Trace

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Trace of an operator: The sum of the diagonal elements of the operator's matrix representation. The "trace" is a number that can be associated with an operator T on Hilbert space, and is usually denoted $\mathrm{tr}(T)$, $\mathrm{tr}\, T$, $\mathrm{Tr}(T)$, or $\mathrm{Tr}\, T$. It can be a complex number, or $+\infty$, or can be undefined (because it is of the type $\infty - \infty$). The set of operators whose trace is a finite complex number is called the *trace class*.

Definition. (i) The trace of an $n \times n$ matrix $A = (a_{ij})_{i,j \leq n}$ is defined as the sum of the entries on the main diagonal:

$$\mathrm{tr}(A) = \sum_{i=1}^{n} a_{ii}\,. \tag{1}$$

(In the sum convention of general relativity, this is written $a_i{}^i$.) For an $n \times m$ matrix with unequal number of rows and columns there is no concept of trace.

(ii) For an infinite matrix $A = (a_{ij})_{i,j \in \mathbb{N}}$, the trace is defined as the series (infinite sum)

$$\mathrm{tr}(A) = \sum_{i=1}^{\infty} a_{ii}\,. \tag{2}$$

The trace is considered well defined if the series converges absolutely.

(iii) For a linear operator T, $\mathrm{tr}(T)$ is defined as the trace of its matrix representation relative to an arbitrary basis. It can be shown that the value of $\mathrm{tr}(T)$ (and whether it is well defined) does not depend on the choice of the basis. In particular, if $\{\phi_1, \phi_2, \ldots\}$ is an orthonormal basis of a Hilbert space $\mathscr{H}$ and T is an operator on $\mathscr{H}$ then

$$\mathrm{tr}(T) = \sum_{n=1}^{\infty} \langle \phi_n | T \phi_n \rangle\,. \tag{3}$$

Properties. (i) The trace is linear:

$$\mathrm{tr}(S + T) = \mathrm{tr}(S) + \mathrm{tr}(T)\,, \quad \mathrm{tr}(\lambda T) = \lambda\, \mathrm{tr}(T) \tag{4}$$

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for all operators S, T from the trace class and all $\lambda \in \mathbb{C}$.

(ii) The trace is invariant under cyclic permutation of factors:

$$\operatorname{tr}(AB \cdots YZ) = \operatorname{tr}(ZAB \cdots Y)\,, \tag{5}$$

in particular $\operatorname{tr}(AB) = \operatorname{tr}(BA)$ and $\operatorname{tr}(ABC) = \operatorname{tr}(CAB)$, which is, however, not always the same as $\operatorname{tr}(CBA)$.

(iii) If an operator T can be diagonalized, i.e., if there exists an orthonormal basis of eigenvectors, then $\operatorname{tr}(T)$ is the sum of the eigenvalues, counted with multiplicity (= degree of degeneracy).

(iv) The trace of the adjoint operator T^* is the complex-conjugate of the trace of T: $\operatorname{tr}(T^*) = \operatorname{tr}(T)^*$.

(v) The trace of a self-adjoint operator T (in the trace class) is real: $\operatorname{tr}(T) \in \mathbb{R}$. A self-adjoint operator lies in the trace class if and only if it is bounded, its spectrum is discrete, all nonzero eigenvalues have finite multiplicity, and the sum of the eigenvalues (with multiplicity) is finite (i.e., converges absolutely).

(vi) The trace of a positive operator $T \geq 0$ is nonnegative: $\operatorname{tr}(T) \geq 0$.

Trace Formula in Quantum Theory. When an observable, given by the self-adjoint operator T, is measured on a system with density matrix ρ then the probability that the outcome Z lies in the set $\Delta \subseteq \mathbb{R}$ is

$$\mathbb{P}(Z \in \Delta) = \operatorname{tr}(\rho\, P_\Delta) \tag{6}$$

with P_Δ the spectral projection of T corresponding to the spectrum in Δ.