Selfadjoint operators and solving the Schrödinger equation

A Tutorial

For some more details and references see: "Stolz 1" on conference site, in particular books by
Achiezer/Glazman, Reed/Simon, Teschl, Weidmann,
as well as ... (insert your own favorite here)

Main Goal:

Why are selfadjoint operators "necessary and sufficient" to do Quantum Mechanics?

Two reasons:

- They are great for mathematics.
- They give the right kind of physics.

Definitions:

$\mathcal{H}$ separable Hilbert space, $\langle \cdot, \cdot \rangle$

$T : D(T) \subset \mathcal{H} \mapsto \mathcal{H}$ linear, densely defined

Adjoint operator:

$$\begin{aligned} D(T^*) &= \{g \in \mathcal{H} : \exists\, h \in \mathcal{H}\, s.t.\ \langle h, f \rangle = \langle g, Tf \rangle\ \forall f \in D(T)\} \\ T^* g &= h \end{aligned}$$

T selfadjoint: $T^* = T$
T hermitean: $\langle Tg, f \rangle = \langle g, Tf \rangle\ \forall\, f, g \in D(T)$
T symmetric: T hermitean and densely defined $\Longleftrightarrow T \subset T^*$

All equivalent if $T \in B(\mathcal{H})$.

Definitions:

Resolvent set:

$$\rho(T) = \{z \in \mathbb{C} : T - z \text{ injective}, (T - z)^{-1} \in B(\mathcal{H})\}$$

Spectrum:

$$\sigma(T) = \mathbb{C} \setminus \rho(T)$$

T symmetric $\implies$ $\sigma(T) \subset \mathbb{R}$

Spectral Family:

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

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

Spectral Theorem:

For every selfadjoint operator T there exists a spectral family E such that

$$T = \int_{\mathbb{R}} t \, dE(t). \tag{1}$$

Conversely, to every spectral family E the right hand side of (1) defines a selfadjoint operator T.

Note: (1) should be interpreted weakly, i.e.

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

for all $f \in D(T)$. Via polarization this can be extended to

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

for all $f, g \in D(T)$.

Stone's Formula:

An explicit way to find the spectral family E for a given selfadjoint operator T (at least in principle) is given by Stone's formula:

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

Applications of the Spectral Theorem:

I. Functional Calculus

T s.a. with spectral family E, $u : \mathbb{R} \to \mathbb{C}$ Borel. Then

$$u(T) := \int u(t)\, dE(t)$$

Properties:

- u bounded $\Longrightarrow u(T) \in B(\mathcal{H})$, $\|u(T)\| \leq \sup |u|$
- $(u \pm v)(T) = u(T) \pm v(T)$, $(uv)(T) = u(T)v(T)$ (modulo domain issues)
- Coincides with other natural definitions where available (e.g. polynomials, power series)

Applications of the Spectral Theorem:

II. Spectral Types

Define *absolutely continuous, singular continuous, pure point spectrum* of T via a.c., s.c, p.p. parts of the spectral measures

$$d\rho_f(t) = d\langle f, E(t)f\rangle.$$

See Notes for details.

Applications of the Spectral Theorem:

III. Solving the Schrödinger equation:

Let H be s.a. in $\mathcal{H}$ and $U(t) := e^{-itH}$ for all $t \in \mathbb{R}$ (in sense of functional calculus).
Then $\psi(t) := U(t)\psi_0$ is the unique solution of the Schrödinger equation

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

Thus: Selfadjointness of the Hamiltonian H (total energy operator) is "sufficient" for Quantum Mechanics!

Unitary Groups:

A family $(U(t))_{t\in\mathbb{R}}$ is called a *strongly continuous one-parameter unitary group* (SCOUG) if

- $U(t)$ 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 $f \in \mathcal{H}$.

Stone's Theorem:

$(U(t))_{t\in\mathbb{R}}$ is a SCOUG if and only if there exists a selfadjoint operator H such that

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

Remark: The "only if" part of Stone's Theorem can be interpreted as "necessity" of selfadjointness of Hamiltonians for Quantum Mechanics:

- Unitarity of the time-evolution $U(t)$ guarantees that the norm of an initial state $\psi_c \in \mathcal{H}$ is preserved in time.
- If $\|\psi_c\|^2 = 1$ and $\mathcal{H} = L^2(X,\mu)$, then this is crucial for the Born interpretation of Quantum Mechanics:
  For all measurable $E \subset X$,

$$\begin{aligned} p_{E,t} &= \|\chi_E \psi(t)\|^2 \\ &= \text{Probability to be in a configuration } x \in E \text{ at time } t \end{aligned}$$

Calculating Time-Evolutions:

Given selfadjoint Hamiltonian H, how does one find $U(t) = e^{-itH}$?

Frequent situation:

- $H = H_0 + V$ (for example: H_0 kinetic energy, V potential energy)
- e^{-itH_0} can be found explicitly:

$$\text{Translation invariance} \Longrightarrow \text{Fouriertransform}$$

- e^{-itH} can be found (studied) by perturbative methods

Continuous and Discrete Laplacians:

Example 1: $H_0 = -\Delta$ in $L^2(\mathbb{R}^d)$ (selfadjoint on $H^2(\mathbb{R}^d)$):

$$\begin{aligned} -\Delta &= F_c |x|^2 F_c^{-1} \\ e^{-it(-\Delta)} &= F_c e^{-it|x|^2} F_c^{-1} \end{aligned}$$

Example 2: $(h_0 f)(x) = -\sum_{y:|x-y|=1} f(y)$ for $f \in \ell^2(\mathbb{Z}^d)$:

$$\begin{aligned} h_0 &= F_d \left(-2 \sum_{j=1}^{d} \cos(x_j) \right) F_d^{-1} \\ e^{-ith_0} &= F_d e^{-it(-2\sum_j \cos(x_j))} F_d^{-1} \end{aligned}$$

Duhamel's Formula:

Theorem

Let $H = H_0 + V$, where H_0 is selfadjoint and V bounded and symmetric in $\mathcal{H}$. Then

$$e^{-itH}\psi_0 = e^{-itH_0}\psi_0 + (-i)\int_0^t e^{-i(t-t_1)H_0} V e^{-it_1 H}\psi_0 \, dt_1$$

Proof.

- Differentiate $e^{itH_0} e^{-itH}\psi_0$.
- Then integrate.

□

Dyson Series:

Theorem

Let $H = H_0 + V$, where H_0 is selfadjoint and V bounded and symmetric, and $\psi_0 \in \mathcal{H}$. Then

$$
\begin{aligned}
& e^{-itH}\psi_0 \\
&= e^{-itH_0}\psi_0 + \sum_{n=1}^{\infty}(-i)^n \int_0^t \int_0^{t_1} \dots \int_0^{t_{n-1}} e^{-i(t-t_1)H_0} V \\
& \quad \left(\prod_{k=1}^{n-1} e^{-i(t_k - t_{k+1})H_0} V\right) e^{-it_n H_0}\psi_0 \, dt_n \dots dt_2 \, dt_1
\end{aligned}
$$

Proof.

Iterate Duhamel. □

Commuting Operators:

If $H = A + B$ with $[A, B] = 0$, then

$$e^{-it(A+B)} = e^{-itA} e^{-itB}$$

Special case: Hamiltonian of a non-interacting quantum system:

$$H = \overline{H_1 \otimes I + I \otimes H_2} \quad \text{in } \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2.$$

Then

$$\begin{aligned} e^{-itH} &= e^{-it(H_1 \otimes I)} e^{-it(I \otimes H_2)} = (e^{-itH_1} \otimes I)(I \otimes e^{-itH_2}) \\ &= e^{-itH_1} \otimes e^{-itH_2} \end{aligned}$$

Baker-Campbell-Hausdorff formula:

Let A, B be bounded and selfadjoint, such that

$$[A,[A,B]] = [B,[A,B]] = 0.$$

Then

$$e^{-it(A+B)} = e^{-itA}e^{-itB}e^{\frac{t^2}{2}[A,B]}$$

Idea of proof: (i) Differentiate $e^{itB}e^{itA}e^{-it(A+B)}$. (ii) Integrate. (iii) Iterate.

Proof extends to the (unbounded) position and momentum operators q and p in $L^2(\mathbb{R})$ (note $[p,q] = -iI$) $\Longrightarrow$

$$\text{Weyl relation:} \quad e^{i(rp+sq)} = e^{-irs/2}e^{irp}e^{isq} \quad \forall r,s \in \mathbb{R}$$

Trotter product formula:

If A, B and $A+B$ are self-adjoint in $\mathcal{H}$, then

$$e^{-it(A+B)}f = \lim_{n\to\infty} \left(e^{-i\frac{t}{n}A}e^{-i\frac{t}{n}B}\right)^n f$$

for all $f \in \mathcal{H}$.

Semi-group version: If A, B and $A+B$ are semi-bounded from below, then

$$e^{-t(A+B)}f = \lim_{n\to\infty} \left(e^{-\frac{t}{n}A}e^{-\frac{t}{n}B}\right)^n$$

for all $f \in \mathcal{H}$ and $t \geq 0$.