

Density matrix

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Abstract. It will discuss the basic properties of the density matrix or density operator as well as the evaluation of the expectation values of the observables, the dynamics of the density operator, also about systems of two states and the Bloch sphere and the representation of the density operator in the Micro-Canonical and Canonical Ensembles ...

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1 Formalism of density operator

The state vector $|\psi\rangle$ in quantum mechanics contains the maximal information about a system. Associated to any state $|\psi\rangle$ it is always possible to define the projector $\hat{P}_\psi = |\psi\rangle\langle\psi|$, but there are situations where the state vector is not known or cases where the system of study is interacting with other system, like a reservoir (a very large system), with which it becomes entangled. It is possible to write state vector for the multi-system but not for a specific system or system of interest.

Quantum states described by state vectors are said to be **pure** states. States that cannot be described by state vectors are said to be in **mixed** states. Introducing the density operator, denoted by $\hat{\rho}$, mixed and pure states are described by the density operator

$$\hat{\rho} = \sum_{i,j} |\psi_i\rangle p_{ij} \langle\psi_j| \quad (1)$$

where the sum is over an ensemble (in the sense of statistical mechanics), consider the case where $\hat{\rho} = \sum_i |\psi_i\rangle p_i \langle\psi_i|$ only for simplicity, then p_i is the probability of the system being in the i th state of the ensemble $|\psi_i\rangle$, where $\langle\psi_i|\psi_i\rangle = 1$. The probabilities satisfy the relations

$$0 \leq p_i \leq 1 \quad \sum_i p_i = 1 \quad \sum_i p_i^2 \leq 1 \quad (2)$$

consider the special case where all the p_i vanish except the j th one, $p_j = \delta_{ij}$, we obtain

$$\hat{\rho} = |\psi_j\rangle\langle\psi_j| \quad (3)$$

the density operator for the **pure** state $|\psi_j\rangle$. Note that the density operator for this case is just the projection operator \hat{P}_{ψ_j} associated with the state $|\psi_j\rangle$, and for the more general case of (1), the density operator is a sum of the projection operators over the ensemble, weighted with the probabilities of each member of the ensemble. Then some assemblies will be considered.

Definition 1. The *trace* of an operator A is given by

$$Tr A = \sum_n \langle n | A | n \rangle \quad (4)$$

where $\{|n\rangle\}$ is an orthonormal basis of compatible observables.

Introducing a complete orthonormal basis $\{|n\rangle\}$ eigenstates of some observable or a complete set of observables, where $\sum_n |n\rangle \langle n| = \hat{I}$ is the identity operator. Then for the i th member of the ensemble we may write

$$|\psi_i\rangle = \sum_n |n\rangle \langle n | \psi_i \rangle = \sum_n c_n^{(i)} |n\rangle \quad (5)$$

where $c_n^{(i)} = \langle n | \psi_i \rangle$ is the coefficient for the n -th term. The matrix element of $\hat{\rho}$ between the n and n' eigenstates is

$$\langle n | \hat{\rho} | n' \rangle = \sum_i \langle n | \psi_i \rangle \rho_i \langle \psi_i | n' \rangle = \sum_i p_i c_n^{(i)} c_{n'}^{(i)*} \quad (6)$$

The quantities $\langle n | \hat{\rho} | n' \rangle$ are the elements of the density matrix. Taking the **trace** of this matrix, we have

$$\begin{aligned} Tr \hat{\rho} &= \sum_n \langle n | \hat{\rho} | n \rangle = \sum_i \sum_n \langle n | \psi_i \rangle p_i \langle \psi_i | n \rangle \\ &= \sum_i \sum_n p_i \langle \psi_i | n \rangle \langle n | \psi_i \rangle = \sum_i p_i = 1 \end{aligned} \quad (7)$$

but if a density operator $\hat{\rho}$ is not normalized, i.e. $Tr \hat{\rho} \neq 1$, but finite, it is always possible to normalize it as follows

$$\hat{\rho}' = \frac{\hat{\rho}}{Tr \hat{\rho}} \quad (8)$$

Notes: There are also cases in which the density matrix is not normalizable, and also note that if the density operator can be expressed as a single projector, then $Tr \hat{\rho}^2 = 1$

Example 1 (Polarization state of a photon). Consider the state

$$|\Phi\rangle = c_+ |+\rangle + c_- |-\rangle \quad (9)$$

where $|+\rangle$ and $|-\rangle$ are states of horizontal and vertical polarization, and $c_+c_+^* + c_-c_-^* = 1$, the density operator is then

$$\begin{aligned}\hat{\rho} &= |\Phi\rangle\langle\Phi| \\ &= c_+c_+|+\rangle\langle+| + c_-c_-|-\rangle\langle-| + c_+c_-^*|+\rangle\langle-| + c_-^*c_+|-\rangle\langle+|\end{aligned}\quad (10)$$

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Since $\hat{\rho}$ is hermitian, the diagonal elements must be real, and it follows from (7) that

$$0 \leq \langle\varphi_n|\hat{\rho}|\varphi_n\rangle \leq 1 \quad (11)$$

Now let us consider the square of the density operator: $\hat{\rho}^2 = \hat{\rho}\hat{\rho}$. For a pure state where $\hat{\rho} = |\psi\rangle\langle\psi|$ it follows that

$$\hat{\rho}^2 = |\psi\rangle\langle\psi|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi| = \hat{\rho} \quad (12)$$

because $\langle\psi|\psi\rangle = 1$ and thus

$$\text{Tr}\hat{\rho}^2 = \text{Tr}\hat{\rho} = 1 \quad (13)$$

For a mixed state

$$\hat{\rho}^2 = \sum_i \sum_j p_i p_j |\psi_i\rangle\langle\psi_i|\psi_j\rangle\langle\psi_j| \quad (14)$$

Taking the trace we have

$$\begin{aligned}\text{Tr}\hat{\rho}^2 &= \sum_n \langle n|\hat{\rho}^2|n\rangle \\ &= \sum_n \sum_i \sum_j p_i p_j \langle n|\psi_i\rangle\langle\psi_i|\psi_j\rangle\langle\psi_j|n\rangle \\ &= \sum_i \sum_j p_i p_j |\langle\psi_i|\psi_j\rangle|^2 \\ &\leq \left[\sum_i p_i \right]^2 = 1\end{aligned}\quad (15)$$

The equality holds only if $|\langle\psi_i|\psi_j\rangle|^2 = 1, \forall |\psi_i\rangle$ and $|\psi_j\rangle$. This is possible only if all the $|\psi_i\rangle$ are collinear in Hilbert space, i.e. equivalent up to an overall phase factor. Thus we can use the following criteria to distinguish between pure and mixed states:

$$\text{Tr}\hat{\rho}^2 = 1, \quad \text{for a pure state}, \quad (16)$$

$$\text{Tr}\hat{\rho}^2 < 1, \quad \text{for a mixed state} \quad (17)$$

For one of the states of the ensemble $|\psi_i\rangle$, by itself pure, the expectation value of some operator \hat{O} is given by

$$\langle \hat{O} \rangle_i = \langle \psi_i | \hat{O} | \psi_i \rangle \quad (18)$$

For the mixed state or statistical mixture, the ensemble average is given by

$$\langle \hat{O} \rangle = \sum_i p_i \langle \psi_i | \hat{O} | \psi_i \rangle \quad (19)$$

which is just the average of the quantum mechanical expectation values weighted with the probabilities p_i . Formally we may write

$$\langle \hat{O} \rangle = \text{Tr}(\hat{\rho} \hat{O}) \quad (20)$$

since

$$\begin{aligned} \text{Tr}(\hat{\rho} \hat{O}) &= \sum_n \langle n | \hat{\rho} \hat{O} | n \rangle \\ &= \sum_n \sum_i p_i \langle n | \psi_i \rangle \langle \psi_i | \hat{O} | n \rangle \\ &= \sum_i \sum_n p_i \langle \psi_i | \hat{O} | n \rangle \langle n | \psi_i \rangle \\ &= \sum_i p_i \langle \psi_i | \hat{O} | \psi_i \rangle \end{aligned} \quad (21)$$

and if we perform a measurement of a physical quantity O associated with the operator \hat{O} , it is easy to see that the probability of finding the eigenvalue o_ω is

$$\mathbf{P}(o_\omega) = \text{Tr}(\hat{\rho} \hat{P}_\omega) \quad (22)$$

After a measurement yielding the value o_ω , the corresponding density operator is therefore

$$\hat{\rho}' = \frac{\hat{P}_\omega \hat{\rho} \hat{P}_\omega}{P(o_\omega)} \quad (23)$$

2 Two state system and the Bloch sphere

For a two-state system, be it a spin-1/2 particle, a two-level atom, or the polarizations of a single photon like the example 1, there always exists a description in terms of the Pauli operators $\hat{\sigma}_1, \hat{\sigma}_2, \hat{\sigma}_3$ satisfying the commutation relations

$$[\hat{\sigma}_i, \hat{\sigma}_j] = 2i\xi_{ijk}\hat{\sigma}_k \quad (24)$$

In the basis where $\hat{\sigma}_3$ and $\hat{\sigma}^2 = \hat{\sigma}_1^2 + \hat{\sigma}_2^2 + \hat{\sigma}_3^2$ are diagonal, these operators can be written in matrix form as

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (25)$$

Any Hermitian 2×2 matrix can be expressed in terms of the Pauli matrices and the 2×2 identity matrix \hat{I} , and this includes, the density operator of a two-state system. That is, we can write

$$\rho = \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 + s_3 & s_1 + is_2 \\ s_1 - is_2 & 1 - s_3 \end{pmatrix} = \frac{1}{2} (\hat{I}_2 + \mathbf{s} \cdot \boldsymbol{\sigma}) \quad (26)$$

where the vector $\mathbf{s} = (s_1, s_2, s_3)$ is known as the Bloch vector. For a pure state $\hat{\rho} = |\Psi\rangle \langle\Psi|$, the Bloch vector has unit length, $\sum_i |s_i|^2 = 1$, and points in some direction specified by the spherical coordinate angles θ and ϕ in a 3-dimensional sphere of the Euclidean space, known as Bloch sphere or Poincar sphere. The associated quantum state can be represented in terms of these angles as

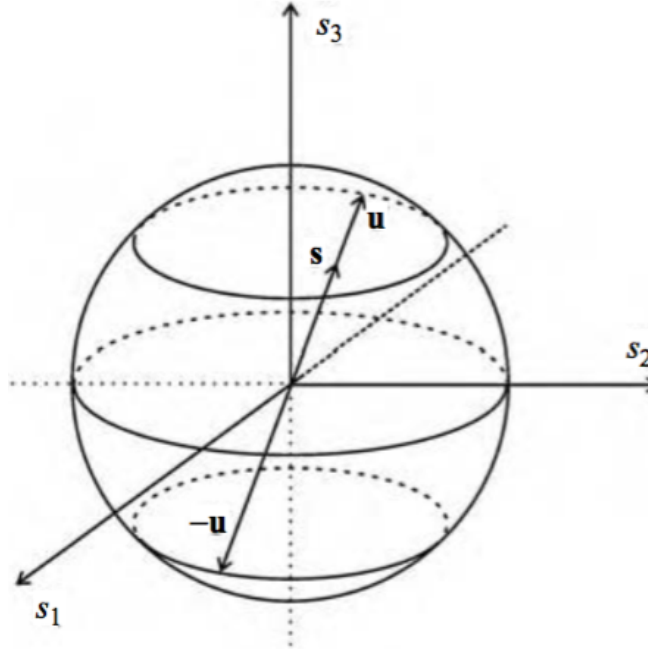


Fig. 1. Bloch sphere and Bloch vector, with the two eigenvectors specified by \mathbf{u} and $-\mathbf{u}$, and the two eigenvalues $(1 \pm |\mathbf{s}|)/2$. vector \mathbf{u} points in the same direction as \mathbf{s}

$$|\Psi\rangle = \cos\left(\frac{\theta}{2}\right) e^{-i\phi/2} |+\rangle + \sin\left(\frac{\theta}{2}\right) e^{i\phi/2} |-\rangle \quad (27)$$

In general, and including the case of mixed states where $|s| \leq 1$, the density operator of the form of equation (26) has the eigenvalues

$$g_1 = \frac{1}{2}[1 + |s|] \quad (28)$$

$$g_2 = \frac{1}{2}[1 - |s|] \quad (29)$$

and its eigenvectors are determined by the two vectors \mathbf{u} and $-\mathbf{u}$ shown in the Bloch sphere in Fig.(1). For pure states ($|s| = 1$), \mathbf{u} coincides with \mathbf{s} , ending on the surface of the Bloch sphere. For a mixed state where $|s| < 1$, vector \mathbf{u} points in the same direction as \mathbf{s} but unlike \mathbf{s} maintains unit length so that its tip always lies on the surface of the Bloch sphere. The equation (27) can be used to express \mathbf{u} and $-\mathbf{u}$ in terms of the vectors in state space.

In optics, for example, the Bloch sphere is useful to represent different types of polarizations. And finally the important point to emphasize here is that every point inside the Bloch sphere is a mixed state and every point on the surface is a pure state.

3 Dynamics of the density operator

In the absence of dissipative interactions and no explicit time dependent interaction, the density operator evolves according to

$$\partial_t \hat{\rho} = \frac{i}{\hbar} [\hat{\rho}, \hat{H}] \quad (30)$$

Proof. Using the fact that each of the states $|\psi_i\rangle$ of the ensemble satisfies the Schrödinger equation:

$$i\hbar \partial_t |\psi_i\rangle = \hat{H} |\psi_i\rangle \quad (31)$$

Differentiating the density operator (1), with the help of the equation (31) and multiplying it by $i\hbar$, then

$$\begin{aligned} i\hbar \partial_t \hat{\rho} &= i\hbar \sum_i p_i (\partial_t |\psi_i\rangle \langle \psi_i| + |\psi_i\rangle \partial_t \langle \psi_i|) \\ &= \sum_i p_i \left(-\frac{i}{\hbar} \hat{H} |\psi_i\rangle \langle \psi_i| + |\psi_i\rangle \langle \psi_i| \frac{i}{\hbar} \hat{H} \right) \\ &= [\hat{H}, \hat{\rho}] \end{aligned} \quad (32)$$

□

Alternatively, applying a unitary evolution operator $\hat{U}(t, t_0)$, we can write

$$\hat{\rho} = \hat{U}(t, 0) \hat{\rho}(0) \hat{U}^\dagger(t, 0) \quad (33)$$

where $t_0 = 0$ and the unitary evolution operator $\hat{U}(t, 0)$ satisfies the equation

$$i\hbar\partial_t\hat{U} = \hat{H}\hat{U} \quad (34)$$

Equation (30) is known as the von Neumann equation, and it is the quantum mechanical analogue to the classical Liouville equation associated with the evolution phase-space probability distributions in statistical mechanics.

4 Degree of mixture

From the equation (17), we find for the smallest value of $Tr\rho^2$ the quotient $\frac{1}{d}$, i.e. the infimum of a set $\{Tr\rho^2\}$, where d is the dimension of the Hilbert space \mathcal{H} . The value $p_i = \frac{1}{d}$ is adopted and belongs to

$$\hat{\rho} = \frac{1}{d}\hat{\mathbf{I}} \quad (35)$$

This completely structureless density operator is called the maximal mixed density operator.

Statistical mixtures are produced operationally in experiments by the "mixing" of states. One can introduce the parameter

$$\Xi \equiv 1 - Tr\hat{\rho}^2 \quad (36)$$

to quantify the degree of mixture which varies between that of a pure state, $\Xi = 0$, and that of maximal mixture, $\Xi = 1 - \frac{1}{d}$:

$$0 \leq \Xi \leq 1 - \frac{1}{d} \quad (37)$$

5 Modified axioms for Quantum Mechanics

It is possible to formulate the principles of quantum mechanics state with the density operator instead of the state vector, then:

Principle 1

For all physical system we can associate a Hilbert space \mathcal{H} . $\forall t$ the state of the system is completely determined by a density operator $\hat{\rho}(t)$. This operator is Hermitian and satisfies $Tr\hat{\rho}(t) = 1$ that is the normalization condition. If the system is in a pure state, $\hat{\rho}(t)$ has one eigenvalue equal to 1 and all the other eigenvalues are zero. But in general all eigenvalues p_i of $\hat{\rho}$ satisfy

$$0 \leq p_i \leq 1 \quad (38)$$

Principles 2 and 3 The equations for measuring the physical quantities and the time evolution of the system are (22)(23)(30)

6 The Micro-Canonical and Canonical Ensembles

For a system where the only available information is:

The system is, with certainty (i. e. with probability 1), a given subspace \mathcal{J} of the total Hilbert space \mathcal{H} . If $\dim(\mathcal{J}) = d > 1$ the system is not in a pure state, and it has to be described by a density operator. First consider a orthonormal basis set $\{|\psi : i = 1, \dots, d\rangle\}$ of \mathcal{J} , the density operator is

$$\hat{\rho} = \frac{1}{d} \sum_{i=1}^d |\psi_i\rangle \langle \psi_i| \quad (39)$$

called the **microcanonical** density operator. We can also write the density operator for the system, with the associated subspace \mathcal{S} , interacting very weakly with a large energy reservoir. Then the density operator of \mathcal{S} is then

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{\text{Tr}(e^{-\beta \hat{H}})} \quad (40)$$

where β is related to the temperature T of the reservoir ($= (\kappa_B T)^{-1}$) and where \hat{H} is the Hamiltonian of \mathcal{S} , it is known as **Canonical** density operator.

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