

# Ralph's density operator

Ralph is exploring accounting implications of quantum information and recognizes sometimes (perhaps, often) the state of the system is only partially known. That is, the state of the system is a mixture of quantum states (or qubits). A convenient way to represent such systems involves density operators. A density operator is a convex combination (non-negative weights that sum to one) of outer products of qubits (ket-bra rather than the inner product, bra-ket) representing the components of the system.

$$\rho_0 = \sum_i w_i |\psi_i\rangle \langle \psi_i|$$

where  $|\psi_i\rangle$  is an arbitrary (ket) qubit (its conjugate-transpose,  $\langle \psi_i|$ , is bra).

**Pure states** If the density operator involves only a pure state, for example  $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ , then the  $w = 1$  and  $\rho_0 = |0\rangle \langle 0|$ . This is effectively a projection matrix as qubits are unit length and a standard projection matrix, for example, is

$$|0\rangle \langle 0|0\rangle \langle 0|^{-1} \langle 0|$$

where the middle term in parenthesis is one. The trace (sum of the diagonal elements) is one.

$$Tr[\rho_0] = 1$$

The trace of the density operator squared is also one,  $Tr[\rho_0 \rho_0] = 1$ . Quantum (von Neumann) entropy is zero where quantum entropy is defined as<sup>1</sup>

$$s(\rho) \equiv -Tr[\rho \ln \rho] = -\lambda \ln \lambda$$

$\ln \rho = U \ln \Lambda U^T$  refers to the logarithm of the matrix  $\rho$  and  $\lambda$  is a vector of eigenvalues associated with the spectral decomposition of the density operator  $\rho = U \Lambda U^T$  ( $\rho$  is always a square, symmetric matrix,  $\Lambda$  is a diagonal matrix, and  $U$  is a unitary matrix).<sup>2</sup>

**Mixed states** On the other hand, a mixed state, for example, is

$$\rho = \frac{1}{2} (|0\rangle \langle 0| + |1\rangle \langle 1|) = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}$$

Again, the trace of a mixed state density operator is one. However, the trace of a mixed state density operator squared is less than one.<sup>3</sup> Further, quantum entropy is positive.

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<sup>1</sup>Recall the sum of the eigenvalues equals the trace of a matrix, then the two entropy expressions are equal.

<sup>2</sup> $0 \ln 0$  is treated as 0 as  $\lim_{\lambda \rightarrow 0} \lambda \ln \lambda \rightarrow 0$ .

<sup>3</sup>A pure state has one eigenvalue equal to one and the remainder zero so squaring the matrix (or its eigenvalues) has no effect. On the other hand, a mixed state density operator has eigenvalues that also sum to one but each eigenvalue is less than one; hence, squaring produces a sum (or trace) less than one.

**Multiple qubit states** Multiple qubit states have similar properties to those discussed above.

$$\rho_{AB} = \sum_{ij} w_{ij} |\psi_i \phi_j\rangle \langle \psi_i \phi_j|$$

They may be pure or mixed, their trace is one, the trace of the square of the density is one for pure states and less than one for mixed states, and quantum entropy is zero for pure states and positive for mixed states. However, other possibilities now arise. For instance, we may be interested in the properties of system A or B individually where A represents the first qubit and B the second qubit.

The above notation applies effectively for product states such as

$$\rho_{01} = \frac{1}{2} (|00\rangle \langle 00| + |11\rangle \langle 11|)$$

where  $|\psi_0\rangle = |\phi_0\rangle = |0\rangle, |\psi_1\rangle = |\phi_1\rangle = |1\rangle, w_{00} = w_{11} = \frac{1}{2}, w_{01} = w_{10} = 0$ . Notice, this is a mixed state.

$$Tr[\rho_{01}\rho_{01}] = \frac{1}{2}$$

and

$$s(\rho_{01}) = \ln 2$$

Suppose we create the reduced density operator for system 1 (the first qubit). This is accomplished by employing the partial trace. The partial trace functions by multiplying the outer product of the target qubit by the inner product of the qubit(s) being traced out.

$$\rho_0 = \frac{1}{2} (|0\rangle \langle 0| \langle 0| 0\rangle + |1\rangle \langle 1| \langle 1| 1\rangle) = \frac{1}{2} I$$

where  $I$  refers to the identity matrix.

The notation also applies to entangled states if we utilize the idea that entangled states are transformations of product states. For instance,

$$|\beta_{00}\rangle = CnotH_1 |00\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$$

Then,

$$\begin{aligned} \rho_{AB} &= CnotH_1 |00\rangle \langle 00| H_1 Cnot \\ \rho_{AB} &= \frac{1}{2} (|00\rangle \langle 00| + |00\rangle \langle 11| + |11\rangle \langle 00| + |11\rangle \langle 11|) \end{aligned}$$

with  $w = 1$ . It is a pure state (the trace of the square of the density operator is one and its entropy is zero).

Suggested:

1. Determine eigenvalues and orthonormal eigenvectors for  $\rho = \frac{1}{2}I_2$  (its spectral decomposition).

2. Suppose Ralph works with accounting observable.

$$O = \begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix}$$
$$= |v_1 \ v_2\rangle \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} \langle v_1^T \ v_2^T |$$

Determine the expected value.

$$\begin{aligned} \langle O \rangle &= Tr[\rho O] \\ &= \sum_i Pr(\lambda_i) \lambda_i \\ &= \sum_i Tr[\rho |v_i\rangle \langle v_i|] \lambda_i \end{aligned}$$

3. Now, suppose Ralph is working with the two qubit state  $\rho_{AB} = |\beta_{00}\rangle \langle \beta_{00}|$  and accounting observable

$$O_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix}$$

Determine the expected value  $\langle O_2 \rangle = Tr[\rho_{AB} O_2]$ .

4. Trace out the second qubit of  $\rho_{AB}$  to determine the reduced density operator  $\rho_A$ .

5. Calculate  $Tr[\rho_A]$ ,  $Tr[\rho_A \rho_A]$ , and quantum entropy  $s(\rho_A)$ . Compare these quantities to their analogs for  $\rho_{AB}$ .