Abstract

In this tutorial we collect facts from the theory of self-adjoint operators, mostly with a view of what is relevant for applications in mathematical quantum mechanics, in particular for solving the Schrödinger equation. Specific topics include the spectral theorem and functional calculus for self-adjoint operators, Stone’s Theorem, Laplacians and Fourier transform, Duhamel’s formula and Dyson series, time-evolution of non-interacting quantum systems, as well as the Baker-Campbell-Hausdorff formula and Trotter product formula.

We assume that the user of these notes is familiar with basic functional analysis and linear operator theory in Hilbert spaces. In most instances we don’t provide proofs. Details on both, basic background as well as proofs, can be found in numerous books, such as [1, 3, 4, 5, 6].

1 Self-Adjoint Operators

Let $\mathcal{H}$ be a separable complex Hilbert space with inner product $\langle \cdot, \cdot \rangle$, which we choose linear in the second argument and conjugate-linear in the first argument. Let $T$ be a densely defined linear operator in $\mathcal{H}$, i.e. $T : D(T) \to \mathcal{H}$ linear with $D(T)$ dense in $\mathcal{H}$.

The adjoint $T^*$ of $T$ is the linear operator in $\mathcal{H}$ defined by

$$D(T^*) = \{ g \in \mathcal{H} : \exists h \in \mathcal{H} \text{ such that } \langle h, f \rangle = \langle g, Tf \rangle \text{ for all } f \in D(T) \}$$

$$T^* g = h.$$  

$T$ is called self-adjoint if $T^* = T$ (which includes the requirement $D(T^*) = D(T)$).

Self-adjoint operators $T$ are hermitean (defined as $\langle Tg, f \rangle = \langle g, Tf \rangle$ for all $f, g \in D(T)$) and symmetric (meaning that $T^*$ is an extension of $T$).

For unbounded operators these three properties are not equivalent. However, if $T \in B(\mathcal{H})$, the bounded and everywhere defined operators on $\mathcal{H}$, then hermitean, symmetric and self-adjoint all have the same meaning.

The resolvent set of a linear operator $T$ in $\mathcal{H}$ is given by

$$\rho(T) = \{ z \in \mathbb{C} : T - z \text{ is injective and } (T - z)^{-1} \in B(\mathcal{H}) \}$$
and \((T - z)^{-1}\) is referred to as the resolvent of \(T\) at \(z\).

The spectrum of \(T\) is the complement of the resolvent set,

\[
\sigma(T) = \mathbb{C} \setminus \rho(T).
\]

The resolvent set is open in \(\mathbb{C}\) and thus the spectrum a closed subset of \(\mathbb{C}\).

For symmetric and, in particular, self-adjoint operators \(T\) the spectrum is real, \(\sigma(T) \subset \mathbb{R}\).

2 The Spectral Theorem for Self-Adjoint Operators

There are at least two good reasons for the prominence of self-adjoint operators in mathematical physics (and for why they are preferred over hermitean and symmetric operators). One reason is mathematical and given by the spectral theorem for self-adjoint operators, discussed in this section. The other reason is physical and given by Stone’s Theorem, discussed in the next section.

2.1 Spectral Theorem

A spectral family \(E\) in \(\mathcal{H}\) is a family of orthogonal projections \(E(t), t \in \mathbb{R}\), in \(\mathcal{H}\) with the properties

(a) \(E(s) \leq E(t)\) if \(s \leq t\) (in the sense that \(\langle f, E(s)f \rangle \leq \langle f, E(t)f \rangle\) for all \(f \in \mathcal{H}\)),
(b) \(E\) is strongly right-continuous, i.e. \(\lim_{\varepsilon \to 0^+} E(t + \varepsilon)f = E(t)f\) for all \(t \in \mathbb{R}\) and \(f \in \mathcal{H}\),
(c) \(E(t) \to 0\) strongly as \(t \to -\infty\) and \(E(t) \to I\) strongly as \(t \to \infty\).

The spectral theorem established a one-to-one correspondence between self-adjoint operators and spectral families:

**Theorem 2.1 (Spectral Theorem).** For every self-adjoint operator \(T\) there exists a spectral family \(E\) such that

\[
T = \int_{\mathbb{R}} t \, dE(t).
\]

Vice versa, to every spectral family \(E\) the right hand side of (5) defines a self-adjoint operator \(T\).

In the case of unbounded self-adjoint operators \(T\), the correct interpretation of (5) needs some care for which we refer to the literature. For bounded self-adjoint \(T\), which are characterized by their associated sesquilinear form \(\langle \cdot, T \cdot \rangle\), (5) is equivalent to its weak form

\[
\langle g, Tf \rangle = \int_{\mathbb{R}} t \, d\langle g, E(t)f \rangle
\]

for all \(f, g \in \mathcal{H}\). Here \(d\langle g, E(\cdot)f \rangle\) is the complex Borel measure on \(\mathbb{R}\) defined via polarization as

\[
\frac{1}{4}(\rho_{g+f} - \rho_{g-f} + i\rho_{g-if} - i\rho_{g+if}),
\]

for all \(f, g \in \mathcal{H}\). Here \(\rho_{g+f}\) denotes the complex spectral measure of \(T\) associated with \(g + f\).
where $\rho_f$ is the bounded Borel measure with distribution function $\rho_f(t) = \langle f, E(t)f \rangle$. As a special case we have

$$\langle f, Tf \rangle = \int t \, d\rho_f(t). \quad (8)$$

For a given self-adjoint operator $T$ the spectral family $E$ can be found from Stone’s formula

$$\langle g, (E(b) - E(a))f \rangle = \lim_{\delta \to 0+} \lim_{\epsilon \to 0+} \frac{1}{2\pi i} \int_{a+\delta}^{b+\delta} \langle g, ((T - t - i\epsilon)^{-1} - (T - t + i\epsilon)^{-1})f \rangle \, dt. \quad (9)$$

This formula (or one of its close relatives) is central to the proof of the Spectral Theorem, where it is shown that (9) indeed defines a spectral family and that (5) holds with this choice of $E$. However, in applications to concrete self-adjoint operators $T$ one usually tries to exploit specific properties of $T$ for a more direct approach to studying its spectral family (see, for example, Section 4 below).

Two of the most important applications of the spectral theorem are the introduction of a functional calculus for self-adjoint operators as well as the definition of spectral types.

### 2.2 Functional Calculus

For Borel functions $u : \mathbb{R} \to \mathbb{C}$ and a self-adjoint operator $T$ with spectral family $E$ one defines the operator

$$u(T) = \int u(t) \, dE(t), \quad (10)$$

which, as above, is best interpreted in weak sense. Among the useful properties of the functional calculus defined via (10) are:

- If $u$ is bounded, then $u(T) \in B(H)$ with $\|u(T)\| \leq \sup |u|$.
- $(u \pm v)(T) = u(T) \pm v(T)$ and $(uv)(T) = u(T)v(T)$ (up to suitable domain considerations if $u$ and/or $v$ are unbounded).
- For functions $u$ where $u(T)$ can be defined in other natural ways, this definition will coincide with the one via the functional calculus, for example
  - If $v_z(t) = \frac{1}{t-z}$ and $z \in \rho(T)$, then $v_z(T) = (T - z)^{-1}$.
  - For polynomials $u(t) = \sum_{j=0}^{n} c_j t^j$ one gets $u(T) = \sum_{j=0}^{n} c_j T^j$.
  - If $T$ is bounded and $u$ is analytic in an open disc $\{ z \in \mathbb{C} : |z - a| < r \}$ containing $\sigma(T)$ and with Taylor series $u(t) = \sum_{j=0}^{\infty} c_j (t - a)^j$, then $u(T) = \sum_{j=0}^{\infty} c_j (T - a)^j$, where the series converges in operator norm.

### 2.3 Spectral Types

The bounded Borel measures $\rho_f$ have unique Lebesgue decompositions

$$\rho_f = \rho_f^{ac} + \rho_f^{sc} + \rho_f^{pp} \quad (11)$$
into absolutely continuous, singular continuous and pure point measures. This can be used to define the \textit{absolutely continuous spectrum} \( \sigma_{ac}(T) \), the \textit{singular continuous spectrum} \( \sigma_{sc}(T) \) and the \textit{pure point spectrum} \( \sigma_{pp}(T) \) of \( T \) via

\[
\sigma_{\bullet}(T) = \bigcup_{f \in \mathcal{H}} \text{supp} \, \rho_f^\bullet
\]

for \( \bullet \in \{ac, sc, pp\} \). Here the support of a Borel measure \( \rho \) on \( \mathbb{R} \) is defined as

\[
\text{supp} \, \rho = \{ t : \rho((t - \varepsilon, t + \varepsilon)) > 0 \text{ for all } \varepsilon > 0 \}.
\]

The set

\[
\mathcal{H}_{ac}(T) = \{ f \in \mathcal{H} : \rho_f \text{ is purely absolutely continuous} \}
\]

is a reducing subspace for \( T \), the \textit{absolutely continuous subspace} of \( \mathcal{H} \) with respect to \( T \). The restriction \( T_{ac} \) of \( T \) to \( \mathcal{H}_{ac}(T) \) is the \textit{absolutely continuous part} of \( T \) and satisfies \( \sigma(T_{ac}) = \sigma_{ac}(T) \).

Similarly, one defines the \textit{singular continuous and pure point subspaces} \( \mathcal{H}_{sc}(T) \) and \( \mathcal{H}_{pp}(T) \), as well as the \textit{singular continuous and pure point parts} \( T_{sc} \) and \( T_{pp} \) of \( T \). One has

\[
\mathcal{H} = \mathcal{H}_{ac}(T) \oplus \mathcal{H}_{sc}(T) \oplus \mathcal{H}_{ac}(T) \quad \text{and} \quad T = T_{ac} \oplus T_{sc} \oplus T_{pp}.
\]

3 \textbf{Solving the Schrödinger Equation and Stone’s Theorem}

In quantum mechanics (at least in its version due to Schrödinger) the state of a quantum mechanical system at time \( t \) is given by a normalized vector \( \psi(t) \) in a Hilbert space \( \mathcal{H} \). For a system in initial state \( \psi_0 \in \mathcal{H} \) at \( t = 0 \) one finds \( \psi(t) \) by solving the \textit{Schrödinger equation}

\[
i \partial_t \psi(t) = H \psi(t), \quad \psi(0) = \psi_0,
\]

where we have set Planck’s constant \( h = 1 \). Here \( H \) is the \textit{Hamiltonian} of the system, a self-adjoint operator in \( \mathcal{H} \) representing the total energy of the system.

One can argue that self-adjointness of the Hamiltonian is necessary as well as sufficient for guaranteeing the existence of a unique solution of the Schrödinger equation which also has properties which one would like to have for physical reasons.

\textit{Sufficiency of self-adjointness} of \( H \) is a consequence of the functional calculus: For all \( t \in \mathbb{R} \) let \( u_t(x) = e^{-itx} \) and define

\[
U(t) = u_t(H) = e^{-itH}
\]

by the functional calculus. It can then be shown that \( \psi(t) = U(t)\psi_0 \) is the unique solution of (16) if \( \psi_0 \in D(H) \) (in this case one finds that \( \psi(t) \in \mathcal{H} \) for all \( t \) and \( \partial_t \psi(t) = -iH\psi(t) \) in the sense of a derivative of an \( \mathcal{H} \)-valued function). For unbounded Hamiltonians \( H \), one generally interprets \( U(t)\psi_0 \) as a solution of the Schrödinger equation even if \( \psi_0 \) is not in the domain of \( H \).
\[ U(t) = e^{-itH} \] is referred to as the time evolution of the Hamiltonian \( H \).

The solution \( \psi(t) = U(t)\psi_0 \) also has properties which one would expect from the time evolution of a state in a closed quantum mechanical system. Mathematically, this is expressed by the fact that \( U = (U(t))_{t \in \mathbb{R}} \) is a strongly continuous one-parameter unitary group (SCOUG). This means that

- \( U(t) \) is unitary in \( \mathcal{H} \) for all \( t \in \mathbb{R} \),
- \( U(0) = I \) and \( U(t+s) = U(t)U(s) \) for all \( t, s \in \mathbb{R} \), and
- \( U(t)f \to U(s)f \) as \( t \to s \) for all \( f \in \mathcal{H} \).

In particular, unitarity of \( U \) means that the solution \( \psi(t) = U(t)\psi_0 \) preserves the norm of \( \psi_0 \), which was assumed to be one. In the canonical case where \( \mathcal{H} \) is an \( L^2 \)-space over the configuration space \( X \) of the system (with suitable measure), preservation of the \( L^2 \)-norm is crucial for the probabilistic (Born) interpretation of quantum mechanical waves. According to this interpretation,

\[ p_{E,t} = \| \chi_E \psi(t) \|^2 \] (18)

is the probability that the system will be in a configuration \( x \in E \) at time \( t \), where \( E \) is any measurable subset of \( X \).

If one works under the reasonable postulate that the time-evolution of a quantum system should be governed by a SCOUG, then the necessity of self-adjointness of the Hamiltonian is a consequence of Stone’s Theorem:

**Theorem 3.1** (Stone). If \( A \) is the infinitesimal generator of a SCOUG, then \( H = iA \) is self-adjoint.

Here the infinitesimal generator \( A \) of \( U \) is defined as

\[ D(A) = \{ f \in \mathcal{H} : g = \lim_{h \to 0} \frac{1}{h} (U(h)f - f) \text{ exists} \}, \quad Af = g. \] (19)

Assume that \( H \) is the Hamiltonian of a quantum system and the Schrödinger equation (16) is solved by \( \psi(t) = U(t)\psi_0 \), where \( \psi_0 \in D(H) \) and \( U(\cdot) \) is a SCOUG with generator \( A \). Then, in particular,

\[ -iH\psi_0 = \psi'(0) = \lim_{h \to 0} \frac{1}{h} (U(h)\psi_0 - \psi_0). \] (20)

Thus \( \psi_0 \in D(A) \) and \( -iH\psi_0 = A\psi_0 \). Vice versa, if \( \psi_0 \in D(A) \), then \( U(t)\psi_0 \) solves (16) with \( H = iA \), meaning that we can only gain by choosing the domain of \( H \) at least as large as the domain of \( A \).

We combine this to get \( D(A) = D(H) \) and \( H = iA \). Thus, by Stone’s Theorem, \( H \) is self-adjoint.
4 Calculating Time-Evolutions

Stone’s formula (9) and the functional calculus (10) can, at least in principle, be used to determine the time-evolution \( U(t) = e^{-itH} \) of a self-adjoint Hamiltonian \( H \). However, in most applications one takes a different approach. This exploits that Hamiltonians can often be written in the form

\[
H = H_0 + V,
\]

where the time-evolution of \( H_0 \) can be found explicitly and \( V \) can be considered as a perturbation of \( H_0 \) (in suitable sense). Often, but not always, \( H_0 \) and \( V \) correspond to the kinetic and potential energy of the quantum mechanical system.

4.1 Fourier transform

Let us discuss only the continuous and discrete Laplacians as the two most important examples of the kinetic energy operator \( H_0 \). Both of these are translation invariant, one in the continuum and one on the lattice \( \mathbb{Z}^d \), meaning that both of them can be diagonalized via Fourier transforms:

The **continuous d-dimensional Laplacian** is the self-adjoint operator

\[
H_0 = -\Delta
\]

in \( \mathcal{H} = L^2(\mathbb{R}^d) \) with domain \( D(H_0) = H^2(\mathbb{R}^d) \), the second order Sobolev space (i.e. the space of those \( L^2 \)-functions whose weak derivatives up to second order are still in \( L^2 \)).

The continuum Fourier transform on \( \mathbb{R}^d \) is the unitary operator \( F_c : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d) \) defined by

\[
(F_c f)(y) = \text{l.i.m.}_{L \to \infty} (2\pi)^{-d/2} \int_{[-L,L]^d} f(x) e^{-iy \cdot x} \, dx,
\]

\[
(F_c^{-1} g)(x) = \text{l.i.m.}_{L \to \infty} (2\pi)^{-d/2} \int_{[-L,L]^d} g(y) e^{-iy \cdot x} \, dy,
\]

where l.i.m. denotes the \( L^2 \)-limit of functions in \( y \) and \( x \), respectively. One has the unitary equivalence

\[
-\Delta = F_c |x|^2 F_c^{-1},
\]

where, somewhat sloppily, \( |x|^2 \) stands for the maximal multiplication operator with the function \( |x|^2 = \sum_{j=1}^d x_j^2 \). This gives the representation

\[
e^{-it(-\Delta)} = F_c e^{-it|x|^2} F_c^{-1}
\]

for the time-evolution of the Laplacian. From this one can derive the explicit formula

\[
(e^{-it(-\Delta)} f)(x) = \text{l.i.m.}_{L \to \infty} (4\pi it)^{-d/2} \int_{[-L,L]^d} e^{i|x-y|^2/4t} f(y) \, dy,
\]

see e.g. [4].
The $d$-dimensional discrete Laplacian is the bounded self-adjoint operator $h_0$ on $\ell^2(\mathbb{Z}^d)$ given by
\begin{equation}
(h_0f)(x) = -\sum_{y \in \mathbb{Z}^d, |x-y|=1} f(y) \quad \text{for all } x \in \mathbb{Z}^d.
\end{equation}
Here $|x| = \sum_j |x_j|$ is the 1-norm. More appropriately, $h_0$ should be referred to as the (negative) adjacency operator on $\mathbb{Z}^d$, as it differs from the “correct” discrete Laplacian by $2dI$. But the effects of this shift are trivial, so that it is frequently neglected.

With the discrete Fourier transform $F_d : L^2([0,2\pi)^d) \to \ell^2(\mathbb{Z}^d)$ given by
\begin{equation}
(F_df)(n) = (2\pi)^{-d/2} \int_{[0,2\pi)^d} f(x) e^{-in \cdot x} \, dx,
\end{equation}
\begin{equation}
(F_d^{-1}g)(x) = \text{l.i.m.}_{L \to \infty} (2\pi)^{-d/2} \sum_{n \in \mathbb{Z}^d, |n| \leq L} g(n) e^{inx},
\end{equation}
one has
\begin{equation}
h_0 = F_d \left( -2 \sum_{j=1}^d \cos(x_j) \right) F_d^{-1}.
\end{equation}
While this allows to represent the time-evolution of $h_0$ as
\begin{equation}
e^{-ith_0} = F_d e^{-it(-2\sum_j \cos(x_j))} F_d^{-1},
\end{equation}
it does not lead to an explicit formula quite as simple as (27).

4.2 Duhamel’s Formula and Dyson Series

Once the “free” time-evolution $e^{-itH_0}$ is well understood, one can study the time evolution of $H = H_0 + V$ by perturbative methods. The basic tool for this is Duhamel’s formula which, for simplicity, we state here only for bounded $V$, while it also holds for certain unbounded perturbations (e.g. those which are relatively $H_0$-bounded with relative bound less than one).

**Theorem 4.1** (Duhamel’s Formula). Let $H_0$ be self-adjoint and $V$ bounded and symmetric in $\mathcal{H}$ and $H = H_0 + V$. Then
\begin{equation}
e^{-itH} \psi_0 = e^{-itH_0} \psi_0 + (-i) \int_0^t e^{-i(t-t_1)H_0} Ve^{-it_1H} \psi_0 \, dt_1
\end{equation}
for every $\psi_0 \in \mathcal{H}$.

Observe that the integrand on the right of (33) is continuous, so that the integral (as well as other integrals appearing below) can be interpreted as a Riemann integral of an $\mathcal{H}$-valued function.

**Proof.** The proof of (33) proceeds by differentiation and subsequent integration: For $\psi_0 \in D(H_0) = D(H)$ one has by an operator version of the product rule
\begin{align}
\frac{d}{dt} e^{itH_0} e^{-itH} \psi_0 &= e^{itH_0} iH_0 e^{-itH} \psi_0 - e^{itH_0} iHe^{-itH} \psi_0 \\
&= -ie^{itH_0} Ve^{-itH} \psi_0.
\end{align}
This is now integrated to yield

\[ e^{itH_0} e^{-itH} \psi_0 - \psi_0 = (-i) \int_0^t e^{it_1 H_0} V e^{-it_1 H} \psi_0 \, dt_1, \quad (36) \]

from which (33) follows after multiplying by \( e^{-itH_0} \). This extends to general \( \psi_0 \), as both sides of (33) are bounded operators.

In some cases (33) can be used directly to obtain information on \( e^{-itH} \) by using bounds on the integral. In other cases, one may exploit that (33) can be iterated, i.e. one may express \( e^{-itH} \psi_0 \) under the integral by another application of Duhamel’s formula. This leads to the Dyson series:

**Theorem 4.2 (Dyson Series).** Let \( H_0 \) be self-adjoint and \( V \) bounded and symmetric, and \( \psi_0 \in \mathcal{H} \). Then

\[ e^{-itH} \psi_0 = e^{-itH_0} \psi_0 + \sum_{n=1}^{\infty} (-i)^n \int_0^t \int_0^{t_1} \ldots \int_0^{t_{n-1}} e^{-i(t-t_1)H_0} V \left( \prod_{k=1}^{n-1} e^{-i(t_k-t_{k+1})H_0} V \right) e^{-it_n H_0} \psi_0 \, dt_n \ldots dt_2 \, dt_1, \quad (37) \]

with convergence of the series in operator norm.

**Proof.** Iterating (33) \( \ell \) times gives a partial sum from \( n = 1 \) to \( n = \ell \) for the series in (37), with the \( \ell \)-th term being replaced by

\[ (-i)^\ell \int_0^t \int_0^{t_1} \ldots \int_0^{t_{\ell-1}} e^{-i(t-t_1)H_0} V \left( \prod_{k=1}^{\ell-1} e^{-i(t_k-t_{k+1})H_0} V \right) e^{-it\ell H} \psi_0 \, dt_\ell \ldots dt_2 \, dt_1, \quad (38) \]

note the \( H \) in the last term under the integral. The integral (38) defines a bounded operator with norm at most \( \frac{\|t\|}{\ell !} \|V\|^{\ell} \). Thus the partial sums converge to the series (37) in operator norm.

\[ \square \]

4.3 **Non-interacting systems, Baker-Campbell-Hausdorff and Trotter**

The simplest case for calculating the time-evolution of an additive Hamiltonian \( H = A + B \) is when \( A \) and \( B \) commute, \([A, B] = 0\). Then

\[ e^{-it(A+B)} = e^{-itA} e^{-itB}. \quad (39) \]

If \( A \) and \( B \) are bounded self-adjoint operators, then this follows with essentially the same proof as for the “ordinary” exponential function (also using the last remark in Section 2.2 above. However, (39) also extends to suitable classes of unbounded self-adjoint operators.

For example, the Hamiltonian of a quantum system consisting of two non-interacting subsystems governed by Hamiltonians \( H_1, H_2 \) in Hilbert spaces \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \) is given by

\[ H = H_1 \otimes I + I \otimes H_2 \quad \text{in} \quad \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2. \quad (40) \]
Here the closure on the right is necessary if \( H_1 \) and \( H_2 \) are both unbounded. \( H_1 \otimes I \) and \( I \otimes H_2 \) commute, which leads to
\[
e^{-itH} = e^{-it(H_1 \otimes I)} e^{-it(I \otimes H_2)} = (e^{-itH_1} \otimes I)(I \otimes e^{-itH_2}) \tag{41}
\]
\[
e^{-itH_1} \otimes e^{-itH_2}. \tag{42}
\]
Of course, this is what must happen physically: The two non-interacting systems evolve separately in their respective Hilbert spaces. This formula for the time-evolution of non-interacting quantum systems extends in an obvious way to systems consisting of an arbitrary finite number of non-interacting subsystems.

In some cases where operators \( A \) and \( B \) don’t commute, one may instead use the Baker-Campbell-Hausdorff formula to find the evolution of \( A + B \). In its simplest version for square matrices (or bounded operators) \( A \) and \( B \) such that \([A, [A, B]] = [B, [A, B]] = 0\), the BCH formula says
\[
e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]]. \tag{43}
\]
Here matrix-exponentials are defined as Taylor series.

A proof of (43) can be sketched along exactly the same lines which were used above to prove Duhamel’s formula and the Dyson series, but with more technical effort: (i) Differentiate \( e^{-tB} e^{-tA} e^{t(A+B)} \), using that \([B, e^{-tA}] = -t[B, A] e^{-tA}\) to simplify the result, (ii) integrate over \( 0 \leq t \leq 1 \), (iii) iterate the first two steps and recognize that the power series of \( e^{t^2[A,B]/2}\) arises.

For self-adjoint \( A \) and \( B \) this gives the time evolution
\[
e^{-it(A+B)} = e^{-itA} e^{-itB} e^{\frac{t^2}{2}[A,B]} \tag{44}
\]
As a special case, at least formally, this leads to the Weyl relation
\[
e^{i(rp+sq)} = e^{-irs/2} e^{irp} e^{isq}. \tag{45}
\]
Here \( r, s \in \mathbb{R} \) and \( p \) and \( q \) are the momentum and position operators in \( L^2(\mathbb{R}) \), i.e. \((pf)(x) = -if'(x), (gf)(x) = xf(x)\). They satisfy \([p, q] = -iI\), and thus, in particular, \([p, [p, q]] = [q, [p, q]] = 0\), so that formally (45) follows from (43). As \( p \) and \( q \) are unbounded operators, the rigorous proof needs a bit more care than for the case of bounded operators, but, using the theory of analytic vectors, follows essentially the same steps, see e.g. Section 5.2.1 in [2] for details.

While the BCH formula (and certain analogues for higher order commutators) apply only in very special cases, a much more generally applicable tool is the Trotter product formula. It says that if \( A, B \) and \( A + B \) (with domain \( D(A) \cap D(B) \)) are self-adjoint in \( \mathcal{H} \), then
\[
e^{-it(A+B)} f = \lim_{n \to \infty} \left( e^{-i\frac{t}{n} A} e^{-i\frac{t}{n} B} \right)^n f \tag{46}
\]
for all \( f \in \mathcal{H} \). For proofs see Theorem VIII.30 in [3] or Theorem 7.40 in [6]. In these references one can also find a semi-group version of the Trotter product formula: If \( A, B \) and \( A + B \) are semi-bounded from below, then
\[
e^{-t(A+B)} f = \lim_{n \to \infty} \left( e^{-\frac{t}{n} A} e^{-\frac{t}{n} B} \right)^n \tag{47}
\]
for all \( f \in \mathcal{H} \) and all \( t \geq 0 \). The latter is relevant, for example, in the proof of the Feynman-Kac formula, but we won’t go into this here, see, e.g., Chapter X.11 of [4].
References


