3 More about Hilbert space

3.1 Unitaries

The “isomorphisms” of Hilbert spaces are called unitaries:

**Definition 3.1.** A linear mapping $U : \mathcal{H}_1 \to \mathcal{H}_2$ is called **unitary** iff it is bijective and preserves inner products,

$$\langle U\psi | U\phi \rangle = \langle \psi | \phi \rangle \quad \forall \psi, \phi \in \mathcal{H}_1.$$  \hfill (3.1)

By the polarization identity, the last condition can be replaced with preserving norms (= being **isometric**),

$$\|U\psi\| = \|\psi\| \quad \forall \psi \in \mathcal{H}_1.$$  \hfill (3.2)

The condition “bijective” can be replaced with “surjective” because any $U$ preserving norms is injective. In case $\mathcal{H}_2 = \mathcal{H}_1 = \mathcal{H}$, $U$ is called a **unitary operator**.

Since the Schrödinger equation entails the conservation of $|\psi|^2$, we expect that for initial data $\psi_0$ with $\|\psi_0\| = 1$ also $\psi_t$ has norm 1; by linearity, the evolution from time 0 to time $t$ (if unique) preserves norms. At this point, however, it is not clear whether the evolution mapping $\psi_0 \mapsto \psi_t$ is surjective, and not even whether it is defined on all of $L^2(\mathbb{R}^{3N})$.

Unitaries can be used to define the notion of a **generalized orthonormal basis** in $\mathcal{H}$ as a unitary $U : \mathcal{H} \to L^2(\Omega, \mathfrak{A}, \mu)$. This allows us to represent every $\psi$ as a function $f(x) = U\psi(x)$ on the set $\Omega$, with $f(x)$ playing the role of the expansion coefficients $c_i$ or $c(k)$. For the momentum representation mentioned before, $U$ corresponds to the Fourier transformation; we will see later that Fourier transformation indeed defines a unitary $U : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$.

3.2 Projections

The **closed subspaces** of a Hilbert space $\mathcal{H}$ are themselves Hilbert spaces (with the same inner product $\langle \cdot | \cdot \rangle$). In contrast, if a subspace $X \subset \mathcal{H}$ is not closed then it is a vector space with an inner product but not a Hilbert space. If $\mathcal{H}$ is finite-dimensional, then all subspaces are closed. But not so if dim $\mathcal{H} = \infty$: For example, consider $\mathcal{H} = \ell^2$ and $X$ the set of all sequences in which only finitely many terms are non-zero,

$$X = \bigcup_{n=1}^{\infty} \left\{ (x_1, \ldots, x_n, 0, 0, 0, \ldots) : x_1, \ldots, x_n \in \mathbb{C} \right\}. \quad (3.3)$$

Since $X$ is closed under addition and scalar multiplication, it is a subspace. Its closure, however, is $\ell^2$ and thus strictly bigger. Indeed, for any element $\psi = (x_1, x_2, \ldots)$ of $\ell^2$ and any $\varepsilon > 0$, there is a $\phi \in X$ with $\|\phi - \psi\| < \varepsilon$; simply set $\phi = (x_1, \ldots, x_n, 0, 0, \ldots)$ with $n$ so large that

$$\|\psi\|^2 = \sum_{i=1}^{\infty} |x_i|^2 < \sum_{i=1}^{n} |x_i|^2 + \varepsilon^2, \quad (3.4)$$

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which exists because the series converges. Then \( \|\phi - \psi\|^2 = \sum_{i=n+1}^{\infty} |x_i|^2 \leq \varepsilon^2 \).

**Proposition 3.2.** For any set \( S \subseteq \mathcal{H} \), its orthogonal complement

\[
S^\perp = \{ \psi \in \mathcal{H} : \langle \psi | \phi \rangle = 0 \forall \phi \in S \}
\]

is a closed subspace of \( \mathcal{H} \).

**Proof.** With \( \psi_1 \) and \( \psi_2 \in S^\perp \), also \( c\psi_1 + \psi_2 \in S^\perp \) for any \( c \in \mathbb{C} \); so \( S^\perp \) is a subspace. Now suppose \( \psi_1, \psi_2, \ldots \in S^\perp \) and \( \psi_n \to \psi \); then, for any \( \phi \in S \), \( 0 = \langle \psi_n | \phi \rangle \to \langle \psi | \phi \rangle \), so \( \psi \in S^\perp \).

**Theorem 3.3.** (Projection theorem) Let \( X \subseteq \mathcal{H} \) be a closed subspace. Then every \( \psi \in \mathcal{H} \) can be decomposed in a unique way as \( \psi = \phi + \chi \) with \( \phi \in X \) and \( \chi \in X^\perp \).

**Proof.** Existence. Let \( \psi \in \mathcal{H} \). We first show that there is a \( \phi \in X \) that is closest to \( \psi \). Let \( d = \inf_{f \in X} \|\psi - f\| \). Choose a sequence \( f_n \in X \) so that \( \|\psi - f_n\| \to d \). We show that \( (f_n) \) is a Cauchy sequence. For this we use the parallelogram law

\[
\|u + v\|^2 + \|u - v\|^2 = 2\|u\|^2 + 2\|v\|^2,
\]

which holds in any vector space with inner product (easy to check). So

\[
\|f_n - f_m\|^2 = \|(f_n - \psi) - (f_m - \psi)\|^2
\]

\[
= 2\|f_n - \psi\|^2 + 2\|f_m - \psi\|^2 - \|(f_n - \psi) + (f_m - \psi)\|^2
\]

\[
= 2\|f_n - \psi\|^2 + 2\|f_m - \psi\|^2 - 4\|\psi + 1/2(f_n + f_m)\|^2
\]

\[
\leq 2\|f_n - \psi\|^2 + 2\|f_m - \psi\|^2 - 4d^2
\]

\[
\overset{m,n \to \infty}{\longrightarrow} 2d^2 + 2d^2 - 4d^2 = 0.
\]

Thus, \( (f_n) \) is a Cauchy sequence, so it converges to \( f \), and \( f \in X \). (This step would fail if \( X \) were not closed.) It follows that \( \|\psi - f\| = d \).

Now set \( \phi = f \) and \( \chi = \psi - f \). Then \( \psi = \phi + \chi \), \( \phi \in X \), and it remains to show that \( \chi \in X^\perp \). For any \( g \in X \) and any \( t \in \mathbb{R} \),

\[
d^2 \leq \|\psi - (f + tg)\|^2 = \|\chi - tg\|^2
\]

\[
= \|\chi\|^2 + t^2\|g\|^2 - 2t\text{Re} \langle \chi | g \rangle,
\]

so \( 0 \leq t^2\|g\|^2 - 2\text{Re} \langle \chi | g \rangle \) for all \( t \in \mathbb{R} \), which implies \( \text{Re} \langle \chi | g \rangle = 0 \). A similar argument using \( ti \) instead of \( t \) shows that \( \text{Im} \langle \chi | g \rangle = 0 \). This completes the proof of existence.

Uniqueness. If \( \phi + \chi = \psi = \phi' + \chi' \) with \( \phi, \phi' \in X \) and \( \chi, \chi' \in X^\perp \) then set \( \Delta \phi = \phi - \phi' \in X \), \( \Delta \chi = \chi - \chi' \in X^\perp \), note \( 0 = \Delta \phi + \Delta \chi \) and thus

\[
0 = \langle \Delta \chi | 0 \rangle = \langle \Delta \chi | \Delta \phi + \Delta \chi \rangle = \langle \Delta \chi | \Delta \phi \rangle + \|\Delta \chi\|^2
\]

so \( \Delta \chi = 0 \); as a consequence, \( \Delta \phi = 0 \). \( \square \)
For two Hilbert spaces \( \mathcal{H}_1, \mathcal{H}_2 \), their direct sum or orthogonal sum \( \mathcal{H}_1 \oplus \mathcal{H}_2 \) is the Cartesian product \( \mathcal{H}_1 \times \mathcal{H}_2 \), equipped with the componentwise addition and scalar multiplication (i.e., the direct sum of vector spaces) and the inner product

\[
\langle (\psi_1, \psi_2), (\phi_1, \phi_2) \rangle_{\mathcal{H}_1 \oplus \mathcal{H}_2} = \langle \psi_1 | \phi_1 \rangle_{\mathcal{H}_1} + \langle \psi_2 | \phi_2 \rangle_{\mathcal{H}_2},
\]

which implies \( \| (\psi_1, \psi_2) \| = \sqrt{\| \psi_1 \|^2 + \| \psi_2 \|^2} \). One easily checks that \( \mathcal{H}_1 \oplus \mathcal{H}_2 \) is again a Hilbert space.

The projection theorem provides a canonical unitary isomorphism \( \mathcal{H} \rightarrow X \oplus X^\perp \), \( \psi \mapsto (\phi, \chi) \). It is common to neglect the difference between \( \mathcal{H} \) and \( X \oplus X^\perp \) in the notation and write \( \mathcal{H} = X \oplus X^\perp \).

**Definition 3.4.** For any closed subspace \( X \subseteq \mathcal{H} \), the mapping \( \psi \mapsto \phi \) is the orthogonal projection (or simply projection) to \( X \) and defines a linear operator \( P_X : \mathcal{H} \rightarrow X \) (or, if we wish, \( P_X : \mathcal{H} \rightarrow \mathcal{H} \)). It has the properties

\[
P_X^2 = P_X
\]

and

\[
\langle P_X u | v \rangle = \langle u | P_X v \rangle.
\]

(This is easily visible from \( \mathcal{H} = X \oplus X^\perp \).)

**Corollary 3.5.** It also follows from the projection theorem that if \( X \) is a closed subspace then \( (X^\perp)^\perp = X \). More generally, for any set \( X \subseteq \mathcal{H} \), \( (X^\perp)^\perp \) is the smallest closed subspace containing \( X \) (i.e., the closure of the linear hull of \( X \), \( \text{span} \ X \)).

*Proof.* of the second statement: \( \text{span} X \perp = X \perp \), so \( X^\perp = (\text{span} X)^\perp \). \( \square \)

**Proposition 3.6.** Every ONS \( B \subset \mathcal{H} \) is an ONB of \( \text{span} B \).

*Proof.* Clearly, \( B = \{ \phi_i : i \in \mathcal{I} \} \) is an ONS also in the Hilbert space \( X = \text{span} B \). If \( B \) were not maximal, then there would exist a unit vector \( \psi \in X \) with \( \langle \phi_j | \psi \rangle = 0 \) for every \( j \in \mathcal{I} \). Since

\[
\psi = \sum_{i \in \mathcal{I}'} c_i \phi_i
\]

with some countable set \( \mathcal{I}' \subseteq \mathcal{I} \),

\[
\langle \phi_j | \psi \rangle = \sum_{i \in \mathcal{I}'} c_i \langle \phi_j | \phi_i \rangle = c_j
\]

for every \( j \in \mathcal{I}' \); thus, all \( c_j = 0 \) and \( \psi = 0 \), in contradiction to \( \| \psi \| = 1 \). \( \square \)
3.3 Classification of Hilbert spaces

The following theorem provides the classification of all Hilbert spaces (modulo unitary equivalence). There is exactly one Hilbert space for every cardinality.

**Theorem 3.7.** Let $B_1$ be an ONB of $\mathcal{H}_1$ and $B_2$ an ONB of $\mathcal{H}_2$. There is a unitary isomorphism $\mathcal{H}_1 \rightarrow \mathcal{H}_2$ if and only if $B_1$ and $B_2$ have equal cardinality. Moreover, for any set $S$, an example of a Hilbert space with an ONB of the same cardinality as $S$ is provided by $L^2(S, \text{all subsets}, \#)$ (with $\#$ the counting measure).

**Lemma 3.8.** All ONBs of a Hilbert space have the same cardinality.


**Proof.** of Theorem 3.7. Suppose $B_1 = \{\phi_i^{(1)} : i \in \mathcal{I}_1\}$ and $B_2 = \{\phi_i^{(2)} : i \in \mathcal{I}_2\}$ have equal cardinality, i.e., there is a bijection $\varphi : B_1 \rightarrow B_2$. Any $\psi \in \mathcal{H}_1$ can, by Theorem 2.9, be written as

$$\psi = \sum_{i \in \mathcal{I}_1} c_i \phi_i^{(1)}.$$  \hspace{1cm} (3.20)

Define $U : \mathcal{H}_1 \rightarrow \mathcal{H}_2$ by

$$U \psi = \sum_{i \in \mathcal{I}_1} c_i \phi_i^{(2)},$$  \hspace{1cm} (3.21)

which exists by Theorem 2.9. Define $V : \mathcal{H}_2 \rightarrow \mathcal{H}_1$ in the analogous way and observe $UV = I_{\mathcal{H}_2}$ and $VU = I_{\mathcal{H}_1}$, which shows that $U$ is surjective. The preservation of inner products follows from (2.29). Thus, $U$ is unitary.

Conversely, if $U : \mathcal{H}_1 \rightarrow \mathcal{H}_2$ is unitary then $UB_1$ is an ONB of $\mathcal{H}_2$ and by Lemma 3.8 has the same cardinality as $B_2$.

For $L^2(S, \#)$, $B = \{\phi_s : s \in S\}$ with $\phi_s(x) = 1$ if $x = s$ and $\phi_s(x) = 0$ if $x \neq s$ is an ONB.

Hilbert spaces whose ONBs are uncountable are rarely considered in quantum physics. A Hilbert space is called *separable* if its ONBs are either finite or countably infinite. So $L^2(\mathbb{R}^d)$ is separable. More generally, a metric space is said to be *separable* if there is a dense countable subset. To see that for Hilbert spaces these two definitions are equivalent, note first that if $\mathcal{H}$ has a finite or countable ONB $\{\phi_n\}$ then the countable set

$$\left\{ \sum_{n=1}^{N} c_n \phi_n \middle| N \in \mathbb{N}, c_n \in \mathbb{Q} + i\mathbb{Q} \right\}$$  \hspace{1cm} (3.22)

is dense in $\mathcal{H}$. Conversely, if the sequence $(\tilde{\phi}_n)_{n \in \mathbb{N}}$ is dense in $\mathcal{H}$ then dilute it to a linearly independent sequence $(\phi_n)_{n \in \mathbb{N}}$ with span$\{\phi_n : n \in \mathbb{N}\} = \text{span}\{\tilde{\phi}_n : n \in \mathbb{N}\}$. Then apply the Gram–Schmidt procedure of orthonormalization.
3.4 Bounded operators

**Definition 3.9.** A linear operator \( L : X \rightarrow Y \) between normed vector spaces \( X \) and \( Y \) is called *bounded* iff there is \( C < \infty \) with

\[
\|L\psi\|_Y \leq C\|\psi\|_X \quad \forall \psi \in X.
\]

(3.23)

The *operator norm* of \( L \) is defined by

\[
\|L\| = \sup_{\|\psi\|_X = 1} \|L\psi\|_Y.
\]

(3.24)

That is, \( \|L\| \) is the smallest possible constant \( C \) in (3.23)

**Example 3.10.** Suppose \( X = Y = \mathcal{H} \) with \( \dim \mathcal{H} = n < \infty \), so \( L \) can be regarded as an \( n \times n \) matrix. Suppose further that \( L \) is diagonalizable with eigenvalues \( \lambda_1, \ldots, \lambda_n \in \mathbb{C} \). Then \( \|L\| = \max\{|\lambda_1|, \ldots, |\lambda_n|\} \).

**Example 3.11.** Projections \( P \) are bounded operators with \( X = Y = \mathcal{H} \) and \( \|P\| = 1 \) (except for \( P = 0 \), which can be regarded as the projection to \( \{0\} \)).

**Theorem 3.12.** Let \( X, Y \) be normed vector spaces, \( L : X \rightarrow Y \) linear. The following statements are equivalent:

(i) \( L \) is continuous at 0.

(ii) \( L \) is continuous.

(iii) \( L \) is bounded.

**Proof.** (iii) \(\Rightarrow\) (i): If \( \|\psi_n\| \rightarrow 0 \) then \( \|L\psi_n\| \leq \|L\|\|\psi_n\| \rightarrow 0 \).

(i) \(\Rightarrow\) (ii): Suppose \( \|\psi_n - \psi\| \rightarrow 0 \) and \( L \) is continuous at 0. Then \( \|L\psi_n - L\psi\| = \|L(\psi_n - \psi)\| \rightarrow 0 \).

(ii) \(\Rightarrow\) (iii): Suppose \( L \) was not bounded. Then there is a sequence \( \psi_n \in X \) with \( \|\psi_n\| = 1 \) and \( \|L\psi_n\| \geq n \). Then \( \phi_n := \psi_n/\|L\psi_n\| \) converges to 0 but \( \|L\phi_n\| = 1 \), so \( L\phi_n \not\rightarrow 0 \), in contradiction to continuity at 0. \(\square\)

**Theorem 3.13.** Let \( X \) be a normed space, \( Y \) a Banach space, \( Z \subset X \) a dense subspace and \( L : Z \rightarrow Y \) bounded linear. Then \( L \) possesses a unique bounded linear continuation \( \tilde{L} : X \rightarrow Y \) with \( \tilde{L}|_Z = L \) and \( \|	ilde{L}\| = \|L\| \).

**Proof.** Let \( x \in X \). By hypothesis there is a sequence \( z_n \in Z \) with \( \|z_n - x\|_X \rightarrow 0 \). Since \( z_n \) converges, it is in particular a Cauchy sequence; because of \( \|Lz_n - Lz_m\|_Y = \|L(z_n - z_m)\|_Y \leq \|L\|\|z_n - z_m\|_X \) we also have that \( (Lz_n) \) is a Cauchy sequence in \( Y \) and thus converges, \( Lz_n \rightarrow y \in Y \). Here, \( y \) does not depend on the choice of \( z_n \) (only of \( x \)): If \( z'_n \) is another sequence in \( Z \) with \( \|z'_n - x\|_X \rightarrow 0 \) then also the sequence \( z_1, z'_1, z_2, z'_2, \ldots \) converges to \( x \) and, by the above argument, \( Lz_1, Lz'_1, Lz_2, Lz'_2, \ldots \) converges to \( \tilde{y} \in Y \). Since any subsequence must have the same limit, \( y = \tilde{y} \). So we can set \( \tilde{L}x := y \).
By construction, \( \tilde{L} \) is linear. It is bounded since
\[
\| \tilde{L} x \|_Y = \lim_{n \to \infty} \| L z_n \|_Y \leq \lim_{n \to \infty} \| L \| \| z_n \|_X = \| L \| \| x \|_X.
\] (3.25)

As a consequence, \( \tilde{L} \) is continuous, and a continuous mapping is uniquely determined by its restriction to a dense subset.

Many relevant operators in quantum mechanics are not bounded. The Coulomb potential \( V = -1/r \) is not bounded, the Laplacian \( -\nabla^2 \) is not bounded. If \( \psi \in L^2(\mathbb{R}^d) \) then \( V \psi \) is not necessarily square-integrable; likewise, if \( \psi \in C^2(\mathbb{R}^d) \cap L^2(\mathbb{R}^d) \) then \( -\nabla^2 \psi \) is not necessarily square-integrable. We thus describe unbounded operators as a pair \( (A, \mathcal{D}) \), where \( \mathcal{D} \subseteq \mathcal{H} \) is a subspace (usually a dense subspace), and \( A : \mathcal{D} \to \mathcal{H} \) is a linear mapping; \( \mathcal{D} \) is called the domain of \( A \). Unlike bounded operators, \( A \) cannot be continued in a natural way to \( \tilde{A} : \mathcal{H} \to \mathcal{H} \). (However, if a linear mapping \( R : \mathcal{H} \to \mathcal{H} \) is given, it may well be an unbounded operator; after all, \( \mathcal{H} \) has a Hamel basis, say \( \{ u_i : i \in \mathcal{I} \} \) (not orthonormal!) and \( R \) can be defined by choosing arbitrary \( v_i \in \mathcal{H} \) for \( i \in \mathcal{I} \) and setting \( Ru_i = v_i \).)