II. Bounded Linear Operators on Hilbert Spaces

II.1. Self-Adjoint, Normal, and Unitary Operators

In this section we collect some basic facts about the spectral theory of bounded linear operators on Hilbert spaces. Note that any Hilbert space $\big(\mathcal{H}, \langle\cdot|\cdot\rangle\big)$ is, in particular, a Banach space with norm $\|x\| = \sqrt{\langle x|x\rangle}$. We recall from (I.8) that

$$\mathcal{B}(\mathcal{H}) \;=\; \Big\{ A : \mathcal{H} \to \mathcal{H} \;\Big|\; A \text{ is linear, } \|A\|_{\mathcal{B}(\mathcal{H})} < \infty \Big\}, \tag{II.1}$$

where

$$\|A\|_{\mathcal{B}(\mathcal{H})} \;:=\; \sup_{x \in \mathcal{H}\setminus\{0\}} \left\{ \frac{\|Ax\|}{\|x\|} \right\} \;=\; \sup_{x\in\mathcal{H}, \|x\|=1} \big\{ \|Ax\| \big\} \;=\; \sup_{x,y\in\mathcal{H}, \|x\|=\|y\|=1} \Big\{ \big|\langle y|Ax\rangle\big| \Big\} \tag{II.2}$$

is the operator norm of A, where the last inequality follows from (I.30).

Fix $A \in \mathcal{B}(\mathcal{H})$. For any $y \in \mathcal{H}$, the map $\ell_y(x) := \langle y|Ax\rangle$ defines a bounded linear functional $\ell_y \in \mathcal{H}^*$ with $\|\ell_y\|_{\mathcal{H}^*} \leq \|y\| \cdot \|A\|_{\mathrm{op}}$. By the Riesz representation theorem I.10 there exists a unique vector $z_y \in \mathcal{H}$ such that

$$\forall\, x \in \mathcal{H} : \qquad \langle y|Ax\rangle \;=\; \ell_y(x) \;=\; \langle z_y|x\rangle\,. \tag{II.3}$$

Definition II.1. Let $\big(\mathcal{H}, \langle\cdot|\cdot\rangle\big)$ be a complex Hilbert space and $A \in \mathcal{B}(\mathcal{H})$ a bounded operator on $\mathcal{H}$.

(i) The map $y \mapsto z_y =: A^*(y)$, where $z_y \in \mathcal{H}$ is the unique vector in (II.3), is linear and defines a bounded operator $A^* \in \mathcal{B}(\mathcal{H})$ called the **adjoint operator to $\boldsymbol{A}$**. This operator is uniquely determined by

$$\forall\, x, y \in \mathcal{H} : \qquad \langle y|Ax\rangle \;=\; \langle A^* y|x\rangle\,. \tag{II.4}$$

(ii) If $A = A^*$ then A is called **self-adjoint**.

(iii) If $AA^* = A^*A$ then A is said to be **normal**.

(iv) A bounded operator A is called **(bounded) invertible** if there exists a bounded operator $A^{-1} \in \mathcal{B}(\mathcal{H})$ such that $AA^{-1} = A^{-1}A = \mathbf{1}_{\mathcal{H}}$. In this case the operator $A^{-1} \in \mathcal{B}(\mathcal{H})$ is called the **inverse of A**. The set of bounded invertible operators on $\mathcal{H}$ form a group with respect to composition, the **automorphism group $\mathrm{Aut}(\mathcal{H})$** $\subseteq \mathcal{B}(\mathcal{H})$.

(v) The **spectrum $\sigma(A)$** $\subseteq \mathbb{C}$ and the **resolvent set $\rho(A)$** $\subseteq \mathbb{C}$ of a bounded operator $A \in \mathcal{B}(\mathcal{H})$ are defined by

$$\sigma(A) := \big\{ \lambda \in \mathbb{C} \;\big|\; A - \lambda \cdot \mathbf{1}_{\mathcal{H}} \text{ is not bounded invertible} \big\}, \tag{II.5}$$

$$\rho(A) := \big\{ \lambda \in \mathbb{C} \;\big|\; A - \lambda \cdot \mathbf{1}_{\mathcal{H}} \text{ is bounded invertible} \big\}, \tag{II.6}$$

i.e., $\rho(A) = \mathbb{C} \setminus \sigma(A)$.

(vi) A bounded invertible operator $U \in \mathrm{Aut}(\mathcal{H})$ is called **unitary** if $U^{-1} = U^*$. The set of unitary operators on $\mathcal{H}$ form a subgroup of $\mathrm{Aut}(\mathcal{H})$, the **unitary group $\mathcal{U}(\mathcal{H})$**.

II.2. Linear Operators on finite-dimensional Hilbert Spaces

We first discuss the finite-dimensional case. Let $d \in \mathbb{N}$ fixed and $\mathcal{H} = \mathbb{C}^d$ equipped with the unitary scalar product (I.16).

- If $d \in \mathbb{N}$, $\{e_1, \ldots, e_d\} \subseteq \mathcal{H} := \mathbb{C}^d$ is the canonical ONB, and $A \in \mathcal{B}(\mathbb{C}^d)$ is a (bounded) linear operator then

$$A = \mathbf{1}_{\mathcal{H}} \, A \, \mathbf{1}_{\mathcal{H}} = \sum_{m,n=1}^{d} |e_m\rangle\langle e_m| \, A \, |e_n\rangle\langle e_n| = \sum_{m,n=1}^{d} A_{m,n} \, |e_m\rangle\langle e_n| , \tag{II.7}$$

  where the matrix elements $A_{m,n}$ of A are given by $A_{m,n} = \langle e_m | A e_n \rangle$.

- In the finite-dimensional case, the spectrum $\sigma(A) \subseteq \mathbb{C}$ of $A \in \mathcal{B}(\mathbb{C}^d)$ coincides with the set of eigenvalues and these, in turn, with the zeroes of the characteristic polynomial,

$$\sigma(A) = \big\{ \lambda \in \mathbb{C} \;\big|\; \lambda \text{ is an eigenvalue of } A \big\} = \big\{ \lambda \in \mathbb{C} \;\big|\; \det[A - \lambda \cdot \mathbf{1}] = 0 \big\} . \tag{II.8}$$

  Note that $\sigma(A)$ is a set of at most d numbers in the complex plane, and $\rho(A)$ is the entire complex plane except for these isolated points.

- In particular, $(A^*)_{m,n} = \overline{A_{n,m}}$, i.e., $A^* = \overline{A^t}$, for (finite-dimensional) matrices.

- If $A = A^* \in \mathcal{B}(\mathbb{C}^d)$ is self-adjoint then A is **diagonalizable**, i.e., there exists an ONB $\{\varphi_1, \ldots, \varphi_d\} \subseteq \mathcal{H} := \mathbb{C}^d$ of eigenvectors and d corresponding eigenvalues

$\{\lambda_1, \ldots, \lambda_d\} \subseteq \mathbb{C}$ such that

$$A \;=\; \sum_{j=1}^{d} \lambda_j \, |\varphi_j\rangle\langle\varphi_j| \,. \tag{II.9}$$

Moreover, all eigenvalues of a self-adjoint operator are real, $\sigma(A) \subseteq \mathbb{R}$.

- Furthermore, if $A = A^* \in \mathcal{B}(\mathbb{C}^d)$ is self-adjoint then

$$\|A\|_{\mathrm{op}} \;=\; \max\big\{ |\lambda| \;:\; \lambda \in \sigma(A) \big\} \,. \tag{II.10}$$

Indeed, if $\{\varphi_1, \ldots, \varphi_d\} \subseteq \mathbb{C}^d$ is an ONB of eigenvectors with corresponding eigenvalues $\{\lambda_1, \ldots, \lambda_d\} = \sigma(A) \subseteq \mathbb{R}$ such that

$$A \;=\; \sum_{j=1}^{d} \lambda_j \, |\varphi_j\rangle\langle\varphi_j| \,, \tag{II.11}$$

then $\|A\varphi_j\| = |\lambda_j|$, for any $j \in \mathbb{Z}_1^d$, and hence $\|A\|_{\mathrm{op}} = \sup_{\|\psi\|=1} \|A\psi\| \geq \max_{1\leq j\leq d} |\lambda_j|$. Conversely, if $\varphi, \psi \in \mathbb{C}^d$ then

$$\begin{aligned} \big|\langle\varphi|A\psi\rangle\big| \;&\leq\; \sum_{j=1}^{d} |\lambda_j| \, \big|\langle\varphi|\varphi_j\rangle \, \langle\varphi_j|\psi\rangle\big| \\ &\leq \Big(\max_{1\leq j\leq d} |\lambda_j|\Big) \bigg(\sum_{j=1}^{d} \big|\langle\varphi|\varphi_j\rangle\big|^2\bigg)^{1/2} \bigg(\sum_{j=1}^{d} \big|\langle\varphi_j|\psi\rangle\big|^2\bigg)^{1/2} \\ &= \Big(\max_{1\leq j\leq d} |\lambda_j|\Big) \, \|\varphi\| \, \|\psi\| \,, \end{aligned} \tag{II.12}$$

which implies that $\|A\|_{\mathrm{op}} \leq \max_{1\leq j\leq d} |\lambda_j|$.

- Note that here and henceforth we count multiplicities, i.e., the eigenvalues are not necessarily distinct. For instance, the unit matrix $(\mathbf{1}_{\mathbb{C}^d})_{m,n} = \delta_{m,n}$ is self-adjoint, its eigenvalues are $\lambda_1 = \ldots = \lambda_d = 1$, and its spectrum consists of a single point $\sigma(\mathbf{1}) = \{1\}$.

- More generally, if $K \in \mathbb{N}$ and $A_1 = A_1^*$, $A_2 = A_2^*$, ..., $A_K = A_K^* \in \mathcal{B}(\mathbb{C}^d)$ are mutually commuting self-adjoint operators,

$$\forall\, k, \ell \in \mathbb{Z}_1^K : \qquad [A_k, A_\ell] \;=\; A_k\, A_\ell \;-\; A_\ell\, A_k \;=\; 0 \,, \tag{II.13}$$

then $A_1, A_2, \ldots, A_K$ are simultaneously diagonalizable. That is, there exists an ONB $\{\varphi_j | j \in \mathbb{Z}_1^d\} \subseteq \mathbb{C}^d$ of joint eigenvectors and $K \cdot d$ corresponding real eigenvalues $\sigma(A_k) = \{\lambda_{k,j} | j \in \mathbb{Z}_1^d\} \subseteq \mathbb{R}$ such that

$$A_k \;=\; \sum_{j=1}^{d} \lambda_{k,j} \, |\varphi_j\rangle\langle\varphi_j| \,. \tag{II.14}$$

- The latter statement (II.14) for $K = 2$ implies that normal operators, i.e., those for which $AA^* = A^*A$, are diagonalizable, too.

  Namely, defining the **real part** $\mathrm{Re}(\boldsymbol{A})$ and the **imaginary part** $\mathrm{Im}(\boldsymbol{A})$ of an operator $A \in \mathcal{B}(\mathcal{H})$ by

$$\mathrm{Re}(A) := \frac{1}{2}\big(A + A^*\big) \quad \text{and} \quad \mathrm{Im}(A) := \frac{1}{2i}\big(A - A^*\big), \tag{II.15}$$

  we observe that

$$A = \mathrm{Re}(A) + i\mathrm{Im}(A), \tag{II.16}$$

  much like $z = \mathrm{Re}(z) + i\mathrm{Im}(z)$ for $z \in \mathbb{C}$ with $\mathrm{Re}(z), \mathrm{Im}(z) \in \mathbb{R}$. It is easy to check that the normality of A is equivalent to $[\mathrm{Re}(A)\,,\, \mathrm{Im}(A)] = 0$. Hence, $\mathrm{Re}(A)$ and $\mathrm{Im}(A)$ are simultaneously diagonalizable, and there exists an ONB $\{\varphi_j | j \in \mathbb{Z}_1^d\} \subseteq \mathbb{C}^d$ of joint eigenvectors and $2d$ real eigenvalues $\{\alpha_1, \beta_1, \ldots, \alpha_d, \beta_d\} \subseteq \mathbb{R}$ such that $\mathrm{Re}(A) = \sum_{j=1}^d \alpha_j \, |\varphi_j\rangle\langle\varphi_j|$ and $\mathrm{Im}(A) = \sum_{j=1}^d \beta_j \, |\varphi_j\rangle\langle\varphi_j|$. Therefore, A is diagonalizable, namely,

$$A = \sum_{j=1}^d (\alpha_j + i\beta_j) \, |\varphi_j\rangle\langle\varphi_j| \,. \tag{II.17}$$

- An important class of normal operators, besides self-adjoint ones, are unitary operators $U \in \mathcal{U}(\mathcal{H})$, since $UU^* = \mathbf{1}_{\mathcal{H}} = U^*U$. It follows that unitary operators are diagonalizable and that their spectra are contained in the unit circle, $\sigma(U) \subseteq \{z \in \mathbb{C} : \ |z| = 1\}$
- If $A_{m,n} = \langle e_m | A e_n \rangle$ is the matrix representation of A with respect to the canonical ONB $\{e_1, \ldots, e_d\} \subseteq \mathbb{C}^d$ then the self-adjointness of A is equivalent to $A_{n,m} = \overline{A_{m,n}}$. Its diagonalizability is equivalent to the existence of a **unitary matrix** $U \in \mathcal{U}(\mathbb{C}^d)$ such that

$$A = U^* \, D \, U \,, \tag{II.18}$$

  where $D \in \mathcal{B}(\mathbb{C}^d)$ is a diagonal matrix,

$$D_{i,j} = \langle e_i | D e_j \rangle = \delta_{i,j} \, \lambda_j \quad \Leftrightarrow \quad D = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \lambda_d \end{pmatrix}. \tag{II.19}$$

  Indeed, if U has the matrix representation $U_{i,n} = \langle e_i | U e_n \rangle$ then $U_{i,n} := \langle \varphi_i | e_n \rangle$ has the desired properties.

The general form to which any operator on a finite-dimensional Hilbert space can be transformed to is given by the **singular value decomposition** described in the following theorem.

Theorem II.2 (Singular Value Decomposition)**.** *Let* $d \in \mathbb{N}$ *and* $\big(\mathcal{H} = \mathbb{C}^d, \langle\cdot|\cdot\rangle = \langle\cdot|\cdot\rangle_{\mathrm{unit}}\big)$ *be the* d*-dimensional complex Hilbert space defined by the unitary scalar product and* $A \in \mathcal{B}(\mathcal{H})$ *a bounded operator on* $\mathcal{H}$*. Then there exist ONB* $\{f_1, \ldots, f_d\}, \{g_1, \ldots, g_d\} \subseteq \mathcal{H}$ *and nonnegative numbers* $\rho_1, \ldots, \rho_d \in \mathbb{R}_0^+$ *called* ***singular values of A*** *such that*

$$A \;=\; \sum_{n=1}^{d} \rho_n \, |f_n\rangle\langle g_n| \,. \tag{II.20}$$

Equivalently, if $A_{m,n} = \langle e_m | A e_n\rangle$ *denote the matrix elements of* A *in the canonical ONB* $\{e_1, \ldots, e_d\} \subseteq \mathcal{H}$ *then there exist unitary matrices* $U, V \in \mathcal{U}(\mathbb{C}^d)$ *such that*

$$A \;=\; U^* \, D \, V \,, \tag{II.21}$$

where $D \in \mathcal{B}(\mathbb{C}^d)$ *is the diagonal matrix,*

$$D \;=\; \begin{pmatrix} \rho_1 & 0 & \cdots & 0 \\ 0 & \rho_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \rho_d \end{pmatrix} , \tag{II.22}$$

with $\rho_1, \ldots, \rho_d \in \mathbb{R}_0^+$*.*

II.3. Positivity and Functional Calculus

Definition II.3 (Functional Calculus)**.** Let $d \in \mathbb{N}$ and $\big(\mathcal{H} = \mathbb{C}^d, \langle\cdot|\cdot\rangle = \langle\cdot|\cdot\rangle_{\mathrm{unit}}\big)$ be the d-dimensional complex Hilbert space defined by the unitary scalar product, $A = A^* \in \mathcal{B}(\mathcal{H})$ a self-adjoint operator on $\mathcal{H}$, and $\{\varphi_1, \ldots, \varphi_d\} \subseteq \mathcal{H}$ an ONB of eigenvectors of A with corresponding eigenvalues $\{\lambda_1, \ldots, \lambda_d\} = \sigma(A) \subseteq \mathbb{R}$, such that

$$A \;=\; \sum_{j=1}^{d} \lambda_j \, |\varphi_j\rangle\langle \varphi_j| \,. \tag{II.23}$$

If $f \in C(\mathbb{R}; \mathbb{C})$ then define

$$f(A) \;:=\; \sum_{j=1}^{d} f(\lambda_j) \, |\varphi_j\rangle\langle \varphi_j| \,. \tag{II.24}$$

- It easy to check that $f(A)$ defined by (II.24) is normal.
- If $f(x) = \alpha_0 + \alpha_1 x + \ldots + \alpha_N x^N$ is a complex polynomial, $\alpha_0, \alpha_1, \ldots, \alpha_N \in \mathbb{C}$, then $f(A)$ defined by (II.24) coincides with $\alpha_0 + \alpha_1 A + \ldots + \alpha_N A^N$.

- Suppose that $(a_k)_{k=0}^{\infty} \in \mathbb{C}^{\mathbb{N}_0}$ is a complex sequence with $\limsup_{k\to\infty} |a_k|^{1/k} := 1/R < \infty$ and $z_0 \in \mathbb{C}$. Then the power series $f(z) := \sum_{k=0}^{\infty} a_k (z-z_0)^k$ converges absolutely in $D(z_0, R) := \{z \in \mathbb{C} : \ |z - z_0| < R\}$. If $\sigma(A) \subseteq D(z_0, R)$ then $f(A)$ defined by (II.24) coincides with the norm-convergent power series

$$f(A) \ = \ \sum_{k=0}^{\infty} a_k \, (A - z_0)^k \, . \tag{II.25}$$

- This way and with $z_0 = 0$ and $R = \infty$, we obtain many elementary functions of self-adjoint operators $A = A^*$, e.g., the matrix exponential function and many others,

$$\exp(A) \ := \ \sum_{k=0}^{\infty} \frac{A^k}{k!} \, , \tag{II.26}$$

$$\sin(A) \ := \ \sum_{k=0}^{\infty} \frac{(-1)^k A^{2k+1}}{(2k+1)!} \, , \tag{II.27}$$

$$\cos(A) \ := \ \sum_{k=0}^{\infty} \frac{(-1)^k A^{2k}}{(2k)!} \, . \tag{II.28}$$

  Eqs. (II.26)-(II.28) define bounded operators on $\mathcal{H}$ as norm-convergent power series.

Definition II.4 (Positivity)**.** Let $\big(\mathcal{H}, \langle \cdot | \cdot \rangle\big)$ be a complex Hilbert space and $A = A^*, B = B^* \in \mathcal{B}(\mathcal{H})$ two self-adjoint operators on $\mathcal{H}$.

$$(i) \quad A \text{ is called } \textbf{positive, } \boldsymbol{A \geq 0} \ :\Leftrightarrow \ \forall \varphi \in \mathcal{H} : \quad \langle \varphi \,|\, A\varphi \rangle \ \geq \ 0 \, . \tag{II.29}$$

$$(ii) \qquad \boldsymbol{A \geq B} \ :\Leftrightarrow \ A - B \geq 0 \, . \tag{II.30}$$

- Using the diagonal form

$$A \ = \ \sum_{j=1}^{d} \lambda_j \, |\varphi_j\rangle\langle\varphi_j| \, , \tag{II.31}$$

  one easily checks that

$$\big\{ A \ \geq \ 0 \big\} \quad \Leftrightarrow \quad \big\{ \sigma(A) \ \subseteq \ \mathbb{R}_0^+ \big\} \, . \tag{II.32}$$

- Hence, if $f \in C(\mathbb{R}_0^+; \mathbb{R})$ and A is positive then $f(A)$ can be defined by (II.24).
- In particular, we have for positive A that

$$\sqrt{A} \ = \ \sum_{j=1}^{d} \sqrt{\lambda_j} \ |\varphi_j\rangle\langle\varphi_j| \, , \tag{II.33}$$

$$A \, \ln(A) \ = \ \sum_{j=1}^{d} \lambda_j \, \ln(\lambda_j) \, |\varphi_j\rangle\langle\varphi_j| \, , \tag{II.34}$$

where we use the convention that $0 \ln(0) = 0$, which is consistent with the continuity of $\lim_{r \searrow 0}\{r \ln(r)\} = 0$ at $r = 0$.

Next, let $d \in \mathbb{N}$ and $\mathcal{H} = \mathbb{C}^d$ be the d-dimensional complex Hilbert space endowed with the unitary scalar product and $A \in \mathcal{B}(\mathcal{H})$ a bounded operator on $\mathcal{H}$. According to Theorem II.2, there exist ONB $\{f_1, \ldots, f_d\}, \{g_1, \ldots, g_d\} \subseteq \mathcal{H}$ and nonnegative numbers $\rho_1, \rho_2, \ldots, \rho_d \geq 0$, such that A assumes its singular value decomposition

$$A \;=\; \sum_{n=1}^{d} \rho_n \, |f_n\rangle\langle g_n| \, . \tag{II.35}$$

Then A^*A is positive,

$$A^*A \;=\; \sum_{m,n=1}^{d} \rho_m \, \rho_n \, |g_m\rangle\langle f_m|f_n\rangle\langle g_n| \;=\; \sum_{n=1}^{d} \rho_n^2 \, |g_n\rangle\langle g_n| \;\geq\; 0 \, , \tag{II.36}$$

which can also be seen directly, as $\langle \varphi | A^*A\varphi\rangle = \langle A\varphi | A\varphi\rangle = \|A\varphi\| \geq 0$. We can thus define the **absolute value $|A|$** of A by (II.33),

$$|A| \;:=\; \sqrt{A^* \, A} \;=\; \sum_{n=1}^{d} \sqrt{\rho_n^2} \; |g_n\rangle\langle g_n| \, , \;=\; \sum_{n=1}^{d} \rho_n \, |g_n\rangle\langle g_n| \, . \tag{II.37}$$

Note that $|A|^* = |A|$, but $|A^*| = \sum_{n=1}^{d} \rho_n |f_n\rangle\langle f_n| \neq |A|$, in general. From these observations and taking $U := \sum_{n=1}^{d} |f_n\rangle\langle g_n|$, we obtain the polar decomposition of A,

Theorem II.5 (Polar Decomposition)**.** *Let $d \in \mathbb{N}$ and $\big(\mathcal{H} = \mathbb{C}^d, \langle\cdot|\cdot\rangle = \langle\cdot|\cdot\rangle_{\mathrm{unit}}\big)$ be the d-dimensional complex Hilbert space defined by the unitary scalar product and $A \in \mathcal{B}(\mathcal{H})$ a bounded operator on $\mathcal{H}$. Then there exist a unitary operator $U \in \mathcal{U}(\mathcal{H})$ such that*

$$A \;=\; U \, |A| \, . \tag{II.38}$$

The right side of (II.38) *is called the **polar decomposition** of A.*

II.4. Traces and Trace Norms

Definition II.6. Let $d \in \mathbb{N}$ and $\big(\mathcal{H} = \mathbb{C}^d, \langle\cdot|\cdot\rangle = \langle\cdot|\cdot\rangle_{\mathrm{unit}}\big)$ be the d-dimensional complex Hilbert space defined by the unitary scalar product, $\{\varphi_1, \ldots, \varphi_d\} \subseteq \mathcal{H}$ an ONB, and $A \in \mathcal{B}(\mathcal{H})$ a bounded operator on $\mathcal{H}$.

(i) The **trace $\mathrm{Tr}(A)$** of A is defined as

$$\mathrm{Tr}(A) \;:=\; \sum_{j=1}^{d} \langle \varphi_j \,|\, A\varphi_j\rangle \, . \tag{II.39}$$

(ii) For $p \in [1, \infty)$ define the **trace norm $\|A\|_p$** of A by

$$\|A\|_p := \big[\mathrm{Tr}\big(|A|^p\big)\big]^{1/p}. \tag{II.40}$$

Remarks and Examples.

- The trace $\mathrm{Tr}(A)$ of $A \in \mathcal{B}(\mathcal{H})$ is well-defined, i.e., independent of the choice of the ONB $\{\varphi_1, \ldots, \varphi_d\} \subseteq \mathcal{H}$. Indeed, if $\{f_1, \ldots, f_d\} \subseteq \mathcal{H}$ is any ONB and $A = \sum_{i,j=1}^N a_{i,j}\, |f_i\rangle\langle f_j|$ then

$$\mathrm{Tr}(A) = \sum_{i,j=1}^d a_{i,j}\, \langle f_j | f_i \rangle = \sum_{i=1}^d a_{i,i} = \sum_{i=1}^d \langle f_i | A f_i \rangle, \tag{II.41}$$

  independent of the choice of the ONB $\{f_1, \ldots, f_d\}$ in $\mathcal{H}$.

- If $\{\lambda_1, \ldots, \lambda_d\} \subseteq \mathbb{C}$ are the zeros of the characteristic polynomial $\chi(\lambda) = \det[A - \lambda \cdot \mathbf{1}] = (\lambda_1 - \lambda) \cdots (\lambda_d - \lambda)$ (counting multiplicities), then $\mathrm{Tr}(A) = \lambda_1 + \ldots + \lambda_d$ is the sum of these zeroes. Indeed, it is easy to check that $\mathrm{Tr}(A) = -\alpha_{d-1} = \lambda_1 + \ldots + \lambda_d$, when writing $\chi(\lambda) = \alpha_0 + \ldots + \alpha_{d-1}\lambda^{d-1} + \lambda^d$.

- If $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_d \geq 0$ are the eigenvalues of $|A|$, then $\|A\|_p = \big(\sum_{n=1}^N \rho_n^p\big)^{1/p}$.

- If $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_d \geq 0$ and $A \neq 0$ then $\rho_1 > 0$. If furthermore $1 \leq q < p < \infty$ then

$$\|A\|_p^p = \sum_{n=1}^N \rho_n^p = \rho_1^p \sum_{n=1}^N \left(\frac{\rho_n}{\rho_1}\right)^p \leq \rho_1^p \sum_{n=1}^N \left(\frac{\rho_n}{\rho_1}\right)^q = \rho_1^{p-q}\, \|A\|_q^q. \tag{II.42}$$

Theorem II.7. *Let $\big(\mathcal{H} = \mathbb{C}^d, \langle\cdot|\cdot\rangle = \langle\cdot|\cdot\rangle_{\mathrm{unit}}\big)$ be a finite-dimensional complex Hilbert space and $A, B \in \mathcal{B}(\mathcal{H})$ two linear operators on $\mathcal{H}$.*

$$(i) \qquad \|AB\|_1 \leq \|A\|_{\mathrm{op}} \cdot \|B\|_1; \tag{II.43}$$

$$(ii) \qquad \|A\|_{\mathrm{op}} = \sup\big\{\mathrm{Tr}(AB) \;\big|\; B \in \mathcal{L}^1(\mathcal{H}),\ \|B\|_1 = 1\big\}. \tag{II.44}$$

$$(iii) \qquad A = A^* \;\Rightarrow\; \|A\|_{\mathrm{op}} = \sup\big\{\mathrm{Tr}(\rho A) \;\big|\rho \in \mathcal{DM}(\mathcal{H})\big\}, \tag{II.45}$$

where

$$\mathcal{DM}(\mathcal{H}) := \big\{\rho \in \mathcal{L}^1(\mathcal{H}) \;\big|\; \rho = \rho^* \geq 0,\ \mathrm{Tr}(\rho) = 1\big\} \subseteq \mathcal{L}^1(\mathcal{H}) \tag{II.46}$$

*is the convex subset of **density matrices**.*

II.5. Tensor Products of Hilbert Spaces

In this section we define tensor products of Hilbert spaces and observe some basic facts about these. To this end we suppose that $\big(\mathcal{H}, \langle\cdot|\cdot\rangle\big)$ and $\big(\mathcal{H}', \langle\cdot|\cdot\rangle'\big)$ are two (separable, complex) Hilbert spaces. For $f \in \mathcal{H}$ and $f' \in \mathcal{H}'$ we define a map $f \otimes f' : \mathcal{H} \times \mathcal{H}' \to \mathbb{C}$ by

$$\forall\, h \in \mathcal{H},\ h' \in \mathcal{H}' : \qquad \big(f \otimes f'\big)[h, h'] := \langle h | f \rangle\, \langle h' | f' \rangle. \tag{II.47}$$

Obviously, $f \otimes f'$ is a bi-antilinear form,

$$\big(f \otimes f'\big)[g + \alpha h, g' + \beta h'] \;=\; \big(f \otimes f'\big)[g, g'] \;+\; \overline{\alpha}\,\big(f \otimes f'\big)[h, g'] \;+\; \overline{\beta}\,\big(f \otimes f'\big)[g, h'] \;+\; \overline{\alpha\,\beta}\,\big(f \otimes f'\big)[h, h'] \,. \tag{II.48}$$

With these bi-antilinear forms we build a complex vector space $\mathcal{G}_{\mathrm{fin}}$ by the usual pointwise operations,

$$\big((f \otimes f') + \alpha(g \otimes g')\big)[h, h'] \;:=\; \big(f \otimes f'\big)[h, h'] \;+\; \alpha\big(g \otimes g'\big)[h, h'] \,. \tag{II.49}$$

This vector space contains all (finite) linear combinations of bilinear forms $f \otimes f'$,

$$\mathcal{G}_{\mathrm{fin}} \;=\; \Big\{ \sum_{j=1}^{L} \alpha_j (f_j \otimes f_j') \;\Big|\; L \in \mathbb{N},\; \forall\, j \in \mathbb{Z}_1^L :\; \alpha_j \in \mathbb{C},\; f_j \in \mathcal{H},\; f_j' \in \mathcal{H}' \Big\} . \tag{II.50}$$

We define a quadratic form $\langle \cdot | \cdot \rangle_{\mathcal{G}} : \mathcal{G}_{\mathrm{fin}} \times \mathcal{G}_{\mathrm{fin}} \to \mathbb{C}$ by continuation by antilinearity of

$$\langle f \otimes f' | g \otimes g' \rangle_{\mathcal{G}} \;:=\; \langle f | g \rangle \, \langle f' | g' \rangle \,, \tag{II.51}$$

i.e.,

$$\Big\langle \sum_{i=1}^{L} \alpha_i \, f_i \otimes f_i' \;\Big|\; \sum_{j=1}^{L} \beta_j \, g_j \otimes g_j' \Big\rangle_{\mathcal{G}} \;:=\; \sum_{i,j=1}^{L} \overline{\alpha_i}\, \beta_j \, \langle f_i | g_j \rangle \, \langle f_i' | g_j' \rangle \,. \tag{II.52}$$

Lemma II.8. *The quadratic form $\langle \cdot | \cdot \rangle_{\mathcal{G}} : \mathcal{G}_{\mathrm{fin}} \times \mathcal{G}_{\mathrm{fin}} \to \mathbb{C}$ as in* (II.51) *defines a scalar product on $\mathcal{G}_{\mathrm{fin}}$.*

Proof. Sesquilinearity and symmetry of $\langle \cdot | \cdot \rangle_{\mathcal{G}}$ are trivial, and we concentrate on its positive definiteness. Let $\{\varphi_k\}_{k=1}^{\infty} \subseteq \mathcal{H}$ and $\{\varphi_\ell'\}_{\ell=1}^{\infty} \subseteq \mathcal{H}'$ be two ONB and assume that $\Psi = \sum_{j=1}^{L} \alpha_j (f_j \otimes f_j') \in \mathcal{G}_{\mathrm{fin}}$. Then

$$\begin{aligned} \langle \Psi | \Psi \rangle_{\mathcal{G}} \;&=\; \sum_{i,j=1}^{L} \overline{\alpha_i}\, \alpha_j \, \langle f_i | f_j \rangle \, \langle f_i' | f_j' \rangle' \;=\; \sum_{k,\ell=1}^{\infty} \sum_{i,j=1}^{L} \overline{\alpha_i}\, \alpha_j \, \langle f_i | \varphi_k \rangle \, \langle \varphi_k | f_j \rangle \, \langle f_i' | \varphi_\ell' \rangle' \, \langle \varphi_\ell' | f_j' \rangle' \\ &=\; \sum_{k,\ell=1}^{\infty} \Big| \sum_{j=1}^{L} \alpha_j \, \big(f_j \otimes f_j'\big)[\varphi_k, \varphi_\ell'] \Big|^2 \;=\; \sum_{k,\ell=1}^{\infty} \big| \Psi[\varphi_k, \varphi_\ell'] \big|^2 \,. \end{aligned} \tag{II.53}$$

This proves that $\langle \Psi | \Psi \rangle_{\mathcal{G}} \geq 0$. Moreover, $\langle \Psi | \Psi \rangle_{\mathcal{G}} = 0$ implies that $\Psi[\varphi_k, \varphi_\ell'] = 0$, for all $k, \ell \in \mathbb{N}$. Since $\{\varphi_k\}_{k=1}^{\infty} \subseteq \mathcal{H}$ and $\{\varphi_\ell'\}_{\ell=1}^{\infty} \subseteq \mathcal{H}'$ are ONB, this in turn yields $\Psi = 0$. $\square$

Definition II.9. Suppose that $\big(\mathcal{H}, \langle \cdot | \cdot \rangle\big)$ and $\big(\mathcal{H}', \langle \cdot | \cdot \rangle'\big)$ are two separable, complex Hilbert spaces. Define $\mathcal{G}_{\mathrm{fin}}$ as in (II.50) and equip it with the scalar product $\langle \cdot | \cdot \rangle_{\mathcal{G}} : \mathcal{G}_{\mathrm{fin}} \times \mathcal{G}_{\mathrm{fin}} \to \mathbb{C}$ as in (II.51). We define a separable, complex Hilbert space $\big(\mathcal{G},\, \langle \cdot | \cdot \rangle_{\mathcal{G}}\big)$ as the completion

$$\mathcal{G} \;:=\; \overline{\mathcal{G}_{\mathrm{fin}}}^{\langle \cdot | \cdot \rangle_{\mathcal{G}}} \tag{II.54}$$

of $\mathcal{G}_{\mathrm{fin}}$ with respect to the norm induced by $\langle \cdot | \cdot \rangle_{\mathcal{G}}$. The Hilbert space $\mathcal{G}$ is called the **tensor product** of $\mathcal{H}$ and $\mathcal{H}'$, and we write $\mathcal{G} =: \boldsymbol{\mathcal{H} \otimes \mathcal{H}'}$ and $\langle \cdot | \cdot \rangle_{\mathcal{G}} =: \boldsymbol{\langle \cdot | \cdot \rangle_{\mathcal{H} \otimes \mathcal{H}'}}$.

Remarks and Examples.

- If $\{\varphi_k\}_{k=1}^{\infty} \subseteq \mathcal{H}$ and $\{\varphi'_\ell\}_{\ell=1}^{\infty} \subseteq \mathcal{H}'$ are ONB then so is $\{\varphi_k \otimes \varphi'_\ell\}_{k,\ell=1}^{\infty} \subseteq \mathcal{H} \otimes \mathcal{H}'$.
- Definition II.9 can be easily generalized to $N \in \mathbb{N}$ factors: If $\big(\mathcal{H}_n, \langle\cdot|\cdot\rangle_n\big)$ is a Hilbert space with an ONB $\{\varphi_{n;k}\}_{k=1}^{\infty} \subseteq \mathcal{H}_n$, for $n \in \mathbb{Z}_1^N$, then $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_N$ is the tensor product of $\mathcal{H}_1, \ldots, \mathcal{H}_N$ and $\big\{\varphi_{1;k_1} \otimes \cdots \otimes \varphi_{N;k_N} \,\big|\, k_1, \ldots, k_N \in \mathbb{N}\big\} \subseteq \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_N$ is an ONB.
- Assume that $\big(\mathcal{H}, \langle\cdot|\cdot\rangle\big)$ is a separable, complex Hilbert space. Then the space $\mathcal{L}^2(\mathcal{H})$ of Hilbert-Schmidt operators on $\mathcal{H}$ is a Hilbert space $\big(\mathcal{L}^2(\mathcal{H}), \langle\cdot|\cdot\rangle_{\mathcal{L}^2(\mathcal{H})}\big)$ with respect to the scalar product
$$\langle A|B\rangle_{\mathcal{L}^2(\mathcal{H})} \;:=\; \mathrm{Tr}_{\mathcal{H}}\big(A^* B\big)\,. \tag{II.55}$$
- Assume that $\big(\mathcal{H}, \langle\cdot|\cdot\rangle\big)$ is a separable, complex Hilbert space. Then the Hilbert space $\big(\mathcal{L}^2(\mathcal{H}), \langle\cdot|\cdot\rangle_{\mathcal{L}^2(\mathcal{H})}\big)$ of Hilbert-Schmidt operators is isomorphic to $\big(\mathcal{H}\otimes\mathcal{H}^*,\, \langle\cdot|\cdot\rangle_{\mathcal{H}\otimes\mathcal{H}^*}\big)$, the isomorphism being
$$J:\; \mathcal{L}^2(\mathcal{H}) \;\to\; \mathcal{H}\otimes\mathcal{H}^*\,, \quad |\varphi\rangle\langle\psi| \;\mapsto\; \varphi\otimes\psi\,. \tag{II.56}$$
- If $(\Omega, \mathfrak{A}, \mu)$ and $(\Omega', \mathfrak{A}', \mu')$ are two measure spaces then $L^2(\Omega\times\Omega', d\mu\otimes d\mu')$ is isomorphic to $L^2(\Omega, d\mu)\otimes L^2(\Omega', d\mu')$. The isomorphism $I: L^2(\Omega, d\mu)\otimes L^2(\Omega', d\mu') \to L^2(\Omega\times\Omega', d\mu\otimes d\mu')$ derives from the extension by linearity and continuity of
$$\varphi\otimes\varphi' \;\mapsto\; \varphi\cdot\varphi'\,, \quad \text{where} \quad (\varphi\cdot\varphi')[x,x'] \;:=\; \varphi(x)\cdot\varphi'(x')\,. \tag{II.57}$$

II.6. SUPPLEMENTARY MATERIAL

II.6.1. Proof of Theorem II.2 - Singular Value Decomposition

Proof. We only prove (II.20). We may assume that $A \neq 0$. Observe that $A^*A \in \mathcal{B}(\mathcal{H})$ is a self-adjoint matrix and, hence, diagonalizable. In other words, there exists an ONB $\{g_1, \ldots, g_d\} \subseteq \mathcal{H}$ of eigenvectors of A^*A and corresponding real eigenvalues $\lambda_1, \ldots, \lambda_d \in \mathbb{R}$ such that
$$A^*A \;=\; \sum_{j=1}^{d} \lambda_j\, |g_j\rangle\langle g_j|\,. \tag{II.58}$$

Note that the eigenvalues $\lambda_j = \langle g_j|A^*Ag_j\rangle = \|Ag_j\|^2 \geq 0$ are nonnegative, and we may define $\rho_j \in \mathbb{R}_0^+$ by $\rho_j := \sqrt{\lambda_j} = \|Ag_j\|$. Moreover, we may assume w.l.o.g. these numbers to be sorted in descending order such that $\rho_1 \geq \ldots \geq \rho_c > \rho_{c+1} = \ldots = \rho_d = 0$, for some $c \in \mathbb{Z}_1^d$. Hence, $\mathrm{Ker}(A) = \mathrm{span}\{g_{c+1}, \ldots, g_d\}$ and $\dim\mathrm{Ker}(A) = d - c$.

Next, by (I.26),

$$A \;=\; \sum_{j=1}^{d} |Ag_j\rangle\langle g_j| \;=\; \sum_{j=1}^{c} |Ag_j\rangle\langle g_j| \;=\; \sum_{j=1}^{c} \rho_j\, |f_j\rangle\langle g_j|\,, \tag{II.59}$$

where $f_j := \rho_j^{-1} A g_j$, for $j \in \mathbb{Z}_1^c$, using that $\rho_j > 0$ in this case. Then $f_1, f_2, \ldots, f_c \in \mathcal{H}$ are normalized, by definition, and for all $1 \leq m < n \leq c$ we observe that

$$\langle f_m | f_n \rangle \;=\; \frac{\langle Ag_m | Ag_n \rangle}{\rho_m \rho_n} \;=\; \frac{\langle g_m | A^* A g_n \rangle}{\rho_m \rho_n} \;=\; \frac{\rho_n \, \langle g_m | g_n \rangle}{\rho_m} \;=\; 0\,. \tag{II.60}$$

It follows that $\{f_1, f_2, \ldots, f_c\} \subseteq \mathcal{H}$ is an orthonormal system which we can complement (e.g., using the Gram-Schmidt orthonormalization procedure) with vectors $f_{c+1}, \ldots, f_d$ to an ONB $\{f_1, f_2, \ldots, f_d\} \subseteq \mathcal{H}$. Using that $\rho_{c+1} = \ldots = \rho_d = 0$, we finally obtain

$$A \;=\; \sum_{j=1}^{c} \rho_j\, |f_j\rangle\langle g_j| \;=\; \sum_{j=1}^{d} \rho_j\, |f_j\rangle\langle g_j|\,, \tag{II.61}$$

as asserted. □

II.6.2. Proof of Theorem II.5 - Polar Decomposition

Proof. Let $\{f_1, \ldots, f_d\}, \{g_1, \ldots, g_d\} \subseteq \mathcal{H}$ be ONB and $\rho_1, \rho_2, \ldots, \rho_d \geq 0$ nonnegative numbers of a polar decomposition of

$$A \;=\; \sum_{n=1}^{d} \rho_n\, |f_n\rangle\langle g_n|\,, \tag{II.62}$$

which exists according to Theorem II.2. We define

$$U \;=\; \sum_{n=1}^{d} |f_n\rangle\langle g_n| \tag{II.63}$$

and observe that $U^* = \sum_{n=1}^{d} |g_n\rangle\langle f_n|$. Thus

$$U^*\, U \;=\; \sum_{m,n=1}^{d} |g_m\rangle\langle f_m | f_n\rangle\langle g_n| \;=\; \sum_{n=1}^{d} |g_n\rangle\langle g_n| \;=\; \mathbf{1}\,, \tag{II.64}$$

and similary $UU^* = \mathbf{1}$, so U is unitary. Moreover,

$$U\, |A| \;=\; \sum_{m,n=1}^{d} \rho_n\, |f_m\rangle\langle g_m | g_n\rangle\langle g_n| \;=\; \sum_{n=1}^{d} \rho_n\, |f_n\rangle\langle g_n| \;=\; A\,, \tag{II.65}$$

as asserted. □

II.6.3. Compact Operators, Trace Class Operators, Hilbert–Schmidt Operators

In this section we pass to infinite-dimensional Hilbert spaces, but we will restrict ourselves to compact operators, which are well-approximated by matrices (as opposed to the identity operator $\mathbf{1}_{\mathcal{H}}$ on $\mathcal{H}$ or differential operators like $-i\nabla$, say).

Definition II.10. Suppose that $\big(\mathcal{H}, \langle\cdot|\cdot\rangle\big)$ is a (separable, complex) Hilbert space.

(i) We define by

$$\boldsymbol{\mathcal{B}_{\mathbf{fin}}(\mathcal{H})} \ := \ \left\{ \sum_{i,j=1}^{N} a_{i,j} \, |f_i\rangle\langle f_j| \ \middle| \ N \in \mathbb{N} \, , \ \{a_{i,j}\}_{i,j=1}^{N} \subseteq \mathbb{C} \, , \ \{f_i\}_{i=1}^{N} \subseteq \mathcal{H} \right\} \ \subseteq \ \mathcal{B}(\mathcal{H}) \tag{II.66}$$

the space of linear operators (on $\mathcal{H}$) of **finite rank**.

(ii) The closure of $\mathcal{B}_{\mathrm{fin}}(\mathcal{H}) \subseteq \mathcal{B}(\mathcal{H})$ in operator norm,

$$\mathbf{Com}(\boldsymbol{\mathcal{H}}) \ := \ \overline{\mathcal{B}_{\mathrm{fin}}(\mathcal{H})}^{\|\cdot\|_{\mathrm{op}}} \ \subseteq \ \mathcal{B}(\mathcal{H}) \, , \tag{II.67}$$

defines the space of **compact operators** (on $\mathcal{H}$).

Remarks and Examples.

- The **rank $\mathbf{rk}(\boldsymbol{A})$** of an operator $A \in \mathcal{B}(\mathcal{H})$ is defined to be the dimension of its range, $\mathrm{rk}(A) := \dim[\mathrm{Ran}(A)] \in \mathbb{N}_0 \cup \{\infty\}$.
- It follows that $\mathcal{B}_{\mathrm{fin}}(\mathcal{H}) = \big\{ A \in \mathcal{B}(\mathcal{H}) \big| \ \mathrm{rk}(A) + \mathrm{rk}(A^*) < \infty \big\}$.
- The set of finite-rank operators $\mathcal{B}_{\mathrm{fin}}(\mathcal{H})$ is a subspace of $\mathcal{B}(\mathcal{H})$ which is not closed in the operator norm topology. Its closure is the space of compact operators $\mathrm{Com}(\mathcal{H})$. That is, $A \in \mathcal{B}(\mathcal{H})$ is compact iff for any $\varepsilon > 0$ there are $N \in \mathbb{N}$, $\{a_{i,j}\}_{i,j=1}^{N} \subseteq \mathbb{C}$, and $\{f_i\}_{i=1}^{N} \subseteq \mathcal{H}$ such that

$$\left\| A \ - \ \sum_{i,j=1}^{N} a_{i,j} \, |f_i\rangle\langle f_j| \right\|_{\mathrm{op}} \ \leq \ \varepsilon \, . \tag{II.68}$$

- Its closure, the set of compact operators $\mathrm{Com}(\mathcal{H})$, is a closed subspace of the Banach space $\big(\mathcal{B}(\mathcal{H}), \|\cdot\|_{\mathrm{op}}\big)$. and, hence, a Banach (sub-)space $\big(\mathrm{Com}(\mathcal{H}), \|\cdot\|_{\mathrm{op}}\big)$ itself. This Banach subspace $\mathrm{Com}(\mathcal{H}) \subseteq \mathcal{B}(\mathcal{H})$ cannot, however, be complemented by another closed subspace $X \subseteq \mathcal{B}(\mathcal{H})$, such that $\mathcal{B}(\mathcal{H}) = \mathrm{Com}(\mathcal{H}) \oplus X$.
- Since this holds true for finite-rank operators, it follows that every compact operator $A \in \mathrm{Com}(\mathcal{H})$ possesses a **singular value decomposition (SVD)**, i.e., there exist ONB $\{f_n\}_{n=1}^{\infty}, \{g_n\}_{n=1}^{\infty} \subseteq \mathcal{H}$ and singular values $\{\rho_n\}_{n=1}^{\infty} \subseteq \mathbb{R}_0^+$ of A with $\rho_n \geq \rho_{n+1}$ such that

$$A \ = \ \sum_{n=1}^{\infty} \rho_n \, |f_n\rangle\langle g_n| \, . \tag{II.69}$$

It is here where the use of Dirac's ket-bra notation pays off: We never have to introduce and use infinitly extended matrices, but only let the summation range extend to infinitly many terms.

- For $p \in [1, \infty)$, the trace norm $\| \cdot \|_p$ in (II.67) defines a norm, indeed, on the complex vector space $\mathcal{B}_{\mathrm{fin}}(\mathcal{H})$ of finite-rank operators.
- The triangle inequality is the only nontrivial part of the latter statement. We only comment on the cases $p = 1$ and $p = 2$. For $p = 1$, it rests on the representation

$$\|A\|_1 \; = \; \sup \left\{ \sum_{n=1}^{\infty} \big| \langle \psi_n | A \varphi_n \rangle \big| \; \middle| \; \{\psi_m\}_{m=1}^{\infty}, \; \{\varphi_n\}_{n=1}^{\infty} \subseteq \mathcal{H} \text{ ONB} \right\}, \tag{II.70}$$

while for $p = 2$, the key ingredient of the proof is the representation

$$\|A\|_2 \; = \; \sup \left\{ \frac{\mathrm{Tr}(B^* A)}{\mathrm{Tr}(B^* B)^{1/2}} \; \middle| \; B \in \mathcal{B}_{\mathrm{fin}}(\mathcal{H}) \setminus \{0\} \right\}. \tag{II.71}$$

To see that (II.70) is the crucial input in the case $p = 1$, let $A, B \in \mathcal{B}_{\mathrm{fin}}(\mathcal{H})$ and observe that

$$\begin{aligned} \|A + B\|_1 \; &= \; \sup \left\{ \sum_{n=1}^{\infty} \big| \langle \psi_n | (A+B) \varphi_n \rangle \big| \; \middle| \; \{\psi_m\}_{m=1}^{\infty}, \; \{\varphi_n\}_{n=1}^{\infty} \subseteq \mathcal{H} \text{ ONB} \right\} \\ &\leq \; \sup \left\{ \sum_{n=1}^{\infty} \big| \langle \psi_n | A \varphi_n \rangle \big| \; \middle| \; \{\psi_m\}_{m=1}^{\infty}, \; \{\varphi_n\}_{n=1}^{\infty} \subseteq \mathcal{H} \text{ ONB} \right\} \\ &\quad + \; \sup \left\{ \sum_{n=1}^{\infty} \big| \langle \psi_n | B \varphi_n \rangle \big| \; \middle| \; \{\psi_m\}_{m=1}^{\infty}, \; \{\varphi_n\}_{n=1}^{\infty} \subseteq \mathcal{H} \text{ ONB} \right\} \\ &= \|A\|_1 + \|B\|_1 \, . \end{aligned} \tag{II.72}$$

The case $p = 2$ uses (II.71) in a similar way.

Definition II.11. Suppose that $\big(\mathcal{H}, \langle \cdot | \cdot \rangle\big)$ is a (separable, complex) Hilbert space and that $1 \leq p < \infty$. We define by

$$\boldsymbol{\mathcal{L}^p(\mathcal{H})} \; := \; \overline{\mathcal{B}_{\mathrm{fin}}(\mathcal{H})}^{\|\cdot\|_p} \; \subseteq \; \mathcal{B}(\mathcal{H}) \, , \tag{II.73}$$

the space of ***p*-summable operators** (on $\mathcal{H}$). Specifically, the Banach space $\big(\mathcal{L}^1(\mathcal{H}), \| \cdot \|_1\big)$ is called the space of **trace class operators**, and the Banach space $\big(\mathcal{L}^2(\mathcal{H}), \| \cdot \|_2\big)$ is called the space of **Hilbert-Schmidt operators**.

Theorem II.12. *Let $\big(\mathcal{H} = \mathbb{C}^d, \langle \cdot | \cdot \rangle = \langle \cdot | \cdot \rangle_{\mathrm{unit}}\big)$ be a complex Hilbert space with an ONB $\{\varphi_j\}_{j=1}^{\infty} \subseteq \mathcal{H}$ and $A \in \mathcal{L}^1(\mathcal{H})$. Then the* ***trace of A***

$$\mathrm{Tr}(A) \; := \; \sum_{j=1}^{\infty} \langle \varphi_j | \, A \varphi_j \rangle \tag{II.74}$$

*exists and is independent of the ONB $\{\varphi_j\}_{j=1}^\infty \subseteq \mathcal{H}$. If $A_1, A_2, \ldots, A_L \in \mathcal{L}^1(\mathcal{H})$ then the trace is **cyclic**,*

$$\mathrm{Tr}(A_1 A_2 \cdots A_{L-1} A_L) \;=\; \mathrm{Tr}(A_L A_1 A_2 \cdots A_{L-1} A_L)\,. \tag{II.75}$$

Proof. Due to (II.70), the sum on the right side of (II.74) exists and is bounded in absolute value by $\|A\|_1$,

$$\Big| \sum_{j=1}^\infty \langle \varphi_j |\, A\varphi_j\rangle \Big| \;\leq\; \|A\|_1\,. \tag{II.76}$$

Let $\{\psi_k\}_{k=1}^\infty \subseteq \mathcal{H}$ be a second ONB. Given $\varepsilon > 0$, we can find a finite-rank operator $A_\varepsilon \in \mathcal{B}_{\mathrm{fin}}(\mathcal{H})$ such that $\|A - A_\varepsilon\|_1 \leq \varepsilon$. Since A_ε is of finite rank,

$$\sum_{j=1}^\infty \langle \varphi_j |\, A_\varepsilon \varphi_j\rangle \;=\; \mathrm{Tr}(A_\varepsilon) \;=\; \sum_{k=1}^\infty \langle \psi_k |\, A_\varepsilon \psi_k\rangle\,. \tag{II.77}$$

It follows from (II.77) and an application of (II.76) to $A - A_\varepsilon$ that

$$\begin{aligned}\Big| \sum_{j=1}^\infty \langle \varphi_j |\, A\varphi_j\rangle \;-\; \sum_{k=1}^\infty \langle \psi_k |\, A\psi_k\rangle \Big| &= \Big| \sum_{j=1}^\infty \langle \varphi_j |\, (A - A_\varepsilon)\varphi_j\rangle \;-\; \sum_{k=1}^\infty \langle \psi_k |\, (A - A_\varepsilon)\psi_k\rangle \Big| \\ &\leq 2\,\|A - A_\varepsilon\|_1 \;\leq\; 2\varepsilon\,. \end{aligned} \tag{II.78}$$

Since $\varepsilon > 0$ can be chosen arbitrarily small, (II.78) implies that

$$\sum_{j=1}^\infty \langle \varphi_j |\, A\varphi_j\rangle \;=\; \sum_{k=1}^\infty \langle \psi_k |\, A\psi_k\rangle\,. \tag{II.79}$$

The proof of cyclicity is similar: First, one observes that it suffices to prove $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$ for two trace-class operators $A, B \in \mathcal{L}^1(\mathcal{H})$. Then both A and B are approximated by finite-rank operators A_ε and B_ε up to errors in trace norm of size $\varepsilon > 0$. For A_ε and B_ε the identity $\mathrm{Tr}(A_\varepsilon B_\varepsilon) = \mathrm{Tr}(B_\varepsilon A_\varepsilon)$ is trivial. Hence,

$$\begin{aligned}\big|\mathrm{Tr}(AB) - \mathrm{Tr}(BA)\big| \;&\leq\; \big|\mathrm{Tr}(AB) - \mathrm{Tr}(A_\varepsilon B_\varepsilon)\big| \;+\; \big|\mathrm{Tr}(B_\varepsilon A_\varepsilon) - \mathrm{Tr}(BA)\big| \\ &\leq 2\big|\mathrm{Tr}[A(B - B_\varepsilon)]\big| \;+\; 2\big|\mathrm{Tr}[(A - A_\varepsilon)B_\varepsilon]\big| \\ &\leq 2\varepsilon\Big(\|A\|_1 + \|B\|_1 + \varepsilon\Big)\,, \end{aligned} \tag{II.80}$$

and $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$ follows in the limit $\varepsilon \to 0$. $\square$