1 Density operator ($\hat{\rho}$) approach for Eq. (2.3-2.4)

In order to calculate Eq. (2.3-2.4), we could have also used the *density operator*, the sum over pure states $\hat{\rho} \equiv \sum_i w_i \left|\alpha^{(i)}\right\rangle \left\langle\alpha^{(i)}\right|$ [10, p. 181, Eq. (3.4.7)], where w_i is the weight or probabilistic distribution with $\sum_i w_i = 1$, and $\left|\alpha^{(i)}\right\rangle$ are the base kets.

We are in a *pure ensemble*, a collection of identically prepared physical systems, on which a great number of measurements are to be performed in order to determine Eq. (2.3-2.4), all characterized by the same ket $|\alpha\rangle$ [10, p. 24, l. 12-15].

Then, $w_i = 1$ for $i = n$ and $w_i = 0$ for all other conceivable state kets. Thus, the density operator corresponding to a pure state such as ours can written as $\hat{\rho} = \left|\alpha^{(n)}\right\rangle \left\langle\alpha^{(n)}\right|$ [10, p. 182, Eq. (3.4.12)]. In this particular case, $\left|\alpha^{(n)}\right\rangle = |\psi\rangle = (2.2)$, and, in the $\{|1\rangle, |0\rangle\}$ basis,

$$\hat{\rho} = |\psi\rangle\langle\psi| \doteq \begin{pmatrix} a \\ b \end{pmatrix} \begin{pmatrix} a^* & b^* \end{pmatrix} = \begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix}. \tag{1.1}$$

The density operator $\hat{\rho}$ must satisfy the following results: [13, p. 134, Eq. (4.2.23.1-3)] [13, p. 101, Theo. 2.5]

1. The density operator $\hat{\rho}$ must be Hermitian: $\hat{\rho} = \hat{\rho}^\dagger \leftrightarrow \hat{\rho}^\dagger \doteq \begin{pmatrix} (|a|^2)^* & (ab^*)^* \\ (a^*b)^* & (|b|^2)^* \end{pmatrix}^T = \begin{pmatrix} |a|^2 & a^*b \\ ab^* & |b|^2 \end{pmatrix}^T = \begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix} \doteq \hat{\rho}$, where the adjoint (or conjugate transpose) is obtained by both transposing and complex conjugating [1, p. 18, l. 28], and the conjugate and transpose operations commute, $(\hat{A}^*)^T = (\hat{A}^T)^*$.

   Clearly, due to $\hat{\rho}$'s Hermiticity –in particular, all Hermitian and all unitary matrices are normal–, it is also *normal*: it commutes with its Hermitian conjugate or, equivalently, $\hat{\rho}\hat{\rho}^\dagger = \hat{\rho}^\dagger\hat{\rho}$. From the *spectral decomposition* theorem [1, p. 72, Theo. 2.1] we know that every normal operator is diagonalizable (its eigenvectors span the space). Let us consider that $\{|j\rangle\}$ is the just mentioned orthonormal basis. Therefore, the density operator can be represented as $\hat{\rho} = \sum_j \lambda_j \, |j\rangle\langle j|$, where λ_j are its real non-negative eigenvalues [1, p. 101, Eq. (2.157)]. The latter is related to the following condition 3.

2. The normalization condition leads to: $\mathrm{Tr}\hat{\rho} = 1$. Proof:

$$\begin{aligned} \mathrm{Tr}\hat{\rho} &= \mathrm{Tr}(\sum_i w_i \left|\alpha^{(i)}\right\rangle\left\langle\alpha^{(i)}\right|) \overset{(1)}{=} \sum_i w_i \, \mathrm{Tr}(\left|\alpha^{(i)}\right\rangle\left\langle\alpha^{(i)}\right|) \overset{(2)}{=} \sum_i w_i \sum_j \left\langle j|\alpha^{(i)}\right\rangle\left\langle\alpha^{(i)}|j\right\rangle \\ &= \sum_i w_i \sum_j \left\langle\alpha^{(i)}|j\right\rangle\left\langle j|\alpha^{(i)}\right\rangle = \sum_i w_i \, \left\langle\alpha^{(i)}|\hat{1}|\alpha^{(i)}\right\rangle = \sum_i w_i \, \left\langle\alpha^{(i)}|\alpha^{(i)}\right\rangle = \sum_i w_i \overset{(3)}{=} 1, \end{aligned} \tag{1.2}$$

   where in (1) we used $\mathrm{Tr}(\mathrm{k}\hat{A}) = \mathrm{k}\,\mathrm{Tr}(\hat{A})$; in (2), $\mathrm{Tr}(\hat{X}) \equiv \sum_{a'} \langle a'|\hat{X}|a'\rangle$ [10, p. 37, Eq. (1.5.14)]; and, in (3), Ref. [10, p. 108, Eq. (3.4.5)].

   In this instance, $\mathrm{Tr}\hat{\rho} \doteq \mathrm{Tr}\begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix} = |a|^2 + |b|^2 = 1$, where the last equality holds from the normalization condition of Eq. (2.2).

3. The density operator $\hat{\rho}$ must have positive or null eigenvalues - or, equivalently, $\hat{\rho}$ ought to be a positive semidefinite matrix, $\hat{\rho} \geq 0$ -, so that (*von Neumann*) *entropy* $S(\hat{\rho}) \equiv -\mathrm{k}\,\mathrm{Tr}(\hat{\rho}\ln\hat{\rho})$ [10, p. 187, Eq. (3.4.35-36) & (3.4.41)] can be defined, where k is the Boltzmann constant. Proof:

   For an arbitrary vector $|\varphi\rangle$, [1, p. 191, Eq. (2.156)]

$$\langle\varphi|\hat{\rho}|\varphi\rangle = \langle\varphi|(\sum_i w_i\,|\alpha^{(i)}\rangle\,\langle\alpha^{(i)}|)|\varphi\rangle = \sum_i w_i\,\langle\varphi|\alpha^{(i)}\rangle\,\langle\alpha^{(i)}|\varphi\rangle = \sum_i w_i\,|\,\langle\varphi|\alpha^{(i)}\rangle\,|^2 \geq 0. \tag{1.3}$$

   We will prove that $\hat{\rho}$ is positive semidefinite ($\hat{\rho} \geq 0$) in this particular case; id est, that all its eigenvalues, λ, are non-negative:
   $|\hat{\rho}-\lambda\hat{1}| = 0 = \begin{vmatrix} |a|^2-\lambda & ab^* \\ a^*b & |b|^2-\lambda \end{vmatrix} = (|a|^2-\lambda)(|b|^2-\lambda)-|a|^2|b|^2 = |a|^2|b|^2-\lambda(|a|^2+|b|^2)+\lambda^2-|a|^2|b|^2 = \lambda^2-\lambda = \lambda(\lambda-1) = 0 \leftrightarrow \lambda = 0,1 \geq 0.$ QED.

   Concretely, if we use the basis in which $\hat{\rho}$ is diagonal, [10, p. 187 Eq. (3.4.36)],[1]

$$S = -\mathrm{k}\,\mathrm{Tr}(\hat{\rho}\ln\hat{\rho}) \doteq -k\sum_k \rho_k^{\mathrm{diag}}\ln\rho_k^{\mathrm{diag}}. \tag{1.4}$$

   Recalling that the matrix representation is diagonal when its eigenfunctions are used as the base kets [10, p. 22, l. 3-5 & p. 36, l. 5-7], the diagonal elements in this basis are its eigenvalues $\lambda = 0,1$: $\hat{\rho} \doteq \begin{pmatrix} 0 & \\ & 1 \end{pmatrix}$. Hence,
   $S = -\mathrm{k}\,\mathrm{Tr}(\hat{\rho}\ln\hat{\rho}) \doteq -k\sum_k \rho_k^{\mathrm{diag}}\ln\rho_k^{\mathrm{diag}} = -k(0\ln(0)+1\ln(1)) = -k(0+0) = 0,$
   as it should be for a pure ensemble [10, p. 187, Eq. (3.4.38)]. As it can be seen, even though $\ln(0)$ diverges to $-\infty$, $0\ln(0)$ is well behaved. In general, $S \in [0, k\,\ln(n)]$, where $n \in \mathbb{N}-\{0\}$ is the dimension of the Hilbert space [10, p. 187, Eq. (3.4.37)]. Simply stated, entropy is a measure of the disorder or mixedness: $S = 0$ for pure states and $S = k\,\ln(n)$ for maximally mixed states of diagonal form $\hat{\rho} = \frac{\hat{1}_n}{n}$, as stated in footnote 25.

4. For a pure ensemble, the density operator $\hat{\rho}$ is idempotent; that is, $\hat{\rho}^2 = \hat{\rho}$ [10, p. 182, Eq. (3.4.13)]. Thus, for a pure ensemble only, we have $\mathrm{Tr}\hat{\rho}^2 = \mathrm{Tr}\hat{\rho} \overset{(1.2)}{=} 1$ [10, p. 182, Eq. (3.4.15)]. Proof:

$$\hat{\rho}^2 \doteq \begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix}\begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix} = \begin{pmatrix} |a|^2(|a|^2+|b|^2) & ab^*(|a|^2+|b|^2) \\ a^*b(|a|^2+|b|^2) & |b|^2(|a|^2+|b|^2) \end{pmatrix} = \begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix} \doteq \hat{\rho}.$$

Then probability of measuring the cell as *alive* or *dead*, as we previously calculated in Eq. (2.3-2.4),

$$\begin{aligned} \mathrm{Pr.}_{|\psi\rangle}(|1\rangle) = \mathrm{Pr.}_{\hat{\rho}}(|1\rangle) &\equiv \mathrm{Tr}(\hat{\rho}\,\hat{\Lambda}_{|1\rangle}) = \mathrm{Tr}(\hat{\rho}\;|1\rangle\,\langle 1|) \doteq \mathrm{Tr}\left(\hat{\rho}\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix}\right) \\ &= \mathrm{Tr}\left(\begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix}\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}\right) = \mathrm{Tr}\begin{pmatrix} |a|^2 & 0 \\ a^*b & 0 \end{pmatrix} = |a|^2, \end{aligned} \tag{1.5}$$

[1] In Information Theory, the expression in the diagonal basis is called the *Shannon entropy*, with the log in base 2.

$$
\begin{aligned}
\Pr._{|\psi\rangle}(|0\rangle) = \Pr._{\hat{\rho}}(|0\rangle) \equiv \operatorname{Tr}(\hat{\rho}\,\hat{\Lambda}_{|0\rangle}) = \operatorname{Tr}(\hat{\rho}\;|0\rangle\langle 0|) \doteq \operatorname{Tr}\left(\hat{\rho}\begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}0 & 1\end{pmatrix}\right) \\
= \operatorname{Tr}\left(\begin{pmatrix}|a|^2 & ab^* \\ a^*b & |b|^2\end{pmatrix}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}\right) = \operatorname{Tr}\begin{pmatrix}0 & ab^* \\ 0 & |b|^2\end{pmatrix} = |b|^2,
\end{aligned} \tag{1.6}
$$

where $\hat{\Lambda}_{|\phi\rangle} \equiv |\phi\rangle\langle\phi|$ is the *projection operator* along the ket $|\phi\rangle$, which selects that portion of the ket $|\psi\rangle$ (from $\hat{\rho} = |\psi\rangle\langle\psi|$) parallel to $|\phi\rangle$ [10, p. 19, Eq. (1.3.15)]. Besides, the probability (Pr.) of measuring a general ensemble (mixed or pure), characterized by the density operator $\hat{\rho}$, in the state ϕ is defined in terms of the projection operator $\hat{\Lambda}$ as $\Pr._{\hat{\rho}}(|\phi\rangle) \equiv \operatorname{Tr}(\hat{\rho}\,\hat{\Lambda}_{|\phi\rangle})$ [13, p. 134, l. 4][1, p. 102, Eq. (2.159)].

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