mathbf{1}_\Theta(\mathcal{V}_J^\pm), \end{aligned}$$

then the limit (6.6) will exist by the chain rule. Moreover, the situation is completely symmetric for the proof of (6.3). Indeed by a density argument it is enough to prove the existence of

$$(6.10) \quad s - \lim_{t \rightarrow \pm\infty} U_0^*(t)e^{-itH}\mathbf{1}_\Theta(P^\pm)\chi(H),$$

for a compact subset Θ defined as above. But using the characterization (5.11) of the asymptotic velocity P^\pm , we see that

$$\begin{aligned} & s - \lim_{t \rightarrow \pm\infty} U_0^*(t)e^{-itH}\mathbf{1}_\Theta(P^\pm)\chi(H) \\ &= s - \lim_{t \rightarrow \pm\infty} U_0^*(t)\mathbf{1}_\Theta(\mathcal{V})e^{-itH}\mathbf{1}_\Theta(P^\pm)\chi(H), \\ &= s - \lim_{t \rightarrow \pm\infty} \mathbf{1}_\Theta(\mathcal{V})U_{0,J}^*(t)U_J(t, 0)U_J(0, t)e^{-itH}\mathbf{1}_\Theta(P^\pm)\chi(H), \end{aligned}$$

where we used $U_0^*(t)\mathbf{1}_\Theta(\mathcal{V}) = \mathbf{1}_\Theta(\mathcal{V})U_{0,J}^*(t)$ by (6.7). Therefore if we prove the existence of the limits

$$\begin{aligned} & s - \lim_{t \rightarrow \pm\infty} U_{0,J}^*(t)U_J(t, 0), \\ & s - \lim_{t \rightarrow \pm\infty} U_J(0, t)e^{-itH}\mathbf{1}_\Theta(P^\pm)\chi(H), \end{aligned}$$

then the limit (6.10) will exist by the chain rule.

If we summarize the previous discussion, we see that we can divide the proof of Theorem 6.1 into three steps. First, for time-dependent

Dirac operators of the following form $H_J(t) = H_0 + V(t, x)$, we have to define the asymptotic velocity \mathcal{V}_J^\pm . This is done in Appendix B where we also obtain propagation estimates for time-dependent Hamiltonians (see Propositions B.1 and B.2). Next, we prove the existence and asymptotic completeness of wave operators for such hamiltonians. Exactly, we prove the lemma

LEMMA 6.2. — *The limits*

$$(6.11) \quad s - \lim_{t \rightarrow \pm\infty} U_J(0, t)U_{0,J}(t),$$

$$(6.12) \quad s - \lim_{t \rightarrow \pm\infty} U_{0,J}^*(t)U_J(t, 0),$$

exist.

For the last step of the proof, we have to make the link between time-dependent and time-independent Hamiltonians. Precisely we show

LEMMA 6.3. — *There exist the limits*

$$(6.13) \quad s - \lim_{t \rightarrow \pm\infty} e^{itH} \chi(H_0)U_J(t, 0)\mathbf{1}_\Theta(\mathcal{V}_J^\pm),$$

$$(6.14) \quad s - \lim_{t \rightarrow \pm\infty} U_J(0, t)e^{-itH} \mathbf{1}_\Theta(P^\pm)\chi(H).$$

Proof (of Lemma 6.2). — Since the proofs are identical, we only treat the case $t \rightarrow +\infty$ for (6.12). The basic tool to prove Lemma 6.2 will be the Helffer-Sjöstrand formula with several variables presented in Appendix A and Cook’s method (Lemma 4.1). Let $\psi \in \mathcal{D}$ where \mathcal{D} is a dense subset of \mathcal{H} that we shall define precisely later. Let us compute the Heisenberg derivative of the expression $U_{0,J}^*(t)U_J(t, 0)\psi$. We obtain

$$\begin{aligned} \frac{d}{dt}U_{0,J}^*(t)U_J(t, 0)\psi &= U_{0,J}^*(t)i\{H_0 + V_J(t, t\mathcal{V}) - H_J(t)\}U_J(t, 0)\psi, \\ &= U_{0,J}^*(t)i\{(V_{1,J}(t, t\mathcal{V}) - V_{1,J}(t, x)) + \Gamma^0(V_{2,J}(t, t\mathcal{V}) \\ &\quad - V_{2,J}(t, x)) + (mH_0^{-1} - \Gamma^0)V_{2,J}(t, t\mathcal{V})\}U_J(t, 0)\psi, \\ &= I_1(t) + I_2(t) + I_3(t). \end{aligned}$$

Let us prove that $I_1(t) = U_{0,J}^*(t)i(V_{1,J}(t, t\mathcal{V}) - V_{1,J}(t, x))U_J(t, 0)\psi$ belongs to $L^1(dt)$. Since the different commutators between the components of x and \mathcal{V} are bounded i.e.

$$[x_k, \mathcal{V}_l] = iH_0^{-1}\delta_{kl} - ip_lH_0^{-1}\Gamma^kH_0^{-1} \in B(\mathcal{H}),$$

we can apply the Helffer-Sjöstrand formula (A.33) and write $I_1(t)$ as

$$I_1(t) = U_{0,J}^*(t)C_1(t)(x - t\mathcal{V})U_J(t, 0)\psi + O(t^{-2}),$$

where $C_1(t)$ is a bounded operator satisfying $C_1(t) \leq Ct^{-2}$. Now observe that if we prove

$$(6.15) \quad (x - t\mathcal{V})U_J(t, 0)\langle x \rangle^{-1} \in O(t^\mu),$$

with $0 < \mu < 1$ then $I_1(t)$ will belong to $L^1(dt)$. Here, we chose $\mathcal{D} = D(\langle x \rangle)$. Unfortunately, for the same technical reasons as in the proof of microlocal velocity estimates, it is not obvious to show (6.15) in such a form. Actually, we shall prove

$$(x_{nw} - t\mathcal{V}_a(t))U_J(t, 0)\langle x \rangle^{-1} \in O(t^\mu),$$

with $0 < \mu < 1$. Indeed, as x and x_{nw} are equal up to a bounded operator Z , we can replace x by x_{nw} in the previous expression without any change. Moreover, we also have to approach the classical velocity operator \mathcal{V} by $\mathcal{V}_a(t) = \frac{1}{2}(pH_J^{-1}(t) + H_J^{-1}(t)p)$. Note that for t large enough, the operator $H_J(t)$ is always invertible and since

$$(6.16) \quad \mathcal{V} - \mathcal{V}_a(t) = \frac{1}{2}pH_0^{-1}V_J(t, x)H_J^{-1}(t) + hc \in O(t^{-1}),$$

we can also replace \mathcal{V} by $\mathcal{V}_a(t)$ in the previous expression. Finally, to prove (6.15), it is enough to show that

$$L(t) := \frac{1}{t^\mu} \frac{d}{dt} (U_J(0, t)(x_{nw} - t\mathcal{V}_a(t))U_J(t, 0)\langle x \rangle^{-1}) \in L^1((1, +\infty), dt).$$

But we have

$$\begin{aligned} L(t) &= \frac{1}{t^\mu} U_J(0, t) \left\{ i[H_J(t), x_{nw} - t\mathcal{V}_a(t)] - \mathcal{V}_a(t) - t \frac{d}{dt} (\mathcal{V}_a(t)) \right\} U_J(t, 0)\langle x \rangle^{-1}, \\ &= \frac{1}{t^\mu} U_J(0, t) \left\{ (\mathcal{V} - \mathcal{V}_a(t)) + i[V_J(t, x), Z] + it[H_J(t), \mathcal{V}_a(t)] \right. \\ &\quad \left. - t \frac{d}{dt} (\mathcal{V}_a(t)) \right\} U_J(t, 0)\langle x \rangle^{-1}. \end{aligned}$$

It remains to show that all the terms between brackets belong to $O(t^{-1})$ for $t \geq 1$. It is obvious for $(\mathcal{V} - \mathcal{V}_a(t))$ and $[V_J(t, x), Z]$ since Z is bounded. Furthermore,

$$(6.17) \quad i[H_J(t), \mathcal{V}_a(t)] = -\frac{1}{2}(\nabla V_J(t, x)H_J^{-1}(t) + H_J(t)^{-1}\nabla V_J(t, x)) \in O(t^{-2}),$$

since $\nabla V_J(t, x) \in O(t^{-2})$ by (6.8). For the last term, we use the fact that

$$(6.18) \quad \begin{aligned} &\frac{d}{dt} (\mathcal{V}_a(t)) \\ &= \frac{1}{2}(pH_J^{-1}(t)\partial_t V_J(t, x)H_J^{-1}(t) + H_J^{-1}(t)\partial_t V_J(t, x)H_J^{-1}(t)p) \in O(t^{-2}), \end{aligned}$$

since $\partial_t V_J(t, x) \in O(t^{-2})$ by (6.9). This ends the proof for $I_1(t)$. The proof for $I_2(t)$ is identical.

Now let us treat the term $I_3(t)$. Let us denote concisely

$$T(e^{-i \int_0^t (V_{1,J}(s, s\mathcal{V}) + mH_0^{-1}V_{2,J}(s, s\mathcal{V})) ds})$$

by $e^{-iX(t)}$. To apply Cook's Lemma, it is enough to show that

$$(6.19) \quad I_{s,u} := \left\| \int_s^u e^{iX(t)} (\partial_t E(t)) e^{itH_0} V_{2,J}(t, t\mathcal{V}) U_J(t, 0) \psi dt \right\|,$$

tends to 0 when $s, u \rightarrow \infty$. From the definition of $E(t)$, it is clear that it anticommutes with H_0 and with \mathcal{V} . Thus we can write $e^{-iX(t)} (\partial_t E(t)) = (\partial_t E(t)) e^{-i\tilde{X}(t)}$ where

$$e^{-i\tilde{X}(t)} = T(e^{-i \int_0^t (V_{1,J}(s, -s\mathcal{V}) - mH_0^{-1}V_{2,J}(s, -s\mathcal{V})) ds}).$$

By an integration by part in (6.19), we obtain

$$\begin{aligned} I_{s,u} \leq & \left\| E(u) e^{-i\tilde{X}(u)} e^{iuH_0} V_{2,J}(u, u\mathcal{V}) U_J(u, 0) \psi \right\| \\ & + \left\| E(s) e^{-i\tilde{X}(s)} e^{isH_0} V_{2,J}(s, s\mathcal{V}) U_J(s, 0) \psi \right\| \\ & + \left\| \int_s^u E(t) \partial_t (e^{-i\tilde{X}(t)} e^{itH_0} V_{2,J}(t, t\mathcal{V}) U_J(t, 0) \psi) dt \right\|. \end{aligned}$$

Using $V_{2,J}(t, t\mathcal{V}) \in O(t^{-1})$ and Lemma 6.1, the first two terms tend to 0 as $s, u \rightarrow \infty$. If we compute the derivative in the last term, we find

$$\begin{aligned} & \partial_t (e^{-i\tilde{X}(t)} e^{itH_0} V_{2,J}(t, t\mathcal{V}) U_J(t, 0) \psi) \\ &= -i(V_{1,J}(t, -t\mathcal{V}) - mH_0^{-1}V_{2,J}(t, -t\mathcal{V})) e^{-i\tilde{X}(t)} e^{itH_0} V_{2,J}(t, t\mathcal{V}) U_J(t, 0) \psi \\ & \quad + e^{-i\tilde{X}(t)} e^{itH_0} (\partial_t V_{2,J}(t, t\mathcal{V}) + \mathcal{V} \nabla V_{2,J}(t, t\mathcal{V})) U_J(t, 0) \psi \\ & \quad - ie^{-i\tilde{X}(t)} e^{itH_0} V_{2,J}(t, t\mathcal{V}) (V_{1,J}(t, x) + V_{2,J}(t, x) \Gamma^0) U_J(t, 0) \psi. \end{aligned}$$

All these terms belong to $O(t^{-2})$ by (6.8) and (6.9). Since $E(t)$ is bounded, the last integral also tends to 0 which concludes the proof of the lemma. \square

Proof (of Lemma 6.3). — Since the proofs are identical, we only treat the case $t \rightarrow +\infty$. Let us consider a function $g \in C_0^\infty(\Theta)$ such that $g = 1$ on the annulus $C(\epsilon_0(\chi), 1)$. It is enough to prove the existence of (6.13) replacing $\mathbf{1}_\Theta(\mathcal{V}_J^+)$ by $g(\mathcal{V}_J^+)$. Let us define two other functions g_1 and g_2 belonging to $C_0^\infty(\Theta)$ such that $g_1 g = g$ and $g_2 g_1 = g_1$. Then using Proposition B.3, we have

$$\begin{aligned} g(\mathcal{V}_J^+) &= s - \lim_{t \rightarrow +\infty} U_J(0, t) g_1 \left(\frac{x}{t} \right) g(\mathcal{V}) U_J(t, 0), \\ &= s - \lim_{t \rightarrow +\infty} U_J(0, t) g_2 \left(\frac{x}{t} \right) g_1 \left(\frac{x}{t} \right) g_2 \left(\frac{x}{t} \right) g(\mathcal{V}) U_J(t, 0). \end{aligned}$$

Now we introduce the operator $M(t) = g_1(\frac{x}{t}) + (\mathcal{V} - \frac{x}{t}) \cdot \nabla g_1(\frac{x}{t})$ and using Proposition B.4, we have

$$g(\mathcal{V}_J^+) = s - \lim_{t \rightarrow +\infty} U_J(0, t) g_2\left(\frac{x}{t}\right) M(t) g_2\left(\frac{x}{t}\right) g(\mathcal{V}) U_J(t, 0).$$

For technical reasons, we have to approach the operator $M(t)$ by $M_a(t) = g_1(\frac{x_{nw}}{t}) + (\mathcal{V}_a - \frac{x_{nw}}{t}) \cdot \nabla g_1(\frac{x_{nw}}{t})$ where $\mathcal{V}_a = \frac{1}{2}(pH^{-1} + H^{-1}p)$ and also the operator $g(\mathcal{V})$ by $g(\mathcal{V}_a(t))$ where $\mathcal{V}_a(t)$ defined as in Lemma 6.2. Using the Helffer-Sjöstrand formula and (6.16), we have

$$(6.20) \quad g(\mathcal{V}) - g(\mathcal{V}_a(t)) \in O(t^{-1}).$$

Hence, by the same arguments as in the proof of Proposition 4.5, we obtain

$$g(\mathcal{V}_J^+) = s - \lim_{t \rightarrow +\infty} U_J(0, t) g_2\left(\frac{x}{t}\right) M_a(t) g_2\left(\frac{x}{t}\right) g(\mathcal{V}_a(t)) U_J(t, 0).$$

Then we define the propagation observable

$$\phi_a(t) = \chi(H) g_2\left(\frac{x}{t}\right) M_a(t) g_2\left(\frac{x}{t}\right) g(\mathcal{V}_a(t)),$$

and it is easy to see that

$$(6.13) = s - \lim_{t \rightarrow +\infty} e^{itH} \phi_a(t) U_J(t, 0).$$

Let us compute the time derivative of this quantity. We obtain

$$\begin{aligned} & \frac{d}{dt} \phi_a(t) + iH\phi_a(t) - i\phi_a(t)H_J(t) \\ (6.21) \quad &= -\frac{1}{t} \chi(H) \left(\nabla g_2\left(\frac{x}{t}\right) \frac{x}{t} M_a(t) g_2\left(\frac{x}{t}\right) + hc \right) g(\mathcal{V}_a(t)) \\ (6.22) \quad &- \frac{1}{t} \chi(H) g_2\left(\frac{x}{t}\right) \left(\mathcal{V}_a - \frac{x_{nw}}{t} \right) \nabla^2 g_1\left(\frac{x_{nw}}{t}\right) \frac{x_{nw}}{t} g_2\left(\frac{x}{t}\right) g(\mathcal{V}_a(t)) \\ (6.23) \quad &+ \chi(H) g_2\left(\frac{x}{t}\right) M_a(t) g_2\left(\frac{x}{t}\right) \frac{d}{dt} (g(\mathcal{V}_a(t))) \\ (6.24) \quad &+ \chi(H) \left(i \left[H_0, g_2\left(\frac{x}{t}\right) \right] M_a(t) g_2\left(\frac{x}{t}\right) + hc \right) g(\mathcal{V}_a(t)) \\ (6.25) \quad &+ \chi(H) g_2\left(\frac{x}{t}\right) i (H M_a(t) - M_a(t) H_J(t)) g_2\left(\frac{x}{t}\right) g(\mathcal{V}_a(t)) \\ (6.26) \quad &+ \chi(H) g_2\left(\frac{x}{t}\right) M_a(t) g_2\left(\frac{x}{t}\right) i [H_J(t), g(\mathcal{V}_a(t))]. \end{aligned}$$

Observing that $i[H_0, g_2(\frac{x}{t})] = \frac{1}{t} \Gamma \cdot \nabla g_2(\frac{x}{t})$, the terms (6.21) and (6.24) can be written after commutation operations and using (6.20) as

$$\frac{1}{t} \chi(H) \eta\left(\frac{x}{t}\right) B(t) \eta\left(\frac{x}{t}\right) g(\mathcal{V}) + O(t^{-2}),$$

where $B(t)$ is a uniformly bounded operator in t and $\eta \in C_0^\infty(\mathbb{R}^3)$ such that $\text{supp } \eta \cap C(\epsilon_0(\chi), 1) = \emptyset$ and $\text{supp } \eta \cap \text{supp } g = \emptyset$. Thus these terms are integrable along the evolution using Propositions 4.2, 4.4 and B.3.

Moreover, combining the Helffer-Sjöstrand formula and using (6.17) and (6.18), the following estimates hold

$$(6.27) \quad i[H_J(t), g(\mathcal{V}_a(t))] \in O(t^{-2}),$$

$$(6.28) \quad \frac{d}{dt}g(\mathcal{V}_a(t)) \in O(t^{-2}).$$

Therefore, the terms (6.23) and (6.26) belong to $O(t^{-2})$ and are integrable in norm.

Now note that $V_J(t, x)g_2(\frac{x}{t}) = V(x)g_2(\frac{x}{t})$. Hence we have

$$g_2\left(\frac{x}{t}\right)i(HM_a(t) - M_a(t)H_J(t))g_2\left(\frac{x}{t}\right) = g_2\left(\frac{x}{t}\right)i[H, M_a(t)]g_2\left(\frac{x}{t}\right)$$

and using Lemma 5.2, the term (6.25) is equal to

$$\begin{aligned} \frac{1}{t}\chi(H)g_2\left(\frac{x}{t}\right)\left(\mathcal{V}_a - \frac{x_{nw}}{t}\right)\nabla^2g_1\left(\frac{x_{nw}}{t}\right)\mathcal{V}g_2\left(\frac{x}{t}\right)g(\mathcal{V}_a(t)) \\ + \chi(H)g_2\left(\frac{x}{t}\right)i[H, \mathcal{V}_a]\nabla g_1\left(\frac{x_{nw}}{t}\right)g_2\left(\frac{x}{t}\right)g(\mathcal{V}_a(t)) + O(t^{-2}). \end{aligned}$$

Repeating the proof of Proposition 4.5, the sum of (6.22) and (6.25) is equal to

$$\frac{1}{t}\chi(H)g_2\left(\frac{x}{t}\right)\left(\mathcal{V} - \frac{x}{t}\right)\nabla^2g_1\left(\frac{x}{t}\right)\left(\mathcal{V} - \frac{x}{t}\right)g_2\left(\frac{x}{t}\right)g(\mathcal{V}_a(t)) + O(t^{-2}).$$

Eventually, using (6.20) once again, we obtain

$$\begin{aligned} \frac{d}{dt}\phi_a(t) + iH\phi_a(t) - i\phi_a(t)H_J(t) \\ = \frac{1}{t}\chi(H)g_2\left(\frac{x}{t}\right)\left(\mathcal{V} - \frac{x}{t}\right)\nabla^2g_1\left(\frac{x}{t}\right)\left(\mathcal{V} - \frac{x}{t}\right)g_2\left(\frac{x}{t}\right)g(\mathcal{V}) + L^1(dt) + O(t^{-2}). \end{aligned}$$

Thus using Propositions 4.5 and B.4, this term is integrable along the evolution and we conclude the proof of (6.13) by Lemma 4.1.

The proof of (6.14) is essentially the same as the previous one. We omit it. □

Therefore, we have constructed the Dollard-modified wave operators Ω^\pm and $\tilde{\Omega}^\pm$. The fact that $(\Omega^\pm)^* = \tilde{\Omega}^\pm$ follows from [8], Lemma B.5.1. It remains to prove the intertwining relations (6.4) and (6.5). Using Proposition 5.1, we see that

$$\begin{aligned} P^\pm \mathbf{1}_{\mathbb{R}^3 \setminus \{0\}}(P^\pm) &= s - \lim_{t \rightarrow \pm\infty} e^{itH} \mathcal{V} e^{-itH} \mathbf{1}_{\mathbb{R}^3 \setminus \{0\}}(P^\pm), \\ &= s - \lim_{t \rightarrow \pm\infty} e^{itH} U_0(t) \mathcal{V} U_0^*(t) e^{-itH} \mathbf{1}_{\mathbb{R}^3 \setminus \{0\}}(P^\pm), \\ &= \Omega^\pm \mathcal{V} (\Omega^\pm)^*, \end{aligned}$$

which proves (6.4). Now (6.5) is equivalent to

$$s - \lim_{t \rightarrow \pm\infty} e^{itH} (H - H_0) e^{-itH} \mathbf{1}_{\mathbb{R}^3 \setminus \{0\}}(P^\pm) = 0.$$

But using Theorem 5.1, it is enough to show that

$$s - \lim_{t \rightarrow \pm\infty} e^{itH} V(x) J\left(\frac{x}{t}\right) e^{-itH} = 0,$$

for any $J \in C_0^\infty(\mathbb{R}^3 \setminus \{0\})$. As $V \in S^{-1}(\mathbb{R}^3)$, $V(x)J(\frac{x}{t}) \in O(t^{-1})$ and the result holds. \square

A. Functions of selfadjoint operators and applications.

In this appendix we give some useful formulae to study functions of selfadjoint operators $f(A)$ and commutators of the following form $[T, f(A)]$. Here, A and T denote two (possibly vectors of) commuting selfadjoint operators acting on a Hilbert space \mathcal{H} . We first consider the case of a function $f \in L^1(\mathbb{R}^3)$; in this case, the Fourier transform is enough to obtain the formulae. For smooth functions $f \in C^\infty(\mathbb{R}^3)$ which are not necessarily integrable, we shall need the Helffer-Sjöstrand formula presented Section A.2.

A.1. Fourier transform.

General setting. — Let A a vector of commuting selfadjoint operators in \mathcal{H} and let us denote by $W(\xi) = \{e^{-i\xi A}\}$ the induced unitary representation of \mathbb{R}^3 in \mathcal{H} . We need the function space $\mathcal{F}^{1,N}(\mathbb{R}^3) = \{f \in L^1(\mathbb{R}^3) / (1 + |\xi|^2)^{\frac{N}{2}} \hat{f}(\xi) \in L^1(\mathbb{R}^3)\}$ for $N \in \mathbb{N}$. Equivalently we have $\mathcal{F}^{1,N}(\mathbb{R}^3) = \{f \in L^1(\mathbb{R}^3) / \widehat{\nabla^k f} \in L^1(\mathbb{R}^3), k = 1, \dots, N\}$. As a first case we consider a bounded operator T in \mathcal{H} and a function $f \in W^{1,1}(\mathbb{R}^3)$. We now define the class $C^1(A; \mathcal{H})$ of regular bounded operators with respect to A by

$$C^1(A; \mathcal{H}) = \{T \in \mathcal{B}(\mathcal{H}) / s \longrightarrow e^{is\xi A} T e^{-is\xi A} \in C^1(\mathbb{R}_s; \mathcal{B}(\mathcal{H}))\}.$$

Then we have the following equivalence (see [1], Proposition 5.2)

$$T \in C^1(A; \mathcal{H}) \iff [T, A] \in \mathcal{B}(\mathcal{H}).$$

In particular, for T a bounded operator belonging to $C^1(A; \mathcal{H})$, we can write

$$\begin{aligned} [T, e^{i\xi A}] &= \int_0^1 \frac{d}{ds} \left(e^{i(1-s)\xi A} T e^{is\xi A} \right) ds, \\ (A.1) \qquad &= (i\xi) \int_0^1 e^{i(1-s)\xi A} [T, A] e^{is\xi A} ds. \end{aligned}$$

Now assume that $f \in \mathcal{F}^{1,1}(\mathbb{R}^3)$. Using the Fourier transform of f denoted by \hat{f} and (A.1), we have

$$\begin{aligned} i[T, f(A)] &= \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\mathbb{R}^3} \hat{f}(\xi) i[T, e^{i\xi A}] d\xi, \\ (A.2) \qquad &= \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\mathbb{R}^3} \widehat{\nabla} f(\xi) \int_0^1 e^{i(1-s)\xi A} i[T, A] e^{is\xi A} ds d\xi, \end{aligned}$$

where the right-hand-sides in the two equalities of (A.2) make sense on $\mathcal{B}(\mathcal{H})$ since $\hat{f} \in L^1(\mathbb{R}^3)$ and $\widehat{\nabla} f \in L^1(\mathbb{R}^3)$ by hypothesis and $[T, A]$ bounded on \mathcal{H} .

Now we consider the case of an unbounded operator T in \mathcal{H} . Let us introduce some definitions and basic results. Let H be another selfadjoint operator in a Hilbert space \mathcal{H} . Assume that the family of unitary operators $\{W(\xi)\}_{\xi \in \mathbb{R}^3}$ leaves invariant the domain $D(H)$ of H . We denote by \mathcal{G}^1 this domain and by \mathcal{G}^s , $0 \leq s \leq 1$, the interpolation space between $\mathcal{G}^0 = \mathcal{H}$ and $\mathcal{G}^1 = D(H)$. We also denote by $\mathcal{G}^{-s} = (\mathcal{G}^s)^*$ the dual Hilbert space of \mathcal{G}^s . We make the usual identification $\mathcal{H}^* = \mathcal{H}$ and thus we have

$$\mathcal{G}^s \hookrightarrow \mathcal{G}^t \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{G}^{-t} \hookrightarrow \mathcal{G}^{-s}, \quad 0 \leq t \leq s \leq 1.$$

At last we denote by $\mathcal{B}(\mathcal{G}^s, \mathcal{G}^t)$ the set of bounded operators between \mathcal{G}^s and \mathcal{G}^t . Then we have the following result (see [4], Proposition 1).

PROPOSITION A.1. — *Let H, T two selfadjoint operators on \mathcal{H} satisfying $T \in \mathcal{B}(\mathcal{G}^1, \mathcal{G}^{-1})$. Let A a vector of commuting selfadjoint operators on \mathcal{H} . Let $-1 \leq t \leq s \leq 1$. Assume that $e^{i\xi A} \mathcal{G}^1 \subset \mathcal{G}^1$ and $[T, A] \in \mathcal{B}(\mathcal{G}^s, \mathcal{G}^t)$. Then one has*

$$(A.3) \qquad i[T, e^{i\xi A}] = i\xi \int_0^1 e^{i(1-s)\xi A} i[T, A] e^{is\xi A} ds,$$

where the right-hand-side is well defined as a strong integral on $\mathcal{B}(\mathcal{G}^s, \mathcal{G}^t)$ i.e. the integral is strongly convergent. As a direct application, we have for all $f \in \mathcal{F}^{1,1}(\mathbb{R}^3)$

$$(A.4) \qquad i[T, f(A)] = \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\mathbb{R}^3} \widehat{\nabla} f(\xi) \int_0^1 e^{i(1-s)\xi A} i[T, A] e^{is\xi A} ds d\xi.$$

Application (Commutator expansion). — Commutator expansions of two selfadjoint operators T, A are formulae which relate the commutator $[T, f(A)]$ with the successive commutators $ad_A^k(T)$ defined by recurrence by $ad_A^1(T) = [T, A]$ and for any $k \geq 1$, $ad_A^k(T) = [ad_A^{k-1}(T), A]$.

PROPOSITION A.2. — *Let H, T two selfadjoint operators on \mathcal{H} such that $T \in \mathcal{B}(\mathcal{G}^1, \mathcal{G}^{-1})$. Let A a vector of commuting selfadjoint operators on \mathcal{H} . Let $f \in \mathcal{F}^{1, N+1}(\mathbb{R}^3)$. Assume that*

$$(H1) \quad e^{i\xi A} \mathcal{G}^1 \subset \mathcal{G}^1;$$

$$(H2) \quad ad_A^k(T) \in \mathcal{B}(\mathcal{H}) \text{ for any } k \leq N + 1.$$

Then we have

$$(A.5) \quad [T, f(A)] = \sum_{k=0}^N \frac{\nabla^k f(A)}{k!} ad_A^k(T) + R_N,$$

where $\|R_N\| \leq c_N(f) \|ad_A^{N+1}(T)\|$. If we replace the operator A by $\frac{A}{t}$ we have the following useful consequence of (A.5)

$$(A.6) \quad \left[T, f\left(\frac{A}{t}\right) \right] = \sum_{k=0}^N \frac{\nabla^k f\left(\frac{A}{t}\right)}{t^k k!} ad_A^k(T) + O(t^{-N-1}).$$

Proof. — In formula (A.4), we commute $[T, A]$ with $e^{is\xi A}$ to obtain

$$[T, f(A)] = \nabla f(A) [T, A] + \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\mathbb{R}^3} \widehat{\nabla} f(\xi) \int_0^1 e^{i(1-s)\xi A} [[T, A], e^{is\xi A}] ds d\xi.$$

Now we use formula (A.3) in this last integral. We repeat the procedure N times to obtain (A.5). \square

The assumption on the stability of the domain $D(H)$ under the action of the unitary group $e^{i\xi A}$ is not easy to prove in general. We already saw that, if $[H, A] \in \mathcal{B}(D(H), \mathcal{H})$ then it suffices to show that $(H - z)^{-1} D(A) \subset D(A)$ for $z \notin \sigma(H)$ (see Lemma 3.4). Actually, when the commutator between $[H, A]$ is bounded, we have the following equivalences

LEMMA A.1. — *Let H, A two selfadjoint operators on \mathcal{H} . Assume that $i[H, A]$ defined as a quadratic form on $D(H) \cap D(A)$ extends to a bounded operator on \mathcal{H} . Then the following assertions are equivalent*

- (i) $(H - z)^{-1} D(A) \subset D(A)$,
- (ii) $e^{i\xi A} D(H) \subset D(H)$,

(iii) $(A - z)^{-1}D(H) \subset D(H)$,

(iv) $e^{isH}D(A) \subset D(A)$.

In particular, if H or A is bounded on \mathcal{H} then the four assertions are automatically satisfied.

Proof. — According to Lemma 3.4, we only need to prove that (ii) implies (iii) and (iv) implies (i). These two implications follow from the same argument. Assume (ii) and $[H, A]$ bounded. Let $\psi \in D(H)$. We have to show that $\|H(A - z)^{-1}\psi\| < \infty$. For we use the resolvent formula

$$H(A - z)^{-1}\psi = i \int_0^\infty e^{izt} H e^{-itA} \psi dt, \quad \text{Im } z > 0.$$

Then we commute H and e^{-itA} under the integral and we use formula (A.3). We obtain

$$\begin{aligned} H(A - z)^{-1}\psi &= i \int_0^\infty e^{izt} e^{-itA} H \psi dt \\ &\quad + i \int_0^\infty e^{izt} (-it) \int_0^1 e^{-i(1-s)tA} [H, A] e^{-istA} \psi ds dt. \end{aligned}$$

Finally one has

$$\|H(A - z)^{-1}\psi\| \leq \|H\psi\| \int_0^\infty e^{-\text{Im } zt} dt + C \|\psi\| \int_0^\infty e^{-\text{Im } zt} |t| dt,$$

since $[H, A]$ is bounded. Both integrals converge then the result holds. \square

We now give some examples needed in the previous sections. H is the massive Dirac operator defined in section 2. In this case, the domain \mathcal{G}^1 of H is equal to $[H^1(\mathbb{R}^3)]^4$.

Example 1. — Let $T = H$ and A the locally conjugate operator defined in section 3. Then the assumptions of Proposition A.1 are obviously satisfied since $e^{i\xi A} \mathcal{G}^1 \subset \mathcal{G}^1$ and $i[H, A] \in \mathcal{B}(\mathcal{H})$. Then we have

$$(A.7) \quad i[H, f(A)] = \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\mathbb{R}^3} \widehat{\nabla} f(\xi) \int_0^1 e^{i(1-s)\xi A} (\mathcal{V}^2 + K) e^{is\xi A} ds d\xi,$$

where K is compact on \mathcal{H} . The right hand side is a bounded operator on \mathcal{H} .

Example 2. — Let $T = H$ and let A be $\mathcal{V}_a = \frac{1}{2}(pH^{-1} + H^{-1}p)$ the approached classical velocity operator defined in section 6. Clearly the commutator $[H, \mathcal{V}_a] = \frac{i}{2}(\nabla V H^{-1} + H^{-1} \nabla V)$ is bounded. Then $e^{i\xi \mathcal{V}_a} \mathcal{G}^1 \subset$

\mathcal{G}^1 is satisfied by Lemma A.1 since \mathcal{V}_a is also bounded. Thus we have

$$(A.8) \quad i[H, f(\mathcal{V}_a)] = \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\mathbb{R}^3} \widehat{\nabla} f(\xi) \int_0^1 e^{i(1-s)\xi \mathcal{V}_a} \frac{i}{2} (\nabla V(x) H^{-1} + H^{-1} \nabla V(x)) e^{is\xi \mathcal{V}_a} ds d\xi.$$

The right hand side is a bounded operator on \mathcal{H} .

Example 3. — Let $T = H$ and let $A = x_{nw}$ the Newton-Wigner operator defined in Section 2. Again we have to check that $e^{i\xi x_{nw}} \mathcal{G}^1 \subset \mathcal{G}^1$. First observe that $[H, x_{nw}] = \mathcal{V} + [V, Z]$ is bounded on \mathcal{H} . Then it is equivalent to show that $(H - z)^{-1} D(x_{nw}) \subset D(x_{nw})$ by Lemma A.1. But $D(x_{nw}) = D(x)$ and the result follows from the domain invariance property proved in Section 2. Finally we have

$$(A.9) \quad i[H, f(x_{nw})] = \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\mathbb{R}^3} \widehat{\nabla} f(\xi) \int_0^1 e^{i(1-s)\xi x_{nw}} \frac{i}{2} (\mathcal{V} + i[V(x), Z]) e^{is\xi x_{nw}} ds d\xi.$$

The right hand side is a bounded operator on \mathcal{H} .

A.2. Helffer-Sjöstrand formula.

In this appendix, we give a brief review of the Helffer-Sjöstrand formula which first appeared in [21] and which is useful to estimate functions of selfadjoint operators $f(A)$ for functions f which are not integrable. We follow the presentation given by Davies in [6] and we state a version needed in Section 6.

First, consider a function f belonging to the class of smooth real-functions

$$S^{-\rho}(\mathbb{R}) = \{f \in C^\infty(\mathbb{R}) : |f^{(k)}(x)| \leq C \langle x \rangle^{-\rho-k}, \forall k \in \mathbb{N}\}, \quad \rho > 0.$$

We call *almost-analytic extension* of f and we denote it by \tilde{f} the following function

$$(A.10) \quad \tilde{f}(z) = \tilde{f}(x + iy) := \left\{ \sum_{k=0}^n f^{(k)}(x) \frac{(iy)^k}{k!} \right\} \tau\left(\frac{y}{\langle x \rangle}\right),$$

where n is an integer larger than 1 and $\tau \in C_0^\infty(\mathbb{R})$ such that $\tau(x) = 1$ for $|x| \leq 1$ and $\tau(x) = 0$ for $|x| \geq 2$. This function satisfies the properties

(see [6])

$$(A.11) \quad \bullet \quad \tilde{f}|_{\mathbb{R}} = f,$$

$$(A.12) \quad \bullet \quad \text{supp } \tilde{f} \subset \{x + iy : |y| \leq C\langle x \rangle\},$$

$$(A.13) \quad \bullet \quad |\partial_{\bar{z}} \tilde{f}(z)| \leq C\langle x \rangle^{-\rho-1-n} |y|^n,$$

$$(A.14) \quad \bullet \quad f(x) = \frac{i}{2\pi} \int_{\mathbb{C}} \partial_{\bar{z}} \tilde{f}(z) (z - x)^{-1} dz \wedge d\bar{z}.$$

Now, given a self-adjoint operator A in a Hilbert space \mathcal{H} , we can define the operator $f(A)$ as follows

$$(A.15) \quad f(A) = \frac{i}{2\pi} \int_{\mathbb{C}} \partial_{\bar{z}} \tilde{f}(z) (z - A)^{-1} dz \wedge d\bar{z},$$

where the integral converges in operator norm in \mathcal{H} by (A.13) and since $\rho > 0$. Moreover, we stress the fact that the operator $f(A)$ does not depend of the choices of $n \geq 1$ and τ (see Lemma 2.2.4 in [6]).

For the applications, we use this formula for time-dependent potentials of the following form. Let $J \in C_0^\infty(\mathbb{R} \setminus \{0\})$. Given a function $f \in S^{-\rho}(\mathbb{R})$, we denote by $f(t, x)$ the time-dependent function defined by

$$f(t, x) = f(x)J\left(\frac{x}{t}\right).$$

With respect to the variable x , this function belongs to $C_0^\infty(K_t) \subset S^{-\rho}(\mathbb{R})$ where K_t denotes a compact subset of \mathbb{R} such that $K_t \subset [-Mt, Mt]$, for M large enough and independent of t . Thus we can define the almost-analytic extension of f with respect to x by

$$(A.16) \quad \tilde{f}(t, z) := \left\{ \sum_{k=0}^n f^{(k)}(t, x) \frac{(iy)^k}{k!} \right\} \tau\left(\frac{y}{\langle x \rangle}\right).$$

This function satisfies the following properties

$$(A.17) \quad \bullet \quad \text{supp } \tilde{f} \subset [-Mt, Mt]^2,$$

$$(A.18) \quad \bullet \quad |\partial_{\bar{z}} \tilde{f}(z)| \leq Ct^{-\rho-1-n} |y|^n,$$

$$(A.19) \quad \bullet \quad f(t, x) = \frac{i}{2\pi} \int_{\mathbb{C}} \partial_{\bar{z}} \tilde{f}(t, z) (z - x)^{-1} dz \wedge d\bar{z}.$$

We can define time-dependent functions of self-adjoint operators A as previously by

$$(A.20) \quad f(t, A) = \frac{i}{2\pi} \int_{\mathbb{C}} \partial_{\bar{z}} \tilde{f}(t, z) (z - A)^{-1} dz \wedge d\bar{z}.$$

Now we are interested in extending this last formula to functions f of several variables. Let us consider f belonging to the class of functions

$$S^{-\rho}(\mathbb{R}^3) = \{f \in C^\infty(\mathbb{R}^3) : |\partial_x^\alpha f(x)| \leq C\langle x \rangle^{-\rho-|\alpha|}, \forall \alpha \in \mathbb{N}^3\}, \quad \rho > 0.$$

We can define the Helffer-Sjöstrand formula for this function with respect to the first variable. If $x = (x_1, x_2, x_3)$, we have

$$\tilde{f}(x_1 + iy_1, x_2, x_3) = \left\{ \sum_{\alpha_1=0}^{n_1} \partial_{x_1}^{\alpha_1} f(x) \frac{(iy_1)^{\alpha_1}}{\alpha_1!} \right\} \tau\left(\frac{y_1}{\langle x_1 \rangle}\right).$$

Using (A.13), we see that the functions $x_2 \rightarrow \tilde{f}(x_1 + iy_1, x_2, x_3)$ (resp. $x_3 \rightarrow \tilde{f}(x_1 + iy_1, x_2, x_3)$) also belong to the class $S^{-\rho}(\mathbb{R})$ uniformly with respect to the other variables. That is to say we have

$$|\partial_{x_j}^{\alpha_j} \tilde{f}(x_1 + iy_1, x_2, x_3)| \leq C \langle x \rangle^{-\rho}, \quad \forall \alpha_j \in \mathbb{N}, \quad j = 2, 3,$$

and the constant C does not depend on the variables x_1, y_1, x_2 (resp. x_1, y_1, x_3). Thus by induction we define the complete almost-analytic extension

$$\begin{aligned} \tilde{f}(z_1, z_2, z_3) = \left\{ \sum_{\alpha \leq \beta} \partial_x^\alpha f(x) \frac{(iy_1)^{\alpha_1}}{\alpha_1!} \frac{(iy_2)^{\alpha_2}}{\alpha_2!} \frac{(iy_3)^{\alpha_3}}{\alpha_3!} \right\} \\ \tau\left(\frac{y_1}{\langle x_1 \rangle}\right) \tau\left(\frac{y_2}{\langle x_2 \rangle}\right) \tau\left(\frac{y_3}{\langle x_3 \rangle}\right), \end{aligned}$$

where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, $\beta = (n_1, n_2, n_3)$ and $n_j \geq 1$, for all $j = 1, 2, 3$. This function satisfies the properties.

(A.21) • $\text{supp } \tilde{f} \subset \{(x, y) \in \mathbb{R}^6 / |y_j| \leq C \langle x_j \rangle, \quad j = 1, 2, 3\},$

(A.22) • $|\partial_{\bar{z}} \tilde{f}(z)| \leq C \langle x \rangle^{-\rho-3-|\alpha|} |y_1|^{n_1} |y_2|^{n_2} |y_3|^{n_3},$

(A.23) • $f(x) = \frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{f}(z) (z_1 - x_1)^{-1} (z_2 - x_2)^{-1} (z_3 - x_3)^{-1} dz \wedge d\bar{z}.$

Here, we denoted $z = (z_1, z_2, z_3) = (x_1 + iy_1, x_2 + iy_2, x_3 + iy_3)$. Moreover, $\partial_{\bar{z}}$ stands for $\partial_{\bar{z}_1} \partial_{\bar{z}_2} \partial_{\bar{z}_3}$ and $dz \wedge d\bar{z}$ for $(dz_1 \wedge d\bar{z}_1) \wedge (dz_2 \wedge d\bar{z}_2) \wedge (dz_3 \wedge d\bar{z}_3)$. The formulae (A.22) and (A.23) follow from (A.13) and (A.14).

Eventually, if A denotes a vector of commuting self-adjoint operators in \mathcal{H} , we can define $f(A)$ as follows

(A.24) $f(A) = \frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{f}(z) (z_1 - A_1)^{-1} (z_2 - A_2)^{-1} (z_3 - A_3)^{-1} dz \wedge d\bar{z}.$

Of course, we have a time dependent version of this last formula. Let us consider a function $J \in C_0^\infty(\mathbb{R}^3 \setminus \{0\})$. Define the time-dependent function $f(t, x) = f(x)J(\frac{x}{t})$ as previously. Thus the almost-analytic extension

$$\begin{aligned} \tilde{f}(t, z_1, z_2, z_3) = \left\{ \sum_{\alpha} \partial_x^\alpha f(t, x) \frac{(iy_1)^{\alpha_1}}{\alpha_1!} \frac{(iy_2)^{\alpha_2}}{\alpha_2!} \frac{(iy_3)^{\alpha_3}}{\alpha_3!} \right\} \\ \tau\left(\frac{y_1}{\langle x_1 \rangle}\right) \tau\left(\frac{y_2}{\langle x_2 \rangle}\right) \tau\left(\frac{y_3}{\langle x_3 \rangle}\right), \end{aligned}$$

satisfies the properties

$$(A.25) \bullet \text{supp } \tilde{f} \subset [-Mt, Mt]_{z_1}^2 \times [-Mt, Mt]_{z_2}^2 \times [-Mt, Mt]_{z_3}^2,$$

$$(A.26) \bullet |\partial_{\bar{z}} \tilde{f}(t, z)| \leq Ct^{-\rho-3-|\alpha|} |y_1|^{\alpha_1} |y_2|^{\alpha_2} |y_3|^{\alpha_3},$$

$$(A.27) \bullet f(t, x) = \frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{f}(t, z) (z_1 - x_1)^{-1} (z_2 - x_2)^{-1} (z_3 - x_3)^{-1} dz \wedge d\bar{z}.$$

Given A a vector of commuting selfadjoint operators on \mathcal{H} , we define

$$(A.28) \quad f(t, A) = \frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{f}(t, z) (z_1 - A_1)^{-1} (z_2 - A_2)^{-1} (z_3 - A_3)^{-1} dz \wedge d\bar{z}.$$

Before to give commutator expansion formula, let us make the following observation. The assumption $f \in S^{-\rho}(\mathbb{R}^3)$ with $\rho > 0$ is only needed to ensure the convergence of the integral in operator norm. Actually, formulae (A.15), (A.20), (A.24), (A.28) hold if we assume $\rho \in \mathbb{R}$ and the almost-analytic extensions satisfy the same properties. When $\rho \leq 0$, the integrals converge for the strong convergence.

Application 1 (Commutator expansion). — Let A a vector of commuting selfadjoint operators on \mathcal{H} and T selfadjoint on \mathcal{H} . Let $f \in S^\rho(\mathbb{R}^3)$ with $\rho \in \mathbb{R}$. Assume that

$$(H3) \quad A \in C^1(T).$$

$$(H4) \quad ad_A^k(T) \in \mathcal{B}(\mathcal{H}), \quad k = 1, 2.$$

Then we have

$$[T, f(A)] = \frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{f}(z) [T, R_1 R_2 R_3] dz \wedge d\bar{z},$$

where $R_j = (z_j - A_j)^{-1}$. The assumption (H3) allows us to expand the commutator under the integral and one obtains

$$(A.29) \quad [T, f(A)] = \frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{f}(z) \left(\sum_{l=1}^3 \left(\prod_{k_1=1}^l R_{k_1} \right) [T, A_l] \left(\prod_{k_2=l}^3 R_{k_2} \right) \right) dz \wedge d\bar{z}.$$

Provided $[T, A_j]$ bounded for $l = 1, 2, 3$, the integral in (A.29) converges in operator norm for $\rho < 1$ by (A.22). Now commuting $[T, A_l]$ with $\prod_{k_2=l}^3 R_{k_2}$ and noting that

$$\frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{f}(z) \left(\sum_{l=1}^3 \left(\prod_{k_1=1}^l R_{k_1} \right) \left(\prod_{k_2=l}^3 R_{k_2} \right) \right) dz \wedge d\bar{z} = \nabla f(A) \cdot [T, A],$$

we get

$$[T, f(A)] = \nabla f(A) \cdot [T, A] + \frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{f}(z) \left(\sum_{l=1}^3 \left(\prod_{k_1=1}^l R_{k_1} \right) \left[[T, A_l], \prod_{k_2=l}^3 R_{k_2} \right] \right) dz \wedge d\bar{z}.$$

Since $ad_A^2(T)$ bounded on \mathcal{H} , this last integral converges in norm of operator for $\rho < 2$. Eventually we have proven that for any $f \in S^\rho(\mathbb{R}^3)$ with $\rho < 2$,

$$(A.30) \quad [T, f(A)] = \nabla f(A) \cdot [T, A] + B,$$

where B bounded on \mathcal{H} .

In many cases we have to deal with functions of time-dependent Hamiltonians of the form $f(\frac{A}{t})$. Therefore under the same hypotheses on f, T, A , we have

$$(A.31) \quad \left[T, f\left(\frac{A}{t}\right) \right] = \frac{1}{t} \nabla f\left(\frac{A}{t}\right) \cdot [T, A] + O(t^{-2}).$$

Application 2. — Given two vectors of selfadjoint operators A and T on \mathcal{H} and a function f belonging to the space $S^\rho(\mathbb{R}^3)$, we would like to express the difference between $f(A)$ and $f(T)$ as the product of an operator C and $A - T$. We apply formula (A.24)

$$f(A) - f(T) = \frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{f}(z) (R_1^A R_2^A R_3^A - R_1^T R_2^T R_3^T) dz \wedge d\bar{z},$$

where $R_j^A = (z_j - A_j)^{-1}$ and $R_j^T = (z_j - T_j)^{-1}$. Using the resolvent identity $R_j^A - R_j^T = R_j^T (A_j - T_j) R_j^A$ which makes sense on $\mathcal{B}(\mathcal{H})$, one obtains

$$f(A) - f(T) = \frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{f}(z) \left(\sum_{l=1}^3 \left(\prod_{k_1=1}^l R_{k_1}^T \right) (A_l - T_l) \left(\prod_{k_2=l}^3 R_{k_2}^A \right) \right) dz \wedge d\bar{z}.$$

Now we want to commute $A_l - T_l$ with $\prod_{k_2=l}^3 R_{k_2}^A$ under the integral. Thus we have to assume that $A \in C^1(T)$. In this case, we get

$$(A.32) \quad f(A) - f(T) = C \cdot (A - T) + B,$$

where

$$C = \frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{f}(z) \left(\sum_{l=1}^3 \left(\prod_{k_1=1}^l R_{k_1}^T \right) \left(\prod_{k_2=l}^3 R_{k_2}^A \right) \right) dz \wedge d\bar{z},$$

is a bounded operator on \mathcal{H} if $\rho < 1$ according to (A.22). Moreover if we suppose $[T, A_j]$ bounded then

$$B = \frac{-i}{(2\pi)^3} \int_{\mathbb{C}^3} \partial_{\bar{z}} \tilde{f}(z) \left(\sum_{l=1}^3 \left(\prod_{k_1=1}^l R_{k_1}^T \right) \left[(A_l - T_l), \prod_{k_2=l}^3 R_{k_2}^A \right] \right) dz \wedge d\bar{z},$$

is bounded if $\rho < 2$ by (A.22) since $A \in C^1(T)$ implies $[T, R_j^A] = R_j^A [T, A_j] R_j^A$.

We end this application by giving a time-dependent version useful for Section 6. Given two self-adjoint operators A and T in a Hilbert space \mathcal{H} and given two functions $f \in S^\rho(\mathbb{R}^3)$ and $J \in C_0^\infty(\mathbb{R}^3)$, we want to express the difference between the functions of operators $f(t, A)$ and $f(t, tT)$ as the product of one operator $C(t)$ and $A - tT$. Moreover, we want to obtain good estimates of $C(t)$ with respect to t when t goes to infinity. Assume that $A \in C^1(T)$ and $[A, T]$ bounded on \mathcal{H} then using formula (A.32), we get

$$(A.33) \quad f(t, A) - f(t, tT) = C(t) \cdot (A - tT) + B(t).$$

From the exact expressions of $C(t)$ and $B(t)$, by (A.26) and (A.25), if we assume $\rho < 1$, we obtain the following estimates

$$\begin{aligned} C(t) &\in O(t^{\rho-1}), \\ B(t) &\in O(t^{\rho-1}). \end{aligned}$$

B. Time-dependent Dirac operator and asymptotic velocity.

In this appendix, we study time-dependent Dirac operators of the form

$$H(t) = H_0 + V(t, x),$$

where $V(t, x) = V_1(t, x) + V_2(t, x)\Gamma^0$ is the sum of a scalar and a matrix-valued time-dependent potentials. The main assumptions on the time decay of $V(t, x)$ will be

$$(B.1) \quad |\partial_t^k V(t, x)| \leq C \langle t \rangle^{-1-k}, \quad k \in \mathbb{N}$$

$$(B.2) \quad |\partial_x^\alpha V(t, x)| \leq C \langle t \rangle^{-1-|\alpha|}, \quad \forall \alpha \in \mathbb{N}^3.$$

For such Hamiltonians, it is possible to define an associated unitary dynamics (see [8], appendix B.3, Proposition B.3.6) which we will denote by $U(t, s)$ and which satisfies

- The map $(t, s) \longrightarrow U(t, s)$ is strongly continuous with values in unitary operators in \mathcal{H} such that

$$U(t, t) = 1, \quad U(t, u)U(u, s) = U(t, s).$$

- If we denote $B = (H_0^2 + 1)^{\frac{1}{2}}$, we have

$$\begin{aligned} \partial_s U(t, s)B^{-1} &= U(t, s)iH(s)B^{-1}, \\ \partial_t B^{-1}U(t, s) &= -iB^{-1}H(t)U(t, s). \end{aligned}$$

We wish to define the asymptotic velocity and to describe some of its properties. Let us first prove the proposition

PROPOSITION B.1. — *Under the previous assumptions, the limit*
 (B.3)
$$s - C_\infty - \lim_{t \rightarrow \pm\infty} U(0, t)\mathcal{V}U(t, 0) =: \mathcal{V}^\pm,$$

exists.

Proof. — By a density argument, it is enough to show that

$$\lim_{t \rightarrow \pm\infty} U(0, t)g(\mathcal{V})U(t, 0)\psi,$$

exists for any $\psi \in \mathcal{H}$ and any $g \in C_0^\infty(\mathbb{R}^3)$. Let us introduce the operator $\mathcal{V}_a(t) = \frac{1}{2}(pH(t)^{-1} + H(t)^{-1}p)$ as in Lemma 6.2. Using (6.20), it is enough to show the existence of $\lim_{t \rightarrow \pm\infty} U(0, t)g(\mathcal{V}_a(t))U(t, 0)\psi$. But we have

$$\frac{d}{dt}U(0, t)g(\mathcal{V}_a(t))U(t, 0)\psi = U(0, t)\left(\frac{d}{dt}g(\mathcal{V}_a(t)) + i[H(t), g(\mathcal{V}_a(t))]\right)U(t, 0)\psi.$$

By (6.27) and (6.28), this term is integrable in norm. Hence the result follows from Proposition 4.1. □

As in the case of time-independent Hamiltonians, we can give an alternative definition of \mathcal{V}^\pm in terms of the position observable. Exactly, we prove the following proposition

PROPOSITION B.2. — *The asymptotic velocity \mathcal{V}^\pm is characterized by*

$$(B.4) \quad \mathcal{V}^\pm = s - C_\infty - \lim_{t \rightarrow \pm\infty} U(0, t)\frac{x}{t}U(t, 0).$$

The first step is to obtain propagation estimates for solutions $U(t, 0)\psi$. The next proposition summarizes the large and minimal velocity estimates in this case as obtained for time-independent hamiltonians.

PROPOSITION B.3. — *Suppose that $j, g \in C_0^\infty(\mathbb{R}^3)$ and $\text{supp } j \cap \text{supp } g = \emptyset$. Then*

$$(B.5) \quad \int_1^\infty \left\| j\left(\frac{x}{t}\right)g(\mathcal{V})U(t, 0)\psi \right\|^2 \frac{dt}{t} \leq C\|\psi\|^2, \quad \forall \psi \in \mathcal{H}.$$

Furthermore, if $J \in C_0^\infty(\mathbb{R}^3)$ such that $J = 1$ on a neighbourhood of $\text{supp } g$, then

$$(B.6) \quad s - \lim_{t \rightarrow \pm\infty} U(0, t)J\left(\frac{x}{t}\right)g(\mathcal{V})U(t, 0) = g(\mathcal{V}^\pm).$$

Proof. — Assume first that $0 \notin \text{supp } g$. Since the intersection of the supports of j and g is empty, by a covering argument we may assume that there exists $v \in \mathbb{R}^3$, $v \neq 0$ such that

$$(B.7) \quad \text{supp } g \subset \{x : \langle v, x \rangle > \theta_2\},$$

$$(B.8) \quad \text{supp } j \subset \{x : \langle v, x \rangle < \theta_1\},$$

where $0 < \theta_1 < \theta_2$. Let us choose a function $\tilde{J} \in C^\infty(\mathbb{R})$ such that $\tilde{J}' \in C_0^\infty(\mathbb{R})$, $\tilde{J}'(x) = 0$ when $x \geq \theta_1$ and

$$(B.9) \quad \tilde{J}'(\langle v, x \rangle) \geq j^2(x),$$

Now we define $J(x) := \tilde{J}(\langle v, x \rangle)$ and the propagation observable

$$\phi(t) = g(\mathcal{V}_a(t))J\left(\frac{x_{nw}}{t}\right)g(\mathcal{V}_a(t)),$$

where $\mathcal{V}_a(t) = \frac{1}{2}(pH(t)^{-1} + H(t)^{-1}p)$. We compute its Heisenberg derivative using Lemma 5.2

$$\begin{aligned} \mathbf{D}\phi(t) &= \left(\frac{d}{dt}g(\mathcal{V}_a(t))\right)J\left(\frac{x_{nw}}{t}\right)g(\mathcal{V}_a(t)) + hc \\ &\quad + i[H(t), g(\mathcal{V}_a(t))]J\left(\frac{x_{nw}}{t}\right)g(\mathcal{V}_a(t)) + hc \\ &\quad + \frac{1}{t}g(\mathcal{V}_a(t))\left(\mathcal{V} - \frac{x_{nw}}{t}\right)\nabla J\left(\frac{x_{nw}}{t}\right)g(\mathcal{V}_a(t)) + O(t^{-2}). \end{aligned}$$

The first two terms are integrable in norm by (6.27) and (6.28). Moreover, we can replace the Newton-Wigner variable x_{nw} by x by Lemma 5.1 and also $g(\mathcal{V}_a(t))$ by $g(\mathcal{V})$ thanks to (6.20). Now we claim that there exists a constant C_0 strictly positive such that

$$\frac{1}{t}g(\mathcal{V})\left(\mathcal{V} - \frac{x}{t}\right)\nabla J\left(\frac{x}{t}\right)g(\mathcal{V}) \geq \frac{C_0}{t}g(\mathcal{V})j^2\left(\frac{x}{t}\right)g(\mathcal{V}).$$

Indeed, observe that if we commute certain terms in this last expression, we obtain, using (B.7), (B.8), (B.9) and the fact that $[\mathcal{V}, f(\frac{x}{t})] \in O(t^{-1})$

$$\begin{aligned} &\frac{1}{t}g(\mathcal{V})\left(\mathcal{V} - \frac{x}{t}\right)\nabla J\left(\frac{x}{t}\right)g(\mathcal{V}) \\ &= \frac{1}{t}g(\mathcal{V})\langle v, \mathcal{V} - \frac{x}{t} \rangle \tilde{J}'\left(\langle v, \frac{x}{t} \rangle\right)g(\mathcal{V}), \\ &\geq \frac{1}{t}\left(\tilde{J}'\left(\langle v, \frac{x}{t} \rangle\right)\right)^{\frac{1}{2}}g(\mathcal{V})\langle v, \mathcal{V} \rangle g(\mathcal{V})\left(\tilde{J}'\left(\langle v, \frac{x}{t} \rangle\right)\right)^{\frac{1}{2}} \\ &\quad - \frac{1}{t}g(\mathcal{V})\left(\tilde{J}'\left(\langle v, \frac{x}{t} \rangle\right)\right)^{\frac{1}{2}}\langle v, \frac{x}{t} \rangle\left(\tilde{J}'\left(\langle v, \frac{x}{t} \rangle\right)\right)^{\frac{1}{2}}g(\mathcal{V}) + O(t^{-2}), \\ &\geq \frac{1}{t}(\theta_2 - \theta_1)g(\mathcal{V})j^2\left(\frac{x}{t}\right)g(\mathcal{V}) + O(t^{-2}). \end{aligned}$$

The constant C_0 is strictly positive since $\theta_2 > \theta_1$. Eventually we have

$$\mathbf{D}\phi(t) \geq \frac{C_0}{t} g(\mathcal{V}) j^2 \left(\frac{x}{t}\right) g(\mathcal{V}) + O(t^{-2}).$$

Thus we can conclude the proof of (B.5) using Proposition 4.1.

If $0 \in \text{supp } g$ then one can find $v \in \mathbb{R}^3$ such that

$$\begin{aligned} \text{supp } j &\subset \{x : \langle v, x \rangle > \theta_2\}, \\ \text{supp } g &\subset \{x : \langle v, x \rangle < \theta_1\}, \end{aligned}$$

where $0 < \theta_1 < \theta_2$. Now we make the same computations with $-\mathbf{D}\phi(t)$ to get the result.

To show (B.6), we consider a function $J \in C^\infty(\mathbb{R}^3)$ such that $\nabla J \in C_0^\infty(\mathbb{R}^3)$ and $\text{supp } \nabla J \cap \text{supp } g = \emptyset$. We claim that the following limit exists and is equal to 0

$$(B.10) \quad s - \lim_{t \rightarrow \infty} U(0, t) J \left(\frac{x}{t}\right) g(\mathcal{V}) U(t, 0),$$

which proves (B.6). Let us denote $\phi(t) = J(\frac{x}{t})g(\mathcal{V}_a(t))$. Then, using (6.27), (6.28) and (6.20), we obtain

$$|(\psi, \mathbf{D}\phi(t)\psi)| \leq \frac{C}{t} \|\tilde{j}\left(\frac{x}{t}\right)\tilde{g}(\mathcal{V})\psi\|^2 + O(t^{-2}),$$

where $\tilde{j}, \tilde{g} \in C_0^\infty(\mathbb{R}^3)$ such that $\text{supp } \tilde{j} \cap \text{supp } \tilde{g} = \emptyset$ and $\tilde{j}\nabla J = \nabla J$ and $\tilde{g}g = g$. Thus the following limit

$$(B.11) \quad s - \lim_{t \rightarrow \infty} U(0, t)\phi(t)U(t, 0),$$

exists by Lemma 4.1 and (B.5). This implies that the limit (B.10) exists by (6.20). Now, assume that $J \in C_0^\infty(\mathbb{R}^3)$ and $\text{supp } J \cap \text{supp } g = \emptyset$. Then we also know that

$$\int_1^\infty \left\| J \left(\frac{x}{t}\right) g(\mathcal{V}) U(t, 0) \psi \right\|^2 \frac{dt}{t} < \infty, \forall \psi \in \mathcal{H}.$$

So in this case the limit (B.10) is zero. To conclude the proof, we need show that there is no propagation for large $\frac{x}{t}$. But this follows by the same limit procedure used in Proposition 4.4. We omit the details. \square

We prove now the “microlocal velocity estimate”.

PROPOSITION B.4. — *Suppose that $g, J \in C_0^\infty(\mathbb{R}^3)$ and $\text{supp } g \cap \text{supp } \nabla J = \emptyset$. Then*

$$(B.12) \quad \int_1^\infty \left\| \left(\frac{x}{t} - \mathcal{V}\right) J \left(\frac{x}{t}\right) g(\mathcal{V}) U(t, 0) \psi \right\|^2 \frac{dt}{t} < \|\psi\|^2, \forall \psi \in \mathcal{H}.$$

Moreover,

$$(B.13) \quad s - \lim_{t \rightarrow \infty} \left(\frac{x}{t} - \mathcal{V} \right) J \left(\frac{x}{t} \right) g(\mathcal{V}) U(t, 0) = 0.$$

Proof. — Let us define the following propagation observables

$$\phi_0(t) = g(\mathcal{V}) J \left(\frac{x}{t} \right) \left(\frac{x}{t} - \mathcal{V} \right)^2 J \left(\frac{x}{t} \right) g(\mathcal{V}),$$

and

$$\phi_a(t) = g(\mathcal{V}_a(t)) J \left(\frac{x}{t} \right) \left\{ \frac{x_{nw}^2}{t^2} - 2 \frac{A(t)}{t} + \mathcal{V}^2 \right\} J \left(\frac{x}{t} \right) g(\mathcal{V}_a(t)),$$

where $A(t) = \frac{1}{2}(x.pH^{-1}(t) + H^{-1}(t)p.x)$ which is well-defined for t large enough. By the same arguments as in Proposition 4.5 and using (6.20), we have $\phi_a(t) = \phi_0(t) + O(t^{-1})$. The Heisenberg derivative of $\phi_a(t)$ equals

$$\mathbf{D}\phi_a(t) = \frac{2}{t} g(\mathcal{V}) J \left(\frac{x}{t} \right) \left(\frac{x}{t} - \mathcal{V} \right)^2 J \left(\frac{x}{t} \right) g(\mathcal{V}) + O(t^{-2}).$$

Thus (B.12) holds by Proposition 4.1. To show (B.13), first observe that it is equivalent to prove that

$$(B.14) \quad s - \lim_{t \rightarrow \infty} U(0, t) \phi_0(t) U(t, 0) = 0.$$

But, by Lemma 4.1 and the previous computation of the Heisenberg derivative of $\phi_a(t)$, we know that the limit

$$s - \lim_{t \rightarrow \infty} U(0, t) \phi_a(t) U(t, 0),$$

exists. Hence, since $\phi_a(t) = \phi_0(t) + O(t^{-1})$, this proves the existence of the limit in (B.14). Moreover, $\phi_0(t) \geq 0$ and thus

$$0 \leq \int_1^\infty (\psi, U(0, t) \phi_0(t) U(t, 0) \psi) \frac{dt}{t} < \infty,$$

by (B.12). Therefore the limit (B.14) is zero. □

We finally give the proof of Proposition B.2. It is enough to show that for any $f, g, J \in C_0^\infty(\mathbb{R}^3)$ such that $J = 1$ on $\text{supp } g$,

$$s - \lim_{t \rightarrow \infty} U(0, t) \left(f \left(\frac{x}{t} \right) - f(\mathcal{V}) \right) J \left(\frac{x}{t} \right) g(\mathcal{V}) U(t, 0) = 0.$$

But we already saw in Proposition 5.1 that

$$f \left(\frac{x}{t} \right) - f(\mathcal{V}) = B \left(\frac{x}{t} - \mathcal{V} \right) + O(t^{-1}),$$

where B is a bounded operator. Thus we conclude the proof using Proposition B.4. □

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