(μ) The Inner Product

The inner product $\langle\phi|\psi\rangle \in \mathbb{C}$ of two vectors in the complex vector space $\mathcal{H}$ is, as the term scalar product suggests, a scalar, that is, a complex number, satisfying certain properties:

Definition. *An* ***inner product*** *(or scalar product) $\langle\phi|\psi\rangle \in \mathbb{C}$ is a form defined on a complex vector space $\mathcal{H}$ satisfying the following three properties:*

- ***linear*** *in the second argument (on the right): for each ϕ, the map $\psi \in \mathcal{H} \mapsto \langle\phi|\psi\rangle \in \mathbb{C}$ is linear:*

$$\langle\phi|\alpha\psi + \beta\psi'\rangle = \alpha\,\langle\phi|\psi\rangle + \beta\,\langle\phi|\psi'\rangle \qquad (\forall\alpha,\beta \in \mathbb{C})$$

- ***conjugate symmetric*** *(or: Hermitian symmetric):*

$$\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$$

- ***positive definite****:*

$$\langle\psi|\psi\rangle > 0$$

for every nonzero vector $\psi \neq 0$.

The space $\mathcal{H}$ is then called a **Hermitian space**.

Remark. The linearity property (with $\alpha = \beta = 0$) implies that the inner product with the zero vector is always zero; in particular $\langle\psi|\psi\rangle = 0$ when $\psi = 0$.

The conjugate-symmetry property already implies that $\langle\psi|\psi\rangle \in \mathbb{R}$, but positive definiteness specifies that $\langle\psi|\psi\rangle$ is in fact a positive real number, which is zero only for a vector that is itself zero.

Conjugate symmetry, together with linearity in the second argument, also implies that the inner product is

- **conjugate-linear** (or: antilinear) in the first argument (on the left):

$$\langle\alpha\phi + \beta\phi'|\psi\rangle = \alpha^*\,\langle\phi|\psi\rangle + \beta^*\,\langle\phi'|\psi\rangle \qquad (\forall\alpha,\beta \in \mathbb{C})$$

More generally, we can therefore expand on both sides simultaneously to obtain the

- **expansion formula for the inner product**:

$$\langle\alpha\phi + \beta\phi'|\gamma\psi + \delta\psi'\rangle = \alpha^*\gamma\,\langle\phi|\psi\rangle + \alpha^*\delta\,\langle\phi|\psi'\rangle + \beta^*\gamma\,\langle\phi'|\psi\rangle + \beta^*\delta\,\langle\phi'|\psi'\rangle$$

The calculation generalizes to several vectors $\phi_1, \phi_2, \ldots, \phi_n$ and $\psi_1, \psi_2, \ldots, \psi_n$:

$$\langle \textstyle\sum_i \alpha_i\phi_i | \sum_j \beta_j\psi_j\rangle = \displaystyle\sum_{i,j} \alpha_i^*\beta_j\,\langle\phi_i|\psi_j\rangle$$

Definition. *The **norm** (induced by the inner product) of $\psi \in \mathcal{H}$ is defined by*

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

*It is sometimes called the **Euclidean** norm and denoted with a subscript "2," as in $\|\psi\|_2$, to distinguish it from other norms.*

Since the inner product is positive definite, the norm is well defined, and is also

- **positive definite**:

$$\|\psi\| \geqslant 0 \quad \text{with } \|\psi\| = 0 \text{ if and only if } \psi = 0$$

By linearity in the second argument and conjugate linearity in the first, the norm satisfies $\|\alpha\psi\|^2 = \langle\alpha\psi|\alpha\psi\rangle = \alpha^*\alpha\,\langle\psi|\psi\rangle = |\alpha|^2\|\psi\|^2$, so it is

- **absolutely homogeneous**:

$$\|\alpha\psi\| = |\alpha|\,\|\psi\| \quad \text{for every scalar } \alpha \in \mathbb{C}$$

(The third property of the norm — the triangle inequality — is presented below.)

Remark. The vector ψ is **normalized** (or is a unit vector) if it has unit norm: $\|\psi\| = 1$. Given a nonzero vector ψ, one can always **normalize** it by dividing it by its norm, because by absolute homogeneity with $\alpha = \frac{1}{\|\psi\|}$, we have:

$$\left\|\frac{\psi}{\|\psi\|}\right\| = \frac{\|\psi\|}{\|\psi\|} = 1$$

so that $\frac{\psi}{\|\psi\|}$ is indeed normalized. In quantum theory, one very often refers to normalized states.

The expansion formula for the inner product (above) gives in particular

$$\langle\phi + \psi|\phi + \psi\rangle = \langle\phi|\phi\rangle + \langle\phi|\psi\rangle + \langle\psi|\phi\rangle + \langle\psi|\psi\rangle\,.$$

We note that

$$\langle\phi|\psi\rangle + \langle\psi|\phi\rangle = \langle\phi|\psi\rangle + \langle\phi|\psi\rangle^* = 2\,\mathrm{Re}\,\langle\phi|\psi\rangle$$

(twice the real part). We therefore obtain the **expansion formula for the squared norm**:

$$\|\phi + \psi\|^2 = \|\phi\|^2 + \|\psi\|^2 + 2\,\mathrm{Re}\,\langle\phi|\psi\rangle$$

For several vectors $\phi_1, \phi_2, \ldots, \phi_n$, we similarly obtain

$$\|\phi_1 + \phi_2 + \cdots + \phi_n\|^2 = \sum_i \|\phi_i\|^2 + 2\sum_{i<j} \mathrm{Re}\,\langle\phi_i|\phi_j\rangle$$

Definition. *Two vectors ϕ and ψ are **orthogonal** if*

$$\langle\phi|\psi\rangle = 0$$

We then write $\phi \perp \psi$.

This relation is symmetric, because $\langle\phi|\psi\rangle = 0$ implies $\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^* = 0$. Several vectors $\phi_1, \phi_2, \dots, \phi_n$ are **orthogonal** (pairwise) if $\phi_i \perp \phi_j$ for all $i \neq j$.

For orthogonal vectors, the expansion formula for the squared norm (above) gives the

Theorem (Pythagorean theorem). *If $\phi \perp \psi$, then $\|\phi+\psi\|^2 = \|\phi\|^2 + \|\psi\|^2$. More generally, if the vectors $\phi_1, \phi_2, \dots, \phi_n$ are pairwise orthogonal, then*

$$\|\phi_1 + \phi_2 + \cdots + \phi_n\|^2 = \|\phi_1\|^2 + \|\phi_2\|^2 + \cdots + \|\phi_n\|^2.$$

Remark. Unlike what happens in a Euclidean space (over $\mathbb{R}$), the converse of the Pythagorean theorem for two vectors ϕ and ψ is false (when $\langle\phi|\psi\rangle$ is purely imaginary).

Definition. *The vectors $\phi_1, \phi_2, \dots, \phi_n$ are **orthonormal** if they are both orthogonal (pairwise) and normalized:*

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

*An **orthonormal basis** of $\mathcal{H}$, or of a subspace $\mathcal{V}$ of $\mathcal{H}$, is a basis consisting of orthonormal vectors.*

Orthonormal vectors $\phi_1, \phi_2, \dots, \phi_n$ are always linearly independent, because $\alpha_1\phi_1 + \cdots + \alpha_n\phi_n = 0$ implies $\alpha_i = \langle\phi_i|\alpha_1\phi_1 + \cdots + \alpha_n\phi_n\rangle = 0$ for every i. They therefore form an orthonormal basis of the subspace $\mathcal{V}_n = \mathrm{Vect}(\phi_1, \phi_2, \dots, \phi_n)$ spanned by these vectors, which has dimension n.

In quantum theory, one generally considers only bases that are orthonormal.

Definition. *A vector ϕ is an **orthogonal projection** of ψ onto the subspace $\mathcal{V}$ if $\phi \in \mathcal{V}$ and the difference $\psi - \phi$ is orthogonal to every vector in $\mathcal{V}$.*

If $\phi_1, \phi_2, \dots, \phi_n$ form an orthonormal basis of $\mathcal{V}_n = \mathrm{Vect}(\phi_1, \phi_2, \dots, \phi_n)$, the orthogonal projection of ψ onto $\mathcal{V}_n$ has the form $\alpha_1\phi_1 + \cdots + \alpha_n\phi_n$, where the coefficients satisfy the condition $\langle\phi_i|\psi - \alpha_1\phi_1 - \cdots - \alpha_n\phi_n\rangle = 0$ for every i, that is, after expanding: $\langle\phi_i|\psi\rangle - \alpha_i = 0$. Consequently, the orthogonal projection of ψ onto $\mathcal{V}_n$, which we denote by $\Pi_n\psi$, is unique and is given by the **expansion formula in the basis** $\phi_1, \phi_2, \dots, \phi_n$:

$$\Pi_n\psi = \langle\phi_1|\psi\rangle\ \phi_1 + \langle\phi_2|\psi\rangle\ \phi_2 + \cdots + \langle\phi_n|\psi\rangle\ \phi_n$$

The linear map $\Pi_n : \mathcal{H} \to \mathcal{V}_n$ is the **orthogonal projector** (or orthogonal projection operator) onto $\mathcal{V}_n$.

If $n < \dim\mathcal{H}$, one can always find a vector $\psi \notin \mathcal{V}_n$ that is linearly independent of $\phi_1, \phi_2, \dots, \phi_n$, and then $\psi \neq \Pi_n\psi$. By definition of Π_n, the nonzero vector $\psi - \Pi_n\psi$ is orthogonal to every vector in $\mathcal{V}_n$, that is, to each of the vectors $\phi_1, \phi_2, \dots, \phi_n$. Normalizing it,

$$\phi_{n+1} = \frac{\psi - \Pi_n\psi}{\|\psi - \Pi_n\psi\|}$$

and adjoining it to the preceding vectors, we obtain $n+1$ orthonormal vectors $\phi_1, \dots, \phi_{n+1}$ that form an orthonormal basis of $\mathcal{V}_{n+1} = \mathrm{Vect}(\phi_1, \phi_2, \dots, \phi_{n+1})$. This is step n in the

Theorem (Gram–Schmidt process). *In a Hermitian space $\mathcal{H}$ of dimension $d = \dim \mathcal{H}$, the successive application of step n described above for $n = 0, 1, \ldots, d-1$ produces an orthonormal basis $\phi_1, \phi_2, \ldots, \phi_d$ of $\mathcal{H}$.*

Remark. This algorithm presupposes that $\mathcal{H}$ has nonzero dimension (is not reduced to the zero vector $\{0\}$); otherwise $d = 0$, no step is necessary, and the basis is empty. Note that if $d > 0$, step 0 simply amounts to choosing a nonzero vector ψ and normalizing it; $\phi_1 = \frac{\psi}{\|\psi\|}$ forms by itself an orthonormal basis of $\mathcal{V}_1 = \mathrm{Vect}(\phi_1)$. After step $d-1$, we do indeed have d orthonormal vectors (therefore linearly independent) that form a basis of the d-dimensional space $\mathcal{H}$.

The Gram–Schmidt process therefore always guarantees the **existence** of an orthonormal basis for every Hermitian space. Any $\psi \in \mathcal{H}$ is its own orthogonal projection onto $\mathcal{H} = \mathrm{Vect}(\phi_1, \phi_2, \ldots, \phi_d)$, so it is given by the **expansion formula in the orthonormal basis**:

$$\psi = \langle \phi_1 | \psi \rangle \; \phi_1 + \langle \phi_2 | \psi \rangle \; \phi_2 + \cdots + \langle \phi_d | \psi \rangle \; \phi_d$$

If one starts from given orthonormal vectors $\phi_1, \phi_2, \ldots, \phi_n$ with $n < d$, steps $n, n+1, \ldots, d-1$ of the Gram–Schmidt process produce $d-n$ additional vectors $\phi_{n+1}, \ldots, \phi_d$ such that $\phi_1, \phi_2, \ldots, \phi_d$ is an orthonormal basis of $\mathcal{H}$. This proves the

Theorem (orthonormal basis extension theorem). *Every orthonormal family $\phi_1, \phi_2, \ldots, \phi_n$ can be extended to an orthonormal basis $\phi_1, \phi_2, \ldots, \phi_n, \ldots \phi_d$ of $\mathcal{H}$.*

Since every subspace $\mathcal{V}$ of $\mathcal{H}$ is also a Hermitian space, it admits an orthonormal basis. The orthogonal projection, denoted $\Pi\psi$, of $\psi \in \mathcal{H}$ onto $\mathcal{V}$ is therefore unique and given by the expansion formula in this basis, as above.

By completing this basis to an orthonormal basis of $\mathcal{H}$, the added basis vectors span a subspace $\mathcal{V}^\perp$, the **orthogonal complement** of $\mathcal{V}$, that is, the space of all vectors orthogonal to those of $\mathcal{V}$. The projection of ψ onto $\mathcal{V}^\perp$ is simply $\psi - \Pi\psi$. Since $\psi - \Pi\psi$ is orthogonal to every vector in $\mathcal{V}$, it is orthogonal to $\Pi\psi$. By the Pythagorean theorem:

$$\|\psi\|^2 = \|\psi - \Pi\psi + \Pi\psi\|^2 = \|\psi - \Pi\psi\|^2 + \|\Pi\psi\|^2 \geqslant \|\Pi\psi\|^2$$

which shows that projection reduces the norm if $\psi \neq \Pi\psi$, that is, if $\psi \notin \mathcal{V}$:

Theorem (Norm reduction by orthogonal projection). *For every orthogonal projector Π onto a subspace $\mathcal{V}$,*

$$\|\Pi\psi\| \leqslant \|\psi\|$$

with equality if and only if $\psi \in \mathcal{V}$.

Apply this result to two nonzero normalized vectors ϕ and ψ: $\|\phi\| = \|\psi\| = 1$, with $\mathcal{V} = \mathrm{Vect}(\phi)$. The expansion formula in the basis consisting of the single vector ϕ gives $\Pi\psi = \langle \phi | \psi \rangle \; \phi$. We obtain $\|\Pi\psi\| = |\langle \phi | \psi \rangle| \leqslant 1$, with equality if and only if ψ and ϕ are collinear. More generally, for two nonzero vectors ϕ and ψ that are not necessarily normalized, we reduce to the preceding case by normalizing them and obtain $|\langle \frac{\phi}{\|\phi\|} | \frac{\psi}{\|\psi\|} \rangle| \leqslant 1$ with the same equality case. We have obtained the

Theorem (Cauchy–Schwarz inequality). *For all vectors ϕ, ψ:*

$$|\langle\phi|\psi\rangle| \leqslant \|\phi\| \, \|\psi\|$$

with equality if and only if ϕ and ψ are collinear. (The case in which one of the vectors is zero is trivial, since both sides of the inequality are then zero.)

Consequently, in the expansion formula for the squared norm,

$$\|\phi + \psi\|^2 = \|\phi\|^2 + \|\psi\|^2 + 2\,\mathrm{Re}\,\langle\phi|\psi\rangle\,,$$

we can bound $\mathrm{Re}\,\langle\phi|\psi\rangle \leqslant |\,\langle\phi|\psi\rangle\,| \leqslant \|\phi\|\,\|\psi\|$ to obtain

$$\|\phi + \psi\|^2 \leqslant \|\phi\|^2 + \|\psi\|^2 + 2\|\phi\|\,\|\psi\| = (\|\phi\| + \|\psi\|)^2.$$

The norm therefore satisfies

- the **triangle inequality** (or: Minkowski inequality):

$$\|\phi + \psi\| \leqslant \|\phi\| + \|\psi\|$$

Remark. From the two inequalities $\mathrm{Re}\,\langle\phi|\psi\rangle \leqslant |\,\langle\phi|\psi\rangle\,| \leqslant \|\phi\|\,\|\psi\|$ that led to the triangle inequality, equality $\|\phi+\psi\| = \|\phi\| + \|\psi\|$ holds if and only if, first, ϕ and ψ are collinear (equality in the Cauchy–Schwarz inequality), and, second, $\mathrm{Re}\,\langle\phi|\psi\rangle = |\,\langle\phi|\psi\rangle\,|$, that is, $\langle\phi|\psi\rangle \geqslant 0$. The equality case in the triangle inequality therefore amounts to saying that ϕ and ψ are positively collinear.