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Density Matrix

Leslie Ballentine

A matrix representation of the ► *state operator*. So named because in the *position* basis its diagonal elements are equal to the position probability density. This name is older than the modern term *state operator*, and is still frequently used in its place, especially in many-electron theory and ► quantum chemistry. The name *density matrix* is not entirely accurate, since in the position basis it is not really a matrix, but rather a function of two continuous variables. If a discrete basis is chosen (such as the *spin* basis), then it becomes a genuine matrix, but its diagonal elements are *probabilities* rather than densities. ► States, pure and mixed, and their representation.

Density Operator

Werner Stulpe

Density operator, an operator used to describe (mixed) quantum states. A *density operator* [1–6], also called *statistical operator* or – somehow misleading – density matrix, is a positive trace-class ► operator ρ of trace 1 acting in some separable complex ► Hilbert space $\mathcal{H}$; i.e., ρ is a linear operator defined on $\mathcal{H}$ with values in $\mathcal{H}$ that satisfies $\rho = \rho^*$, $\langle\phi|\rho\phi\rangle \geqslant 0$ for all $\phi \in \mathcal{H}$, and $\operatorname{tr}\rho = \sum_i \langle\phi_i|\rho\phi_i\rangle = 1$, $\phi_1, \phi_2, \ldots$ being a complete orthonormal system in $\mathcal{H}$. In particular, ρ is a compact self-adjoint ► operator; in consequence, a density operator has the spectral decomposition $\rho = \sum_i \lambda_i P_{\chi_i}$ (► self-adjoint operator) where $\lambda_1, \lambda_2, \ldots$ are the nonzero eigenvalues of ρ, counted according to their multiplicity and arranged according to $\lambda_1 \geqslant \lambda_2 \geqslant \ldots > 0$, $\sum_i \lambda_i = 1$, $\chi_1, \chi_2, \ldots$ is an orthonormal system