

Solution 3.2.

We want to show that ρ is a pure state if and only if

$$\rho = \rho^\dagger, \quad \text{tr}(\rho^2) = 1, \quad \text{tr}(\rho^3) = 1.$$

A pure state clearly satisfies these properties, so all we need to show is sufficiency.

Since ρ is Hermitian, it has an eigendecomposition, $\rho = \sum_j \lambda_j |e_j\rangle\langle e_j|$, where the eigenvalues λ_j are real (we cannot assume they are nonnegative). The condition,

$$1 = \text{tr}(\rho^2) = \sum_j \lambda_j^2,$$

shows that $0 \leq \lambda_j^2 \leq 1$ or, equivalently, that $0 \leq |\lambda_j| \leq 1$. We can use this result and the trace conditions to write

$$1 = \text{tr}(\rho^3) = \sum_j \lambda_j^3 \leq \sum_j |\lambda_j| \lambda_j^2 \leq \sum_j \lambda_j^2 = 1.$$

The bookending inequalities imply that the inequalities must be saturated. The first inequality is saturated if and only if all the eigenvalues are nonnegative, giving us $0 \leq \lambda_j \leq 1$, and the second if and only if there is one eigenvalue equal to 1, with all the others equal to 0. Thus ρ is a pure state.