

Review of Quantum Mechanics

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6 Coherence and Decoherence at a Glance

Coherence refers to many meanings in different circumstances. We consider its usages in the context of physics. Roughly speaking, coherence means that two (or more than two) states (waves, particles) have a well defined correlation as time t or positions x change. For example, in the two-slit experiment, coherent light source is required to produce interference. Let the two waves through the two slits be $\psi_1(x_1, t_1)$ and $\psi_2(x_2, t_2)$. The fully coherence means that if we know the wave $\psi_1(x_1, t_1)$, we can know the $\psi_2(x_2, t_2)$ at any time and position. In this definition, it seems that every two sinusoidal waves $\exp(ik_1x - \omega_1t + \phi_1)$ and $\exp(ik_2x - \omega_2t + \phi_2)$ are coherent. However, we also require $k_1 = k_2$ and $\omega_1 = \omega_2$. The reason is as the following. When we measure the interference, frequently we collect the data for a long time over many periods. The interference signal is the an time average of the product $\psi_1^*(t)\psi_2(t)$. $|\psi_1(t)|^2$ and $|\psi_2(t)|^2$ are the background intensity. The time-averaged interference is

$$I_{\text{interference}} = \lim_{T \rightarrow \infty} \frac{\int_0^T 2\text{Re}[\psi_1^*(t)\psi_2(t)]}{T}. \quad (103)$$

If the two waves have different frequencies, the time-average vanishes.

Another question is that are any two waves fully coherent if they have the same frequencies. The answer is not necessary. Why? It is because the phase ψ_1 and ψ_2 can fluctuate. The coherence implies that $\delta = \phi_1 - \phi_2$ is a constant as time t and position x changes. In practical situations, as the waves propagate, the environment provides noises to the phases. As a result, the time-average becomes smaller. This process is called “**decoherence**” Typically, a system gradually loses its coherence as t increases or traveled length x increases.

A more realistic system consists of many waves (states, particles)¹,

$$\psi(x, t) = \psi_1(x, t) + \psi_2(x, t) + \psi_3(x, t) + \dots \quad (104)$$

The interference involves all the cross-product terms $\psi_1^*(t)\psi_2(t)$, $\psi_2^*(t)\psi_3(t)$, $\psi_3^*(t)\psi_4(t)$, and so on. To deal with a system containing a large number of particles, it is more convenient to use a statistical tool than listing all the states. The idea is to use probabilities to describe distributions of states. This is the motivation of the density operator (matrix) formulation.

¹We use the terms “particle”, “waves”, and “states” interchangeably.

7 Density Operator Formulation

Let's introduce the concepts of an ensemble.

Note 1: Ensemble

An ensemble is a statistical tool to describe a system of many particles. An ensemble consists of a large number of virtual copies of a particle. Ideally, the number of states is infinite. Each copy represents a possible state that a particle can be in. A specific ensemble is specified by assigning the probability in each state.

For example, a photon state $|\text{photon}\rangle$ is decomposed as

$$|\text{photon}\rangle = \alpha|L\rangle + \beta|R\rangle, \quad (105)$$

where $|L\rangle$ ($|R\rangle$) is the left(right)-polarized state. In an ensemble, there are many photons. Let p_L and p_R be the probabilities of the left-polarized state and the right-polarized state, respectively, where

$$p_L + p_R = 1. \quad (106)$$

The probabilities p_L and p_R define the ensemble. We can not use the following expression to describe an ensemble,

$$\cancel{|\text{ensemble}\rangle = p_L|L\rangle + p_R|R\rangle}, \quad (107)$$

since this expression is used for one single state. The mathematical tool to describe an ensemble is the density matrix $\hat{\rho}$,

$$\hat{\rho} = p_L|L\rangle\langle L| + p_R|R\rangle\langle R|. \quad (108)$$

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7.1 Density Operators

In a general case, the density matrix $\hat{\rho}$ can be defined as

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \quad (111)$$

$$\sum_i p_i = 1, \quad (112)$$

$$0 \leq p_i \leq 1, \quad (113)$$

where $|\psi_i\rangle$ are the basis states, and p_i is the probability to find the particle at the i th state. Most times, $|\psi_i\rangle$ are chosen to be orthonormal vectors. In the definition by Eq. (111), the density matrix is a diagonal matrix. However, a density matrix can have nonzero off-diagonal elements. Consider a new set of orthonormal bases $|a_i\rangle$, obtained by the unitary transformation

$$|a_i\rangle = \sum_j U_{ij} |\psi_j\rangle. \quad (114)$$

where $U^\dagger U = \mathbb{1}$. The matrix element U_{ij} can be obtained explicitly by multiplying $\langle\psi_j|$ on the both sides of Eq. (114),

$$U_{ij} = \langle\psi_j|a_i\rangle. \quad (115)$$

The inverse transforms are

$$|\psi_i\rangle = \sum_j U_{ij}^\dagger |a_j\rangle, \quad (116)$$

$$\langle\psi_i| = \sum_{j'} U_{j'i} \langle a_j|. \quad (117)$$

In the new basis,

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i| \quad (118)$$

$$= \sum_i p_i \left(\sum_j U_{ij}^\dagger |a_j\rangle \right) \left(\sum_{j'} U_{j'i} \langle a_j| \right) \quad (119)$$

$$= \sum_{j,j'} \left(\sum_i p_i U_{ij}^\dagger U_{j'i} \right) |a_j\rangle\langle a_j| \quad (120)$$

$$\equiv \sum_{j,j'} \rho_{jj'} |a_j\rangle\langle a_j|, \quad (121)$$

where the element $\rho_{jj'}$ is given by

$$\rho_{jj'} = \sum_i U_{j'i} p_i U_{ij}^\dagger \quad (122)$$

$$= (UPU^\dagger)^T, \quad (123)$$

where P is a diagonal matrix whose diagonal elements are p_i . In the new bases $|a_j\rangle$, the off-diagonal element $\rho_{jj'}$ can be nonzero. Indeed, the off-diagonal element $\rho_{jj'}$ is related to the correlation between the two states $|a_j\rangle$ and $|a_{j'}\rangle$.

Example 1: Two-Level System

Let's work out an example of a two-basis density matrix. Consider an ensemble of the density matrix

$$\rho = 0|L\rangle\langle L| + 1|R\rangle\langle R|, \quad (124)$$

or in the matrix form

$$\rho = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \quad (125)$$

Keep in mind that the matrix in Eq. (125) is written in the definitions

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv |L\rangle, \quad (126)$$

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv |R\rangle. \quad (127)$$

Now we consider new bases $|X\rangle$ and $|Y\rangle$ (linear polarized states)

$$|L\rangle = \frac{1}{\sqrt{2}} (|X\rangle - i|Y\rangle), \quad (128)$$

$$|R\rangle = \frac{1}{\sqrt{2}} (|X\rangle + i|Y\rangle). \quad (129)$$

The unitary transformation is

$$\begin{pmatrix} |L\rangle \\ |R\rangle \end{pmatrix} = U^\dagger \begin{pmatrix} |X\rangle \\ |Y\rangle \end{pmatrix}, \quad (130)$$

where

$$U^\dagger = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix}, \quad (131)$$

$$U = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{pmatrix}. \quad (132)$$

In the new bases, using Eq. (123) the density matrix is

$$\hat{\rho} = \left[\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \right]^T \quad (133)$$

$$= \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \quad (134)$$

Note that the matrix in Eq. (134) is written in the definitions

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv |X\rangle, \quad (135)$$

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv |Y\rangle. \quad (136)$$

The off-diagonal element $\rho_{YX} = \frac{i}{\sqrt{2}}$ reflects the fact that for a right-circular-polarized state $|R\rangle$, the phase difference between $|X\rangle$ and $|Y\rangle$ is $\pi/2$ (the phase factor $\exp \frac{i\pi}{2} = i$).

Exercise 1: Density Matrix

Consider an ensemble of the density matrix

$$\rho = \frac{1}{4}|L\rangle\langle L| + \frac{3}{4}|R\rangle\langle R|. \quad (137)$$

Calculate the density matrix in the bases $|X\rangle$ and $|Y\rangle$.

If we measure an observable A on the ensemble, the expectation value is called “ensemble average”,

$$\langle A \rangle = \sum_i p_i \langle \psi_i | A | \psi_i \rangle \quad (138)$$

$$= \sum_{i,j} p_i \langle \psi_i | \psi_j \rangle \langle \psi_j | A | \psi_i \rangle \quad (139)$$

$$= \sum_j \langle \psi_j | A \underbrace{\sum_i |\psi_i\rangle p_i \langle \psi_i|}_{\text{This term is } A\rho} | \psi_j \rangle \quad (140)$$

$$= \sum_j \langle \psi_j | A \rho | \psi_j \rangle \quad (141)$$

$$= \text{Tr}(A\rho). \quad (142)$$

Although we derive the ensemble average Eq. (142) in the $|\psi_i\rangle$ bases, the trace of a matrix is

independent of the bases. Thus, Eq. (142) is valid in any basis. This basis-free property is the big advantage of using a trace. One direct application is when $A = \mathbb{1}$,

$$\text{Tr}(\rho) = \sum_i p_i = 1, \quad (143)$$

which tells the trace of a density matrix is the total probability.

Exercise 2: Properties of Density Matrix

Some important properties of density matrix are listed below:

- (a) $\rho = \rho^\dagger$
- (b) $\text{Tr}(\rho) = 1$
- (c) $0 < \text{Tr}(\rho^2) \leq 1$

Prove that the above properties are true in any set of bases.

Note 2: Pure and Mixed Ensemble

We start with the bases $|\psi_i\rangle$, where ρ is diagonal. A pure ensemble is specified by $p_i = 1$ of the $|\psi_i\rangle$ and all other $p_j = 0$ for $j \neq i$. The equivalent condition of a pure ensemble is

$$\text{Tr}(\rho^2) = 1, \quad (144)$$

which applies to a density matrix in any basis. The condition of a mixed ensemble is

$$\text{Tr}(\rho^2) < 1. \quad (145)$$

One particle state is always a pure ensemble. One common mistake is to be confused by the superposition of one particle and the mixed ensemble.² Consider a one-particle state (qubit) composed of the superposition of $|0\rangle$ and $|1\rangle$.

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle. \quad (146)$$

One might think that this state has a density matrix $\rho = |\alpha|^2|0\rangle\langle 0| + |\beta|^2|1\rangle\langle 1|$. **But, this is wrong!** The correct density matrix is

$$\rho = |\psi\rangle\langle\psi| \quad (147)$$

$$= (\alpha|0\rangle + \beta|1\rangle)(\alpha^*\langle 0| + \beta^*\langle 1|) \quad (148)$$

$$= |\alpha|^2|0\rangle\langle 0| + |\beta|^2|1\rangle\langle 1| + \alpha\beta^*|0\rangle\langle 1| + \alpha^*\beta|1\rangle\langle 0| \quad (149)$$

$$= \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{pmatrix}, \quad (150)$$

where

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv |0\rangle, \quad (151)$$

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv |1\rangle. \quad (152)$$

It is possible to find the bases where ρ is diagonal, since ρ is a hermitian matrix. The off-diagonal elements in Eq. (150) describe the correlations between the states $|0\rangle$ and $|1\rangle$. An example of a mixed ensemble of qubits is

$$\rho = |\alpha|^2 |0\rangle\langle 0| + |\beta|^2 |1\rangle\langle 1| \quad (153)$$

$$= \begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix}, \quad (154)$$

where both $|\alpha|^2$ and $|\beta|^2$ are nonzero. In this mixed ensemble, the off-diagonal elements are zero. This means that there is no correlation between the states $|0\rangle$ and $|1\rangle$.

If the number of bases is N , the most random mixed ensemble is

$$\rho_{\text{MR}} = \frac{1}{N} \sum_{i=1}^N |\psi_i\rangle\langle\psi_i| \quad (155)$$

$$= \frac{1}{N} \mathbb{1}_{N \times N}, \quad (156)$$

where $\mathbb{1}_{N \times N}$ is the N -by- N identity. The off-diagonal elements of the ensemble ρ_{MR} are always zero, i.e., there is not any correlation between the basis states.

Exercise 3: Pure Ensemble

Which density matrices are pure ensembles?

(a)

$$\rho = \begin{pmatrix} 0.5 & 0 \\ 0 & 0.5 \end{pmatrix}$$

(b)

$$\rho = \begin{pmatrix} \cos^2 \theta & \cos \theta \sin \theta \\ \cos \theta \sin \theta & \sin^2 \theta \end{pmatrix}$$

(c)

$$\rho = \begin{pmatrix} \cos^2 \theta & \cos \theta \sin \theta e^{i\phi} \\ \cos \theta \sin \theta e^{-i\phi} & \sin^2 \theta \end{pmatrix}$$

²In many places, mixed states are called instead of mixed ensemble, although the latter is properer.

(d)

$$\rho = \begin{pmatrix} \cos^2 \theta & \frac{1}{2} \cos \theta \sin \theta \\ \frac{1}{2} \cos \theta \sin \theta & \sin^2 \theta \end{pmatrix}$$

7.2 Dynamics of Density Operators

First, the density operator is not an observable, so we can not use the Heisenberg's picture to obtain its dynamics. Let's begin with a density matrix in the diagonal form,

$$\rho(t) = \sum_i p_i |\psi_i(t)\rangle \langle \psi_i(t)|, \quad (157)$$

where the dynamics of the states can be obtained with Schrödinger Picture

$$i\hbar \frac{\partial}{\partial t} |\psi_i(t)\rangle = \mathcal{H} |\psi_i(t)\rangle, \quad (158)$$

$$-i\hbar \frac{\partial}{\partial t} \langle \psi_i(t)| = \langle \psi_i(t)| \mathcal{H}. \quad (159)$$

Using Eqs. (157), (158) and (159), we obtain

$$\frac{\partial \rho(t)}{\partial t} = \frac{i}{\hbar} [\rho(t), \mathcal{H}]. \quad (160)$$

This equation is known as the von Neumann equation or quantum Liouville equation. Equation (160) describes a closed system where $\text{Tr}(\rho^2)$ is a constant in time. This means that the coherence of the system is not changed. How could a system have dissipation and decoherence? When a system is open to the environment, the interaction between the system and the environment leads to dissipation and decoherence. The idea is to write $\mathcal{H} = \mathcal{H}_{\text{sys}} + \mathcal{H}_{\text{env}}$ and to derive an equation only about the reduced density matrix

$$\frac{\partial \rho(t)_{\text{sys}}}{\partial t} = \frac{i}{\hbar} [\rho(t)_{\text{sys}}, \mathcal{H}_{\text{sys}}] + \text{environment terms}, \quad (161)$$

where the reduced density matrix is obtained by the partial trace

$$\rho(t)_{\text{sys}} = \text{Tr}_{\text{env}}(\rho(t)). \quad (162)$$

There is not a unique answer how to write the environment terms since that depends on what kind of environment it is and the interaction. The discussions of the environment terms belong to the subject "Open Quantum Systems", which is not the main interest here. We will adopt the phenomenological methods later.

Exercise 4: Quantum Liouville Equation

Derive the von Neumann equation, Eq. (160). The first step is to differentiate Eq. (157).

Example 2: Dynamics of a Two Level System

Let the unperturbed Hamiltonian be

$$\mathcal{H} = \begin{pmatrix} E_c & 0 \\ 0 & E_v \end{pmatrix}, \quad (163)$$

and write the density matrix in this basis

$$\rho = \begin{pmatrix} \rho_{cc} & \rho_{cv} \\ \rho_{vc} & \rho_{vv} \end{pmatrix}. \quad (164)$$

Using the von Neumann equation, Eq. (160), we can obtain four first-order differential equations. Two of them are redundant because $\rho_{cc} + \rho_{vv} = 1$ and $\rho_{cv} = \rho_{vc}^*$. We need only two equations

$$\frac{\partial}{\partial t} \rho_{cc} = 0, \quad (165)$$

$$\frac{\partial}{\partial t} \rho_{cv} = \frac{i}{\hbar} \rho_{cv} (E_v - E_c), \quad (166)$$

with the solutions

$$\rho_{cc}(t) = \rho_{cc}(0), \quad (167)$$

$$\rho_{vv}(t) = \rho_{vv}(0), \quad (168)$$

$$\rho_{cv}(t) = \rho_{cv}(0) e^{-i\omega_{cv}t}, \quad (169)$$

$$(170)$$

with $\omega_{cv} = \frac{E_c - E_v}{\hbar}$. The populations ρ_{cc} and ρ_{vv} are unchanged in a unperturbed system. The off-diagonal element ρ_{cv} has a constant amplitude and a linearly-growing phase in time. This means that the coherence of the system is unchanged. In a realistic situation, the system will be dephased. A phenomenological way to add the dephasing is to add $-\gamma\rho_{cv}$ in Eq. (166),

$$\frac{\partial}{\partial t} \rho_{cv} = \frac{i}{\hbar} \rho_{cv} (E_v - E_c) - \gamma \rho_{cv}, \quad (171)$$

with the solution

$$\rho_{cv}(t) = \rho_{cv}(0) e^{-i\omega_{cv}t - \gamma t}, \quad (172)$$

$$(173)$$

and γ is called the dephasing rate.

Exercise 5: Quantum Liouville Equation

Derive Eqs. (165) and (166).