The Density Matrix

The quantum space of states is a Hilbert space $\mathcal{H}$. Any state vector $|\psi\rangle \in \mathcal{H}$ is a pure state. Since any linear combination of elements of $\mathcal{H}$ are also an element of $\mathcal{H}$, it follows that any linear combination of pure states is again a pure state.

But, in the real world we also encounter mixed states. These are described by the density operator,

$$\rho \equiv \sum_k p_k |\psi_k\rangle \langle\psi_k| \,, \tag{1}$$

which characterizes an ensemble of N states, of which n_k (on average) are in the state $|\psi_k\rangle$, and $p_k \equiv n_k/N$ is simply the probability that a state of the ensemble is observed to be in the state $|\psi_k\rangle$. By assumption, the state $|\psi_k\rangle$ is normalized to unity, i.e. $\langle\psi_k|\psi_k\rangle = 1$. The probabilities, p_k must sum to 1,

$$\sum_k p_k = 1\,. \tag{2}$$

The matrix elements of the density matrix with respect to an orthonormal basis $\{|i\rangle\}$ are then given by,

$$\rho_{ij} = \langle i|\,\rho\,|j\rangle = \sum_k p_k \langle i|\psi_k\rangle \langle\psi_k|j\rangle\,. \tag{3}$$

Given a self-adjoint operator Ω that acts on the Hilbert space $\mathcal{H}$, we can define an ensemble average,

$$\langle\overline{\Omega}\rangle \equiv \sum_k p_k \langle\psi_k|\,\Omega\,|\psi_k\rangle = \mathrm{Tr}(\Omega\rho)\,.$$

To verify the last step above, recall that the matrix elements of Ω with respect to an orthonormal basis $\{|i\rangle\}$ are given by $\Omega_{ij} \equiv \langle i|\,\Omega\,|j\rangle$. Thus, by definition of the trace,

$$\begin{aligned}\mathrm{Tr}(\Omega\rho) &= \sum_{ij} \Omega_{ij}\rho_{ji} = \sum_{ij} \langle i|\,\Omega\,|j\rangle \sum_k p_k \langle j|\psi_k\rangle\langle\psi_k|i\rangle \\ &= \sum_k p_k \sum_{ij} \langle\psi_k|i\rangle\langle i|\,\Omega\,|j\rangle\langle j|\psi_k\rangle = \sum_k p_k \langle\psi_k|\,\Omega\,|\psi_k\rangle = \langle\overline{\Omega}\rangle\,,\end{aligned}$$

after using the completeness relation to sum over i and j.

Since Ω is self-adjoint, it possesses real eigenvalues. Suppose ω is one of the possible eigenvalues of Ω. Then, ω is the possible outcome of an experiment that measures the observable corresponding to Ω. Given an ensemble defined by the density operator ρ, the probability $P(\omega)$ of obtaining ω in a measurement is given by

$$P(\omega) = \mathrm{Tr}(P_\omega\rho) = \sum_k p_k |\langle\omega|\psi_k\rangle|^2\,, \tag{4}$$

where $P_\omega \equiv |\omega\rangle\langle\omega|$ is the projection operator that projects onto the one-dimensional subspace of states spanned by $|\omega\rangle$. To verify the last step of eq. (4), we use $(P_\omega)_{ij} = \langle i|\omega\rangle\langle\omega|j\rangle$. It then follows that,

$$\mathrm{Tr}(P_\omega \rho) = \sum_{ij}(P_\omega)_{ij}\rho_{ji} = \sum_{ij}\langle i|\omega\rangle\langle\omega|j\rangle \sum_k p_k \langle j|\psi_k\rangle\langle\psi_k|i\rangle$$

$$= \sum_k p_k \sum_{ij}\langle\psi_k|i\rangle\langle i|\omega\rangle\langle\omega|j\rangle\langle j|\psi_k\rangle = \sum_k p_k |\langle\omega|\psi_k\rangle|^2 .$$

The properties of the density operator are listed below.

1. $\rho^\dagger = \rho$.

Using eq. (3)

$$\rho^*_{ji} = \sum_k p_k \langle j|\psi_k\rangle^* \langle\psi_k|i\rangle^* = \sum_k p_k \langle\psi_k|j\rangle\langle i|\psi_k\rangle = \rho_{ij} .$$

Hence, ρ is hermitian.

2. ρ is positive semi-definite.

For any state χ, we have

$$\langle\chi|\,\rho\,|\chi\rangle = \sum_k p_k \langle\chi|\psi_k\rangle\langle\psi_k|\chi\rangle = \sum_k p_k |\langle\chi|\psi_k\rangle|^2 \geq 0\,,$$

where we have used the fact that the probabilities p_k are real and non-negative.

3. $\mathrm{Tr}\,\rho = 1$.

Using the completeness of the $\{|i\rangle\}$ and $\langle\psi_k|\psi_k\rangle = 1$, it follows that

$$\mathrm{Tr}\,\rho = \sum_i \rho_{ii} = \sum_k p_k \sum_i \langle\psi_k|i\rangle\langle i|\psi_k\rangle = \sum_k p_k = 1\,,$$

after employing eq. (2).

4. For a pure quantum state, $\rho^2 = \rho$, which implies that $\mathrm{Tr}\,\rho^2 = 1$ in light of property 3 above.

For a pure quantum state, we can always find some element of the Hilbert space, $|\psi\rangle$, which is normalized to unity, such that $\rho = |\psi\rangle\langle\psi|$. Then, we trivially obtain

$$\rho^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \rho\,.$$

5. For a mixed quantum state, $0 < \mathrm{Tr}\,\rho^2 < 1$.

First we note that in light of property 1 above, $\rho^2 = \rho\rho^\dagger$, which is a non-negative hermitian operator. Thus, all the eigenvalues of ρ^2 are non-negative. Denoting the eigenvalues of ρ^2 by λ_i, it follows that

$$\mathrm{Tr}\,\rho^2 = \sum_i \lambda_i > 0\,.$$

Note that it is not possible for all of the eigenvalues of ρ^2 to be zero, since this would imply that $\rho = 0$.[1]

To prove that $\operatorname{Tr}\rho^2 < 1$, we start from eq. (3),[2]

$$\operatorname{Tr}\rho^2 = \sum_{k,\ell} p_k p_\ell \sum_{i,n} \langle i|\psi_k\rangle \langle\psi_k|n\rangle \langle n|\psi_\ell\rangle \langle\psi_\ell|i\rangle = \sum_{k,\ell} p_k p_\ell \langle\psi_\ell|\psi_k\rangle \langle\psi_k|\psi_\ell\rangle = \sum_{k,\ell} p_k p_\ell |\langle\psi_\ell|\psi_k\rangle|^2\,, \tag{5}$$

after summing over the two complete sets of states, $\{|i\rangle\}$ and $\{|n\rangle\}$. We now make use of the Schwarz inequality, $|\langle\psi_\ell|\psi_k\rangle|^2 \leq \langle\psi_\ell|\psi_\ell\rangle \langle\psi_k|\psi_k\rangle$. Since $|\psi_k\rangle$ is normalized to unity, we obtain $|\langle\psi_\ell|\psi_k\rangle|^2 \leq 1$. It then follows that

$$\operatorname{Tr}\rho^2 = \sum_{k,\ell} p_k p_\ell |\langle\psi_\ell|\psi_k\rangle|^2 \leq 1\,, \tag{6}$$

after making use of eq. (2). Moreover, the Schwarz inequality is saturated only when $|\psi_k\rangle$ and $|\psi_\ell\rangle$ are proportional for any choice of k and ℓ. Since these are normalized states, they can only differ by a multiplicative phase. But, this case, $|\psi_k\rangle\langle\psi_k|$ in eq. (1) would be independent of k, which means one can simply write $\rho = |\psi\rangle\langle\psi|$, corresponding to a pure state. Thus, for a mixed state, the Schwarz inequality is not saturated, and we conclude that $\operatorname{Tr}\rho^2 < 1$. Thus, we can conclude that for a mixed state, $0 < \operatorname{Tr}\rho^2 < 1$.

6. For a uniform distribution over N states, $\rho = N^{-1}I$, where I is the $N \times N$ identity operator. This is a mixed quantum state. An example of such a quantum state would be unpolarized light.

Using $\operatorname{Tr} I = N$, we easily verify the first three properties above. Moreover, $\operatorname{Tr}\rho^2 = 1/N$ which satisfies the fifth property above for any $N > 1$. Note that by taking $N \gg 1$, we can obtain an arbitrarily small value of $\operatorname{Tr}\rho^2$.

Pure states are governed by the time-dependent Schrodinger equation. A pure state will evolve into a pure state. So, how does one create mixed states? One way to produce a mixed state is to consider a system that is sensitive only to a subset of the full quantum Hilbert space. For example, consider a system that is made up of two separate subsystems. We will perform measurements using operators that are only sensitive to one of the two subsystems. In particular, consider two subsystems called subsystem 1 and subsystem 2. Corresponding to each subsystem is an orthonormal basis $\{|n, 1\rangle\}$ and $\{|m, 2\rangle\}$, respectively. Mathematically, the total Hilbert space is a direct product of two subsystem Hilbert spaces, $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$.

[1]In general, if an $n \times n$ matrix M is diagonalizable, then it possesses n linearly independent eigenvectors. In this case, there exists an invertible matrix S such that $D = S^{-1}MS$, where D is a diagonal matrix whose diagonal elements are the eigenvalues of M. Hence, if all the eigenvalues of M are zero, then it follows that $M = 0$. Note that this argument does not apply to matrices that are not diagonalizable, as the famous example $\left(\begin{smallmatrix} 0 & 1 \\ 0 & 0 \end{smallmatrix}\right)$ attests. Finally, by noting that all hermitian matrices are diagonalizable, we can conclude that for any density matrix (which is necessarily nonzero), $\operatorname{Tr}\rho > 0$.

[2]Given that $p_k \geq 0$, eq. (2) implies that at least one of the p_k appearing in eq. (5) is positive. Hence, it follows that $\operatorname{Tr}\rho^2 \geq p_k^2$. This provides another argument for $\operatorname{Tr}\rho > 0$.

A generic pure state of $\mathcal{H}$ is of the form

$$|\psi\rangle = \sum_n \sum_m c_{nm} |n, 1\rangle \otimes |m, 2\rangle \ , \tag{7}$$

where $\langle\psi|\psi\rangle = 1$ implies that

$$\sum_{m,n} |c_{mn}|^2 = 1 \, . \tag{8}$$

The corresponding density operator is

$$\rho = |\psi\rangle \langle\psi| = \sum_{n,m} \sum_{n',m'} c_{nm} c^*_{n'm'} |n, 1\rangle \otimes |m, 2\rangle \langle n', 1| \otimes \langle m', 2| \ . \tag{9}$$

Consider an operator Ω that is only sensitive to subsystem 1. That is, when Ω acts on $|\psi\rangle$ given by eq. (7), it has no effect on $\{|m, 2\rangle\}$. Using the direct product notation, Ω actually means $\Omega \otimes I$, where Ω acts on subsystem 1, and the identity operator I acts on subsystem 2. Then, the ensemble average of Ω is given by

$$\langle\overline{\Omega}\rangle = \mathrm{Tr}_1\, \mathrm{Tr}_2(\rho\, \Omega) = \mathrm{Tr}_1\big[(\mathrm{Tr}_2\, \rho)\Omega\big] \, ,$$

where Tr_i ($i = 1, 2$) is carried out by summing over the subsystem i part of the total system. Thus, we can express the ensemble average of the operator $\Omega \otimes I$ as

$$\langle\overline{\Omega}\rangle = \mathrm{Tr}_1(\hat{\rho}\, \Omega) \, , \tag{10}$$

where

$$\hat{\rho} \equiv \mathrm{Tr}_2\, \rho \, , \tag{11}$$

is the effective density matrix for subsystem 1. Even though there are typically quantum correlations between the two subsystems, observers (by assumption) are only sensitive to subsystem 1. Thus, in computing an ensemble average of a quantum state of subsystem 1, we must define the ensemble average solely in terms of subsystem 1 quantities; that is, as a trace over subsystem 1 as in eq. (10). It is now a simple matter to compute

$$\hat{\rho} = \mathrm{Tr}_2\, \rho = \sum_j \langle j, 2|\, \rho\, |j, 2\rangle \ , \tag{12}$$

where ρ is given by eq. (9). Using eq. (12), we then find,

$$\begin{aligned}\hat{\rho} = \sum_j \langle j, 2|\, \rho\, |j, 2\rangle &= \sum_{n,m} \sum_{n',m'} c_{nm} c^*_{n'm'} \sum_j |n, 1\rangle \langle j, 2|m, 2\rangle \langle m', 2|j, 2\rangle \langle n', 1| \\ &= \sum_{n,m} \sum_{n',m'} c_{nm} c^*_{n'm'} \sum_j |n, 1\rangle \langle n', 1|\, \delta_{jm} \delta_{jm'} \, . \end{aligned} \tag{13}$$

Performing the sums over j and m' is now trivial due to the two Knonecker deltas, and we end up with

$$\hat{\rho} = \sum_{n,m} \sum_{n'} c_{nm} c^*_{n'm} |n, 1\rangle \langle n', 1| \ .$$

This is the relevant density matrix for subsystem 1. Note that in general it corresponds to a mixed state, since the original state $|\psi\rangle$ can possess non-trivial quantum correlations between the two subsystems as previously noted. But, that information is lost in $\hat{\rho}$, which only knows about subsystem 1.

The only way for $\hat{\rho}$ to correspond to a pure state is if we can decompose c_{nm} as follows,

$$c_{nm} = b_n d_m \,, \tag{14}$$

where

$$\sum_n |b_n|^2 = \sum_m |d_m|^2 = 1\,. \tag{15}$$

In this case, it is straightforward to verify that $\hat{\rho}^2 = \hat{\rho}$, which indicates that the quantum subsystem 1 is a pure state. Indeed, if eq. (14) holds, then we can write eq. (7) as

$$|\psi\rangle = \left(\sum_n b_n \,|n,1\rangle\right)\left(\sum_m d_m \,|m,2\rangle\right) .$$

in which case, $|\psi\rangle$ can be decomposed into a direct product of two pure states,

$$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \ ,$$

where

$$|\psi_1\rangle = \sum_n b_n \,|n,1\rangle \ , \qquad\qquad |\psi_2\rangle = \sum_m d_m \,|n,1\rangle \ .$$

Thus, $\hat{\rho} = |\psi_1\rangle \langle\psi_1|$, which is clearly a pure state. In contrast, if one cannot write c_{mn} in the form given by eq. (14), then $\hat{\rho}$ satisfies $0 < \mathrm{Tr}_1\, \hat{\rho}^2 < 1$, and we conclude that subsystem 1 is a mixed quantum state state.

More explicitly,

$$\begin{aligned}
\mathrm{Tr}_1\, \hat{\rho}^2 &= \sum_{n,m,n'} \sum_{j,k,j'} c_{nm} c^*_{n'm} c_{jk} c^*_{j'k} \,\langle i,1|n,1\rangle \,\langle n',1|\ell,1\rangle \,\langle \ell,1|j,1\rangle \,\langle j',1|i,1\rangle \\
&= \sum_{n,m,n'} \sum_{j,k,j'} c_{nm} c^*_{n'm} c_{jk} c^*_{j'k} \delta_{in} \delta_{\ell n'} \delta_{\ell j} \delta_{ij'} \\
&= \sum_{n,n'} \left(\sum_m c_{nm} c^*_{n'm}\right)\left(\sum_k c_{n'k} c^*_{nk}\right) ,
\end{aligned}$$

which we can write as

$$\mathrm{Tr}_1\, \hat{\rho}^2 = \sum_{n,n'} \left|\sum_m c_{nm} c^*_{n'm}\right|^2 . \tag{16}$$

Note that $\mathrm{Tr}_1\, \hat{\rho}^2 > 0$. We can reinterpret eq. (16) by defining the vectors c_n, whose components are given by c_{nm}. Then, we can rewrite eq. (16) as

$$\mathrm{Tr}_1\, \hat{\rho}^2 = \sum_{n,n'} |\,\langle c_n|c_{n'}\rangle\,|^2 \,, \tag{17}$$

where $\langle c_n|c_{n'}\rangle$ is the complex inner product of the vectors c_n and $c_{n'}$. We can now employ the Schwarz inequality,

$$|\langle c_n|c_{n'}\rangle|^2 \leq \langle c_n|c_n\rangle \langle c_{n'}|c_{n'}\rangle \,, \tag{18}$$

to eq. (17). We then obtain,

$$\mathrm{Tr}_1\, \hat{\rho}^2 \leq \left(\sum_n \langle c_n|c_n\rangle\right)^2 .$$

Finally, we note that eq. (8) is equivalent to

$$\sum_n \langle c_n|c_n\rangle = 1 \,.$$

Hence, we conclude that $0 < \mathrm{Tr}_1\, \hat{\rho}^2 \leq 1$. Note that the inequality is saturated only when the Schwarz inequality [cf. eq. (18)] is saturated, i.e. when the all the vectors c_1, c_2, $c_3, \ldots$ are proportional to the same vector, which we shall denote by d. That is, the inequality is saturated if and only if

$$c_n = b_n d \,, \tag{19}$$

where b_n is the proportionality constant relating the vectors c_n and d. Recall that the components of the vector c_n were denoted by c_{mn}. Then, if we denote the components of the vector d by d_m, then, eq. (19) is equivalent to eq. (14). The conclusion of this analysis is that $0 < \mathrm{Tr}_1\, \hat{\rho}^2 < 1$, corresponding to a mixed quantum state, unless eq. (14) is satisfied.

If $c_{nm} = b_n d_m$, then the inequality is saturated and $\mathrm{Tr}_1\, \hat{\rho}^2 = 1$, corresponding to a pure quantum state. We can verify this result explicitly by inserting $c_{nm} = b_n d_m$ directly into eq. (16),

$$\mathrm{Tr}_1\, \hat{\rho}^2 = \sum_{n,n'} \left| b_n b^*_{n'} \sum_m |d_m|^2 \right|^2 = \sum_n |b_n|^2 \sum_{n'} |b_{n'}|^2 = 1 \,,$$

after making use of eq. (15). It should be noted that the condition $c_{nm} = b_n d_m$ is very strong. As shown in the Appendix, if the matrix elements of a matrix C are $c_{nm} = b_n d_m$, then C is a rank-one matrix with zero determinant.

APPENDIX: Properties of a matrix that satisfies $C_{ij} = a_i b_j$

Consider the $n \times n$ non-zero matrix C, whose matrix elements are given by $C_{ij} = a_i b_j$. More explicitly,

$$C = \begin{pmatrix} a_1 b_1 & a_1 b_2 & \cdots & a_1 b_n \\ a_2 b_1 & a_2 b_2 & \cdots & a_2 b_n \\ \vdots & \vdots & \ddots & \vdots \\ a_n b_1 & a_n b_2 & \cdots & a_n b_n \end{pmatrix} .$$

It is a simple matter to check that the following $n-1$ vectors,

$$\begin{pmatrix} b_2 \\ -b_1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad \begin{pmatrix} b_3 \\ 0 \\ -b_1 \\ \vdots \\ 0 \end{pmatrix}, \quad ,\cdots, \quad \begin{pmatrix} b_n \\ 0 \\ 0 \\ \vdots \\ -b_1 \end{pmatrix}, \tag{20}$$

are linearly independent eigenvectors of C, each with an associated zero eigenvalue. Using the fact that $\operatorname{Tr} C$ is the sum of the eigenvalues, it follows that the (potentially) nonzero eigenvalue of C must be equal to $\sum_i a_i b_i$, and the corresponding eigenvector is

$$\begin{pmatrix} a_1 \\ a_2 \\ 0 \\ \vdots \\ a_n \end{pmatrix}, \tag{21}$$

as is easily verified. If $\sum_i a_i b_i \neq 0$, then 0 is an $(n-1)$-fold degenerate eigenvalue of C. That is, C has $n-1$ zero eigenvalues and one non-zero eigenvalue. Moreover, all n eigenvectors listed above are linearly independent. In contrast, if $\sum_i a_i b_i = 0$, then C has n zero eigenvalues. In this case the eigenvector shown in eq. (21) can be written as a linear combination of the eigenvectors listed in eq. (20).

In light of these results, one can immediately conclude that C is a rank-1 matrix with zero determinant. The latter follows from the fact that C possesses a zero eigenvalue, since $\det C$ is a product of its eigenvalues. Moreover, if $\sum a_i b_i \neq 0$, then C possesses n linearly independent eigenvalues, which implies that C is diagonalizable. In the case where $\sum a_i b_i = 0$, C possesses n zero eigenvalues, but only $n-1$ linearly independent eigenvectors.[3]

[3]The only $n \times n$ matrix that possesses n zero eigenvalues and n linearly independent eigenvectors is the $n \times n$ zero matrix [cf. footnote 1].