Chapter 5

Scattering theory

In this chapter we introduce the basic tools of scattering theory. This theory deals with the unitary group generated by any self-adjoint operator and corresponds to a comparison theory. More precisely, if A and B are self-adjoint operators in a Hilbert space $\mathcal{H}$, and if the corresponding unitary groups are denoted by $\{U_t\}_{t\in\mathbb{R}}$ and $\{V_t\}_{t\in\mathbb{R}}$, then one typically considers the product operator $V_t^*U_t$ and study its behavior for large $|t|$. Understanding the limit $\lim_{t\to\pm\infty} V_t^*U_t$ in a suitable sense, provides many information on the relation between the operator A and B.

Scattering theory was first developed in close relation with physics. However, it is now a mathematical subject on its own, and new developments are currently taking place in a more interdisciplinary framework.

5.1 Evolution groups

Let A be a self-adjoint operator in a Hilbert space $\mathcal{H}$. The elements of the corresponding strongly continuous unitary group $\{U_t\}_{t\in\mathbb{R}}$ provided by Stone's theorem in Theorem 4.2.11 are often denoted by $U_t = \mathrm{e}^{-itA}$. This group is called *the evolution group* associated with A. Let us also recall that if $\{U_t\}_{t\in\mathbb{R}}$ is a strongly continuous unitary group, then its *generator* corresponds to the self-adjoint operator $\big(A, \mathsf{D}(A)\big)$ defined by

$$\mathsf{D}(A) := \Big\{f \in \mathcal{H} \mid \exists\, s - \lim_{t\to 0} \frac{1}{t}[U_t - 1]f\Big\}$$

and for $f \in \mathsf{D}(A)$ by $Af = s - \lim_{t\to0} \frac{i}{t}[U_t - 1]f$. Obviously, the relation $U_t = \mathrm{e}^{-itA}$ then holds, and the domain $\mathsf{D}(A)$ is left invariant by the action of U_t for any $t \in \mathbb{R}$.

Given a strongly continuous unitary group $\{U_t\}_{t\in\mathbb{R}}$ it is often not so simple to compute explicitly $\mathsf{D}(A)$. However, in applications one can often guess a smaller domain $\mathcal{D} \subset \mathcal{H}$ on which the computation of $s - \lim_{t\to0} \frac{1}{t}[U_t - 1]f$ is well-defined. The following statement provides a criterion for checking if the domain $\mathcal{D}$ is large enough for defining entirely the operator A.

Proposition 5.1.1 (Nelson's criterion)**.** *Let $\{U_t\}_{t\in\mathbb{R}}$ be a strongly continuous unitary group, and let A denotes its self-adjoint generator. Let $\mathcal{D}$ be a dense linear submanifold of $\mathcal{H}$ such that $\mathcal{D}$ is invariant under the action of U_t for any $t \in \mathbb{R}$ and such that $s - \lim_{t\to 0} \frac{1}{t}[U_t - 1]f$ has a limit for any $f \in \mathcal{D}$. Then A is essentially self-adjoint on $\mathcal{D}$.*

Proof. Let us denote by A_0 the restriction of A to $\mathcal{D}$. Since A is self-adjoint, A_0 is clearly symmetric. In order to show that A_0 is essentially self-adjoint, we shall use the criterion (ii) of Proposition 2.1.15. More precisely, A_0 is essentially self-adjoint if $\mathsf{Ran}(A_0 \pm i)$ are dense in $\mathcal{H}$, or equivalently if $\mathsf{Ker}(A_0^* \mp i) = \{0\}$. Note that we have also used Lemma 2.1.10 for the previous equivalence.

Let us show that $\mathsf{Ker}(A_0^* - i) = \{0\}$. For that purpose, assume that $h \in \mathsf{Ker}(A_0^* - i)$, *i.e.* $h \in \mathsf{D}(A_0^*)$ and $A_0^* h = ih$. For any $f \in \mathcal{D}$ one has

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle U_t f, h\rangle &= \langle -iAU_t f, h\rangle = i\langle A_0 U_t f, h\rangle \\ &= i\langle U_t f, A_0^* h\rangle = i\langle U_t f, ih\rangle = -\langle U_t f, h\rangle\end{aligned}$$

where the invariance of $\mathcal{D}$ under U_t has been used for the second equality. Thus if one sets $\phi(t) := \langle U_t f, h\rangle$ one gets the differential equation $\phi'(t) = -\phi(t)$, whose solution is $\phi(t) = \phi(0)\,\mathrm{e}^{-t}$. If $\phi(0) \neq 0$ it follows that $|\phi(t)| \to \infty$ as $t \to -\infty$ which is impossible since $|\phi(t)| \leq \|f\|\,\|h\|$. One deduces that $\phi(0) = 0$ which means that $\langle f, h\rangle = 0$. It follows that h is perpendicular to $\mathcal{D}$, but by density of $\mathcal{D}$ in $\mathcal{H}$ one concludes that $h = 0$. □

Remark 5.1.2. *Dealing with the group $\{\mathrm{e}^{-itA}\}_{t\in\mathbb{R}}$ let us provide two formulas which could also have been introduced in the previous chapter, namely*

$$(A - z)^{-1} = i\int_0^\infty \mathrm{e}^{izt}\,\mathrm{e}^{-itA}\,\mathrm{d}t, \qquad \textit{for } \Im(z) > 0\ , \tag{5.1}$$

$$(A - z)^{-1} = -i\int_{-\infty}^0 \mathrm{e}^{izt}\,\mathrm{e}^{-itA}\,\mathrm{d}t, \qquad \textit{for } \Im(z) < 0\ . \tag{5.2}$$

Since the map $t \mapsto \mathrm{e}^{izt}\,\mathrm{e}^{-itA}$ is strongly continuous and integrable in norm, the above integrals exist in the strong sense by Proposition 1.5.3. Their equality with the resolvent of A at z can be checked directly, as shown for example in the proof of [Amr, Prop. 5.1].

Let us now present a few examples of evolution groups and their corresponding self-adjoint generators.

Example 5.1.3. *In the Hilbert space $\mathcal{H} := L^2(\mathbb{R})$ we consider the* translation group, *namely $[U_t f](x) := f(x - t)$ for any $f \in \mathcal{H}$ and $x \in \mathbb{R}$. It is easily checked that $\{U_t\}_{t\in\mathbb{R}}$ defines a strongly continuous unitary group in $\mathcal{H}$. In addition, its self-adjoint generator can by computed on $C_c^\infty(\mathbb{R})$, according to Proposition 5.1.1. One then finds that the generator is $-i\frac{\mathrm{d}}{\mathrm{d}x}$, or in other words the operator D already considered in Chapter 3. Note that the operator D is indeed essentially self-adjoint on $C_c^\infty(\mathbb{R})$.*

Example 5.1.4. *In $\mathcal{H} := L^2(\mathbb{R}^d)$ we consider the* dilation group *acting on any $f \in \mathcal{H}$ by $[U_t f](x) = \mathrm{e}^{dt/2} f(\mathrm{e}^t x)$ for any $x \in \mathbb{R}^d$. It is also easily checked that $\{U_t\}_{t\in\mathbb{R}}$ defines a strongly continuous unitary group in $\mathcal{H}$. The self-adjoint generator of this group can by computed on the Schwartz space $\mathcal{S}(\mathbb{R}^d)$, according to Proposition 5.1.1. A direct computations shows that this generator A is given on $\mathcal{S}(\mathbb{R}^d)$ by the expression*

$$A = -\frac{1}{2}\sum_{j=1}^{d}(X_j D_j + D_j X_j) \equiv -\frac{1}{2}(X \cdot D + D \cdot X).$$

Example 5.1.5. *Consider the Hilbert space $\mathcal{H} := L^2(\mathbb{R}^d)$ and the Laplace operator $-\Delta = D^2$, as already introduced in equation (3.3). The unitary group generated by this operator has obviously a very simple expression once a Fourier transformation is performed, or more precisely $\big[\mathcal{F}\,\mathrm{e}^{-itD^2} f\big](\xi) = \mathrm{e}^{-it\xi^2}[\mathcal{F}f](\xi)$ for any $f \in \mathcal{H}$ and $\xi \in \mathbb{R}^d$. Without this Fourier transformation, this operator corresponds to the following integral operator:*

$$\big[\mathrm{e}^{-itD^2} f\big](x) = \frac{1}{(4\pi it)^{d/2}}\int_{\mathbb{R}^d} \mathrm{e}^{\frac{i|x-y|^2}{4t}} f(y)\mathrm{d}y$$

with the square root given by

$$\Big(\frac{4\pi it}{|4\pi it|}\Big)^{-n/2} = \begin{cases} \mathrm{e}^{-in\pi/4} & \text{if} \quad t > 0, \\ \mathrm{e}^{+in\pi/4} & \text{if} \quad t < 0. \end{cases}$$

Exercise 5.1.6. *Work on the details of the results presented in the previous three examples.*

Later on, we shall often have to compute the derivative with respect to t of the product of two unitary groups. Since the generators of these groups are often unbounded operators, some care is necessary. In the next Lemma, we provide some conditions in order to deal with the Leibnitz rule in this setting. The proof of this Lemma is provided for example in [Amr, Prop. 5.5]. Note that the first statement can even be used in the special case $B = \mathbf{1}$.

Lemma 5.1.7. *Let $\big(A, \mathsf{D}(A)\big)$ and $\big(B, \mathsf{D}(B)\big)$ be self-adjoint operators in a Hilbert space $\mathcal{H}$.*

(i) Let $C \in \mathscr{B}(\mathcal{H})$ be such that $C\mathsf{D}(B) \subset \mathsf{D}(A)$. Then for any $f \in \mathsf{D}(B)$ the map $t \mapsto \mathrm{e}^{itA}\, C\, \mathrm{e}^{-itB} f$ is strongly differentiable and

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{itA}\, C\, \mathrm{e}^{-itB} f = i\,\mathrm{e}^{itA}\big(AC - CB\big)\,\mathrm{e}^{-itB} f\ . \tag{5.3}$$

(ii) Let C be B-bounded and such that $C\mathsf{D}(B^2) \subset \mathsf{D}(A)$. Then for any $f \in \mathsf{D}(B^2)$ the map $t \mapsto \mathrm{e}^{itA}\, C\, \mathrm{e}^{-itB} f$ is strongly differentiable and its derivative is again given by (5.3).

In the next statements, we study the asymptotic behavior of different parts of the Hilbert space under the evolution group. First of all, we consider the absolutely continuous subspace.

Proposition 5.1.8. *Let A be a self-adjoint operator and let $\{U_t\}_{t\in\mathbb{R}}$ be the corresponding unitary group. Let also $f \in \mathcal{H}_{ac}(A)$. Then,*

(i) $U_t f$ converges weakly to 0 as $t \to \pm\infty$,

(ii) If $B \in \mathscr{B}(\mathcal{H})$ is A-compact, then $\|BU_t f\| \to 0$ as $t \to \pm\infty$.

Proof. i) For any $h \in \mathcal{H}_{ac}(A)$ and since $m_h(\mathbb{R}) = \int_{\mathbb{R}} m_h(\mathrm{d}\lambda) = \|h\|^2$, one infers that there exists a non-negative function $\theta \in L^1(\mathbb{R})$ such that $m_h(V) = \int_V \theta(\lambda)\mathrm{d}\lambda$ for any $V \in \mathcal{A}_B$. It thus follows that

$$\varphi(t) := \langle h, U_t h\rangle = \int_{\mathbb{R}} \mathrm{e}^{-it\lambda}\, m_h(\mathrm{d}\lambda) = \int_{\mathbb{R}} \mathrm{e}^{-it\lambda}\, \theta(\lambda)\mathrm{d}\lambda.$$

Thus, φ is the Fourier transform of the function $\theta \in L^1(\mathbb{R})$, and consequently belongs to $C_0(\mathbb{R})$ by the Riemann-Lebesgue lemma. It follows that $\lim_{t\to\pm\infty}\langle h, U_t h\rangle = 0$.

We now show that $\lim_{t\to\pm\infty}\langle g, U_t f\rangle = 0$ for any $g \in \mathcal{H}$ and $f \in \mathcal{H}_{ac}(A)$. Since $U_t f \in \mathcal{H}_{ac}(A)$ for any $t \in \mathbb{R}$ it follows that $\langle g, U_t f\rangle = 0$ if $g \in \mathcal{H}_s(A) := \mathcal{H}_{ac}(A)^\perp$. Thus, one can assume that $g \in \mathcal{H}_{ac}(A)$. By the polarization identity, one then obtains that $\langle g, U_t f\rangle$ is the sum of four terms of the form $\langle g + \alpha f, U_t(g + \alpha f)\rangle$ for some $\alpha \in \mathbb{C}$, and since $g + \alpha f$ belongs to $\mathcal{H}_{ac}(A)$ one infers from the previous paragraph that these four contributions converge to 0 as $t \to \pm\infty$, and this proves the statement (i).

ii) Observe first that it is sufficient to prove the statement (ii) for a dense set of elements of $\mathcal{H}_{ac}(A)$. Let us take for this dense set the linear manifold $\mathcal{H}_{ac}(A) \cap \mathsf{D}(A)$, and for any f in this set we define $g := (A + i)f$. Clearly $g \in \mathcal{H}_{ac}(A)$ and one has $f = (A + i)^{-1}g$. It follows that

$$BU_t f = BU_t(A + i)^{-1}g = B(A + i)^{-1}U_t g. \tag{5.4}$$

Since $U_t g$ converges weakly to 0 by the statement (i) and since $B(A + i)^{-1}$ belongs to $\mathscr{K}(\mathcal{H})$, one deduces from Proposition 1.4.12 that $B(A+i)^{-1}U_t g$ converges strongly to 0 as $t \to \pm\infty$. By (5.4), it means that $BU_t f$ converges strongly to 0, as stated in (ii). ☐

For $f \in \mathcal{H}_{sc}(A)$, the previous result does not hold in general. However, once a certain average is taken, similar results can be deduced. Since t is often interpreted as the time, one speaks about a temporal mean. We state the result for arbitrary $f \in \mathcal{H}_c(A)$, and refer to [Amr, Prop. 5.9] for its proof.

Proposition 5.1.9. *Let A be a self-adjoint operator and let $\{U_t\}_{t\in\mathbb{R}}$ be the corresponding unitary group. Let also $f \in \mathcal{H}_c(A)$. Then,*

(i) For any $h \in \mathcal{H}$ one has

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T |\langle h, U_t f\rangle|^2 \mathrm{d}t = 0 \quad \textit{and} \quad \lim_{T\to\infty} \frac{1}{T}\int_{-T}^0 |\langle h, U_t f\rangle|^2 \mathrm{d}t = 0.$$

(ii) If $B \in \mathscr{B}(\mathcal{H})$ is A-compact, then one has

$$\lim_{T\to\infty} \int_0^T \frac{1}{T}\|BU_tf\|^2 \mathrm{d}t = 0 \quad \textit{and} \quad \lim_{T\to\infty} \frac{1}{T}\int_{-T}^0 \|BU_tf\|^2 \mathrm{d}t = 0.$$

The first result can in fact be deduced from a stronger statement, usually called *RAGE theorem* in honor of its authors Ruelle, Amrein, Georgescu and Enss.

Theorem 5.1.10 (RAGE Theorem)**.** *Let A be a self-adjoint operator and let $\{U_t\}_{t\in\mathbb{R}}$ be the corresponding unitary group. Let also $E(\{0\})$ denote the spectral projection onto $\mathsf{Ker}(A)$. Then for any $f \in \mathcal{H}$ one has*

$$s - \lim_{T\to\pm\infty} \frac{1}{T}\int_0^T U_t f\,\mathrm{d}t = E(\{0\})f.$$

In particular, if $f \perp \mathsf{Ker}(A)$, then the previous limit is 0.

Exercise 5.1.11. *Provide a proof of RAGE theorem, see for Example [RS3, Thm XI.115].*

Let us close this section with one more result about U_tf for any $f \in \mathcal{H}_c(A)$. Its proof can be found in [RS3, Corol. p. 343]. We emphasize that in the statement, the family $\{t_k\}$ can be chosen independently of the element $f \in \mathcal{H}_c(A)$.

Corollary 5.1.12. *Let A be a self-adjoint operator and let $\{U_t\}_{t\in\mathbb{R}}$ be the corresponding unitary group. Then there exists a sequence $\{t_k\}_{k\in\mathbb{N}} \subset \mathbb{R}$ with $t_k \to \infty$ as $k \to \infty$ such that $w - \lim_{k\to\infty} U_{t_k} f = 0$ for any $f \in \mathcal{H}_c(A)$. In addition, if $B \in \mathscr{B}(\mathcal{H})$ is A-compact, then $\lim_{k\to\infty} \|BU_{t_k}f\| = 0$ for any $f \in \mathcal{H}_c(A)$.*

5.2 Wave operators

Scattering theory is mainly a comparison theory. Namely, given a self-adjoint operator H on a Hilbert space $\mathcal{H}$ one wonders if the evolution group $\{\mathrm{e}^{-itH}\}_{t\in\mathbb{R}}$ can be approximated by a simpler evolution group $\{\mathrm{e}^{-itH_0}\}_{t\in\mathbb{R}}$ as $t \to \pm\infty$. More precisely, let $f \in \mathcal{H}$ and consider the family of elements $\mathrm{e}^{-itH} f \in \mathcal{H}$. The previous question reduces to looking for a "simpler" operator H_0 and for two elements $f_\pm \in \mathcal{H}$ such that

$$\lim_{t\to\pm\infty} \big\| \mathrm{e}^{-itH} f - \mathrm{e}^{-itH_0} f_\pm \big\| = 0. \tag{5.5}$$

Obviously, one has to be more precise in what "simpler" means, and about the set of f which admit such an approximation.

Observe first that there is not a single procedure which leads to a natural candidate for H_0. Such a choice depends on the framework and on the problem. However, the initial question can be rephrased very precisely. By using the unitarity of e^{itH}, observe that (5.5) is equivalent to

$$\lim_{t\to\pm\infty} \big\| f - e^{itH} e^{-itH_0} f_\pm \big\| = 0. \tag{5.6}$$

For that reason, a natural object to consider is $s - \lim_{t\to\pm\infty} e^{itH} e^{-itH_0}$. However, this limit has a better chance to exist if considered only on a subspace of the Hilbert space. So let E be an orthogonal projection and assume that $E\, e^{-itH_0} = e^{-itH_0} E$ for any $t \in \mathbb{R}$. Equivalently, this means that the subspace $E\mathcal{H}$ is left invariant by the unitary group $\{e^{-itH_0}\}_{t\in\mathbb{R}}$. We say in that case that E commutes with the evolution group $\{e^{-itH_0}\}_{t\in\mathbb{R}}$. Note that we have chosen the notation E for this projection because in most of the applications E is related to the spectral family of H_0. However, other choices can also appear.

Definition 5.2.1. *Let H, H_0 be two self-adjoint operators in a Hilbert space $\mathcal{H}$, and let E be an orthogonal projection which commutes with $\{e^{-itH_0}\}_{t\in\mathbb{R}}$. The* wave operators *are defined by*

$$W_\pm(H, H_0, E) := s - \lim_{t\to\pm\infty} e^{itH} e^{-itH_0} E \tag{5.7}$$

whenever these limits exit. If $E = \mathbf{1}$ then these operators are denoted by $W_\pm(H, H_0)$.

Note that we could have chosen two different projections $E_\pm$ for $t \to \pm\infty$. Since the general theory is not more difficult in this case, we do not mention it in the sequel. However, in applications this slight extension is often useful. We now provide some information about these operators. Recall that some properties of isometries and partial isometries have be introduced in Propositions 1.4.6 and 1.4.8.

Proposition 5.2.2. *Let $W := W_\pm(H, H_0, E)$ be one of the wave operators. Then*

(i) W is a partial isometry, with initial set $E\mathcal{H}$. In particular, W is an isometry if $E = \mathbf{1}$,

(ii) W intertwines the two operators H_0 and H, or more precisely $e^{-itH} W = W e^{-itH_0}$ for any $t \in \mathbb{R}$. More generally, $E^H(V)W = WE^{H_0}(V)$ for any Borel set V, and $\varphi(H)W = W\varphi(H_0)$ for any $\varphi \in C_b(\mathbb{R})$. The following equality also holds:

$$HWf = WH_0 f \qquad \forall f \in \mathsf{D}(H_0). \tag{5.8}$$

Proof. In this proof we consider only $W := W_+(H, H_0, E)$, the case $W = W_-(H, H_0, E)$ being similar.

i) If $f \perp E\mathcal{H}$ then clearly $Wf = 0$. On the other hand, if $f \in E\mathcal{H}$ then $\|Wf\| = \lim_{t\to\infty} \| e^{itH} e^{-itH_0} f\| = \lim_{t\to\infty} \|f\| = \|f\|$, where Lemma 1.1.5 has been used for the first equality. It follows that W is a partial isometry, or an isometry if $E = \mathbf{1}$.

ii) Observe that

$$\begin{aligned}
\mathrm{e}^{-itH} W &= \mathrm{e}^{-itH}\, s-\lim_{s\to\infty} \mathrm{e}^{isH}\,\mathrm{e}^{-isH_0} E \\
&= s-\lim_{s\to\infty} \mathrm{e}^{i(s-t)H}\,\mathrm{e}^{-isH_0} E \\
&= s-\lim_{s'\to\infty} \mathrm{e}^{-is'H}\,\mathrm{e}^{-i(s'+t)H_0} E \\
&= W\,\mathrm{e}^{-itH_0}
\end{aligned}$$

where we have used that E and e^{-itH_0} commute. This proves the first part of the statement (ii). Then, by multiplying this equality with $\pm i\,\mathrm{e}^{izt}$ and by integrating with respect to t on $[0,\infty)$ for $\Im(z)>0$ or on $(-\infty,0]$ if $\Im(z)<0$, one gets as in Remark 5.1.2 the equality

$$(H-z)^{-1}W = W(H_0-z)^{-1} \qquad \text{for any } z\in\mathbb{C}\setminus\mathbb{R}.$$

One then also deduces for any $\alpha,\beta\in\mathbb{R}$ that

$$\begin{aligned}
&\int_\alpha^\beta \big((H-\lambda-i\varepsilon)^{-1}-(H-\lambda+i\varepsilon)^{-1}\big)W\,\mathrm{d}\lambda \\
&= W\int_\alpha^\beta \big((H_0-\lambda-i\varepsilon)^{-1}-(H_0-\lambda+i\varepsilon)^{-1}\big)\,\mathrm{d}\lambda
\end{aligned}$$

Thus, by considering $\alpha=a+\delta$, $\beta=b+\delta$ and by taking consecutively the two limits $\lim_{\varepsilon\searrow 0}$ and then $\lim_{\delta\searrow 0}$ one infers that $E^H\big((a,b]\big)W = WE^{H_0}\big((a,b]\big)$ for any $a<b$. Considering the limit $a\to-\infty$ one finds $E^H_\lambda W = WE^{H_0}_\lambda$ for any $\lambda\in\mathbb{R}$. The equality mentioned in the statement for any Borel set follows then from the equality for any elements of the spectral family. The equality $\varphi(H)W=W\varphi(H_0)$ follows also from the previous equality and from the definition of the function of an operator.

For (5.8) observe that if $f\in\mathsf{D}(H_0)$, then $W\,\mathrm{e}^{-itH_0} f$ is strongly differentiable at $t=0$, with derivative $-iWH_0f$. However, since $W\,\mathrm{e}^{-itH_0} f = \mathrm{e}^{-itH}\,Wf$, this function is also strongly differentiable at $t=0$. It then follows from Stone's theorem that $Wf\in\mathsf{D}(H)$ and that the derivative at $t=0$ is given by $-iHWf$. The equality (5.8) follows then directly. □

Note that the properties mentioned in the point (ii) are usually referred to as the *intertwining properties* of the wave operators. Note also that the different steps presented in the proof, namely how to go from an intertwining relation for the unitary group to an intertwining relation for arbitrary continuous and bounded functions, is a quite common procedure. One can prove similarly that if $B\in\mathscr{B}(\mathcal{H})$ satisfies $CU_t=U_tC$ for an arbitrary unitary group, then $C\varphi(A)=\varphi(A)C$ for any bounded and continuous function of its generator A.

Let us now state some additional properties of the wave operators.

Proposition 5.2.3. *Let $W_\pm := W_\pm(H, H_0, E)$ be the wave operators for the pair (H, H_0) and the initial set projection E. Let $F_\pm$ be the final range projection,* i.e. *the orthogonal projection on $\mathsf{Ran}(W_\pm)$ which is given by $F_\pm := W_\pm W_\pm^*$. Then $F_\pm$ commute with the elements of the unitary group $\{\mathrm{e}^{-itH}\}_{t\in\mathbb{R}}$ and the limits*

$$W_\pm(H_0, H, F_\pm) := s - \lim_{t\to\pm\infty} \mathrm{e}^{itH_0}\,\mathrm{e}^{-itH}\,F_\pm$$

exist and satisfy $W_\pm(H_0, H, F_\pm) = W_\pm(H, H_0, E)^*$. In addition, the following implications hold:

$$\begin{aligned} E\mathcal{H} \subset \mathcal{H}_{ac}(H_0) &\Longrightarrow F_\pm\mathcal{H} \subset \mathcal{H}_{ac}(H), \\ E\mathcal{H} \subset \mathcal{H}_{c}(H_0) &\Longrightarrow F_\pm\mathcal{H} \subset \mathcal{H}_{c}(H). \end{aligned}$$

Proof. In this proof we consider only $W := W_+(H, H_0, E)$, the case $W = W_-(H, H_0, E)$ being similar. Accordingly, we simply write F for F_+.

i) Recall first that $\mathrm{e}^{-itH}\,W = W\,\mathrm{e}^{-itH_0}$ for any $t \in \mathbb{R}$. By taking the adjoint on both sides, and by switching t to $-t$ one infers that $W^*\,\mathrm{e}^{-itH} = \mathrm{e}^{-itH_0}\,W^*$ for any $t \in \mathbb{R}$. It then follows that

$$\mathrm{e}^{-itH}\,F = \mathrm{e}^{-itH}\,WW^* = W\,\mathrm{e}^{-itH_0}\,W^* = WW^*\,\mathrm{e}^{-itH} = F\,\mathrm{e}^{-itH},$$

which corresponds to the expected commutation relation.

ii) Let us now consider $g \in \mathsf{Ran}(W)$. There exists thus $f \in E\mathcal{H}$ such that $g = Wf$. Then we have

$$\begin{aligned} \|\,\mathrm{e}^{itH_0}\,\mathrm{e}^{-itH}\,g - f\| &= \big\|\,\mathrm{e}^{itH}\,\mathrm{e}^{-itH_0}\,\big(\mathrm{e}^{itH_0}\,\mathrm{e}^{-itH}\,g - f\big)\big\| \\ &= \|g - \mathrm{e}^{itH}\,\mathrm{e}^{-itH_0}\,f\| = \|Wf - \mathrm{e}^{itH}\,\mathrm{e}^{-itH_0}\,f\|, \end{aligned}$$

which converges to 0 as $t \to +\infty$. It thus follows that the operator $W_+(H_0, H, F)$ exists. One also deduces from the previous equalities that $s - \lim_{t\to+\infty} \mathrm{e}^{itH_0}\,\mathrm{e}^{-itH}\,W = E$, and as a consequence

$$\begin{aligned} W_+(H_0, H, F) &= s - \lim_{t\to+\infty} \mathrm{e}^{itH_0}\,\mathrm{e}^{-itH}\,F \\ &= s - \lim_{t\to+\infty} \mathrm{e}^{itH_0}\,\mathrm{e}^{-itH}\,WW^* = EW^* = (WE)^* = W^*, \end{aligned}$$

as mentioned in the statement.

iii) Let again $g \in \mathsf{Ran}(W)$ and let $f \in E\mathcal{H}$ such that $Wf = g$. One then infers from Proposition 5.2.2 that for any $V \in \mathcal{A}_B$ one has

$$\langle g, E^H(V)g\rangle = \langle Wf, E^H(V)Wf\rangle = \langle W^*Wf, E^{H_0}(V)f\rangle = \langle f, E^{H_0}(V)f\rangle.$$

Thus, if the measure $m_f^{H_0}$ is absolutely continuous, then the same property holds for the measure m_g^H. Similarly, if f belongs to $\mathcal{H}_c(H_0)$, then $g = Wf$ belongs to $\mathcal{H}_c(H)$. $\square$

Up to now, we have studied some properties of the wave operators by assuming their existence. In the next statement, we give a criterion which ensures their existence. Its use is often quite easy, especially if the evolution group generated by H_0 is simple enough.

Proposition 5.2.4 (Cook criterion)**.** *Let H_0, H be two self-adjoint operators in a Hilbert space $\mathcal{H}$, let $\mathcal{M}$ be a subspace of $\mathcal{H}$ invariant under the group $\{\mathrm{e}^{-itH_0}\}_{t\in\mathbb{R}}$, and let $\mathcal{D}$ be a linear subset of $\mathcal{M}$ satisfying*

(i) The linear combinations of elements of $\mathcal{D}$ span a dense set in $\mathcal{M}$,

(ii) $\mathrm{e}^{-itH_0} f \in \mathsf{D}(H) \cap \mathsf{D}(H_0)$ for any $f \in \mathcal{D}$ and $t \in \mathbb{R}$,

(iii) $\int_{\pm 1}^{\pm\infty} \|(H - H_0)\,\mathrm{e}^{-i\tau H_0} f\|\mathrm{d}\tau < \infty$ for any $f \in \mathcal{D}$.

Then $W_\pm(H, H_0, E)$ exists, with E the orthogonal projection on $\mathcal{M}$.

Proof. As in the previous proofs, we consider only $W_+(H, H_0, E)$, the proof for the other wave operator being similar.

For any $f \in \mathcal{D}$ and by the assumption (ii) one infers that

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\big(\mathrm{e}^{itH}\,\mathrm{e}^{-itH_0} f\big) &= \big(\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{itH}\big)\,\mathrm{e}^{-itH_0} f + \mathrm{e}^{itH}\,\big(\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{-itH_0} f\big)\\ &= i\,\mathrm{e}^{itH}(H - H_0)\,\mathrm{e}^{-itH_0} f.\end{aligned}$$

By the result of Proposition 1.2.3.(iii) and for any $t > s > 1$ one gets that

$$\begin{aligned}\mathrm{e}^{itH}\,\mathrm{e}^{-itH_0} f - \mathrm{e}^{isH}\,\mathrm{e}^{-isH_0} f &= \int_s^t \frac{\mathrm{d}}{\mathrm{d}\tau}\big(\mathrm{e}^{i\tau H}\,\mathrm{e}^{-i\tau H_0} f\big)\mathrm{d}\tau\\ &= i\int_s^t \mathrm{e}^{i\tau H}(H - H_0)\,\mathrm{e}^{-i\tau H_0} f\mathrm{d}\tau\end{aligned}$$

from which one infers that

$$\begin{aligned}\big\|\,\mathrm{e}^{itH}\,\mathrm{e}^{-itH_0} f - \mathrm{e}^{isH}\,\mathrm{e}^{-isH_0} f\big\| &= \Big\|\int_s^t \frac{\mathrm{d}}{\mathrm{d}\tau}\big(\mathrm{e}^{i\tau H}\,\mathrm{e}^{-i\tau H_0} f\big)\mathrm{d}\tau\Big\|\\ &\leq \int_s^t \big\|\,\mathrm{e}^{i\tau H}(H - H_0)\,\mathrm{e}^{-i\tau H_0} f\big\|\mathrm{d}\tau\\ &= \int_s^t \big\|(H - H_0)\,\mathrm{e}^{-i\tau H_0} f\big\|\mathrm{d}\tau\ .\end{aligned}$$

Since the latter expression is arbitrarily small for s and t large enough, one deduces that the map $t \mapsto \mathrm{e}^{itH}\,\mathrm{e}^{-itH_0} f$ is strongly Cauchy for any $f \in \mathcal{D}$, and thus strongly convergent for any $f \in \mathcal{D}$. The strong convergence on $\mathcal{M}$ directly follows by a simple density argument. □

Let us still mention a rather famous result about trace-class perturbations, see also Extension 1.4.14. For its proof we refer for example to [Kat, Thm. X.4.4].

Theorem 5.2.5 (Kato-Rosenblum theorem). *Let H and H_0 be two self-adjoint operators in a Hilbert space such that $H - H_0$ is a trace class operator (or in particular a finite rank operator). Then the wave operators $W_\pm\big(H, H_0, E_{ac}(H_0)\big)$ exist.*

Extension 5.2.6. *Work on this theorem and on its proof.*

Let us now provide a few examples for which the existence of the wave operators has been shown. Note that most the time, the existence is proved by using Proposition 5.2.4 or a slightly improved version of it. The first example corresponds to a Schrödigner operator with a short-range potential.

Example 5.2.7. *In the Hilbert space $\mathcal{H} := L^2(\mathbb{R}^d)$, let H_0 be the Laplace operator $-\Delta$ and let $H := H_0 + V(X)$ with $V(X)$ a multiplication operator by a real valued measurable function which satisfies*

$$|V(x)| \leq c\,\frac{1}{(1+|x|)^{1+\varepsilon}}$$

for some constant $c > 0$ and some $\varepsilon > 0$. Then the projection E can be chosen equal to $\mathbf{1}$ and the wave operators $W_\pm(H, H_0)$ exist. Note that such a result is part of the folklore of scattering theory for Schrödinger operators and that the proof of such a statement can be found in many textbooks.

The second example is a very simple system on which all the computations can be performed explicitly, see [Yaf, Sec. 2.4].

Example 5.2.8. *Let $\mathcal{H} := L^2(\mathbb{R})$ and consider the operator H_0 defined by the operator D. The corresponding unitary group acts as $[\mathrm{e}^{-itH_0} f](x) = f(x-t)$ as mentioned in Example 5.1.3. Let also $q : \mathbb{R} \to \mathbb{R}$ belong to $L^1(\mathbb{R})$ and consider the unitary operator V defined by $[Vf](x) = \mathrm{e}^{-i\int_0^x q(y)\mathrm{d}y} f(x)$ for any $f \in \mathcal{H}$ and $x \in \mathbb{R}$. By setting $H := VH_0V^*$ one checks that H is the operator defined on*

$$\mathsf{D}(H) := \big\{ f \in \mathcal{H} \mid f \text{ is absolutely continuous and } -if' + qf \in L^2(\mathbb{R}) \big\}$$

with $Hf = -if' + qf$ for any $f \in \mathsf{D}(H)$. The unitary group generated by H can then be computed explicitly and one gets

$$[\mathrm{e}^{itH}\,\mathrm{e}^{-itH_0} f](x) = [V\,\mathrm{e}^{itH_0}\,V^*\,\mathrm{e}^{-itH_0} f](x) = \mathrm{e}^{i\int_x^{x+t} q(y)\mathrm{d}y} f(x).$$

We can then conclude that the wave operators $W_\pm(H, H_0)$ exist and are given by

$$[W_\pm(H, H_0)f](x) = \mathrm{e}^{i\int_x^{\pm\infty} q(y)\mathrm{d}y} f(x).$$

We add one more example for which all computations can be done explicitly and refer to [Ric, Sec. 2] for the details.

Example 5.2.9. *Let $\mathcal{H} := L^2(\mathbb{R}_+)$ and consider the Dirichlet Laplacian H_D on $\mathbb{R}_+$. More precisely, we set $H_\mathrm{D} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ with the domain $\mathsf{D}(H_\mathrm{D}) = \{f \in \mathcal{H}^2(\mathbb{R}_+) \mid f(0) = 0\}$. Here $\mathcal{H}^2(\mathbb{R}_+)$ means the usual Sobolev space on $\mathbb{R}_+$ of order 2. For any $\alpha \in \mathbb{R}$, let us also consider the operator H^α defined by $H^\alpha = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ with $\mathsf{D}(H^\alpha) = \{f \in \mathcal{H}^2(\mathbb{R}_+) \mid f'(0) = \alpha f(0)\}$. It can easily be checked that if $\alpha < 0$ the operator H^α possesses only one eigenvalue, namely $-\alpha^2$, and the corresponding eigenspace is generated by the function $x \mapsto \mathrm{e}^{\alpha x}$. On the other hand, for $\alpha \geq 0$ the operators H^α have no eigenvalue, and so does H_D.*

Let us also recall the action of the dilation group in $\mathcal{H}$, as already introduced in Example 5.1.4. This unitary group $\{U_t\}_{t\in\mathbb{R}}$ acts on $f \in \mathcal{H}$ as

$$[U_t f](x) = \mathrm{e}^{t/2} f\big(\mathrm{e}^t x\big), \qquad \forall x \in \mathbb{R}_+.$$

Its self-adjoint generator is denoted by A. For this model, the following equality can be proved

$$W_-(H^\alpha, H_\mathrm{D}) = 1 + \tfrac{1}{2}\big(1 + \tanh(\pi A) - i\cosh(\pi A)^{-1}\big)\Big[\frac{\alpha + i\sqrt{H_\mathrm{D}}}{\alpha - i\sqrt{H_\mathrm{D}}} - 1\Big]. \tag{5.9}$$

and a similar formula holds for $W_+(H^\alpha, H_\mathrm{D})$. Let us still mention that the function of A in the above formula is linked to the Hilbert transform.

5.3 Scattering operator and completeness

In this section we consider again two self-adjoint operators H and H_0 in a Hilbert space $\mathcal{H}$, and assume that the wave operators $W_\pm(H, H_0)$ exist. Note that for simplicity we have set $E = \mathbf{1}$ but the general theory can be considered without much additional efforts.

Definition 5.3.1. *In the framework mentioned above, the operator*

$$S \equiv S(H, H_0) := \big(W_+(H, H_0)\big)^* W_-(H, H_0)$$

is called the scattering operator *for the pair (H, H_0).*

We immediately state and prove some properties of this operator. For simplicity, we shall simply write $W_\pm$ for $W_\pm(H, H_0)$.

Proposition 5.3.2. *(i) The scattering operator commutes with H_0, or more precisely*

$$[S, \mathrm{e}^{-itH_0}] = 0 \qquad \forall t \in \mathbb{R}, \tag{5.10}$$

and for any $f \in \mathsf{D}(H_0)$ one has $Sf \in \mathsf{D}(H_0)$ and $SH_0 f = H_0 S f$.

(ii) S is an isometric operator if and only if $\mathsf{Ran}(W_-) \subset \mathsf{Ran}(W_+)$,

(iii) S is a unitary operator if and only if $\mathsf{Ran}(W_-) = \mathsf{Ran}(W_+)$.

Proof. i) The first statement directly follows from the intertwining relations as presented in Proposition 5.2.2 and in its proof for the adjoint operators. Indeed one has

$$S\,\mathrm{e}^{-itH_0} = W_+^* W_-\,\mathrm{e}^{-itH_0} = W_+^*\,\mathrm{e}^{-itH}\,W_- = \mathrm{e}^{-itH_0}\,W_+^* W_- = \mathrm{e}^{-itH_0}\,S.$$

Then, for any $f \in \mathsf{D}(H_0)$ observe that $\frac{i}{t}S(\mathrm{e}^{-itH_0} - 1)f = \frac{i}{t}(\mathrm{e}^{-itH_0} - 1)Sf$, and since the l.h.s. converges to SH_0f, the r.h.s. must also converge and it converges then to H_0Sf, which proves the second part of the statement (i).

ii) Let us set $F_\pm$ for the final range projection, *i.e.* $F_\pm := W_\pm W_\pm^*$. The assumption $\mathsf{Ran}(W_-) \subset \mathsf{Ran}(W_+)$ means $F_+W_- = W_-$. Under this hypothesis one has

$$S^*S = W_-^* W_+ W_+^* W_- = W_-^* F_+ W_- = W_-^* W_- = \mathbf{1},$$

which means that S is isometric. On the other hand if $\mathsf{Ran}(W_-) \subset \mathsf{Ran}(W_+)$ is not satisfied, then there exists $g \in \mathsf{Ran}(W_-)$ with $g \notin \mathsf{Ran}(W_+) \equiv \mathsf{Ran}(F_+)$. By setting $f = W_-^* g$ (so that $g = W_- f$) one infers that $\|F_+g\| < \|g\| = \|W_-f\| = \|f\|$, since W_- is an isometry. It follows that

$$\|Sf\| = \|W_+^* W_- f\| = \|W_+^* g\| = \|W_+ W_+^* g\| = \|F_+ g\| < \|f\|,$$

which means that S can not be isometric.

iii) S is unitary if and only if S and S^* are isometric. By (ii) S is isometric if and only if $\mathsf{Ran}(W_-) \subset \mathsf{Ran}(W_+)$. Since $S^* = W_-^* W_+$ one infers by exchanging the role of the two operators that S^* is isometric if and only if $\mathsf{Ran}(W_+) \subset \mathsf{Ran}(W_-)$. This naturally leads to the statement (iii). □

In relation with the previous statement, let us assume that H_0 is purely absolutely continuous. In that case, one often says that the scattering system for the pair (H, H_0) is *complete*[1] if $\mathsf{Ran}(W_-) = \mathcal{H}_{ac}(H)$ or if $\mathsf{Ran}(W_+) = \mathcal{H}_{ac}(H)$. We also say that *the asymptotic completeness* holds if $\mathsf{Ran}(W_-) = \mathsf{Ran}(W_+) = \mathcal{H}_p(H)^\perp$. Note that this latter requirement is a very strong condition. In particular it implies that H has not singular continuous spectrum, and that for any $f \in \mathcal{H}_{ac}(H)$ there exists $f_\pm$ such that

$$\lim_{t\to\pm\infty} \big\|\,\mathrm{e}^{-itH} f - \mathrm{e}^{-itH_0} f_\pm\big\| = 0. \tag{5.11}$$

In other words, the evolution of any element of $\mathcal{H}_{ac}(H)$ can be described asymptotically by the simpler evolution e^{-itH_0} on a vector $f_\pm$.

In the Examples 5.2.7, 5.2.8 and 5.2.9, the corresponding scattering systems are asymptotically complete. Note also that the Kato-Rosenblum theorem leads to the existence and to the completeness of the wave operators. On the other hand, Cook criterion, as presented in Proposition 5.2.4, does not provide any information about the completeness or the asymptotic completeness of the wave operators.

[1] Be aware that this terminology is not completely fixed and can still depend on the authors.

Let us close this section with a variant of the spectral theorem. The following formulation is a little bit imprecise because a fully rigorous version needs some more information on the structure of direct integrals of Hilbert spaces and on the notion of the multiplicity theory. We refer to [BM, Chap. 2] for the notion of multiplicity, and to the same book but Chapter 4 and 5 for more information on direct integral of Hilbert spaces and of operators. We also refer to [Yaf, Sec. 1.5] for a very short presentation of the same material.

For a σ-finite measure m on $(\mathbb{R}, \mathcal{A}_B)$ we define

$$\mathscr{H} := \int_{\mathbb{R}}^{\oplus} \mathfrak{H}(\lambda)\, m(\mathrm{d}\lambda) \tag{5.12}$$

as the Hilbert space of equivalence class of vector-valued functions $\mathbb{R} \ni \lambda \mapsto \mathfrak{f}(\lambda) \in \mathfrak{H}(\lambda)$ taking values in the Hilbert space $\mathfrak{H}(\lambda)$ and which are measurable and square integrable with respect to the measure m. The scalar product in $\mathscr{H}$ is given by

$$\langle \mathfrak{f}, \mathfrak{g} \rangle_{\mathscr{H}} := \int_{\mathbb{R}} \langle \mathfrak{f}(\lambda), \mathfrak{g}(\lambda) \rangle_\lambda\, m(\mathrm{d}\lambda)$$

with $\langle \cdot, \cdot \rangle_\lambda$ the scalar product in $\mathfrak{H}(\lambda)$. If the fiber $\mathfrak{H}(\lambda)$ is a constant Hilbert space $\mathfrak{H}$ independent of λ, then the above construction corresponds to $L^2(\mathbb{R}, m; \mathfrak{H}) \cong L^2(\mathbb{R}, m) \otimes \mathfrak{H}$.

In this context, one of the formulation of the spectral theorem can be expressed as a decomposition of any self-adjoint operator into a direct integral of operator. More precisely, for any self-adjoint operator H in a Hilbert space $\mathcal{H}$ there exists a measure σ-finite measure m on $\mathbb{R}$ and a unitary transformation $\mathscr{F} : \mathcal{H} \to \mathscr{H}$ such that

$$\langle E(V) f, g \rangle_{\mathcal{H}} = \int_V \langle [\mathscr{F} f](\lambda), [\mathscr{F} g](\lambda) \rangle_\lambda\, m(\mathrm{d}\lambda),$$

where $E(\cdot)$ is the spectral measure associated with H and V is any Borel set on $\mathbb{R}$. A different way of writing the same information is by saying that H is a diagonal operator in the direct integral representation provided by $\mathscr{H}$. In other words, the following equality holds:

$$\mathscr{F} H \mathscr{F}^* = \int_{\mathbb{R}}^{\oplus} \lambda\, m(\mathrm{d}\lambda).$$

Note that such a decomposition is called *the direct integral representation of H*. This representation is often highly non-unique, but in applications some natural choices often appear. In addition, if H is purely absolutely continuous, then the measure m can be chosen as the Lebesgue measure, as mentioned in [BM, Sec. 5.2.4]. In any case, the support of the measure m coincides with the spectrum of H, and thus we can restrict the above construction to the spectrum $\sigma(H)$ of H.

Once the notion of a direct integral Hilbert space $\mathscr{H}$ is introduced, as in (5.12), direct integral operators operators acting on this Hilbert space can naturally be studied.

We refer again to [BM] for more information, or to [RS4, XIII.16] for a short introduction to this theory and a few important results. Our only aim in this direction is the statement of the following result. Note that its proof is based on the commutation relation provided in (5.10) and that such an argument is quite standard.

Proposition 5.3.3. *Let H_0 be an absolutely continuous self-adjoint operator in a Hilbert space $\mathcal{H}$ and let $\mathscr{F}_0$ and $\mathscr{H}_0$ be a direct integral representation of H_0,* i.e. *$\mathscr{H}_0$ is a direct integral Hilbert space as constructed in* (5.12) *with m the Lebesgue measure, and $\mathscr{F}_0 : \mathcal{H} \to \mathscr{H}_0$ is a unitary map satisfying $\mathscr{F}_0 H_0 \mathscr{F}_0^* = \int_{\sigma(H_0)}^{\oplus} \lambda \,\mathrm{d}\lambda$. Let H be another self-adjoint operator in $\mathcal{H}$ such that the wave operators $W_\pm(H, H_0)$ exist and are asymptotically complete. Then there exists a family $\{S(\lambda)\}_{\lambda\in\sigma(H_0)}$ of unitary operator in $\mathfrak{H}(\lambda)$ for almost every λ such that*

$$\mathscr{F} S \mathscr{F}^* = \int_{\sigma(H_0)}^{\oplus} S(\lambda)\,\mathrm{d}\lambda.$$

The operator $S(\lambda)$ is called the *scattering matrix at energy* λ even if $S(\lambda)$ is usually not a matrix but a unitary operator in $\mathfrak{H}(\lambda)$. Note that there also exist expressions for the operators S and the operator $S(\lambda)$ in terms of the difference of the resolvent of H and the resolvent of H_0 on the real axis. Such expressions are usually referred to as *the stationary approach of scattering theory*. This approach will not be developed here, but the reference [Yaf] is one of the classical book on the subject.

Extension 5.3.4. *Work on the notion of multiplicity and on the theory of direct integral of Hilbert spaces and direct integral of operators.*