The State-Operator Formulation of Quantum Mechanics

- The *state operator* or *density operator* ρ is a Hermitian operator acting in the Hilbert space used to describe a system (or ensemble of systems). Its fundamental property is that the expectation value of any observable operator Ω in the state ρ is given by

$$\langle\Omega\rangle = \mathrm{Tr}(\rho\Omega) \equiv \mathrm{Tr}(\Omega\rho). \tag{1}$$

Special cases:

$$\begin{aligned} \Omega = I: &\qquad \mathrm{Tr}\,\rho &=& \ 1. \\ \Omega = P_\omega: &\qquad \mathrm{Prob}(\omega) &=& \ \mathrm{Tr}(\rho P_\omega). \end{aligned}$$

- The state operator for a *pure state* (or *pure ensemble*) described by the unit-normalized state vector $|\psi\rangle$ is

$$\rho = |\psi\rangle\langle\psi|.$$

It has the following properties:

1. Whereas the state vector is arbitrary up to an overall phase, $|\psi\rangle$ and $e^{i\theta}|\psi\rangle$ being physically equivalent for real θ, the state operator is unique:

$$e^{-i\theta}|\psi\rangle\langle\psi|e^{i\theta} = |\psi\rangle\langle\psi|.$$

2. The expectation value of Ω is indeed given by Eq. (1):

$$\begin{aligned} \langle\Omega\rangle &= \langle\psi|\Omega|\psi\rangle = \sum_j \langle\psi|j\rangle\langle j|\Omega|\psi\rangle = \sum_j \langle j|\Omega|\psi\rangle\langle\psi|j\rangle \\ &= \mathrm{Tr}(\Omega\rho) \equiv \mathrm{Tr}(\rho\Omega). \end{aligned}$$

3. ρ has a complete orthonormal basis of eigenkets. It has one eigenvalue equal to 1 with eigenket $|\psi\rangle$. The remaining eigenvalues are all equal to 0.
4. In the Schrödinger picture,

$$\rho(t) = U(t)|\psi(0)\rangle\langle\psi(0)|U^\dagger(t) = U(t)\rho(0)U^\dagger(t).$$

Therefore,

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H(t), \rho(t)] \qquad \text{(note the overall sign of the RHS).}$$

In the Heisenberg picture, by contrast,

$$\rho_H(t) = \rho(0) \quad \text{while} \quad \Omega_H(t) = U(t)^\dagger \Omega U(t).$$

5. The matrix representation of the state operator in a particular orthonormal basis is called the *density matrix*.

   In the specific case of a point-like particle in one spatial dimension,

$$\langle x|\rho|x'\rangle = \langle x|\psi\rangle\langle\psi|x'\rangle = \psi(x)\psi^*(x'),$$

   so the diagonal matrix elements give the probability density $|\psi(x)|^2$.

- The most general state operator, describing a *mixed state* (or *mixed ensemble*), can be cast in the form

$$\rho = \sum_{k=1}^{m} w_k |\psi_k\rangle\langle\psi_k|,$$

  where each of the real weights w_k satisfies $0 \leq w_k \leq 1$. It is not necessary that different $|\psi_k\rangle$'s be orthogonal, or that m be less than n, the dimension of the vector space.

  A general state operator has the following properties:

  1. Normalization: from Eq. (1),

$$\mathrm{Tr}\,\rho = 1 \qquad \Rightarrow \qquad \sum_k w_k = 1.$$

  2. Positive semi-definiteness:

$$\langle\phi|\rho|\phi\rangle \geq 0 \quad \text{for all possible } |\phi\rangle.$$

  3. Time evolution (Schrödinger picture):

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H(t), \rho(t)], \qquad \rho(t) = U(t)\rho(0)U^\dagger(t).$$

  4. Diagonalization: ρ has a complete orthonormal eigenbasis $\{|p_j\rangle\}$, such that

$$\rho = \sum_{j=1}^{n} p_j |p_j\rangle\langle p_j|.$$

     Properties 1 and 2 imply that $\sum_j p_j = 1$ and $p_j \geq 0$. It follows that

$$0 \leq p_j \leq 1 \quad \text{and} \quad \mathrm{Tr}\,\rho^2 = \sum_j p_j^2 \leq 1.$$

  5. $\mathrm{Tr}\,\rho^2 = 1$ only in a pure state, for which $p_j = \delta_{j,m}$ and $\rho = |p_m\rangle\langle p_m|$.

     $\mathrm{Tr}\,\rho^2 < 1$ is the signature of a mixed state, in which the state operator cannot be cast as a single projection operator, i.e., $\rho \neq |\psi\rangle\langle\psi|$.

  6. Since $\mathrm{Tr}(A+B) = \mathrm{Tr}\,A + \mathrm{Tr}\,B$,

$$\langle\Omega\rangle = \sum_k w_k \langle\psi_k|\Omega|\psi_k\rangle = \sum_j p_j \langle p_j|\Omega|p_j\rangle,$$

     i.e., each expectation value in a mixed state is the weighted average of the corresponding expectation values in the pure states forming the mixture. The averaging process is essentially classical: there are no quantum-mechanical interference terms between the different pure states.