Quantum dynamics

As in the finite dimensional case, the solution of the Schrödinger equation

$$\mathrm{i}\frac{d}{dt}\psi(t) = H\psi(t) \tag{5.1}$$

is given by

$$\psi(t) = \exp(-\mathrm{i}tH)\psi(0). \tag{5.2}$$

A detailed investigation of this formula will be our first task. Moreover, in the finite dimensional case the dynamics is understood once the eigenvalues are known and the same is true in our case once we know the spectrum. Note that, like any Hamiltonian system from classical mechanics, our system is not hyperbolic (i.e., the spectrum is not away from the real axis) and hence simple results such as all solutions tend to the equilibrium position cannot be expected.

5.1. The time evolution and Stone's theorem

In this section we want to have a look at the initial value problem associated with the Schrödinger equation (2.12) in the Hilbert space $\mathfrak{H}$. If $\mathfrak{H}$ is one-dimensional (and hence A is a real number), the solution is given by

$$\psi(t) = \mathrm{e}^{-\mathrm{i}tA}\psi(0). \tag{5.3}$$

Our hope is that this formula also applies in the general case and that we can reconstruct a one-parameter unitary group $U(t)$ from its generator A (compare (2.11)) via $U(t) = \exp(-\mathrm{i}tA)$. We first investigate the family of operators $\exp(-\mathrm{i}tA)$.

Theorem 5.1. *Let A be self-adjoint and let $U(t) = \exp(-\mathrm{i}tA)$.*

(i) *$U(t)$ is a strongly continuous one-parameter unitary group.*

(ii) *The limit* $\lim_{t\to 0}\frac{1}{t}(U(t)\psi - \psi)$ *exists if and only if* $\psi \in \mathfrak{D}(A)$ *in which case* $\lim_{t\to 0}\frac{1}{t}(U(t)\psi - \psi) = -\mathrm{i}A\psi$.

(iii) $U(t)\mathfrak{D}(A) = \mathfrak{D}(A)$ *and* $AU(t) = U(t)A$.

Proof. The group property (i) follows directly from Theorem 3.1 and the corresponding statements for the function $\exp(-\mathrm{i}t\lambda)$. To prove strong continuity, observe that

$$\lim_{t\to t_0} \|\mathrm{e}^{-\mathrm{i}tA}\psi - \mathrm{e}^{-\mathrm{i}t_0 A}\psi\|^2 = \lim_{t\to t_0}\int_{\mathbb{R}} |\mathrm{e}^{-\mathrm{i}t\lambda} - \mathrm{e}^{-\mathrm{i}t_0\lambda}|^2 d\mu_\psi(\lambda)$$
$$= \int_{\mathbb{R}} \lim_{t\to t_0} |\mathrm{e}^{-\mathrm{i}t\lambda} - \mathrm{e}^{-\mathrm{i}t_0\lambda}|^2 d\mu_\psi(\lambda) = 0$$

by the dominated convergence theorem.

Similarly, if $\psi \in \mathfrak{D}(A)$, we obtain

$$\lim_{t\to 0} \|\frac{1}{t}(\mathrm{e}^{-\mathrm{i}tA}\psi - \psi) + \mathrm{i}A\psi\|^2 = \lim_{t\to 0}\int_{\mathbb{R}} |\frac{1}{t}(\mathrm{e}^{-\mathrm{i}t\lambda} - 1) + \mathrm{i}\lambda|^2 d\mu_\psi(\lambda) = 0$$

since $|\mathrm{e}^{\mathrm{i}t\lambda} - 1| \le |t\lambda|$. Now let $\tilde{A}$ be the generator defined as in (2.11). Then $\tilde{A}$ is a symmetric extension of A since we have

$$\langle\varphi, \tilde{A}\psi\rangle = \lim_{t\to 0}\langle\varphi, \frac{\mathrm{i}}{t}(U(t) - 1)\psi\rangle = \lim_{t\to 0}\langle\frac{\mathrm{i}}{-t}(U(-t) - 1)\varphi, \psi\rangle = \langle\tilde{A}\varphi, \psi\rangle$$

and hence $\tilde{A} = A$ by Corollary 2.2. This settles (ii).

To see (iii), replace $\psi \to U(s)\psi$ in (ii). □

For our original problem this implies that formula (5.3) is indeed the solution to the initial value problem of the Schrödinger equation. Moreover,

$$\langle U(t)\psi, AU(t)\psi\rangle = \langle U(t)\psi, U(t)A\psi\rangle = \langle\psi, A\psi\rangle \tag{5.4}$$

shows that the expectations of A are time independent. This corresponds to conservation of energy.

On the other hand, the generator of the time evolution of a quantum mechanical system should always be a self-adjoint operator since it corresponds to an observable (energy). Moreover, there should be a one-to-one correspondence between the unitary group and its generator. This is ensured by Stone's theorem.

Theorem 5.2 (Stone)**.** *Let* $U(t)$ *be a weakly continuous one-parameter unitary group. Then its generator* A *is self-adjoint and* $U(t) = \exp(-\mathrm{i}tA)$.

Proof. First of all observe that weak continuity together with item (iv) of Lemma 1.12 shows that $U(t)$ is in fact strongly continuous.

Next we show that A is densely defined. Pick $\psi \in \mathfrak{H}$ and set

$$\psi_\tau = \int_0^\tau U(t)\psi dt$$

(the integral is defined as in Section 4.1) implying $\lim_{\tau\to 0} \tau^{-1}\psi_\tau = \psi$. Moreover,

$$\begin{aligned}
\frac{1}{t}(U(t)\psi_\tau - \psi_\tau) &= \frac{1}{t}\int_t^{t+\tau} U(s)\psi ds - \frac{1}{t}\int_0^\tau U(s)\psi ds \\
&= \frac{1}{t}\int_\tau^{\tau+t} U(s)\psi ds - \frac{1}{t}\int_0^t U(s)\psi ds \\
&= \frac{1}{t}U(\tau)\int_0^t U(s)\psi ds - \frac{1}{t}\int_0^t U(s)\psi ds \to U(\tau)\psi - \psi
\end{aligned}$$

as $t \to 0$ shows $\psi_\tau \in \mathfrak{D}(A)$. As in the proof of the previous theorem, we can show that A is symmetric and that $U(t)\mathfrak{D}(A) = \mathfrak{D}(A)$.

Next, let us prove that A is essentially self-adjoint. By Lemma 2.7 it suffices to prove $\mathrm{Ker}(A^* - z^*) = \{0\}$ for $z \in \mathbb{C}\backslash\mathbb{R}$. Suppose $A^*\varphi = z^*\varphi$. Then for each $\psi \in \mathfrak{D}(A)$ we have

$$\frac{d}{dt}\langle\varphi, U(t)\psi\rangle = \langle\varphi, -\mathrm{i}AU(t)\psi\rangle = -\mathrm{i}\langle A^*\varphi, U(t)\psi\rangle = -\mathrm{i}z\langle\varphi, U(t)\psi\rangle$$

and hence $\langle\varphi, U(t)\psi\rangle = \exp(-\mathrm{i}zt)\langle\varphi,\psi\rangle$. Since the left-hand side is bounded for all $t \in \mathbb{R}$ and the exponential on the right-hand side is not, we must have $\langle\varphi,\psi\rangle = 0$ implying $\varphi = 0$ since $\mathfrak{D}(A)$ is dense.

So A is essentially self-adjoint and we can introduce $V(t) = \exp(-\mathrm{i}t\overline{A})$. We are done if we can show $U(t) = V(t)$.

Let $\psi \in \mathfrak{D}(A)$ and abbreviate $\psi(t) = (U(t) - V(t))\psi$. Then

$$\lim_{s\to 0}\frac{\psi(t+s) - \psi(t)}{s} = \mathrm{i}\overline{A}\psi(t)$$

and hence $\frac{d}{dt}\|\psi(t)\|^2 = 2\,\mathrm{Re}\langle\psi(t), \mathrm{i}A\psi(t)\rangle = 0$. Since $\psi(0) = 0$, we have $\psi(t) = 0$ and hence $U(t)$ and $V(t)$ coincide on $\mathfrak{D}(A)$. Furthermore, since $\mathfrak{D}(A)$ is dense, we have $U(t) = V(t)$ by continuity. □

As an immediate consequence of the proof we also note the following useful criterion.

Corollary 5.3. *Suppose $\mathfrak{D} \subseteq \mathfrak{D}(A)$ is dense and invariant under $U(t)$. Then A is essentially self-adjoint on $\mathfrak{D}$.*

Proof. As in the above proof it follows that $\langle\varphi,\psi\rangle = 0$ for any $\psi \in \mathfrak{D}$ and $\varphi \in \mathrm{Ker}(A^* - z^*)$. □

Note that by Lemma 4.9 two strongly continuous one-parameter groups commute,

$$[\mathrm{e}^{-\mathrm{i}tA}, \mathrm{e}^{-\mathrm{i}sB}] = 0, \tag{5.5}$$

if and only if the generators commute.

Clearly, for a physicist, one of the goals must be to understand the time evolution of a quantum mechanical system. We have seen that the time evolution is generated by a self-adjoint operator, the Hamiltonian, and is given by a linear first order differential equation, the Schrödinger equation. To understand the dynamics of such a first order differential equation, one must understand the spectrum of the generator. Some general tools for this endeavor will be provided in the following sections.

Problem 5.1. *Let $\mathfrak{H} = L^2(0, 2\pi)$ and consider the one-parameter unitary group given by $U(t)f(x) = f(x - t \mod 2\pi)$. What is the generator of U?*

5.2. The RAGE theorem

Now, let us discuss why the decomposition of the spectrum introduced in Section 3.3 is of physical relevance. Let $\|\varphi\| = \|\psi\| = 1$. The vector $\langle\varphi, \psi\rangle\varphi$ is the projection of ψ onto the (one-dimensional) subspace spanned by φ. Hence $|\langle\varphi, \psi\rangle|^2$ can be viewed as the part of ψ which is in the state φ. The first question one might raise is, how does

$$|\langle\varphi, U(t)\psi\rangle|^2, \qquad U(t) = \mathrm{e}^{-\mathrm{i}tA}, \tag{5.6}$$

behave as $t \to \infty$? By the spectral theorem,

$$\hat{\mu}_{\varphi,\psi}(t) = \langle\varphi, U(t)\psi\rangle = \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}t\lambda} d\mu_{\varphi,\psi}(\lambda) \tag{5.7}$$

is the **Fourier transform** of the measure $\mu_{\varphi,\psi}$. Thus our question is answered by Wiener's theorem.

Theorem 5.4 (Wiener). *Let μ be a finite complex Borel measure on $\mathbb{R}$ and let*

$$\hat{\mu}(t) = \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}t\lambda} d\mu(\lambda) \tag{5.8}$$

be its Fourier transform. Then the Cesàro time average of $\hat{\mu}(t)$ has the limit

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T |\hat{\mu}(t)|^2 dt = \sum_{\lambda\in\mathbb{R}} |\mu(\{\lambda\})|^2, \tag{5.9}$$

where the sum on the right-hand side is finite.

Proof. By Fubini we have

$$\begin{aligned}\frac{1}{T}\int_0^T |\hat{\mu}(t)|^2 dt &= \frac{1}{T}\int_0^T \int_{\mathbb{R}}\int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}(x-y)t} d\mu(x) d\mu^*(y) dt\\ &= \int_{\mathbb{R}}\int_{\mathbb{R}} \left(\frac{1}{T}\int_0^T \mathrm{e}^{-\mathrm{i}(x-y)t} dt\right) d\mu(x) d\mu^*(y).\end{aligned}$$

The function in parentheses is bounded by one and converges pointwise to $\chi_{\{0\}}(x-y)$ as $T\to\infty$. Thus, by the dominated convergence theorem, the limit of the above expression is given by

$$\int_{\mathbb{R}}\int_{\mathbb{R}} \chi_{\{0\}}(x-y) d\mu(x) d\mu^*(y) = \int_{\mathbb{R}} \mu(\{y\}) d\mu^*(y) = \sum_{y\in\mathbb{R}} |\mu(\{y\})|^2,$$

which finishes the proof. □

To apply this result to our situation, observe that the subspaces $\mathfrak{H}_{ac}$, $\mathfrak{H}_{sc}$, and $\mathfrak{H}_{pp}$ are invariant with respect to time evolution since $P^{xx}U(t) = \chi_{M_{xx}}(A)\exp(-\mathrm{i}tA) = \exp(-\mathrm{i}tA)\chi_{M_{xx}}(A) = U(t)P^{xx}$, $xx \in \{ac, sc, pp\}$. Moreover, if $\psi \in \mathfrak{H}_{xx}$, we have $P^{xx}\psi = \psi$, which shows $\langle\varphi, f(A)\psi\rangle = \langle\varphi, P^{xx} f(A)\psi\rangle = \langle P^{xx}\varphi, f(A)\psi\rangle$ implying $d\mu_{\varphi,\psi} = d\mu_{P^{xx}\varphi,\psi}$. Thus if μ_ψ is *ac*, *sc*, or *pp*, so is $\mu_{\varphi,\psi}$ for every $\varphi\in\mathfrak{H}$.

That is, if $\psi \in \mathfrak{H}_c = \mathfrak{H}_{ac}\oplus\mathfrak{H}_{sc}$, then the Cesàro mean of $\langle\varphi, U(t)\psi\rangle$ tends to zero. In other words, the average of the probability of finding the system in any prescribed state tends to zero if we start in the continuous subspace $\mathfrak{H}_c$ of A.

If $\psi\in\mathfrak{H}_{ac}$, then $d\mu_{\varphi,\psi}$ is absolutely continuous with respect to Lebesgue measure and thus $\hat{\mu}_{\varphi,\psi}(t)$ is continuous and tends to zero as $|t|\to\infty$. In fact, this follows from the Riemann-Lebesgue lemma (see Lemma 7.6 below).

Now we want to draw some additional consequences from Wiener's theorem. This will eventually yield a dynamical characterization of the continuous and pure point spectrum due to Ruelle, Amrein, Gorgescu, and Enß. But first we need a few definitions.

An operator $K\in\mathfrak{L}(\mathfrak{H})$ is called a **finite rank operator** if its range is finite dimensional. The dimension

$$\mathrm{rank}(K) = \dim \mathrm{Ran}(K)$$

is called the **rank** of K. If $\{\psi_j\}_{j=1}^n$ is an orthonormal basis for $\mathrm{Ran}(K)$, we have

$$K\psi = \sum_{j=1}^n \langle\psi_j, K\psi\rangle\psi_j = \sum_{j=1}^n \langle\varphi_j, \psi\rangle\psi_j, \tag{5.10}$$

where $\varphi_j = K^*\psi_j$. The elements φ_j are linearly independent since $\mathrm{Ran}(K) = \mathrm{Ker}(K^*)^\perp$. Hence every finite rank operator is of the form (5.10). In addition, the adjoint of K is also finite rank and is given by

$$K^*\psi = \sum_{j=1}^n \langle\psi_j, \psi\rangle\varphi_j. \tag{5.11}$$

The closure of the set of all finite rank operators in $\mathfrak{L}(\mathfrak{H})$ is called the set of **compact operators** $\mathfrak{C}(\mathfrak{H})$. It is straightforward to verify (Problem 5.2)

Lemma 5.5. *The set of all compact operators $\mathfrak{C}(\mathfrak{H})$ is a closed $*$-ideal in $\mathfrak{L}(\mathfrak{H})$.*

There is also a weaker version of compactness which is useful for us. The operator K is called **relatively compact** with respect to A if

$$KR_A(z) \in \mathfrak{C}(\mathfrak{H}) \tag{5.12}$$

for one $z \in \rho(A)$. By the first resolvent formula this then follows for all $z \in \rho(A)$. In particular we have $\mathfrak{D}(A) \subseteq \mathfrak{D}(K)$.

Now let us return to our original problem.

Theorem 5.6. *Let A be self-adjoint and suppose K is relatively compact. Then*

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \|K\mathrm{e}^{-\mathrm{i}tA}P^c\psi\|^2 dt = 0 \qquad \text{and} \qquad \lim_{t\to\infty} \|K\mathrm{e}^{-\mathrm{i}tA}P^{ac}\psi\| = 0 \tag{5.13}$$

for every $\psi \in \mathfrak{D}(A)$. If, in addition, K is bounded, then the result holds for any $\psi \in \mathfrak{H}$.

Proof. Let $\psi \in \mathfrak{H}_c$, respectively, $\psi \in \mathfrak{H}_{ac}$, and drop the projectors. Then, if K is a rank one operator (i.e., $K = \langle\varphi_1, .\rangle\varphi_2$), the claim follows from Wiener's theorem, respectively, the Riemann-Lebesgue lemma. Hence it holds for any finite rank operator K.

If K is compact, there is a sequence K_n of finite rank operators such that $\|K - K_n\| \le 1/n$ and hence

$$\|K\mathrm{e}^{-\mathrm{i}tA}\psi\| \le \|K_n\mathrm{e}^{-\mathrm{i}tA}\psi\| + \frac{1}{n}\|\psi\|.$$

Thus the claim holds for any compact operator K.

If $\psi \in \mathfrak{D}(A)$, we can set $\psi = (A-\mathrm{i})^{-1}\varphi$, where $\varphi \in \mathfrak{H}_c$ if and only if $\psi \in \mathfrak{H}_c$ (since $\mathfrak{H}_c$ reduces A). Since $K(A+\mathrm{i})^{-1}$ is compact by assumption, the claim can be reduced to the previous situation. If K is also bounded, we can find a sequence $\psi_n \in \mathfrak{D}(A)$ such that $\|\psi - \psi_n\| \le 1/n$ and hence

$$\|K\mathrm{e}^{-\mathrm{i}tA}\psi\| \le \|K\mathrm{e}^{-\mathrm{i}tA}\psi_n\| + \frac{1}{n}\|K\|,$$

concluding the proof. □

With the help of this result we can now prove an abstract version of the RAGE theorem.

Theorem 5.7 (RAGE). *Let A be self-adjoint. Suppose $K_n \in \mathfrak{L}(\mathfrak{H})$ is a sequence of relatively compact operators which converges strongly to the identity. Then*

$$\begin{aligned}\mathfrak{H}_c &= \{\psi \in \mathfrak{H} | \lim_{n\to\infty} \lim_{T\to\infty} \frac{1}{T}\int_0^T \|K_n \mathrm{e}^{-\mathrm{i}tA}\psi\| dt = 0\},\\ \mathfrak{H}_{pp} &= \{\psi \in \mathfrak{H} | \lim_{n\to\infty} \sup_{t\geq 0} \|(\mathbb{I} - K_n)\mathrm{e}^{-\mathrm{i}tA}\psi\| = 0\}.\end{aligned} \tag{5.14}$$

Proof. Abbreviate $\psi(t) = \exp(-\mathrm{i}tA)\psi$. We begin with the first equation.

Let $\psi \in \mathfrak{H}_c$. Then

$$\frac{1}{T}\int_0^T \|K_n\psi(t)\| dt \leq \left(\frac{1}{T}\int_0^T \|K_n\psi(t)\|^2 dt\right)^{1/2} \to 0$$

by Cauchy–Schwarz and the previous theorem. Conversely, if $\psi \notin \mathfrak{H}_c$, we can write $\psi = \psi^c + \psi^{pp}$. By our previous estimate it suffices to show $\|K_n\psi^{pp}(t)\| \geq \varepsilon > 0$ for n large. In fact, we even claim

$$\lim_{n\to\infty} \sup_{t\geq 0} \|K_n\psi^{pp}(t) - \psi^{pp}(t)\| = 0. \tag{5.15}$$

By the spectral theorem, we can write $\psi^{pp}(t) = \sum_j \alpha_j(t)\psi_j$, where the ψ_j are orthonormal eigenfunctions and $\alpha_j(t) = \exp(-\mathrm{i}t\lambda_j)\alpha_j$. Truncate this expansion after N terms. Then this part converges uniformly to the desired limit by strong convergence of K_n. Moreover, by Lemma 1.14 we have $\|K_n\| \leq M$, and hence the error can be made arbitrarily small by choosing N large.

Now let us turn to the second equation. If $\psi \in \mathfrak{H}_{pp}$, the claim follows by (5.15). Conversely, if $\psi \notin \mathfrak{H}_{pp}$, we can write $\psi = \psi^c + \psi^{pp}$ and by our previous estimate it suffices to show that $\|(\mathbb{I} - K_n)\psi^c(t)\|$ does not tend to 0 as $n \to \infty$. If it did, we would have

$$\begin{aligned}0 &= \lim_{T\to\infty} \frac{1}{T}\int_0^T \|(\mathbb{I} - K_n)\psi^c(t)\|^2 dt\\ &\geq \|\psi^c(t)\|^2 - \lim_{T\to\infty} \frac{1}{T}\int_0^T \|K_n\psi^c(t)\|^2 dt = \|\psi^c(t)\|^2,\end{aligned}$$

a contradiction. □

In summary, regularity properties of spectral measures are related to the long time behavior of the corresponding quantum mechanical system. However, a more detailed investigation of this topic is beyond the scope of this manuscript. For a survey containing several recent results, see [**28**].

It is often convenient to treat the observables as time dependent rather than the states. We set

$$K(t) = \mathrm{e}^{\mathrm{i}tA} K \mathrm{e}^{-\mathrm{i}tA} \tag{5.16}$$

and note

$$\langle \psi(t), K\psi(t)\rangle = \langle \psi, K(t)\psi\rangle, \qquad \psi(t) = \mathrm{e}^{-\mathrm{i}tA}\psi. \tag{5.17}$$

This point of view is often referred to as the **Heisenberg picture** in the physics literature. If K is unbounded, we will assume $\mathfrak{D}(A) \subseteq \mathfrak{D}(K)$ such that the above equations make sense at least for $\psi \in \mathfrak{D}(A)$. The main interest is the behavior of $K(t)$ for large t. The strong limits are called **asymptotic observables** if they exist.

Theorem 5.8. *Suppose A is self-adjoint and K is relatively compact. Then*

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}tA} K \mathrm{e}^{-\mathrm{i}tA}\psi dt = \sum_{\lambda\in\sigma_p(A)} P_A(\{\lambda\}) K P_A(\{\lambda\})\psi, \quad \psi \in \mathfrak{D}(A). \tag{5.18}$$

If K is in addition bounded, the result holds for any $\psi \in \mathfrak{H}$.

Proof. We will assume that K is bounded. To obtain the general result, use the same trick as before and replace K by $KR_A(z)$. Write $\psi = \psi^c + \psi^{pp}$. Then

$$\lim_{T\to\infty} \frac{1}{T}\| \int_0^T K(t)\psi^c dt\| \le \lim_{T\to\infty} \frac{1}{T}\int_0^T \|K(t)\psi^c dt\| = 0$$

by Theorem 5.6. As in the proof of the previous theorem we can write $\psi^{pp} = \sum_j \alpha_j \psi_j$ and hence

$$\sum_j \alpha_j \frac{1}{T}\int_0^T K(t)\psi_j dt = \sum_j \alpha_j \left(\frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}t(A-\lambda_j)} dt\right) K\psi_j.$$

As in the proof of Wiener's theorem, we see that the operator in parentheses tends to $P_A(\{\lambda_j\})$ strongly as $T \to \infty$. Since this operator is also bounded by 1 for all T, we can interchange the limit with the summation and the claim follows. □

We also note the following corollary.

Corollary 5.9. *Under the same assumptions as in the RAGE theorem we have*

$$\lim_{n\to\infty}\lim_{T\to\infty} \frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}tA} K_n \mathrm{e}^{-\mathrm{i}tA}\psi dt = P^{pp}\psi, \tag{5.19}$$

respectively,

$$\lim_{n\to\infty}\lim_{T\to\infty} \frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}tA} (\mathbb{I} - K_n) \mathrm{e}^{-\mathrm{i}tA}\psi dt = P^{c}\psi. \tag{5.20}$$

Problem 5.2. *Prove Lemma 5.5.*

Problem 5.3. *Prove Corollary 5.9.*

5.3. The Trotter product formula

In many situations the operator is of the form $A+B$, where $\mathrm{e}^{\mathrm{i}tA}$ and $\mathrm{e}^{\mathrm{i}tB}$ can be computed explicitly. Since A and B will not commute in general, we cannot obtain $\mathrm{e}^{\mathrm{i}t(A+B)}$ from $\mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{\mathrm{i}tB}$. However, we at least have

Theorem 5.10 (Trotter product formula)**.** *Suppose A, B, and $A+B$ are self-adjoint. Then*

$$\mathrm{e}^{\mathrm{i}t(A+B)} = \operatorname*{s-lim}_{n\to\infty} \left(\mathrm{e}^{\mathrm{i}\frac{t}{n}A}\,\mathrm{e}^{\mathrm{i}\frac{t}{n}B}\right)^n. \tag{5.21}$$

Proof. First of all note that we have

$$\begin{aligned}&\left(\mathrm{e}^{\mathrm{i}\tau A}\mathrm{e}^{\mathrm{i}\tau B}\right)^n - \mathrm{e}^{\mathrm{i}t(A+B)}\\ &\quad= \sum_{j=0}^{n-1}\left(\mathrm{e}^{\mathrm{i}\tau A}\,\mathrm{e}^{\mathrm{i}\tau B}\right)^{n-1-j}\left(\mathrm{e}^{\mathrm{i}\tau A}\,\mathrm{e}^{\mathrm{i}\tau B} - \mathrm{e}^{\mathrm{i}\tau(A+B)}\right)\left(\mathrm{e}^{\mathrm{i}\tau(A+B)}\right)^j,\end{aligned}$$

where $\tau = \frac{t}{n}$, and hence

$$\|(\mathrm{e}^{\mathrm{i}\tau A}\mathrm{e}^{\mathrm{i}\tau B})^n - \mathrm{e}^{\mathrm{i}t(A+B)}\psi\| \le |t| \max_{|s|\le|t|} F_\tau(s),$$

where

$$F_\tau(s) = \|\frac{1}{\tau}(\mathrm{e}^{\mathrm{i}\tau A}\,\mathrm{e}^{\mathrm{i}\tau B} - \mathrm{e}^{\mathrm{i}\tau(A+B)})\mathrm{e}^{\mathrm{i}s(A+B)}\psi\|.$$

Now for $\psi \in \mathfrak{D}(A+B) = \mathfrak{D}(A)\cap\mathfrak{D}(B)$ we have

$$\frac{1}{\tau}(\mathrm{e}^{\mathrm{i}\tau A}\,\mathrm{e}^{\mathrm{i}\tau B} - \mathrm{e}^{\mathrm{i}\tau(A+B)})\psi \to \mathrm{i}A\psi + \mathrm{i}B\psi - \mathrm{i}(A+B)\psi = 0$$

as $\tau\to 0$. So $\lim_{\tau\to0} F_\tau(s) = 0$ at least pointwise, but we need this uniformly with respect to $s\in[-|t|,|t|]$.

Pointwise convergence implies

$$\|\frac{1}{\tau}(\mathrm{e}^{\mathrm{i}\tau A}\,\mathrm{e}^{\mathrm{i}\tau B} - \mathrm{e}^{\mathrm{i}\tau(A+B)})\psi\| \le C(\psi)$$

and, since $\mathfrak{D}(A+B)$ is a Hilbert space when equipped with the graph norm $\|\psi\|^2_{\Gamma(A+B)} = \|\psi\|^2 + \|(A+B)\psi\|^2$, we can invoke the uniform boundedness principle to obtain

$$\|\frac{1}{\tau}(\mathrm{e}^{\mathrm{i}\tau A}\,\mathrm{e}^{\mathrm{i}\tau B} - \mathrm{e}^{\mathrm{i}\tau(A+B)})\psi\| \le C\|\psi\|_{\Gamma(A+B)}.$$

Now

$$\begin{aligned}|F_\tau(s) - F_\tau(r)| &\le \|\frac{1}{\tau}(\mathrm{e}^{\mathrm{i}\tau A}\,\mathrm{e}^{\mathrm{i}\tau B} - \mathrm{e}^{\mathrm{i}\tau(A+B)})(\mathrm{e}^{\mathrm{i}s(A+B)} - \mathrm{e}^{\mathrm{i}r(A+B)})\psi\|\\ &\le C\|(\mathrm{e}^{\mathrm{i}s(A+B)} - \mathrm{e}^{\mathrm{i}r(A+B)})\psi\|_{\Gamma(A+B)}\end{aligned}$$

shows that $F_\tau(.)$ is uniformly continuous and the claim follows by a standard $\frac{\varepsilon}{2}$ argument. □

If the operators are semi-bounded from below, the same proof shows

Theorem 5.11 (Trotter product formula)**.** *Suppose A, B, and $A+B$ are self-adjoint and semi-bounded from below. Then*

$$\mathrm{e}^{-t(A+B)} = \operatorname*{s-lim}_{n\to\infty} \left(\mathrm{e}^{-\frac{t}{n}A}\,\mathrm{e}^{-\frac{t}{n}B}\right)^n, \quad t \geq 0. \tag{5.22}$$

Problem 5.4. *Prove Theorem 5.11.*