Orthonormal Basis

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Orthonormal basis (plural orthonormal bases): a set B of vectors in Euclidean or Hilbert space such that every vector can be written as a (finite or infinite) linear combination of vectors from B, while all vectors from B have length 1 and any two of them are orthogonal. The number of vectors in B then equals the dimension of the space, which can be finite or infinite.

In the infinite-dimensional Hilbert spaces considered in quantum physics, the appropriate sense of linear combination is that of a *convergent series*

$$\psi = \sum_{n=1}^{\infty} c_n \, \phi_n \,, \tag{1}$$

where $B = \{\phi_1, \phi_2, \ldots\}$ and c_n are complex coefficients, called the *expansion coefficients* of ψ relative to B. (A basis in the sense that linear combinations are convergent series is called a *Schauder basis*, whereas a basis in the sense that linear combinations can only involve finitely many terms is a called a *Hamel basis*.) Thus, an orthonormal basis in Hilbert space is a set $B = \{\phi_1, \phi_2, \ldots\}$ of vectors such that every vector ψ can be written in the form (1), and

$$\langle \phi_n | \phi_m \rangle = \delta_{nm} \,, \tag{2}$$

where $\delta_{nm} = 1$ if $n = m$ and $\delta_{nm} = 0$ otherwise.

A set of vectors that satisfies (2) but does not permit to represent every vector in the form (1) is called an *orthonormal set* or *orthonormal sequence*; it is an orthonormal basis of a closed subspace. A set of vectors that permits to represent every vector in the form (1) but does not satisfy (2) is called a *basis* (but not orthonormal). The word "orthonormal" means pairwise orthogonal ($\langle \phi_n | \phi_m \rangle = 0$ for all $n \neq m$) and normalized ($\langle \phi_n | \phi_n \rangle = 1$ for all n).

If ψ has expansion coefficients c_n—as expressed in (1)—and ψ' has expansion coefficients c'_n then

$$\langle \psi | \psi' \rangle = \sum_{n=1}^{\infty} c_n^* \, c'_n \,, \tag{3}$$

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where * denotes the complex conjugate. The coefficients can be computed according to

$$c_n = \langle \phi_n | \psi \rangle \,. \tag{4}$$

Just as a vector ψ is represented, relative to an orthonormal basis, by a sequence of numbers c_n, an operator T is represented by an (infinite) matrix $T_{nm} = \langle \phi_n | T\, \phi_m \rangle$. An operator T is *diagonal* in an orthonormal basis if $T_{nm} = 0$ for $n \neq m$. A self-adjoint operator T can be diagonalized (i.e., an orthonormal basis can be found in which T is diagonal) if and only if T has pure point spectrum. To diagonalize a self-adjoint operator T with continuous spectrum, one needs the concept of a *generalized orthonormal basis*: in this case, the basis elements are themselves not contained in the Hilbert space. For example, the generalized orthonormal basis diagonalizing the quantum-mechanical position operator on the Hilbert space $L^2(\mathbb{R})$ of square-integrable functions consists of Dirac delta functions, not contained in $L^2(\mathbb{R})$, and the generalized orthonormal basis diagonalizing the momentum operator consists of plane waves e^{ikx}, which are not square-integrable either. A generalized orthonormal basis can be defined rigorously as a unitary isomorphism between the given Hilbert space and $L^2(\Omega, \mu)$, where Ω is the index set of the generalized basis ($\Omega = \mathbb{R}$ in the examples above), and μ is a measure on Ω (the Lebesgue volume measure in the examples above).