The Density Matrix
A Note

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For a pure state, using the wave function $|\Psi\rangle$ the density matrix is given by

$$\rho_{tot} = |\Psi\rangle\langle\Psi|.$$

In a generic quantum system such as one at finite temperature the wave function if a mixed state for example

$$\rho_{tot} = \frac{e^{-\beta H}}{\mathrm{Tr}[e^{-\beta H}]}$$

for the canonical ensemble.

Suppose a system consists of two non-interacting subsystems A and B. The combined system has a wavefunction

$$\Psi = \Psi(\alpha, \beta)$$

where α and β are the commuting variables for the subsystems A and B respectively.

For a moment, only consider the subsystem A. A complete description of all measurements of A is provided by the density matrix $\rho_A(\alpha, \alpha')$ as

$$\rho_A(\alpha, \alpha') = \sum_{\beta} \Psi^*(\alpha, \beta)\Psi_A(\alpha', \beta).$$

Likewise

$$\rho_B(\beta, \beta') = \sum_{\alpha} \Psi^*(\alpha, \beta)\Psi_A(\alpha, \beta').$$

The rule for computing an expectation value of te an operator $\mathcal{A}$ composed of A degrees of freedom is

$$\langle \mathcal{A} \rangle = \mathrm{Tr}\, \mathcal{A}\rho_A.$$

Density matrices satisfy

- $\mathrm{Tr}\,\rho = 1$
  Total probability is equal to 1
- $\rho = \rho^\dagger$
- $\rho_j \geq 0$
  All eigenvalues are non-negative.

The eigenvalues ρ_j can be considered to be probabilities that the system j-th state.

A quantitative measure of departure from the pure stater is provided by the von Neumann entropy

$$S = -\,\mathrm{Tr}\,\rho \log \rho.$$

S is zero if and only if all the eigenvalues but one are zero. The one non-vanishing eigenvalue is equal to 1 by the trace condition on ρ. The entropy is also a measure of the degree of entanglement between A and B. Hence the name entanglement entropy.

The opposite scenario to the pure state is a completely incoherent density matrix in which all the eigenvalues are equal to

$$\frac{1}{N}$$

where N is the dimensionality of the Hilbert space. In this case S takes its maximum value

$$S = \log N.$$

Note. The von Neumann entropy should not be confused with the thermal entropy of the second law of thermodynamics.