Preliminaries

These notes assume familiarity with basic linear algebra over the field of complex numbers. For convenience, we quickly recall the concepts that will be relevant, and we fix notation. As is common in the field, we use Dirac's so-called bra-ket notation

0.1 Dirac's Bra-ket Notation

Let $\mathbb{C}$ be the field of complex numbers, and let $\mathcal{H}$ be a finite-dimensional **Hilbert space** over $\mathbb{C}$. Vectors in $\mathcal{H}$ are denoted as **ket-vectors** $|\varphi\rangle$. Given $\mathcal{H}$, we consider the following two related spaces. The **dual** vector space $\mathcal{H}^*$ of $\mathcal{H}$, i.e., the vector space of linear functionals $\mathcal{H} \to \mathbb{C}$; the elements of $\mathcal{H}^*$ are denoted as **bra-vectors** $\langle\psi|$. And, second, the algebra $\mathcal{L}(\mathcal{H})$ of linear maps $\mathcal{H} \to \mathcal{H}$, with the identity map denoted as $\mathbb{I}$ (or as $\mathbb{I}_{\mathcal{H}}$, if we want to make $\mathcal{H}$ explicit). More generally, for (finite-dimensional complex) Hilbert spaces $\mathcal{H}$ and $\mathcal{H}'$, we write $\mathcal{L}(\mathcal{H},\mathcal{H}')$ for the vector space of linear maps $\mathcal{H} \to \mathcal{H}'$. An element of $\mathcal{L}(\mathcal{H})$ or $\mathcal{L}(\mathcal{H},\mathcal{H}')$ is called an **operator**. We also consider operators in $\mathcal{L}\big(\mathcal{L}(\mathcal{H})\big)$ or $\mathcal{L}\big(\mathcal{L}(\mathcal{H}),\mathcal{L}(\mathcal{H}')\big)$, which are then refered to as **superoperators**. The identity superoperator in $\mathcal{L}\big(\mathcal{L}(\mathcal{H})\big)$ is denoted by *id*.

By considering a fixed orthonormal basis of $\mathcal{H}$ (see Section 0.2) and setting $d := \dim \mathcal{H}$, ket-vectors $|\varphi\rangle \in \mathcal{H}$ can be represented by *column vectors* in $\mathbb{C}^d$ and bra-vectors $\langle\psi| \in \mathcal{H}^*$ by *row vectors* in $\mathbb{C}^d$. Similarly, operators $R \in \mathcal{L}(\mathcal{H})$ are then represented by *matrices* in $\mathbb{C}^{d\times d}$, and correspondingly for $R \in \mathcal{L}(\mathcal{H},\mathcal{H}')$. The standard matrix multiplication is then consistent with how the elements of $\mathbb{C}$, $\mathcal{H}$, $\mathcal{H}^*$ and $\mathcal{L}(\mathcal{H})$ naturally act upon each other in an associative and linear way. For instance, a bra-vector $\langle\psi| \in \mathcal{H}^*$ acts on a ket-vector $|\varphi\rangle \in \mathcal{H}$, resulting in a scalar, which we then write as

$$\langle\psi|\varphi\rangle := \langle\psi||\varphi\rangle \in \mathbb{C}\,.$$

Similarly, we have

$$R|\varphi\rangle \in \mathcal{H}\;, \quad \langle\psi|R \in \mathcal{H}^* \quad \text{and} \quad |\varphi\rangle\langle\psi| \in \mathcal{L}(\mathcal{H})\;,$$

etc.

We now bring the **inner product** $(\cdot,\cdot)$ into the picture, which makes the vector space $\mathcal{H}$ a Hilbert space.[1] For ket-vectors $|\psi\rangle, |\varphi\rangle \in \mathcal{H}$, given as column vectors

$$|\psi\rangle = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_d \end{bmatrix} \in \mathbb{C}^d \qquad \text{and} \qquad |\varphi\rangle = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_d\;, \end{bmatrix} \in \mathbb{C}^d\;,$$

the inner product is

$$(|\psi\rangle,|\varphi\rangle) = \sum_i \bar{\alpha}_i\beta_i \in \mathbb{C}\,,$$

[1] Since we are in finite dimension, *completeness* is automatically ensured.

where, for any scalar $\alpha \in \mathbb{C}$, $\bar{\alpha}$ denotes its complex conjugate.[2] Clearly, $\overline{(|\psi\rangle, |\varphi\rangle)} = (|\varphi\rangle, |\psi\rangle)$. For any such ket-vector $|\psi\rangle \in \mathcal{H}$ there exists a (unique) bra-vector in $\mathcal{H}^*$, denoted by $\langle\psi|$ then, such that

$$\langle\psi||\varphi\rangle = (|\psi\rangle, |\varphi\rangle)$$

for any $|\varphi\rangle \in \mathcal{H}$, and vice versa. Obviously, in the matrix view, $\langle\psi| = \big[\bar{\alpha}_1, \bar{\alpha}_2, \cdots, \bar{\alpha}_d\big]$ is the claimed bra-vector. This also means that we may understand $\langle\psi|\varphi\rangle$, our short hand for $\langle\psi||\varphi\rangle$, as an alternative notiation for the *inner product* $(|\psi\rangle, |\varphi\rangle)$ of $|\psi\rangle$ and $|\varphi\rangle$. In line with this, $|\varphi\rangle\langle\psi|$ is called the **outer product** of $|\varphi\rangle$ and $|\psi\rangle$.[3]

More generally, for any operator $R \in \mathcal{L}(\mathcal{H}, \mathcal{H}')$ there exists a (unique) $R^\dagger \in \mathcal{L}(\mathcal{H}', \mathcal{H})$, called the **adjoint** of R, so that $(R|\psi\rangle, |\varphi'\rangle) = (|\psi\rangle, R^\dagger|\varphi'\rangle)$ for all $|\psi\rangle \in \mathcal{H}$ and $|\varphi'\rangle \in \mathcal{H}'$. When given as a matrix, $R^\dagger$ is the **conjugate transpose** of R. Thus, we may actually write

$$|\varphi\rangle^\dagger = \langle\varphi| \qquad \text{and} \qquad \langle\varphi|^\dagger = |\varphi\rangle\,,$$

and, similarly, $\alpha^\dagger = \bar{\alpha}$ for any scalar $\alpha \in \mathbb{C}$. Together with basic properties of the adjoint, namely that $(RL)^\dagger = L^\dagger R^\dagger$, this also shows that, for instance, the bra-vector defined by the ket-vector $R|\varphi\rangle \in \mathcal{H}$ is given by $(R|\varphi\rangle)^\dagger = \langle\varphi|R^\dagger$.

Finally, we point out that in the context of Dirac's bra-ket notation, it is convenient to define the **trace** as the unique linear functional $\mathrm{tr} : \mathcal{L}(\mathcal{H}) \to \mathbb{C}$ with the property that

$$\mathrm{tr}(|\varphi\rangle\langle\psi|) = \langle\psi|\varphi\rangle$$

for all $|\psi\rangle, |\varphi\rangle \in \mathcal{H}$. It is not too hard to show (see also the next section) that this is equivalent to the standard definition of the trace of an operator. We recall that the trace is cyclic, i.e.,

$$\mathrm{tr}(RL) = \mathrm{tr}(LR)$$

for all $R, L \in \mathcal{L}(\mathcal{H})$, which actually can be seen very easily from our way of defining the trace.

We can carry over the inner product from the Hilbert space $\mathcal{H}$ to the dual vector space $\mathcal{H}^*$ by setting $(\langle\varphi|, \langle\psi|) = \langle\psi|\varphi\rangle$, and we can lift it to $\mathcal{L}(\mathcal{H})$, and more generally to $\mathcal{L}(\mathcal{H}, \mathcal{H}')$, by setting $(R, L) = \mathrm{tr}(R^\dagger L)$ for $R, L \in \mathcal{L}(\mathcal{H}, \mathcal{H}')$. The latter is called **Hilbert-Schmidt** (or **Frobenius**) **inner product**, and it is consistent with the inner products in $\mathcal{H}$, $\mathcal{H}^*$ and $\mathbb{C}$ when considering the respective special cases $\mathcal{L}(\mathbb{C}, \mathcal{H})$, $\mathcal{L}(\mathcal{H}, \mathbb{C})$ and $\mathcal{L}(\mathbb{C}, \mathbb{C})$.

0.2 Basic Linear Algebra

We recall some basic concepts and facts from linear algebra, which will be of importance for us; more details can be found in standard linear-algebra textbooks. Recall that $\mathcal{H}$ denotes a Hilbert space, $\mathcal{H}^*$ its dual, and $\mathcal{L}(\mathcal{H})$ the algebra of operators $\mathcal{H} \to \mathcal{H}$, and it is from now on understood that by a "Hilbert space" we always mean a finite-dimensional complex Hilbert space.

As is standard, we write $\|\cdot\|$ for the **norm** induced by the inner product, i.e.,

$$\||\varphi\rangle\| = \sqrt{\langle\varphi|\varphi\rangle}$$

for any $|\varphi\rangle \in \mathcal{H}$.

[2] Note that this is opposite to the convention typically used in mathematics, where the inner product is usually considered to be *linear* in the *first* argument and *conjugate-linear* in the *second*.

[3] Typically $|\varphi\rangle, |\psi\rangle \in \mathcal{H}$, but $|\varphi\rangle\langle\psi|$ is well defined also for $|\psi\rangle \in \mathcal{H}$ and $|\varphi\rangle \in \mathcal{H}'$, as operator in $\mathcal{L}(\mathcal{H}, \mathcal{H}')$ then.

Proposition 0.1 (Cauchy-Schwarz inequality)**.** *For any* $|\varphi\rangle, |\psi\rangle \in \mathcal{H}$*:*

$$|\langle\varphi|\psi\rangle| \leq \||\varphi\rangle\| \cdot \||\psi\rangle\|$$

with equality if and only if $|\varphi\rangle = \alpha|\psi\rangle$ *for some* $\alpha \in \mathbb{C}$*.*

A family $\{|e_i\rangle\}_{i\in I}$ of ket-vectors[4] is an **orthonormal basis** of $\mathcal{H}$ if it is a basis of $\mathcal{H}$, i.e., the vectors are *linearly independent* and *span* all of $\mathcal{H}$, and

$$\langle e_i|e_j\rangle = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

for all $i, j \in I$. Similarly, we can define orthonormal bases of $\mathcal{H}^*$ and $\mathcal{L}(\mathcal{H})$, and we observe that if $\{|e_i\rangle\}_{i\in I}$ is an orthonormal basis of $\mathcal{H}$ then $\{\langle e_i|\}_{i\in I}$ is an orthonormal basis of $\mathcal{H}^*$ and $\{|e_i\rangle\langle e_j|\}_{i,j\in I}$ is an orthonormal basis of $\mathcal{L}(\mathcal{H})$.

It is an easy exercise to show that a basis $\{|e_i\rangle\}_{i\in I}$ of $\mathcal{H}$ is orthonormal if and only if

$$\sum_{i\in I} |e_i\rangle\langle e_i| = \mathbb{I}\,.$$

This in particular implies that for any $R \in \mathcal{L}(\mathcal{H})$ and any orthonormal basis $\{|e_i\rangle\}_{i\in I}$ of $\mathcal{H}$

$$\mathrm{tr}(R) = \sum_{i\in I} \mathrm{tr}(R|e_i\rangle\langle e_i|) = \sum_{i\in I} \langle e_i|R|e_i\rangle\,;$$

thus, our definition of the trace coincides with the standard one.

When using Dirac's bra-ket notation, it is common and convenient to denote an orthonormal basis by $\{|i\rangle\}_{i\in I}$ instead of, say, $\{|e_i\rangle\}_{i\in I}$. In other words, we may use the indices as "names" of the vectors. The indices may be integers or reals, but also abstract symbols. For instance, the orthonormal basis vectors $\binom{1}{0}$ and $\binom{0}{1}$ of $\mathcal{H} = \mathbb{C}^2$ will be denoted by $|0\rangle$ and $|1\rangle$, respectively, and $\frac{1}{\sqrt{2}}\binom{1}{1}$ and $\frac{1}{\sqrt{2}}\binom{1}{-1}$ by $|+\rangle$ and $|-\rangle$, respectively.

Let $R \in \mathcal{L}(\mathcal{H})$. We recall the following standard notions. The **image** of R is the subspace of $\mathcal{H}$ defined by $\mathrm{im}(R) := \{R|\varphi\rangle \in \mathcal{H} \,|\, |\varphi\rangle \in \mathcal{H}\}$, and the **kernel** of R is the subspace of $\mathcal{H}$ defined by $\ker(R) := \{|\varphi\rangle \in \mathcal{H} \,|\, R|\varphi\rangle = 0\}$. Furthermore, the **support** $\mathrm{supp}(R)$ of R is the orthogonal complement of the kernel, i.e., $\mathrm{supp}(R) := \{|\psi\rangle \in \mathcal{H} \,|\, \langle\psi|\varphi\rangle = 0 \;\forall\, |\varphi\rangle \in \ker(R)\}$, and the **rank** is the dimension of the support, i.e., $\mathrm{rank}(R) := \dim(\mathrm{supp}(R))$.

It is easy to see that $\mathrm{rank}(R) = 1$ if and only if $R = |\psi\rangle\langle\varphi|$ for non-zero $|\psi\rangle, |\varphi\rangle \in \mathcal{H}$, and we then obviously have that $|\varphi\rangle$ spans $\mathrm{supp}(R)$ and $|\psi\rangle$ spans $\mathrm{im}(R)$.

We conclude by recalling some important classes of operators and some of their properties. An operator $R \in \mathcal{L}(\mathcal{H})$ is called **normal** if

$$R^\dagger R = R R^\dagger\,,$$

and it is called **Hermitian** (or **self-adjoint**) if

$$R^\dagger = R\,.$$

It is not too hard to show that $R \in \mathcal{L}(\mathcal{H})$ is Hermitian if and only if $\langle\varphi|R|\varphi\rangle \in \mathbb{R}$ for all $|\varphi\rangle \in \mathcal{H}$. Furthermore, $R \in \mathcal{L}(\mathcal{H})$ is **positive-semidefinite**, denoted by $R \geq 0$, if

$$\langle\varphi|R|\varphi\rangle \geq 0 \quad \forall\, |\varphi\rangle \in \mathcal{H}\,;$$

[4] Such a family $\{|e_i\rangle\}_{i\in I}$ of vectors (or later matrices) stands for the function $I \to \mathcal{H}$, $i \mapsto |e_i\rangle$, but we think of it as a (unordered) list of vectors with indices in I. We may also write $\{|e_1\rangle, \ldots, |e_d\rangle\}$ instead of $\{|e_i\rangle\}_{i\in\{1,\ldots,d\}}$.

this in particular implies that R is Hermitian. We set $\mathcal{P}(\mathcal{H}) := \{R \in \mathcal{L}(\mathcal{H}) \,|\, R \geq 0\}$, and for $R, L \in \mathcal{L}(\mathcal{H})$ we write $R \geq L$ to express that $R - L \geq 0$. This is known as **Loewner order**.

For Hilbert spaces $\mathcal{H}$ and $\mathcal{H}'$ with $\dim(\mathcal{H}) = \dim(\mathcal{H}')$, $U \in \mathcal{L}(\mathcal{H}, \mathcal{H}')$ is **unitary** if

$$U^\dagger U = \mathbb{I}_{\mathcal{H}} \qquad \text{and} \qquad UU^\dagger = \mathbb{I}_{\mathcal{H}'} \,.$$

We write $\mathcal{U}(\mathcal{H}, \mathcal{H}')$ and $\mathcal{U}(\mathcal{H})$ for the respective sets of unitary operators $U \in \mathcal{L}(\mathcal{H}, \mathcal{H}')$ and $U \in \mathcal{L}(\mathcal{H})$. For $\mathcal{H}$ and $\mathcal{H}'$ as above, it is well known that if $U \in \mathcal{L}(\mathcal{H}, \mathcal{H}')$ maps *some* orthonormal basis of $\mathcal{H}$ into an orthonormal basis of $\mathcal{H}'$ then $U \in \mathcal{U}(\mathcal{H}, \mathcal{H}')$ is unitary, and, vice versa, if $U \in \mathcal{U}(\mathcal{H}, \mathcal{H})$ then U maps *every* orthonormal basis of $\mathcal{H}$ into an orthonormal basis of $\mathcal{H}'$.

For Hilbert spaces $\mathcal{H}$ and $\mathcal{H}'$ with $\dim(\mathcal{H}) \leq \dim(\mathcal{H}')$, $V \in \mathcal{L}(\mathcal{H}, \mathcal{H}')$ is called an **isometry** if $V^\dagger V = \mathbb{I} \in \mathcal{L}(\mathcal{H})$. Similarly to a unitary, an isometry maps any orthonormal basis of $\mathcal{H}$ into an orthonormal basis of $\mathrm{im}(V) \subseteq \mathcal{H}'$, and vice versa. It is easy thus easy to see that for any two isometries $V, W \in \mathcal{L}(\mathcal{H}, \mathcal{H}')$ there exists a unitary $U \in \mathcal{U}(\mathcal{H}')$ with $W = UV$.

Finally, an operator $P \in \mathcal{L}(\mathcal{H})$ is called a **projection**[5] if

$$P^\dagger = P \qquad \text{and} \qquad P^2 = P \,,$$

and two such projections $P, Q \in \mathcal{L}(\mathcal{H})$ are **mutually orthogonal** if $PQ = 0$ (and thus also $QP = 0$). This notion of orthogonality coincides with the orthogonality with respect to the Hilbert-Schmidt inner product, as can e.g. be seen by means of the following characterization.

Lemma 0.2. *$P \in \mathcal{L}(\mathcal{H})$ is a projection if and only if*

$$P = \sum_{i=1}^{r} |e_i\rangle\langle e_i|$$

for some orthonormal basis $\{|e_1\rangle, \ldots, |e_d\rangle\}$ of $\mathcal{H}$ and $0 \leq r \leq d$.

Proof. The "if"-direction is straightforward. For the "only if"-direction, let $\{|e_1\rangle, \ldots, |e_d\rangle\}$ be an orthonormal basis such that $\{|e_1\rangle, \ldots, |e_r\rangle\}$ spans the image of P. It follows that $P|e_i\rangle = |e_i\rangle$ for every $0 \leq i \leq r$; indeed, $|e_i\rangle = P|\varphi_i\rangle$ for some $|\varphi_i\rangle \in \mathcal{H}$ and thus $P|e_i\rangle = P^2|\varphi_i\rangle = P|\varphi_i\rangle = |e_i\rangle$. On the other hand, for $0 \leq i \leq r < j \leq d$, we see that $\langle e_i|P|e_j\rangle = \langle e_i|P^\dagger|e_j\rangle = \langle e_i|e_j\rangle = 0$, i.e., $P|e_j\rangle \in \mathrm{im}(P)$ is orthogonal to $\mathrm{im}(P)$, and hence must be zero. $\square$

0.3 Spectral Decomposition

An important concept is *spectral decomposition*, which we briefly recall here. We start with the following well-known notions. Let $R \in \mathcal{L}(\mathcal{H})$. A non-zero $|\varphi\rangle \in \mathcal{H}$ is called an **eigenvector** of R if $R|\varphi\rangle = \lambda|\varphi\rangle$ for some $\lambda \in \mathbb{C}$, called the corresponding **eigenvalue**. For any eigenvalue λ of R, the subspace $\{|\varphi\rangle \in \mathcal{H} \,|\, R|\varphi\rangle = \lambda|\varphi\rangle\}$ is called the **eigenspace** corresponding to λ.

If $R \in \mathcal{L}(\mathcal{H})$ is Hermitian, then all eigenvalues of R are real, and eigenvectors $|\varphi\rangle$ and $|\psi\rangle$ with *different* eigenvalues satisfy $\langle\varphi|\psi\rangle = 0$. More generally, the following holds.

Theorem 0.3 (Spectral decomposition)**.** *Let $R \in \mathcal{L}(\mathcal{H})$ be normal and $d = \dim(\mathcal{H})$. Then*

$$R = \sum_{i=1}^{d} \lambda_i |e_i\rangle\langle e_i|$$

with $\lambda_1, \ldots, \lambda_d \in \mathbb{C}$ and where $\{|e_1\rangle, \ldots, |e_d\rangle\}$ forms an orthonormal basis of $\mathcal{H}$. Furthermore, if R is Hermitian then $\lambda_1, \ldots, \lambda_d \in \mathbb{R}$.

[5] In the literature, this is sometimes also referred to as an *orthogonal* or *Hermitian* projection.

As a matter of fact, the λ_i's are the eigenvalues of R and the $|e_i\rangle$'s the corresponding eigenvectors. We remark that even though the spectral decomposition of a normal operator R is not unique, in that there is freedom in the ordering of the eigenvalues λ_i and in choosing the bases for the eigenspaces, we typically speak of *the* spectral decomposition of R.

Proof. The characteristic polynomial of R has at least one root $\lambda \in \mathbb{C}$, and thus R has at least one (normalized) eigenvector $|\varepsilon\rangle \in \mathcal{H}$. Then, R acts like $\lambda|\varepsilon\rangle\langle\varepsilon|$ on any multiple of $|\varepsilon\rangle$. Furthermore, in case R is Hermitian, we see that $\bar{\lambda} = \overline{\langle\varepsilon|R|\varepsilon\rangle} = \langle\varepsilon|R^\dagger|\varepsilon\rangle = \langle\varepsilon|R|\varepsilon\rangle = \lambda$, and hence $\lambda \in \mathbb{R}$. Therefore, in case $d = 1$ we are done. Otherwise, we observe that $|\varepsilon\rangle$ is also an eigenvector of $R^\dagger$ with eigenvalue λ; indeed, $R^\dagger|\varepsilon\rangle - \lambda|\varepsilon\rangle$ has norm $\langle\varepsilon|(R - \bar{\lambda})(R^\dagger - \lambda)|\varepsilon\rangle = \langle\varepsilon|(R^\dagger - \bar{\lambda})(R - \lambda)|\varepsilon\rangle = 0$. As a consequence, for every $|\varphi\rangle$ that is orthogonal to $|\varepsilon\rangle$, we have that $\langle\varepsilon|R|\varphi\rangle = \bar{\lambda}\langle\varepsilon|\varphi\rangle = 0$. Hence, we can consider R as an operator in $\mathcal{L}(\mathcal{H}')$ with $\mathcal{H}'$ the orthogonal complement of (the span of) $|\varepsilon\rangle$, and then conclude by induction. $\square$

The following can now be easily seen. If $R \in \mathcal{L}(\mathcal{H})$ is normal then $R \geq 0$ if and only if all its eigenvalues are ≥ 0. Also, if $R \in \mathcal{L}(\mathcal{H})$ is normal, with spectral decomposition as above, then,

$$\ker(R) = \mathrm{span}(\{|e_i\rangle \mid \lambda_i = 0\}) \qquad \text{and} \qquad \mathrm{supp}(R) = \mathrm{im}(R) = \mathrm{span}(\{|e_i\rangle \mid \lambda_i \neq 0\}),$$

and thus $\mathrm{rank}(R) = |\{i \mid \lambda_i \neq 0\}|$.

This family $\{\lambda_1, \ldots, \lambda_d\}$ of eigenvalues, where each eigenvalue is counted according to the dimension of the corresponding eigenspace, is called the **spectrum** of R. Related to the eigenvalues are the **singular values** of an operator $R \in \mathcal{L}(\mathcal{H})$, which are the respective square roots of the eigenvalues of $R^\dagger R$. We also note the following.

Lemma 0.4. *Let $R \in \mathcal{L}(\mathcal{H}, \mathcal{H}')$. Then, $R^\dagger R$ and $RR^\dagger$ have the same non-zero eigenvalues.*

Proof. Let $|\varphi\rangle$ be eigenvector of $R^\dagger R$ with eigenvalue $\lambda \neq 0$. Then, $|\psi\rangle := R|\varphi\rangle$ is an eigenvector of $RR^\dagger$ with eigenvalue λ too: $RR^\dagger|\psi\rangle = RR^\dagger R|\varphi\rangle = \lambda R|\varphi\rangle = \lambda|\psi\rangle$. Furthermore, for two such eigenvectors $|\varphi\rangle, |\varphi'\rangle$ of $R^\dagger R$ with eigenvalues λ, λ', if $|\varphi\rangle$ and $|\varphi'\rangle$ are orthogonal then so are $|\psi\rangle := R|\varphi\rangle$ and $|\psi'\rangle := R|\varphi'\rangle$; indeed, $\langle\psi|\psi'\rangle = \langle\varphi|R^\dagger R|\varphi'\rangle = \lambda'\langle\varphi|\varphi'\rangle = 0$. The corresponding also holds the other way round; this then proves the claim. $\square$

0.4 Matrix Functions

Given a function $f : \mathbb{C} \supseteq D \to \mathbb{C}$, we want to have a meaningful way to apply f to an *operator* $R \in \mathcal{L}(\mathcal{H})$. For some functions, like multiplication with a scalar, or raising to some integer power, this is quite obvious, e.g., we understand well what we mean by $7R$ or R^3, but for other functions it is less clear, e.g., what should $\log(R)$ be? For normal R, this can be done as follows.

Definition 0.1. *Let $f : \mathbb{C} \supseteq D \to \mathbb{C}$ be an arbitrary function. Then, for any normal $R \in \mathcal{L}(\mathcal{H})$ with spectrum in D, we define*

$$f(R) := \sum_{i=1}^{d} f(\lambda_i)|e_i\rangle\langle e_i|,$$

where $R = \sum_{i=1}^{d} \lambda_i|e_i\rangle\langle e_i|$ is the spectral decomposition of R.

Remark 0.1. Understanding the spectral decomposition to be the sum over the *non-zero* eigenvalues λ_i, it is sufficent to require the non-zero eigenvalues to be in D for the above to make sense. This for instance allows us to define R^{-1} (or any other negative power) for *singular* normal operators; this is called the **pseudo-inverse** of R.

Remark 0.2. Also, R^0 is then well defined to be the projection into $\text{supp}(R)$. In particular, for normal $L, R \in \mathcal{L}(\mathcal{H})$ with $\text{supp}(L) \subseteq \text{supp}(R)$ it holds that $LR^0 = L = R^0 L$.

Remark 0.3. For $0 \leq R \in \mathcal{L}(\mathcal{H})$, Defintion 0.1 in particular shows existence of $0 \leq \sqrt{R} \in \mathcal{L}(\mathcal{H})$ with $\sqrt{R}^2 = R$. Writing $\langle\varphi|R|\varphi\rangle = \langle\varphi|\sqrt{R}^2|\varphi\rangle = \langle\varphi|\sqrt{R}^\dagger\sqrt{R}|\varphi\rangle = \big\|\sqrt{R}|\varphi\rangle\big\|^2$, and using basic properties of the norm, it then follows that for $0 \leq R \in \mathcal{L}(\mathcal{H})$:

$$|\varphi\rangle \in \ker(R) \iff \langle\varphi|R|\varphi\rangle = 0\,.$$

The restriction on R to be normal can be avoided, for instance by using the so-called Jordan canonical form of R, or, if f is analytic on and inside a closed contour that encloses the spectrum, via the Cauchy integral, but this is beyond what we need. The only exception is the following.

Definition 0.2. *For any $R \in \mathcal{L}(\mathcal{H})$, we define the* **modulus** *of R to be the operator*

$$|R| := \sqrt{R^\dagger R} \in \mathcal{P}(\mathcal{H})\,.$$

Obviously, in case of a normal R, the above two definitions are consistent.

0.5 The Tensor Product

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be (finite-dimensional complex) Hilbert spaces, considered as vector spaces for now. Then, an explicit way to define the tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$ of $\mathcal{H}_1$ and $\mathcal{H}_2$ is by setting it to be the vector space of bilinear maps $\mathcal{H}_1^* \times \mathcal{H}_2^* \to \mathbb{C}$. Furthermore, for $|\varphi_1\rangle \in \mathcal{H}_1$ and $|\varphi_2\rangle \in \mathcal{H}_2$, one then defines $|\varphi_1\rangle \otimes |\varphi_2\rangle$ to be the element in $\mathcal{H}_1 \otimes \mathcal{H}_2$ that maps

$$\mathcal{H}_1^* \times \mathcal{H}_2^* \ni (\langle\psi_1|, \langle\psi_2|) \mapsto \langle\psi_1|\varphi_1\rangle\langle\psi_2|\varphi_2\rangle \in \mathbb{C}\,.$$

Every element in $\mathcal{H}_1 \otimes \mathcal{H}_2$ can then be written (non-uniquely) as a finite linear combination of vectors $|\varphi_1\rangle \otimes |\varphi_2\rangle$ with $|\varphi_1\rangle \in \mathcal{H}_1$ and $|\varphi_2\rangle \in \mathcal{H}_2$, and the following equalities hold:

$$\big(|\varphi_1\rangle + |\psi_1\rangle\big) \otimes |\varphi_2\rangle = |\varphi_1\rangle \otimes |\varphi_2\rangle + |\psi_1\rangle \otimes |\varphi_2\rangle\,,$$

$$|\varphi_1\rangle \otimes \big(|\varphi_2\rangle + |\psi_2\rangle\big) = |\varphi_1\rangle \otimes |\varphi_2\rangle + |\varphi_1\rangle \otimes |\psi_2\rangle$$

and

$$\big(\lambda|\varphi_1\rangle\big) \otimes |\varphi_2\rangle = \lambda\big(|\varphi_1\rangle \otimes |\varphi_2\rangle\big) = |\varphi_1\rangle \otimes \big(\lambda|\varphi_2\rangle\big)$$

hold for all $|\varphi_1\rangle, |\psi_1\rangle \in \mathcal{H}_1$ and $|\varphi_2\rangle, |\psi_2\rangle \in \mathcal{H}_2$ and $\lambda \in \mathbb{C}$.

Despite the explicit definition given, it will be convenient to think of $\mathcal{H}_1 \otimes \mathcal{H}_2$ as an abstract vector space with the above properties.

Along the same lines, we can define the tensor product $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_1') \otimes \mathcal{L}(\mathcal{H}_2, \mathcal{H}_2')$ of two operator spaces, and the tensor product $\mathcal{H}_1^* \otimes \mathcal{H}_2^*$ of two dual spaces; after all, these are again vector spaces.

A tensor product $R \otimes L \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_1') \otimes \mathcal{L}(\mathcal{H}_2, \mathcal{H}_2')$ of operators R in $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_1')$ and L in $\mathcal{L}(\mathcal{H}_2, \mathcal{H}_2')$ naturally acts on a tensor product $|\psi_1\rangle \otimes |\psi_2\rangle$ of ket vectors $|\psi_1\rangle \in \mathcal{H}_1$ and $|\psi_2\rangle \in \mathcal{H}_2$ as

$$(R \otimes L)(|\psi_1\rangle \otimes |\psi_2\rangle) = R|\psi_1\rangle \otimes L|\psi_2\rangle\,.$$

It is straightforward to verify that by linear extension this induces a well-defined natural isomorphism between $\mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2, \mathcal{H}_1' \otimes \mathcal{H}_2')$ and $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_1') \otimes \mathcal{L}(\mathcal{H}_2, \mathcal{H}_2')$, and so by convention we will not distinguish between the two.

Similarly, a tensor product of bra-vectors acts on a tensor product of ket-vectors as

$$(\langle\varphi_1| \otimes \langle\varphi_2|)(|\psi_1\rangle \otimes |\psi_2\rangle) = \langle\varphi_1||\psi_1\rangle \otimes \langle\varphi_2||\psi_2\rangle = \langle\varphi_1|\psi_1\rangle \otimes \langle\varphi_2|\psi_2\rangle = \langle\varphi_1|\psi_1\rangle\langle\varphi_2|\psi_2\rangle\,,$$

inducing a natural isomorphism between $(\mathcal{H}_1 \otimes \mathcal{H}_2)^*$ and $\mathcal{H}_1^* \otimes \mathcal{H}_2^*$. Above, we additionally exploited the natural isomorphism $\mathbb{C} \otimes \mathbb{C} \to \mathbb{C}$, $\alpha \otimes \beta \mapsto \alpha\beta$, and thus by convention we do not distinguish between the two.[6] Along the same lines, a tensor product of ket-vectors acts on a tensor product of bra-vectors as

$$(|\psi_1\rangle \otimes |\psi_2\rangle)(\langle\varphi_1| \otimes \langle\varphi_2|) = |\psi_1\rangle\langle\varphi_1| \otimes |\psi_2\rangle\langle\varphi_2|\,.$$

From our definition of the trace as "turning an outer product into an inner product", it then follows that $\mathrm{tr}(|\psi_1\rangle\langle\varphi_1| \otimes |\psi_2\rangle\langle\varphi_2|) = \mathrm{tr}(|\psi_1\rangle\langle\varphi_1|) \cdot \mathrm{tr}(|\psi_2\rangle\langle\varphi_2|)$, and thus

$$\mathrm{tr}(R \otimes L) = \mathrm{tr}(R) \cdot \mathrm{tr}(L)$$

for all $R \in \mathcal{L}(\mathcal{H}_1)$ and $L \in \mathcal{L}(\mathcal{H}_2)$. We can also "mix-and-match", and for instance consider $R \otimes \langle\varphi_2| \in \mathcal{L}(\mathcal{H}_1) \otimes \mathcal{H}_2^*$, which then acts on $|\psi_1\rangle \otimes |\psi_2\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ as

$$(R \otimes \langle\varphi_2|)(|\psi_1\rangle \otimes |\psi_2\rangle) = R|\psi_1\rangle \otimes \langle\varphi_2|\psi_2\rangle = R|\psi_1\rangle\langle\varphi_2|\psi_2\rangle\,,$$

or $R \otimes |\psi_2\rangle \in \mathcal{L}(\mathcal{H}_1) \otimes \mathcal{H}_2$, which then acts on $|\psi_1\rangle \in \mathcal{H}_1 = \mathcal{H}_1 \otimes \mathbb{C}$ as

$$(R \otimes |\psi_2\rangle)|\psi_1\rangle = R|\psi_1\rangle \otimes |\psi_2\rangle\,.$$

Along the same lines as above, a tensor product of superoperators naturally acts on a tensor product of operators.

In order to turn the vector space $\mathcal{H}_1 \otimes \mathcal{H}_2$ into a Hilbert space, we fix an inner product.[7] The canonical choice is

$$\big(|\varphi_1\rangle|\varphi_2\rangle, |\psi_1\rangle|\psi_2\rangle\big) = \langle\varphi_1|\psi_1\rangle\langle\varphi_2|\psi_2\rangle$$

for $|\varphi_1\rangle|\varphi_2\rangle, |\psi_1\rangle|\psi_2\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$, plus (conjugate-)linear extension, where we make use of the common convention to write $|\varphi_1\rangle|\varphi_2\rangle$ as a short hand for $|\varphi_1\rangle \otimes |\varphi_2\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ (and similarly for bra-vectors). This choice of inner product ensures that the bra-vector of a tensor product $|\varphi_1\rangle|\varphi_2\rangle$ of ket-vectors $|\varphi_1\rangle$ and $|\varphi_2\rangle$ is the tensor product $\langle\varphi_1|\langle\varphi_2|$ of the corresponding bra-vectors. More generally, for $R \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_1')$ and $L \in \mathcal{L}(\mathcal{H}_2, \mathcal{H}_2')$, it then holds that

$$(R \otimes L)^\dagger = R^\dagger \otimes L^\dagger\,.$$

This choice also has the obvious property that if $\{|e_i\rangle\}_{i\in I}$ and $\{|f_j\rangle\}_{j\in J}$ are orthonormal bases of $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, then $\{|e_i\rangle \otimes |f_j\rangle\}_{i\in I, j\in J}$ is an orthonormal basis of $\mathcal{H}_1 \otimes \mathcal{H}_2$. This in particular also implies that if $\mathcal{V}_2$ is a subspace of $\mathcal{H}_2$, then $(\mathcal{H}_1 \otimes \mathcal{V}_2)^\perp = \mathcal{H}_1 \otimes \mathcal{V}_2^\perp$.

0.6 Labeled Hilbert Spaces

When considering multiple Hilbert spaces, instead of referring to them as $\mathcal{H}_1, \mathcal{H}_2$ etc., it is common to denote them by $\mathcal{H}_A, \mathcal{H}_B$ etc. instead. We then think of A, B etc. as a label that is

[6] More generally, for any Hilbert space $\mathcal{H}$, we can (and will) identify elements in $\mathbb{C} \otimes \mathcal{H}$ with elements in $\mathcal{H}$.

[7] We rely here on the convention that the Hilbert spaces we consider are finite dimensional; in general, the vector space $\mathcal{H}_1 \otimes \mathcal{H}_2$ needs to be completed.

"attached" to the respective Hilbert space and to any object related to the respective Hilbert space. We may then write $|\varphi\rangle_A$ to emphasize that $|\varphi\rangle \in \mathcal{H}_A$ and R_A for $R \in \mathcal{L}(\mathcal{H}_A)$.[8]

Given two such labeled Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$, the Hilbert space $\mathcal{H}_{AB}$ with label AB is then by default set to be the tensor product $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$, and similarly for more than two. The Hilbert space labeled by the "empty label" $\emptyset$ is set to $\mathcal{H}_\emptyset = \mathbb{C}$. To simplify notation, we will often just write A instead of $\mathcal{H}_A$, in particular we tend to write $\mathcal{L}(A)$ for $\mathcal{L}(\mathcal{H}_A)$, $\mathcal{L}(AB)$ for $\mathcal{L}(\mathcal{H}_{AB}) = \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$ (which we identify with $\mathcal{L}(\mathcal{H}_A) \otimes \mathcal{L}(\mathcal{H}_B)$), $\mathcal{U}(A)$ for $\mathcal{U}(\mathcal{H}_A)$, etc.

Any operator $R \in \mathcal{L}(\mathcal{H}_A)$ may now be naturally understood as an operator in $\mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$, for any other Hilbert space $\mathcal{H}_B$, by identifying R with $R \otimes \mathbb{I} \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$. We emphasize that this identification is *unambiguous* even if $\mathcal{H}_A = \mathcal{H}_B$, since R is by default assigned to the label A and understood to act on Hilbert space $\mathcal{H}_A$, even if $\mathcal{H}_A = \mathcal{H}_B$.[9] In particular, for $|\Omega\rangle \in \mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$ and $L \in \mathcal{L}(\mathcal{H}_{AB})$ it is understood that

$$R_A|\Omega\rangle_{AB} = (R_A \otimes \mathbb{I}_B)|\Omega\rangle_{AB} \qquad \text{and} \qquad R_A L_{AB} = (R_A \otimes \mathbb{I}_B) L_{AB}\,,$$

etc. This obviously extends to superoperators: any $\mathfrak{T} \in \mathcal{L}\big(\mathcal{L}(\mathcal{H}_A), \mathcal{L}(\mathcal{H}_{A'})\big)$, written as $\mathfrak{T}_A$ or $\mathfrak{T}_{A\to A'}$ if we want to emphasize the domain (and range), acts on $\mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$ as $\mathfrak{T}_A \otimes id_B$.

These labels also allow us to distinguish between the different components in a tensor product, and so we may for instance identify $|\Omega\rangle_{AB} \in \mathcal{H}_A \otimes \mathcal{H}_B$ with $|\Omega\rangle_{BA} \in \mathcal{H}_B \otimes \mathcal{H}_A$, obtained by "flipping the two components" of the tensor product, and similarly for L_{AB} etc.

0.7 The Transpose, and Vector-Representation of Operators

We consider arbitrary but fixed orthonormal bases $\{|i\rangle\}_{i\in I}$ and $\{|k\rangle\}_{k\in K}$ of two respective Hilbert spaces $\mathcal{H}$ and $\mathcal{H}'$. We emphasize that the following definitions are basis-dependent.

Definition 0.3. *The* **transposition map** $\mathcal{L}(\mathcal{H}, \mathcal{H}') \to \mathcal{L}(\mathcal{H}', \mathcal{H})$, $R \mapsto R^T$ *is defined as the superoperator that maps* $|k\rangle\langle i|$ *into* $|i\rangle\langle k|$, *i.e.,*

$$R^T = \sum_{i,k} |i\rangle\langle k|R|i\rangle\langle k|\,.$$

We emphaszie that this should not be confused with the adjoining operation $(\cdot)^\dagger$, which is *conjugate* linear and thus not a superoperator, but is basis independent. Related to the transposition is the following.

Definition 0.4. *The* **complex conjugate** *of a ket-vector* $|\varphi\rangle \in \mathcal{H}$ *and, more generally, of an operator* $R \in \mathcal{L}(\mathcal{H}, \mathcal{H}')$ *is respectively given by*

$$|\bar\varphi\rangle = \sum_i |i\rangle\overline{\langle i|\varphi\rangle} = \sum_i |i\rangle\langle\varphi|i\rangle \in \mathcal{H} \qquad \textit{and} \qquad \bar R = \sum_{i,k} |k\rangle\overline{\langle k|R|i\rangle}\langle i| = (R^\dagger)^T\,.$$

It is easy to see that the actions of $\bar{(\cdot)}$, $(\cdot)^T$ and $(\cdot)^\dagger$ all commute. Furthermore, $\bar R|\bar\varphi\rangle = \overline{R|\varphi\rangle}$, and thus $R^T|\bar\varphi\rangle = \overline{R|\varphi\rangle}$ for Hermitian R, implying that R and R^T have the same eigenvalues then: if $R|\varphi\rangle = \lambda|\varphi\rangle$ then $R^T|\bar\varphi\rangle = \bar\lambda|\bar\varphi\rangle = \lambda|\bar\varphi\rangle$, given that λ must be real for Hermition R.

We also introduce the following (still basis-dependent) notation.

[8] Formally, this can be achieved by declaring that, as a set, $\mathcal{H}_A$ consists of all functions $\{A\} \to \mathcal{H}$ for some Hilbert space $\mathcal{H}$, and, correspondingly, $\mathcal{H}_B$ consists of all functions $\{B\} \to \mathcal{H}'$ for some Hilbert space $\mathcal{H}'$, etc. Then, $\mathcal{H}_A$ and $\mathcal{H}_B$ coincide as Hilbert spaces whenever $\mathcal{H} = \mathcal{H}'$, but nevertheless feature distinct elements.

[9] This is not an exclusively strict rule though: in some occasions we encounter $R \in \mathcal{L}(\mathcal{H}_A)$ and $|\varphi\rangle \in \mathcal{H}_B$ with $\mathcal{H}_A = \mathcal{H}_B$ and consider $R|\varphi\rangle$ defined in the conventional way.

Definition 0.5. *The* **ket-vector representation** $|R\rangle$ *of an operator* R *is given by means of the isomorphism*

$$\mathcal{L}(\mathcal{H},\mathcal{H}') \to \mathcal{H}' \otimes \mathcal{H}\,,\ R \mapsto |R\rangle$$

that maps $|k\rangle\langle i|$ *to* $|k\rangle|i\rangle$.

The following properties are straightforward to verify:

$$R|i\rangle = (\mathbb{I} \otimes \langle i|)|R\rangle\ , \quad R^T|k\rangle = (\langle k| \otimes \mathbb{I})|R\rangle \qquad \text{and} \qquad \langle R|L\rangle = \mathrm{tr}(R^\dagger L)$$

for all $R \in \mathcal{L}(\mathcal{H},\mathcal{H}')$ and respective basis vectors $|i\rangle$ and $|k\rangle$, as well as

$$(R \otimes L)|X\rangle = |RXL^T\rangle$$

for all $R \in \mathcal{L}(\mathcal{H})$, $L \in \mathcal{L}(\mathcal{H}')$ and $X \in \mathcal{L}(\mathcal{H}',\mathcal{H})$. In particular, the following holds.

Corollary 0.5. $\langle X|(R \otimes L)|Y\rangle = \mathrm{tr}(X^\dagger R\,Y L^T)$ *for all* $R\in\mathcal{L}(\mathcal{H})$, $L\in\mathcal{L}(\mathcal{H}')$, $X, Y\in\mathcal{L}(\mathcal{H}',\mathcal{H})$.