DENSITY OPERATOR AND APPLICATIONS IN NONLINEAR AND QUANTUM OPTICS

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Contents

I. GENERAL THEORY OF THE DENSITY OPERATOR

1. Concept of a statistial mixture of states

Consider a quantum system. If we have complete information about the system, the state of the system can be described by a state vector (wave function), denoted by $|\psi\rangle$. Such a state is called a pure state.

It often happens that we don't know the exact state vector of the system. In this case, we say that we have incomplete information about the system. For example, a photon emitted by a source of natural light can have any polarization state with equal probability. Similarly, a system in thermal equilibrium at a temperature T has a probability proportional to $e^{-E_n/kT}$ of being in a state of energy E_n.

More generally, the incomplete information usually presents itself in the following way: the state of this system may be either the state $|\psi_1\rangle$ with a probability p_1 or the state $|\psi_2\rangle$ with a probability p_2, etc... Obviously, we have

$$p_1 + p_2 + ... = \sum_n p_n = 1. \tag{1}$$

We then say that we have a statistical mixture of states $|\psi_1\rangle$, $|\psi_2\rangle$, ... with probabilities p_1, p_2, ... A statistical mixture of two or more than two different states is called a mixed state. In general, a quantum state can be either a pure state or a mixed state.

We emphasize that a system described by a statistical mixture of states must not be confused with a system whose state $|\psi\rangle$ is a linear superposition of states:

$$|\psi\rangle = \sum_n C_n |\psi_n\rangle. \tag{2}$$

For a linear superposition of states, there exist, in general, interference effects between these component states. Such effects are due to the cross terms of the type $C_n C_{n'}^*$, obtained when the modulus of the wave function is squared. Meanwhile, for a statistical mixture of states $|\psi_n\rangle$, we can never obtain interference terms between these component states.

We illustrate the above statements by considering a single particle in the coordinate space R of the position vector $\mathbf{r}$.

If the particle is in a linear superposition state $\psi(\mathbf{r}) = \sum_n C_n \psi_n(\mathbf{r})$, the probability of finding the particle at a given point $\mathbf{r}$ is

$$P(\mathbf{r}) = |\psi(\mathbf{r})|^2 = |\sum_n C_n \psi_n(\mathbf{r})|^2 = \sum_{nn'} C_n C_{n'}^* \psi_n(\mathbf{r}) \psi_{n'}^*(\mathbf{r}). \tag{3}$$

The above expression involves cross terms of the type $C_n C_{n'}^*$, which describe interference between the component states $\psi_n(\mathbf{r})$.

However, if the particle is in a statistical mixture of states $|\psi_n\rangle$ with weight factors p_k, the probability of finding the particle at a given point $\mathbf{r}$ is

$$P(\mathbf{r}) = \sum_n p_n |\psi_n(\mathbf{r})|^2. \tag{4}$$

The above expression shows no interference between the component states $\psi_n(\mathbf{r})$.

2. Pure states. Introduction of the density operator

We first examine the simple case where the state vector of the system is perfectly known, that is, all the probabilities p_n are zero, except one. The system is then said to be in a pure state.

a) Description by a state vector (wave function)

i. State space

A pure quantum state of any physical system is characterized by a state vector, belonging to a linear space S which is called the state space of the system.

ii. Ket vectors

An element, or vector, of the state space S is called a ket vector. It is represented by the symbol $|\phi\rangle$.

iii. Scalar product

With each pair of ket vectors $|\phi\rangle$ and $|\phi'\rangle$, taken in this order, we associate a complex number, which is denoted by $(|\phi\rangle, |\phi'\rangle)$ and satisfies the various properties

$$(|\phi\rangle, |\phi'\rangle) = (|\phi'\rangle, |\phi\rangle)^*,$$
$$(|\phi\rangle, \lambda_1 |\phi_1\rangle + \lambda_2 |\phi_2\rangle) = \lambda_1 (|\phi\rangle, |\phi_1\rangle) + \lambda_2 (|\phi\rangle, |\phi_2\rangle), \tag{5}$$
$$(\lambda_1 |\phi_1\rangle + \lambda_2 |\phi_2\rangle, |\phi\rangle) = \lambda_1^* (|\phi_1\rangle, |\phi\rangle) + \lambda_2^* (|\phi_2\rangle, |\phi\rangle).$$

This complex number is called the scalar or inner product. The linear space with this type of scalar products is called a Hilbert space.

iv. Bra vectors and dual space

Each ket vector $|\phi\rangle$ is associated with a bra vector, denoted by the symbol $\langle\phi|$, which associates every ket vector $|\phi'\rangle$ with a complex number which is denoted by $\langle\phi|\phi'\rangle$ and is equal to $(|\phi\rangle, |\phi'\rangle)$. The set of bra vectors constitutes a vector space called the dual space of the state space S.

v.   Basic properties of the ket and bra vectors

(1) $\langle \phi | \phi' \rangle = \langle \phi' | \phi \rangle^*.$

(2)   If $|\phi\rangle = \lambda_1 |\phi_1\rangle + \lambda_2 |\phi_2\rangle$ then $\langle \phi | = \lambda_1^* \langle \phi_1 | + \lambda_2^* \langle \phi_2 |.$

(6)

More generally, for the superposition state vector $|\psi\rangle = \sum_n C_n |u_n\rangle$, we have

$$\langle \psi | = \sum_n \langle u_n | C_n^*. \tag{7}$$

In the case of a single particle in the coordinate space R of the position vector $\mathbf{r}$, the ket vector $|\phi\rangle$ and the bra vector $\langle \phi |$ are represented by the complex functions $\phi(\mathbf{r})$ and $\phi^*(\mathbf{r})$, respectively, and the scalar product $\langle \phi | \phi' \rangle$ is defined as $\langle \phi | \phi' \rangle = \int \phi^*(\mathbf{r}) \phi'(\mathbf{r}) d\mathbf{r}$. It is clear that $\langle \phi | \phi' \rangle^* = \langle \phi' | \phi \rangle$.

vi.   Orthonormal basis

The state of a pure-state system can be described by a state vector $|\psi\rangle$. The set of state vectors $|u_n\rangle$ is a basis set if an arbitrary state vector $|\psi\rangle$ can be decomposed as

$$|\psi\rangle = \sum_n C_n |u_n\rangle. \tag{8}$$

The set of basis states $|u_n\rangle$ is an orthonormal basis set if

$$\langle u_n | u_m \rangle = \delta_{nm}. \tag{9}$$

The coefficients C_n in Eq. (8) are called the probability amplitudes of the superposition state $|\psi\rangle$ in the basis $\{|u_n\rangle\}$. More exactly, we say that C_n is the probability amplitude of the basis state $|u_n\rangle$ in the superposition state $|\psi\rangle$.

It follows from the expansion (8) and the orthonormality (9) of the basis states $|u_n\rangle$ that the coefficients C_n of the state vector $|\psi\rangle$ can be determined as

$$C_n = \langle u_n | \psi \rangle. \tag{10}$$

We say that the state vector $|\psi\rangle$ is normalized if $\langle \psi | \psi \rangle = 1$. If the state vector $|\psi\rangle$ is normalized, its coefficients satisfy the normalization condition

$$\sum_n |C_n|^2 = 1. \tag{11}$$

From now we consider only normalized state vectors.

Note that the bra vector $\langle \psi |$ associated with the ket vector $|\psi\rangle$ can be decomposed in the form

$$\langle \psi | = \sum_n \langle u_n | C_n^*. \tag{12}$$

With the use of the orthonormality of the basis states $|u_n\rangle$, we find

$$C_n^* = \langle \psi | u_n \rangle = \langle u_n | \psi \rangle^*. \tag{13}$$

vii. Projection operators

We introduce the operator

$$P_{|u_n\rangle} \equiv |u_n\rangle\langle u_n |, \tag{14}$$

whose action on an arbitrary vector $|V\rangle$ is defined as

$$\begin{aligned}
P_{|u_n\rangle} |V\rangle &= (|u_n\rangle\langle u_n |) |V\rangle \\
&= |u_n\rangle(\langle u_n |V\rangle) = |u_n\rangle\langle u_n |V\rangle.
\end{aligned} \tag{15}$$

As seen, the action of $P_{|u_n\rangle}$ on $|V\rangle$ gives a vector parallel to $|u_n\rangle$. In addition, we have

$$\begin{aligned}
P_{|u_n\rangle}^2 &= P_{|u_n\rangle} P_{|u_n\rangle} \\
&= (|u_n\rangle\langle u_n |)(|u_n\rangle\langle u_n |) \\
&= |u_n\rangle(\langle u_n |u_n\rangle)\langle u_n | \\
&= |u_n\rangle\langle u_n | \\
&= P_{|u_n\rangle}.
\end{aligned} \tag{16}$$

The operator $P_{|u_n\rangle} \equiv |u_n\rangle\langle u_n |$ is called the projection operator onto the basis vector $|u_n\rangle$.

viii. Completeness of the basis

The completeness of the set of the basis states $|u_n\rangle$ means that

$$\sum_n P_{|u_n\rangle} = P_{|u_1\rangle} + P_{|u_2\rangle} + ... = 1, \tag{17}$$

that is,

$$\sum_n |u_n\rangle\langle u_n | = |u_1\rangle\langle u_1 | + |u_2\rangle\langle u_2 | + ... = 1. \tag{18}$$

From now we use only the orthonormal basis. The properties of this basis are summarized below:

$$\begin{aligned}
\langle u_n | u_m \rangle &= \delta_{nm}, \\
\sum_n |u_n\rangle\langle u_n | &= 1.
\end{aligned} \tag{19}$$

ix. Linear operators

A linear operator O associates each ket vector $|\phi\rangle$ with a ket vector $|\phi'\rangle = O|\phi\rangle$ and satisfies the linearity

$$O(\lambda_1 | \phi_1 \rangle + \lambda_2 | \phi_2 \rangle) = \lambda_1 O | \phi_1 \rangle + \lambda_2 O | \phi_2 \rangle. \tag{20}$$

Similarly, the linear operator O associates each bra vector $\langle \phi |$ with a bra vector $\langle \phi' | = \langle \phi | O$ and satisfies the linearity

$$(\lambda_1 \langle \phi_1 | + \lambda_2 \langle \phi_2 |)O = \lambda_1 \langle \phi_1 | O + \lambda_2 \langle \phi_2 | O. \tag{21}$$

For the superposition state vector $| \psi \rangle = \sum_n C_n | u_n \rangle$, we have

$$O | \psi \rangle = O \left(\sum_n C_n | u_n \rangle \right) = \sum_n C_n \left(O | u_n \rangle \right) = \sum_n C_n O | u_n \rangle,$$

$$\langle \psi | O = \left(\sum_n C_n^* \langle u_n | \right) O = \sum_n C_n^* \left(\langle u_n | O \right) = \sum_n C_n^* \langle u_n | O. \tag{22}$$

We consider the operator

$$O = | A \rangle \langle B |, \tag{23}$$

whose action on ket and bra vectors is defined as

$$O | \phi \rangle = \left(| A \rangle \langle B | \right) | \phi \rangle = | A \rangle \left(\langle B | \phi \rangle \right) = | A \rangle \langle B | \phi \rangle,$$

$$\langle \phi | O = \langle \phi | \left(| A \rangle \langle B | \right) = \left(\langle \phi | A \rangle \right) \langle B | = \langle \phi | A \rangle \langle B |. \tag{24}$$

We can show that

$$\langle \phi | \left(O | \phi' \rangle \right) = \left(\langle \phi | O \right) | \phi' \rangle = \langle \phi | A \rangle \langle B | \phi' \rangle \equiv \langle \phi | O | \phi' \rangle. \tag{25}$$

x.   Matrix form of a linear operator

With the help of the completeness relation (18), we can represent an arbitrary operator O in the form

$$O = \left(\sum_n | u_n \rangle \langle u_n | \right) O \left(\sum_m | u_m \rangle \langle u_m | \right)$$

$$= \sum_{nm} | u_n \rangle \langle u_n | (O | u_m \rangle) \langle u_m | = \sum_{nm} | u_n \rangle (\langle u_n | O) | u_m \rangle \langle u_m | \tag{26}$$

$$= \sum_{nm} \langle u_n | (O | u_m \rangle) | u_n \rangle \langle u_m | = \sum_{nm} (\langle u_n | O) | u_m \rangle | u_n \rangle \langle u_m |.$$

Hence, we find

$$\langle u_n | (O | u_m \rangle) = (\langle u_n | O) | u_m \rangle \equiv \langle u_n | O | u_m \rangle \equiv O_{nm}. \tag{27}$$

The matrix $O_{nm} = \langle u_n | O | u_m \rangle$ is called the matrix form of the linear operator O. Every operator O can be represented by a matrix O_{nm}.

Every matrix O_{nm} represents an operator O. Indeed, it follows from Eqs. (26) and (27) that

$$O = \sum_{nm} O_{nm} |u_n\rangle\langle u_m|. \tag{28}$$

We can generalize Eq. (27) to obtain

$$\langle \phi_1 | (O | \phi_2\rangle) = (\langle \phi_1 | O) | \phi_2\rangle \equiv \langle \phi_1 | O | \phi_2\rangle. \tag{29}$$

xi.   Hermitian conjugate

Every operator O is associated with an operator $O^\dagger$, whose matrix is

$$(O^\dagger)_{nm} = (O_{mn})^* = (O^T)^*_{nm} \Leftrightarrow \langle u_n | O^\dagger | u_m\rangle = \langle u_m | O | u_n\rangle^*. \tag{30}$$

Here the upper label T means the matrix transpose and the symbol * means the complex conjugate. The operator $O^\dagger$ is called the Hermitian conjugate of the operator O.

For $O = \sum_{nm} O_{nm} |u_n\rangle\langle u_m|$, we have

$$\begin{aligned}
O^\dagger &= \sum_{nm} O^\dagger_{nm} |u_n\rangle\langle u_m| \\
&= \sum_{nm} O^*_{mn} |u_n\rangle\langle u_m| \\
&= \sum_{nm} O^*_{nm} |u_m\rangle\langle u_n|.
\end{aligned} \tag{31}$$

Note that $\left(O^\dagger\right)^\dagger = O$.

We can show that

$$\langle \phi | O = \langle O^\dagger \phi |, \tag{32}$$

where $\langle O^\dagger \phi |$ is the bra vector associated with the ket vector $|O^\dagger \phi\rangle = O^\dagger | \phi\rangle$. Indeed, since $O = \sum_{nm} O_{nm} |u_n\rangle\langle u_m|$, we have

$$\langle \phi | O = \langle \phi | \sum_{nm} O_{nm} |u_n\rangle\langle u_m| = \sum_{nm} O_{nm} \langle \phi | u_n\rangle\langle u_m|. \tag{33}$$

On the other hand, since $O^\dagger = \sum_{nm} O^*_{nm} |u_m\rangle\langle u_n|$, we find

$$\begin{aligned}
|O^\dagger \phi\rangle = O^\dagger | \phi\rangle &= \left(\sum_{nm} O^*_{nm} |u_m\rangle\langle u_n| \right) | \phi\rangle \\
&= \sum_{nm} O^*_{nm} |u_m\rangle\langle u_n | \phi\rangle \\
&= \sum_{nm} O^*_{nm} \langle u_n | \phi\rangle | u_m\rangle,
\end{aligned} \tag{34}$$

which yields

$$\langle O^\dagger \phi | = \sum_{nm} O_{nm} \langle \phi | u_n\rangle\langle u_m|. \tag{35}$$

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Comparison of Eq. (35) with Eq. (33) gives Eq. (32). Thus, $\langle \phi | O$ is a bra vector that is associated with the ket vector $O^\dagger | \phi \rangle$. In the same way, we can say that the ket vector $O | \phi \rangle$ is associated with the bra vector $\langle \phi | O^\dagger$.

Several useful properties of the Hermitian conjugates:

Property 1:

$$\text{If } \langle \phi | = \langle \psi | O$$
$$\text{then } | \phi \rangle = O^\dagger | \psi \rangle. \tag{36}$$

Property 2:

$$\text{If } | \phi \rangle = O | \psi \rangle$$
$$\text{then } \langle \phi | = \langle \psi | O^\dagger. \tag{37}$$

Property 3:

$$\langle \phi | O | \phi' \rangle^* = \langle \phi' | O^\dagger | \phi \rangle. \tag{38}$$

Property 4:

$$\text{If } O = \alpha O_1 O_2 \cdots O_n$$
$$\text{then } O^\dagger = \alpha^* O_n^\dagger O_{n-1}^\dagger \cdots O_1^\dagger, \tag{39}$$

where α is a complex number and O_1, O_2, …, O_n are arbitrary operators.

Property 5:

$$\text{If } O = f(\alpha A)$$
$$\text{then } O^\dagger = f(\alpha^* A^\dagger), \tag{40}$$

where *f* is a real function, *A* is an arbitrary operator, and α is a complex number.

xii.   Hermitian operators

An operator O is called Hermitian if it is equal to its Hermitian conjugate $O^\dagger$, that is,

$$O^\dagger = O \qquad \text{or} \qquad O_{mn}^* = O_{nm}. \tag{41}$$

xiii.   Mean values of observables

Every observable is described by a Hermitian operator. Consider an observable described by a Hermitian operator A. The matrix elements of the operator A in the basis $\{|u_n\rangle\}$ are given by

$$A_{nm} = \langle u_n | A | u_m \rangle = \langle u_n | (A | u_m \rangle) = (\langle u_n | A) | u_m \rangle. \tag{42}$$

Since A is a Hermitian operator, we have

$$A_{nm} = A_{mn}^*. \tag{43}$$

The mean value of A is

$$\langle A \rangle = \langle \psi \,|\, A \,|\, \psi \rangle$$
$$= \left(\sum_n C_n^* \langle u_n \,| \right) A \left(\sum_m C_m \,| u_m \rangle \right)$$
$$= \sum_{nm} C_n^* C_m \langle u_n \,|\, A \,|\, u_m \rangle \tag{44}$$
$$= \sum_{nm} C_n^* C_m A_{nm}.$$

xiv.   Schrödinger equation and Schrödinger picture of quantum mechanics

The time evolution of the state vector $|\psi(t)\rangle$ of the quantum system is described by the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H \,|\psi(t)\rangle, \tag{45}$$

where H is the Hamiltonian operator of the system. The Hamiltonian is the energy, an observable. Therefore, it must be a Hermitian operator, that is, $H^\dagger = H$.

The solution to the Schrödinger equation (45) is given by

$$|\psi(t)\rangle = \exp(-iHt / \hbar) \,|\psi(0)\rangle. \tag{46}$$

The corresponding bra vector is

$$\langle \psi(t) \,| = \langle \psi(0) \,|\, \exp(iHt / \hbar). \tag{47}$$

The time-dependent mean value of the observable A is

$$\langle A(t) \rangle = \langle \psi(t) \,|\, A \,|\, \psi(t) \rangle. \tag{48}$$

Consider the initial state vector $|\psi(0)\rangle = \sum_n C_n(0) \,|u_n\rangle$. The probability amplitude $C_n(0)$ is given by $C_n(0) = \langle u_n \,|\, \psi(0) \rangle$. For an arbitrary time t, we have

$$|\psi(t)\rangle = \sum_n C_n(t) \,|u_n\rangle, \tag{49}$$

where

$$C_n(t) = \langle u_n \,|\, \psi(t) \rangle. \tag{50}$$

Inserting Eq. (49) into Eq. (45) gives

$$i\hbar \sum_n \frac{d}{dt} C_n(t) \,|u_n\rangle = \sum_m C_m(t) H \,|u_m\rangle$$
$$= \sum_{mn} C_m(t) \,|u_n\rangle \langle u_n \,|\, H \,|\, u_m \rangle \tag{51}$$
$$= \sum_{mn} C_m(t) \langle u_n \,|\, H \,|\, u_m \rangle \,|u_n\rangle.$$

Hence, we obtain

$$i\hbar \frac{d}{dt}C_n(t) = \sum_m H_{nm}C_m(t). \tag{52}$$

Here $H_{nm} = \langle u_n | H | u_m \rangle$ is the matrix of the Hamiltonian.

In terms of the probability amplitudes $C_n(t)$, the mean value of the observable A at the time t is given by

$$\langle A(t) \rangle = \langle \psi(t) | A | \psi(t) \rangle = \sum_{nm} C_n^*(t)C_m(t)A_{nm}. \tag{53}$$
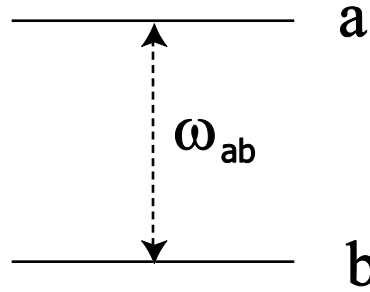
xv. Example of a two-level system

Figure 1: A two-level system.

The simplest quantum system is a two-level system, see Fig. 1. Such a system has two stationary energy levels, denoted by $E_a = \hbar\omega_a$ (upper level) and $E_b = \hbar\omega_b$ (lower level). The wave functions of these two levels are denoted by the state vectors $|a\rangle$ (upper state) and $|b\rangle$ (lower state). These state vectors are normalized in modulus to unity and are orthogonal to each other:

$$\begin{aligned} \langle a | a \rangle &= \langle b | b \rangle = 1, \\ \langle a | b \rangle &= \langle b | a \rangle = 0. \end{aligned} \tag{54}$$

The completeness of the basis requires

$$|a\rangle\langle a| + |b\rangle\langle b| = 1. \tag{55}$$

In general, any state vector (wave function) of the two-level system can be written in the form

$$|\psi\rangle = C_a |a\rangle + C_b |b\rangle. \tag{56}$$

Here C_a and C_b are the probability amplitudes of finding the system in states $|a\rangle$ and $|b\rangle$, respectively. They satisfy the normalization condition

$$|C_a|^2 + |C_b|^2 = 1. \tag{57}$$

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The bra vector $\langle \psi |$ associated with the ket vector $| \psi \rangle$ can be written in the form

$$\langle \psi | = \langle a | C_a^* + \langle b | C_b^*. \tag{58}$$

The mean value of an observable A is

$$
\begin{aligned}
\langle A \rangle &= \langle \psi | A | \psi \rangle \\
&= \left(\langle a | C_a^* + \langle b | C_b^* \right) A \left(C_a | a \rangle + C_b | b \rangle \right) \\
&= | C_a |^2 \langle a | A | a \rangle + | C_b |^2 \langle b | A | b \rangle + C_a^* C_b \langle a | A | b \rangle + C_b^* C_a \langle b | A | a \rangle \\
&= | C_a |^2 A_{aa} + | C_b |^2 A_{bb} + C_a^* C_b A_{ab} + C_b^* C_a A_{ba}.
\end{aligned}
\tag{59}
$$

The total Hamiltonian is

$$H = H_0 + H_I, \tag{60}$$

where H_0 and H_I are the free (unperturbed) and interaction parts, respectively. The upper state $| a \rangle$ and the lower state $| b \rangle$ are the eigenstates of the free Hamiltonian H_0, that is, $H_0 | j \rangle = E_j | j \rangle$, where $j = a, b$. We can represent H_0 in the form

$$H_0 = \hbar \omega_a | a \rangle \langle a | + \hbar \omega_b | b \rangle \langle b |. \tag{61}$$

Why does H_0 have the above form? The reason is the following: since $\sum_j | j \rangle \langle j | = | a \rangle \langle a | + | b \rangle \langle b | = 1$ and $H_0 | j \rangle = E_j | j \rangle$, we can expand H_0 as

$$
\begin{aligned}
H_0 &= \sum_{i,j} (| i \rangle \langle i |) H_0 (| j \rangle \langle j |) \\
&= \sum_{i,j} | i \rangle \langle j | (\langle i | H_0 | j \rangle) \\
&= \sum_{i,j} | i \rangle \langle j | (\langle i | j \rangle E_j) = \sum_{i,j} E_j \delta_{i,j} | i \rangle \langle j | \\
&= \sum_i E_i | i \rangle \langle i | = \sum_i \hbar \omega_i | i \rangle \langle i |.
\end{aligned}
\tag{62}
$$

We consider a particular case where the two-level system is free, i.e., $H_I = 0$. In this case, the Schrödinger equation is

$$
\begin{aligned}
i\hbar \frac{d}{dt} | \psi \rangle &= H_0 | \psi \rangle \\
&= (\hbar \omega_a | a \rangle \langle a | + \hbar \omega_b | b \rangle \langle b |) | \psi \rangle.
\end{aligned}
\tag{63}
$$

It gives

$$
\begin{aligned}
&i \frac{d}{dt} \left(C_a | a \rangle + C_b | b \rangle \right) = (\omega_a | a \rangle \langle a | + \omega_b | b \rangle \langle b |) \left(C_a | a \rangle + C_b | b \rangle \right) \\
&\Rightarrow \\
&i \dot{C}_a | a \rangle + i \dot{C}_b | b \rangle = \omega_a C_a | a \rangle + \omega_b C_b | b \rangle.
\end{aligned}
\tag{64}
$$

Hence, we find

$$\frac{d}{dt}C_a = -i\omega_a C_a,$$

$$\frac{d}{dt}C_b = -i\omega_b C_b. \tag{65}$$

The solutions to the above equations are

$$C_a(t) = e^{-i\omega_a t}C_a(0),$$

$$C_b(t) = e^{-i\omega_b t}C_b(0). \tag{66}$$

Consequently, the explicit time-dependent expression for the state vector (wave function) of the free two-level system is

$$|\psi(t)\rangle = C_a(t)|a\rangle + C_b(t)|b\rangle = e^{-i\omega_a t}C_a(0)|a\rangle + e^{-i\omega_b t}C_b(0)|b\rangle. \tag{67}$$

Note that the probabilities of finding the free two-level system in the upper and lower levels are $|C_a(t)|^2 = |C_a(0)|^2$ and $|C_b(t)|^2 = |C_b(0)|^2$, respectively. They are independent of time. In the contrary, the interference described by the cross term $C_a(t)C_b^*(t) = C_a(0)C_b^*(0)e^{-i(\omega_a-\omega_b)t}$ oscillates in time.

The mean value of an observable A at an arbitrary time t is

$$\begin{aligned}\langle A(t)\rangle &= \langle\psi(t)|A|\psi(t)\rangle = \sum_{nm}C_n^*(t)C_m(t)A_{nm}\\ &= \sum_{nm}C_n^*(0)C_m(0)e^{i(\omega_n-\omega_m)t}A_{nm}\\ &= |C_a(0)|^2 A_{aa} + |C_b(0)|^2 A_{bb}\\ &\quad + C_a^*(0)C_b(0)e^{i\omega_{ab}t}A_{ab} + C_b^*(0)C_a(0)e^{-i\omega_{ab}t}A_{ba}.\end{aligned} \tag{68}$$

Here $\omega_{ab} = \omega_a - \omega_b$ is the transition frequency.

If the initial state is $|\psi(0)\rangle = |a\rangle$, then $C_a(0) = 1$ and $C_b(0) = 0$. In this case, the state vector at an arbitrary time is $|\psi(t)\rangle = e^{-i\omega_a t}|a\rangle$ and the mean value of an observable A at an arbitrary time is $\langle A(t)\rangle = A_{aa} = \langle a|A|a\rangle$. The mean value is independent of time because the initial state $|a\rangle$ is an eigenstate of the system.

If the initial state is $|\psi(0)\rangle = |b\rangle$, then $C_b(0) = 1$ and $C_a(0) = 0$. In this case, the state vector at an arbitrary time is $|\psi(t)\rangle = e^{-i\omega_b t}|b\rangle$ and the mean value of an observable A at an arbitrary time is $\langle A(t)\rangle = A_{bb} = \langle b|A|b\rangle$. The mean value is independent of time because the initial state $|b\rangle$ is an eigenstate of the system.

If the initial state is a superposition state of $|a\rangle$ and $|b\rangle$, with $C_a(0) \neq 0$ and $C_b(0) \neq 0$, then $\langle A(t)\rangle$ in general varies in t.

Exercises

Exercise 1: Consider a two-level system. Suppose that σ is an operator such that $\sigma|a\rangle = |b\rangle$ and $\sigma|b\rangle = 0$. Show that σ can be written in the form $\sigma = |b\rangle\langle a|$.

Exercise 2: By definition $(O^\dagger)_{kl} = O^*_{lk}$, where O is an arbitrary operator and $O^\dagger$ is its Hermitian conjugate. Suppose $O = |u_n\rangle\langle u_m|$. Show that $O^\dagger = |u_m\rangle\langle u_n|$.

Exercise 3: Suppose $O = |A\rangle\langle B|$, where $|A\rangle$ and $|B\rangle$ are two arbitrary vectors. The action of $O = |A\rangle\langle B|$ on an arbitrary vector Q is defined as $O|Q\rangle = (|A\rangle\langle B|)|Q\rangle = |A\rangle(\langle B|Q\rangle) = |A\rangle\langle B|Q\rangle$. Show that $O^\dagger = |B\rangle\langle A|$.

Exercise 4: By definition $O^\dagger = O^{T*}$. Suppose $O = O_1 O_2$. Show that $O^\dagger = O_2^\dagger O_1^\dagger$.

Solutions

Exercise 1:

Since $\sigma|a\rangle = |b\rangle$ and $\sigma|b\rangle = 0$, we have

$$\sigma|a\rangle\langle a| = |b\rangle\langle a|$$

and

$$\sigma|b\rangle\langle b| = 0.$$

When we sum up the last two equations, we obtain

$$\sigma(|a\rangle\langle a| + |b\rangle\langle b|) = |b\rangle\langle a|.$$

On the other hand, the completeness of the basis means that

$$|a\rangle\langle a| + |b\rangle\langle b| = 1.$$

Hence, we find

$$\sigma = |b\rangle\langle a|.$$

Using the orthonormality of $|a\rangle$ and $|b\rangle$, namely $\langle a|a\rangle = 1$ and $\langle a|b\rangle = 0$, we can confirm that the operator $\sigma = |b\rangle\langle a|$ satisfies the relations $\sigma|a\rangle = |b\rangle$ and $\sigma|b\rangle = 0$.

Exercise 2:

For $O = |u_n\rangle\langle u_m|$, we find

$$O_{kl} = \delta_{kn}\delta_{lm}.$$

For $X \equiv |u_m\rangle\langle u_n|$, we have

$$X_{kl} = \delta_{km}\delta_{ln}.$$

We see that

$$X_{kl} = O_{lk}^* \equiv O^{\dagger}{}_{kl}.$$

Hence, we obtain $O^{\dagger} = X$, that is,

$$O^{\dagger} = |u_m\rangle\langle u_n|.$$

Exercise 3:

For $O = |A\rangle\langle B|$, we have

$$O_{kl} = a_k b_l^*,$$

where $a_k = \langle u_k | A \rangle$ and $b_l = \langle u_l | B \rangle$.

For $X = | B \rangle \langle A |$, we have

$$X_{kl} = b_k a_l^*.$$

We see that

$$X_{kl} = O_{lk}^* \equiv O^\dagger{}_{kl}.$$

Hence, we obtain $O^\dagger = X$, that is,

$$O^\dagger = | B \rangle \langle A |.$$

Exercise 4:

For $O = O_1 O_2$, we have

$$O^\dagger = (O_1 O_2)^\dagger = (O_1 O_2)^{T*} = (O_2^T O_1^T)^* = O_2^{T*} O_1^{T*} = O_2^\dagger O_1^\dagger.$$

Generalization:

For $O = \alpha O_1 O_2 \cdots O_n$, where α is a complex number and O_1, O_2, …, O_n are arbitrary operators. Using the result of the above exercise, we can easily show that

$$O^\dagger = \alpha^* O_n^\dagger O_{n-1}^\dagger \cdots O_1^\dagger.$$

b) Description by a density matrix

The relation

$$\langle A \rangle = \langle \psi \mid A \mid \psi \rangle = \sum_{nm} C_n^* C_m A_{nm} \tag{69}$$

shows that the coefficients C_n enter into the mean values through quadratic expressions of the type $C_n^* C_m$. These quadratic expressions are simply the matrix elements of the operator $|\psi\rangle\langle\psi|$, which is the projector onto the ket vector $|\psi\rangle$. Indeed, since

$$
\begin{aligned}
|\psi\rangle &= \sum_n C_n \mid u_n \rangle, \\
\langle \psi \mid &= \sum_n \langle u_n \mid C_n^*,
\end{aligned} \tag{70}
$$

we have

$$
\begin{aligned}
C_n &= \langle u_n \mid \psi \rangle, \\
C_n^* &= \langle \psi \mid u_n \rangle.
\end{aligned} \tag{71}
$$

Hence, we find

$$C_n^* C_m = \langle u_m \mid \psi \rangle\langle \psi \mid u_n \rangle. \tag{72}$$

It is therefore natural to introduce the density operator

$$\rho = |\psi\rangle\langle\psi|. \tag{73}$$

The density operator is represented in the $\{|u_n\rangle\}$ basis by a matrix called the density matrix whose elements are

$$
\begin{aligned}
\rho_{mn} &= \langle u_m \mid \rho \mid u_n \rangle \\
&= \langle u_m \mid \psi \rangle\langle \psi \mid u_n \rangle \\
&= C_n^* C_m.
\end{aligned} \tag{74}
$$

The mean value of the observable A is then given by

$$\langle A \rangle = \langle \psi \mid A \mid \psi \rangle = \sum_{nm} C_n^* C_m A_{nm} = \sum_{nm} \rho_{mn} A_{nm} = \mathrm{Tr}\{\rho A\} = \mathrm{Tr}\{A\rho\}. \tag{75}$$

Mathematically, the operator $|\psi\rangle\langle\psi|$ is the projector onto the ket vector $|\psi\rangle$. Indeed, with the use of the notation

$$P_{|\psi\rangle} \equiv |\psi\rangle\langle\psi|, \tag{76}$$

we see that the action of $P_{|\psi\rangle}$ on an arbitrary vector $|V\rangle$ gives a vector aligned along $|\psi\rangle$, namely,

$$
\begin{aligned}
P_{|\psi\rangle} |V\rangle &= (|\psi\rangle\langle\psi|) |V\rangle \\
&= |\psi\rangle(\langle\psi|V\rangle).
\end{aligned} \tag{77}
$$

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In addition, we have

$$
\begin{aligned}
P_{|\psi\rangle}^2 &= P_{|\psi\rangle} P_{|\psi\rangle} \\
&= (|\psi\rangle\langle\psi|)(|\psi\rangle\langle\psi|) \\
&= |\psi\rangle(\langle\psi|\psi\rangle)\langle\psi| \\
&= |\psi\rangle\langle\psi| \\
&= P_{|\psi\rangle}.
\end{aligned}
\tag{78}
$$

The above properties indicate that $P_{|\psi\rangle} \equiv |\psi\rangle\langle\psi|$ is a projection operator. Since $P_{|\psi\rangle}^2 = P_{|\psi\rangle}$, we find that, in the case of pure states, we have $\rho^2 = \rho$ and hence, $\mathrm{Tr}\rho^2 = \mathrm{Tr}\rho = 1$ [see Eq. (80)].

Note that the matrix ρ_{mn} is a Hermitian matrix. Indeed, we have

$$
\begin{aligned}
\rho_{mn}^* &= C_m^* C_n = \rho_{nm} \\
&\leftrightarrow \\
\rho^\dagger &= \rho.
\end{aligned}
\tag{79}
$$

The specification of ρ suffices to characterize the quantum state of the system. In other words, the density operator ρ enables us to obtain all the physical predictions that can be calculated from $|\psi\rangle$. To show this, we express in terms of the operator ρ the conservation law of probability, the mean value of an observable, and the time evolution of a quantum state.

i. Conservation law of probability

We find from the conservation law of probability that

$$
\mathrm{Tr}\,\rho = \sum_n \rho_{nn} = \sum_n |C_n|^2 = 1.
\tag{80}
$$

Thus, the sum of the diagonal elements of the density matrix is equal to 1.

ii. Mean value of an observable

For the mean value of an observable, we have the formula

$$
\begin{aligned}
\langle A \rangle &= \langle\psi|A|\psi\rangle = \sum_{nm} C_n^* C_m A_{nm} = \sum_{nm} \rho_{mn} A_{nm} \\
&= \mathrm{Tr}\{\rho A\} = \mathrm{Tr}\{A\rho\}.
\end{aligned}
\tag{81}
$$

iii. Schrödinger equation

We derive the time evolution equation for the density operator ρ. As known, the Schrödinger equation is

$$
\frac{d}{dt}|\psi\rangle = \frac{1}{i\hbar} H|\psi\rangle.
\tag{82}
$$

The Hermitian conjugate form of the above equation reads

$$\frac{d}{dt}\langle\psi| = -\frac{1}{i\hbar}\langle\psi|H^\dagger = -\frac{1}{i\hbar}\langle\psi|H. \tag{83}$$

Hence, we have

$$\begin{aligned}
\frac{d}{dt}\rho &= \frac{d}{dt}|\psi\rangle\langle\psi| \\
&= \left(\frac{d}{dt}|\psi\rangle\right)\langle\psi| + |\psi\rangle\left(\frac{d}{dt}\langle\psi|\right) \\
&= \frac{1}{i\hbar}H|\psi\rangle\langle\psi| + \frac{1}{-i\hbar}|\psi\rangle\langle\psi|H \\
&= \frac{1}{i\hbar}(H\rho - \rho H) \\
&= \frac{1}{i\hbar}[H,\rho].
\end{aligned} \tag{84}$$

Here

$$[O_1, O_2] = O_1 O_2 - O_2 O_1 \tag{85}$$

is the commutator between the operators O_1 and O_2. Thus, the time evolution of the density operator ρ is governed by the equation

$$i\hbar\frac{d}{dt}\rho = [H,\rho]. \tag{86}$$

This equation is called the generalized Schrödinger equation.

iv. Summary of the properties of the density operator of a pure state

- The properties of the density operator in the case of pure states are

$$\begin{cases}
\rho^\dagger = \rho, \\
\mathrm{Tr}\,\rho = 1, \\
\langle A\rangle = \mathrm{Tr}\,\{\rho A\} = \mathrm{Tr}\,\{A\rho\}, \\
i\hbar\frac{d}{dt}\rho = [H,\rho].
\end{cases} \tag{87}$$

The above properties are general, i.e., they are true also in the case of mixed states.

- In the case of pure states, there are two specific properties:

$$\begin{cases}
\rho^2 = \rho, \\
\mathrm{Tr}\,\rho^2 = 1.
\end{cases} \tag{88}$$

These properties can be used as criteria to find out if a state is a pure state or not.

v. Advantages of the description in terms of the density operator

A pure state can be described by a density operator as well as by a state vector (wave function). Both descriptions are equivalent. However, the density operator presents a number of advantages:

- First of all, two state vectors $|\psi\rangle$ and $e^{i\theta}|\psi\rangle$ describe the same quantum state. In other words, there exists an arbitrary global phase factor for the state vector. However, the state vectors $|\psi\rangle$ and $e^{i\theta}|\psi\rangle$ correspond to the same density operator

$$
\begin{aligned}
\rho &= |\psi\rangle\langle\psi| \\
&= e^{i\theta}|\psi\rangle\langle\psi|e^{-i\theta}.
\end{aligned}
\tag{89}
$$

Thus, the use of the density operator eliminates the global phase.

- Second, the equation

$$
\langle A\rangle = \mathrm{Tr}\{\rho A\} = \mathrm{Tr}\{A\rho\}
\tag{90}
$$

is linear with respect to the density operator ρ.

However, the equation

$$
\langle A\rangle = \langle\psi|A|\psi\rangle
\tag{91}
$$

is quadratic with respect to $|\psi\rangle$.

vi. Example: the density operator of a pure state of a two-level system

We consider a two-level system in a pure state described by the state vector (wave function)

$$
|\psi\rangle = C_a|a\rangle + C_b|b\rangle.
\tag{92}
$$

The density operator of the system is

$$
\rho = |\psi\rangle\langle\psi| = (C_a|a\rangle + C_b|b\rangle)(C_a^*\langle a| + C_b^*\langle b|).
\tag{93}
$$

Taking the matrix elements, we get

$$
\begin{aligned}
\rho_{aa} &= |C_a|^2, \\
\rho_{ab} &= C_a C_b^*, \\
\rho_{ba} &= \rho_{ab}^*, \\
\rho_{bb} &= |C_b|^2.
\end{aligned}
\tag{94}
$$

The matrix form of the density operator is

$$
\rho = \begin{pmatrix} \rho_{aa} & \rho_{ab} \\ \rho_{ba} & \rho_{bb} \end{pmatrix} = \begin{pmatrix} |C_a|^2 & C_a C_b^* \\ C_b C_a^* & |C_b|^2 \end{pmatrix}.
\tag{95}
$$

We see that $\rho_{nm}^* = \rho_{mn}$, that is, $\rho^\dagger = \rho$. In addition, we have

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$$\text{Tr}\rho \equiv \rho_{aa} + \rho_{bb} = |C_a|^2 + |C_b|^2 = 1. \tag{96}$$

The average value of an observable A is given by

$$\begin{aligned}
\langle A \rangle &= \text{Tr}\{\rho A\} = \text{Tr}\{A\rho\} \\
&= \sum_{nm} \rho_{mn} A_{nm} \\
&= \rho_{aa} A_{aa} + \rho_{bb} A_{bb} + \rho_{ab} A_{ba} + \rho_{ba} A_{ab}.
\end{aligned} \tag{97}$$

It is obvious that the diagonal matrix elements ρ_{aa} and ρ_{bb} are the probabilities of being in the upper and lower states, respectively. The off-diagonal matrix elements ρ_{ab} and ρ_{ba}, where $\rho_{ab} = \rho_{ba}^*$, describe the interference between the upper level $|a\rangle$ and the lower level $|b\rangle$ in the state ρ. To illustrate more clearly the physical meaning of the off-diagonal elements, we use the fact that the atomic polarization (average dipole moment) of a single two-level atom is given by

$$\begin{aligned}
P &= e\langle x \rangle = e\langle \psi | x | \psi \rangle \\
&= e(|C_a|^2 x_{aa} + |C_b|^2 x_{bb} + C_a^* C_b x_{ab} + C_b^* C_a x_{ba}) \\
&= e(C_a^* C_b x_{ab} + C_b^* C_a x_{ba}) \\
&= \rho_{ba} d_x + \rho_{ab} d_x^*,
\end{aligned} \tag{98}$$

where e is the electric charge of the electron and

$$d_x = ex_{ab} \tag{99}$$

is the dipole matrix element. Here we have used the property $x_{aa} = x_{bb} = 0$, which is a consequence of the fact that x is an odd function while $|\varphi_n(x)|^2$ (with $n = a,b$) is, in the case of atoms, an even function. The probability density $|\varphi_n(x)|^2$ is an even function because so is the Coulomb potential in the atom. Thus, in the case of two-level atoms, the off-diagonal elements ρ_{ab} and ρ_{ba} determine the atomic polarization.

As known, for a free two-level system, the Hamiltonian is

$$H_0 = \hbar\omega_a |a\rangle\langle a| + \hbar\omega_b |b\rangle\langle b| \tag{100}$$

and the time evolution of the probability amplitudes is governed by the equations

$$\begin{aligned}
\frac{d}{dt} C_a &= -i\omega_a C_a, \\
\frac{d}{dt} C_b &= -i\omega_b C_b.
\end{aligned} \tag{101}$$

When we use the relation $\rho_{\alpha\beta} = C_\alpha C_\beta^*$, we can easily show that the evolution equations for the density-operator matrix elements of the free two-level system are

$$\frac{d}{dt}\rho_{aa} = 0,$$

$$\frac{d}{dt}\rho_{bb} = 0, \qquad (102)$$

$$\frac{d}{dt}\rho_{ab} = -i(\omega_a - \omega_b)\rho_{ab}.$$

We can also derive the above equations directly from the generalized Schrödinger equation (86). The solutions to Eqs. (102) are

$$\begin{cases} \rho_{aa}(t) = \text{constant}, \\ \rho_{bb}(t) = \text{constant}, \\ \rho_{ab}(t) = e^{-i(\omega_a - \omega_b)t}\rho_{ab}(0). \end{cases} \qquad (103)$$

As seen, when the two-level system is free, the diagonal matrix elements of the density operator are constant. However, the off-diagonal matrix elements oscillate in time.

3. Statistical mixtures of states

a) Definition of the density operator

We now return to the general case where the system is in a mixture of states $|\psi_1\rangle, |\psi_2\rangle, ..., |\psi_k\rangle, ...$, with probabilities $p_1, p_2, ..., p_k, ...$, where

$$\begin{cases} 0 \le p_k \le 1, \\ \sum_k p_k = 1. \end{cases} \qquad (104)$$

The state vectors $|\psi_k\rangle$ of the components are normalized, that is, $\langle \psi_k | \psi_k \rangle = 1$. However, they are not necessarily orthogonal to each other.

The density operator of the statistical mixture of states is defined as

$$\rho = \sum_k p_k \rho_k, \qquad (105)$$

where ρ_k is the density operator corresponding to the state $|\psi_k\rangle$, i.e.,

$$\rho_k = |\psi_k\rangle\langle\psi_k|. \qquad (106)$$

b) Properties of the density operator

i. Hermitivity

Since the coefficients p_k are real, ρ is obviously a Hermitian operator like each of the ρ_k:

$$\rho^\dagger = \sum_k p_k^* \rho_k^\dagger = \sum_k p_k \rho_k = \rho. \tag{107}$$

ii.   Probability conservation law

The conservation law of probability gives

$$\begin{aligned} \mathrm{Tr}\,\rho &= \sum_k p_k \mathrm{Tr}\,\rho_k \\ &= \sum_k p_k = 1. \end{aligned} \tag{108}$$

iii.   Mean values

The expression for the mean value of an observable is

$$\begin{aligned} \langle A \rangle &= \sum_k p_k \langle A \rangle_k \\ &= \sum_k p_k \mathrm{Tr}\{A\rho_k\} \\ &= \mathrm{Tr}\{A \sum_k p_k \rho_k\} \\ &= \mathrm{Tr}\{A\rho\}. \end{aligned} \tag{109}$$

The averaging by means of the density operator, expressed by Eq. (109), has a twofold nature. It comprises both the averaging due to the probabilistic nature of quantum mechanics (even when the information about the object is complete) and the statistical averaging necessitated by the incompleteness of our information. For a pure state, only the first averaging remains. For a mixed state, both types of averaging are always present.

iv.   Schrödinger equation for the density operator

We now derive an equation for the time evolution of the density operator. We assume that the Hamiltonian H of the system is known. The state $|\psi_k\rangle$ satisfies the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi_k\rangle = H |\psi_k\rangle. \tag{110}$$

Therefore, ρ_k obeys the evolution equation

$$i\hbar \frac{d}{dt} \rho_k = [H, \rho_k]. \tag{111}$$

Using the linearity of Eqs. (105) and (111), we find the following evolution equation for the density operator ρ:

$$ i\hbar \frac{d}{dt}\rho = i\hbar \frac{d}{dt}\sum_k p_k \rho_k = \sum_k p_k \left(i\hbar \frac{d}{dt}\rho_k \right) $$
$$ = \sum_k p_k [H, \rho_k] = [H, \sum_k p_k \rho_k] \tag{112} $$
$$ = [H, \rho]. $$

v.   Positivity

We see from the definition $\rho = \sum_k p_k \rho_k$ that, for any ket $|u\rangle$, we have

$$ \langle u | \rho | u \rangle = \sum_k p_k \langle u | \rho_k | u \rangle $$
$$ = \sum_k p_k |\langle u | \psi_k \rangle|^2 \tag{113} $$

and, consequently,

$$ \langle u | \rho | u \rangle \geq 0. \tag{114} $$

Equation (114) means that the density operator ρ is a positive operator.

vi.   Summary of the properties of the density operator of a general quantum state

Thus, for pure states as well as statistical mixtures of states, we have

$$ \begin{cases} \rho^\dagger = \rho, \\ \mathrm{Tr}\,\rho = 1, \\ \langle A \rangle = \mathrm{Tr}\,\{\rho A\} = \mathrm{Tr}\,\{A\rho\}, \\ i\hbar \dfrac{d}{dt}\rho = [H, \rho]. \end{cases} \tag{115} $$

vii.   Differences between the density operator of a mixed quantum state and that of a pure state

The equations

$$ \rho^2 = \rho, $$
$$ \mathrm{Tr}\,\rho^2 = 1 \tag{116} $$

are true for pure states but not true for mixed states. For mixed states, since ρ is no longer a projector, we have

$$ \rho^2 \neq \rho \tag{117} $$

and, consequently, $\mathrm{Tr}\,\rho^2 \neq 1$. For a mixed state, according to comments (i) and (iii) at the end of this section (see pages 26 and 27), we have

$$ \mathrm{Tr}\,\rho^2 < 1. \tag{118} $$

Thus, we have, in general, for pure and mixed states,

$$\text{Tr}\,\rho^2 \le 1. \tag{119}$$

The above equation can be used as a criterion to find out if a state is a pure state ($\text{Tr}\,\rho^2 = 1$) or a mixed state ($\text{Tr}\,\rho^2 < 1$).

c) Populations and coherences

What is the physical meaning of the matrix elements of the density operator ρ in the basis $\{|u_n\rangle\}$?

First, we consider the diagonal element ρ_{nn}. We have

$$\begin{aligned}
\rho_{nn} &= \langle u_n \,|\, \rho \,|\, u_n \rangle \\
&= \sum_k p_k \langle u_n \,|\, \rho_k \,|\, u_n \rangle \\
&= \sum_k p_k \langle u_n \,|\, \psi_k \rangle \langle \psi_k \,|\, u_n \rangle \\
&= \sum_k p_k \,|\langle u_n \,|\, \psi_k \rangle|^2 .
\end{aligned} \tag{120}$$

We express the state $|\psi_k\rangle$ in terms of the basis $\{|u_n\rangle\}$ as

$$|\psi_k\rangle = \sum_n c_n^{(k)} |u_n\rangle. \tag{121}$$

This gives

$$c_n^{(k)} = \langle u_n \,|\, \psi_k \rangle. \tag{122}$$

Then Eq. (120) becomes

$$\rho_{nn} = \sum_k p_k \,|\,c_n^{(k)}\,|^2. \tag{123}$$

It follows from Eq. (123) that ρ_{nn} is a positive real number. The squared modulus $|\,c_n^{(k)}\,|^2$ is the probability of $|u_n\rangle$ in the pure state $|\psi_k\rangle$. Therefore, Eq. (123) means that ρ_{nn} is the probability of $|u_n\rangle$ in the state ρ. For this reason, the diagonal matrix element ρ_{nn} is called the population of the state $|u_n\rangle$. If the same measurement is carried out N times under the same initial condition, where N is a large number, $N\rho_{nn}$ systems will be found in the state $|u_n\rangle$.

Now, we consider the non-diagonal element ρ_{nm}. A calculation analogous to the preceding one gives the following expression for ρ_{nm}:

$$\begin{aligned}
\rho_{nm} &= \langle u_n \,|\, \rho \,|\, u_m \rangle \\
&= \sum_k p_k \langle u_n \,|\, \rho_k \,|\, u_m \rangle \\
&= \sum_k p_k \langle u_n \,|\, \psi_k \rangle \langle \psi_k \,|\, u_m \rangle \\
&= \sum_k p_k c_n^{(k)} c_m^{(k)*}.
\end{aligned} \tag{124}$$

The term $c_n^{(k)} c_m^{(k)*}$ is a cross term. It expresses the interference effects between the states $|u_n\rangle$ and $|u_m\rangle$ that can appear when the state $|\psi_k\rangle$ is a coherent linear superposition of these states. According to Eq. (124), ρ_{nm} is the average of these cross terms, taken over all the possible states of the statistical mixture. If ρ_{nm} is zero, this means that the statistical average has canceled out any interference effects between $|u_n\rangle$ and $|u_m\rangle$. On the other hand, if ρ_{nm} is different from zero, a certain coherence subsists between these states. This is why the non-diagonal elements of ρ are often called coherences.

COMMENTS:

(i) The distinction between populations and coherences obviously depends on the choice of the basis $\{|u_n\rangle\}$. Since ρ is Hermitian, it is always possible to find an orthonormal basis $\{|\chi_n\rangle\}$ where ρ is diagonal. In this basis, ρ can be written as

$$\rho = \sum_l \pi_l \,|\, \chi_l \rangle \langle \chi_l \,|. \tag{125}$$

The density operator ρ can thus be considered to describe a statistical mixture of the orthonormal states $|\chi_n\rangle$ with the probabilities π_l. There are no coherences between the states $|\chi_n\rangle$ in this mixture. We have

$$\begin{aligned}
\mathrm{Tr}\rho^2 &= \sum_l \pi_l^2 \\
&\leq \sum_l \pi_l = 1.
\end{aligned} \tag{126}$$

When one of the coefficients π_l is equal to 1, all the other coefficients must be zero. In this case, the state ρ is a pure state and $\mathrm{Tr}\,\rho^2 = 1$. When all the coefficients π_l are smaller than 1, the state ρ is a mixed state and $\mathrm{Tr}\,\rho^2 < 1$.

(ii) Assume that the Hamiltonian H is time-independent. If $|u_n\rangle$ are eigenvectors of H, then

$$\begin{aligned}
H\,|u_n\rangle &= E_n\,|u_n\rangle, \\
\langle u_n\,|\,H &= \langle u_n\,|\,E_n.
\end{aligned} \tag{127}$$

Hence, we obtain from Eq. (112)

$$i\hbar \frac{d}{dt} \langle u_n \mid \rho \mid u_m \rangle = \langle u_n \mid H\rho - \rho H \mid u_m \rangle$$
$$= \langle u_n \mid E_n \rho - \rho E_m \mid u_m \rangle \qquad (128)$$
$$= (E_n - E_m) \langle u_n \mid \rho \mid u_m \rangle,$$

that is,

$$i\hbar \frac{d}{dt} \rho_{nm} = (E_n - E_m) \rho_{nm}. \qquad (129)$$

The solution to the above equation is

$$\rho_{nm}(t) = e^{-\frac{i}{\hbar}(E_n - E_m)t} \rho_{nm}(0). \qquad (130)$$

In particular, we have $\rho_{nn}(t) = \text{constant}$.

Thus, the populations are constant, and the coherences oscillate at the Bohr frequencies of the system.

(iii) We can easily prove that

$$\rho_{nn} \rho_{mm} \geq \mid \rho_{nm} \mid^2 . \qquad (131)$$

Indeed, according to Eqs. (123) and (124) and to the generalized Cauchy-Scharz-Buniakowsky inequality, we have

$$\rho_{nn} \rho_{mm} = \left(\sum_k p_k \mid c_n^{(k)} \mid^2 \right) \left(\sum_k p_k \mid c_m^{(k)} \mid^2 \right)$$
$$\geq \left(\sum_k p_k \mid c_n^{(k)} c_m^{(k)} \mid \right)^2 \qquad (132)$$
$$\geq \left| \sum_k p_k c_n^{(k)} c_m^{(k)} \right|^2 = \mid \rho_{nm} \mid^2 .$$

It follows from Eq. (131) that ρ can have coherences only between states whose populations are not zero.

It also follows from Eq. (131) that

$$\text{Tr} \rho^2 = \sum_{nm} \mid \rho_{nm} \mid^2$$
$$\leq \sum_{nm} \rho_{nn} \rho_{mm}$$
$$= \sum_n \rho_{nn} \sum_m \rho_{mm} \qquad (133)$$
$$= 1,$$

see Eq. (119).

Exercises

Exercise 1: Consider a two-level system with density operator

$$\rho = \frac{1}{4}|a\rangle\langle a| + \frac{3}{4}|b\rangle\langle b| = \begin{pmatrix} \frac{1}{4} & 0 \\ 0 & \frac{3}{4} \end{pmatrix}.$$

Show that the state of the system is a mixed state.

Exercise 2: Consider a two-level system with density operator

$$\rho = \frac{1}{4}|a\rangle\langle a| + \frac{3}{4}|b\rangle\langle b| + \frac{\sqrt{3}}{4}|a\rangle\langle b| + \frac{\sqrt{3}}{4}|b\rangle\langle a| = \begin{pmatrix} \frac{1}{4} & \frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{4} & \frac{3}{4} \end{pmatrix}.$$

Show that the state ρ is a pure state.

Exercise 3: Consider two orthonormal vectors $|a\rangle$ and $|b\rangle$. Consider a quantum system (ensemble) Q_1 that is prepared in the state $|a\rangle$ with probability 1/4 and in the state $|b\rangle$ with probability 3/4.

Suppose we define

$$|0\rangle = \sqrt{\frac{1}{4}}|a\rangle + \sqrt{\frac{3}{4}}|b\rangle,$$

$$|1\rangle = \sqrt{\frac{1}{4}}|a\rangle - \sqrt{\frac{3}{4}}|b\rangle.$$

Consider a quantum system (ensemble) Q_2 that is prepared in the state $|0\rangle$ with probability 1/2 and in the state $|1\rangle$ with probability 1/2. Show that the quantum systems Q_1 and Q_2 correspond to the same density operator.

Exercise 4: Consider two arbitrary vectors $|A\rangle$ and $|B\rangle$. Show that $\text{Tr}\,|A\rangle\langle B| = \langle B|A\rangle$.

Solutions

Exercise 1:

The square of the density operator of the system is

$$\rho^2 = \frac{1}{16}|a\rangle\langle a| + \frac{9}{16}|b\rangle\langle b| = \begin{pmatrix} \frac{1}{16} & 0 \\ 0 & \frac{9}{16} \end{pmatrix}.$$

We find $\mathrm{Tr}\rho^2 = 1/16 + 9/16 = 10/16 = 5/8 < 1$. This inequality indicates that the state of the system is a mixed state.

Exercise 2:

The square of the density operator of the system is

$$\rho^2 = \frac{1}{4}|a\rangle\langle a| + \frac{3}{4}|b\rangle\langle b| + \frac{\sqrt{3}}{4}|a\rangle\langle b| + \frac{\sqrt{3}}{4}|b\rangle\langle a|$$

$$= \begin{pmatrix} \frac{1}{4} & \frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{4} & \frac{3}{4} \end{pmatrix}$$

$$= \rho.$$

Hence we find $\mathrm{Tr}\rho^2 = \mathrm{Tr}\rho = 1$. These equalities indicate that the state of the system is a pure state.

Exercise 3:

The density operator of the system Q_1 is

$$\rho_1 = \frac{1}{4}|a\rangle\langle a| + \frac{3}{4}|b\rangle\langle b|.$$

The density operator of the system Q_2 is

$$\rho_2 = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|.$$

We can easily show that

$$\rho_2 = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$$

$$= \frac{1}{2}\left(\sqrt{\frac{1}{4}}|a\rangle + \sqrt{\frac{3}{4}}|b\rangle\right)\left(\sqrt{\frac{1}{4}}\langle a| + \sqrt{\frac{3}{4}}\langle b|\right) + \frac{1}{2}\left(\sqrt{\frac{1}{4}}|a\rangle - \sqrt{\frac{3}{4}}|b\rangle\right)\left(\sqrt{\frac{1}{4}}\langle a| - \sqrt{\frac{3}{4}}\langle b|\right)$$

$$= \frac{1}{4}|a\rangle\langle a| + \frac{3}{4}|b\rangle\langle b|$$

$$= \rho_1.$$

Thus, two different realizations may correspond to the same statistical quantum ensemble.

Since $|a\rangle$ and $|b\rangle$ are orthogonal to each other, they are the eigenstates of the density operator $\rho = \rho_1 = \rho_2$. In the contrary, $|0\rangle$ and $|1\rangle$ are not orthogonal to each other. Therefore, $|0\rangle$ and $|1\rangle$ are not the eigenstates of the density operator ρ. In general, the eigenvectors and eigenvalues of a density operator just indicate one of many possible realizations that may give rise to a specific density operator.

Exercise 4:

With the help of the formula

$$\sum_n |u_n\rangle\langle u_n| = 1,$$

we find

$$\text{Tr }|A\rangle\langle B| = \sum_n \langle u_n | A\rangle\langle B | u_n\rangle$$
$$= \sum_n \langle B | u_n\rangle\langle u_n | A\rangle$$
$$= \langle B | A\rangle.$$

4. Applications of the density operator

a) System in thermal equilibrium

The first example we consider is borrowed from quantum statistical mechanics. Consider a system in thermal equilibrium at the absolute temperature T. According to quantum statistical mechanics, the density operator of the system is

$$\rho = Z^{-1} e^{-H/kT}. \tag{134}$$

Here H is the Hamiltonian operator of the system, k is the Boltzmann constant, and Z is a normalization constant chosen so as to make the trace of ρ equal to 1, that is,

$$Z = \mathrm{Tr}\,\{e^{-H/kT}\}. \tag{135}$$

We use the basis from the eigenvectors $|u_n\rangle$ of H. In this basis, we have

$$\rho_{nn} = Z^{-1}\langle u_n | e^{-H/kT} | u_n\rangle = Z^{-1} e^{-E_n/kT} \tag{136}$$

and

$$\rho_{nm} = Z^{-1}\langle u_n | e^{-H/kT} | u_m\rangle = 0 \qquad \text{for } n \neq m. \tag{137}$$

At thermal equilibrium, the populations of the stationary states are exponentially decreasing functions of the energy, and the coherences between stationary states are zero.

b) Description of a part of a physical system

The most important application of the density operator is as a descriptive tool for subsystems of a composite quantum system. Such a description is provided by the reduced density operator. The reduced density operator is indispensable in the analysis of composite quantum systems.

Suppose we have a composition of physical systems A and B. The state space of the combined system AB is the direct product of the state spaces of the subsystems A and B. By definition, the state space of AB contains the vectors of the type

$$|V^{AB}\rangle = |V^A V^B\rangle = |V^A\rangle \otimes |V^B\rangle = |V^A\rangle |V^B\rangle \tag{138}$$

and also their superpositions, where $|V^A\rangle$ and $|V^B\rangle$ are arbitrary vectors in the state spaces of A and B, respectively. The vector $|V^{AB}\rangle$ has two parts, one belongs to A and the other belongs to B. We have $|V^{AB}\rangle = |V^{BA}\rangle$, $|V^A V^B\rangle = |V^B V^A\rangle$, $|V^A\rangle \otimes |V^B\rangle = |V^B\rangle \otimes |V^A\rangle$, and $|V^A\rangle |V^B\rangle = |V^B\rangle |V^A\rangle$. The dimension of the state space of AB is the sum of the dimensions of the state spaces of A and B.

The basis states of the combined system AB are

$$|u^{AB}\rangle = |u^A u^B\rangle = |u^A\rangle \otimes |u^B\rangle = |u^A\rangle |u^B\rangle \tag{139}$$

where $|u^A\rangle$ and $|u^B\rangle$ are the basis states of the subsystems A and B, respectively.

To label the individual basis states of the subsystems A and B, we use indices n_A and n_B, respectively. Then, we can label the basis states of the combined system AB as

$$|u^{AB}_{n_A n_B}\rangle = |u^A_{n_A} u^B_{n_B}\rangle = |u^A_{n_A}\rangle \otimes |u^B_{n_B}\rangle = |u^A_{n_A}\rangle |u^B_{n_B}\rangle. \tag{140}$$

We describe the state of the composite system AB by a density operator ρ^{AB}. The matrix form of the density operator ρ^{AB} is given by

$$\begin{aligned}
\rho^{AB}_{n_A n_B, m_A m_B} &\equiv \langle u^{AB}_{n_A n_B} | \rho^{AB} | u^{AB}_{m_A m_B}\rangle \\
&= \langle u^A_{n_A} u^B_{n_B} | \rho^{AB} | u^A_{m_A} u^B_{m_B}\rangle \\
&= \left(\langle u^B_{n_B} | \langle u^A_{n_A} |\right) \rho^{AB} \left(| u^A_{m_A}\rangle | u^B_{m_B}\rangle\right) \\
&= \langle u^B_{n_B} | \langle u^A_{n_A} | \rho^{AB} | u^A_{m_A}\rangle | u^B_{m_B}\rangle.
\end{aligned} \tag{141}$$

We assume that only part A is observed. Then information about part B is lost. This is the so-called incomplete detection. Therefore, a statistical average over part B is necessary. The state of part A is described by the reduced density operator

$$\begin{aligned}
\rho^A &= \mathrm{Tr}_B\,(\rho^{AB}) \\
&\equiv \sum_n \langle u^B_n | \rho^{AB} | u^B_n\rangle,
\end{aligned} \tag{142}$$

where Tr_B is a map of operators known as the partial trace over system B. In the matrix form, we have

$$\rho^A_{n_A m_A} = \sum_{n_B} \rho^{AB}_{n_A n_B, m_A n_B}. \tag{143}$$

Note that the partial trace of an operator of the type $O^{AB} = |a_1\rangle\langle a_2 | \otimes | b_1\rangle\langle b_2 |$ is given by

$$\begin{aligned}
\mathrm{Tr}_B(| a_1\rangle\langle a_2 | \otimes | b_1\rangle\langle b_2 |) &\equiv | a_1\rangle\langle a_2 | \mathrm{Tr}_B(| b_1\rangle\langle b_2 |) \\
&= | a_1\rangle\langle a_2 | \langle b_2 | b_1\rangle.
\end{aligned} \tag{144}$$

Here $|a_1\rangle$ and $|a_2\rangle$ are any two vectors in the state space of A, and $|b_1\rangle$ and $|b_2\rangle$ are any two vectors in the state space of B. In deriving the above expression, we have used the formula $\mathrm{Tr} | \Psi_1\rangle\langle \Psi_2 | = \langle \Psi_2 | \Psi_1\rangle$.

If the composite system is in a pure state, the incomplete detection process may cause a part of the system to be in a statistical mixture. As an example, consider a two-level atom initially prepared in the excited state. Assume that the atom interacts with a single-mode radiation field that is initially prepared in the vacuum state.

The excited and ground states of the atom are indicated by $|a\rangle$ and $|b\rangle$, respectively. The n-photon state of the field is denoted by $|n\rangle$, where $n = 0, 1, 2, \dots$. The basis states of the composite system "atom+field" are $|a;0\rangle$, $|a;1\rangle$, $|a;2\rangle$, ... , $|a;n\rangle$, ... , and $|b;0\rangle$, $|b;1\rangle$, $|b;2\rangle$, ... , $|b;n\rangle$, ...

The initial state of the composite system is $|a;0\rangle$. After a short time the atom has a probability to make a transition to the ground state by spontaneous emission of a photon. The state vector of the composite system at an arbitrary time t is then given by

$$|\psi^{AB}\rangle = \alpha\,|a;0\rangle + \beta\,|b;1\rangle. \tag{145}$$

The density operator of the composite atom+photon system is

$$\begin{aligned}
\rho^{AB} &= |\psi^{AB}\rangle\langle\psi^{AB}| \\
&= \left(\alpha\,|a;0\rangle + \beta\,|b;1\rangle\right)\left(\langle a;0|\,\alpha^* + \langle b;1|\,\beta^*\right) \\
&= |\alpha|^2\,|a;0\rangle\langle a;0| + |\beta|^2\,|b;1\rangle\langle b;1| \\
&\quad + \alpha\beta^*\,|a;0\rangle\langle b;1| + \alpha^*\beta\,|b;1\rangle\langle a;0|.
\end{aligned} \tag{146}$$

If we observe the state of the atom but not the emitted photon, then the atom will be found in either the excited $|a\rangle$ or the ground state $|b\rangle$; however, it will no longer be in a pure state. The new state can be described by the reduced density operator

$$\begin{aligned}
\rho_{\text{atom}} &= \text{Tr}_{\text{ph}}\rho^{AB} = \text{Tr}_{\text{ph}}\,|\psi^{AB}\rangle\langle\psi^{AB}| \\
&= |\alpha|^2\,|a\rangle\langle a| + |\beta|^2\,|b\rangle\langle b|.
\end{aligned} \tag{147}$$

Basic properties of the reduced density operator

<u>Hermitivity</u>: We can show that

$$\left(\rho^A\right)^\dagger = \rho^A,$$
$$\text{or,} \tag{148}$$
$$\left(\rho^A_{nn'}\right)^* = \rho^A_{n'n}.$$

Indeed, the matrix elements of the reduced density operator ρ^A are given by

$$\begin{aligned}
\rho^A_{nn'} &= \langle u^A_n | \rho^A | u^A_{n'}\rangle \\
&= \langle u^A_n | \sum_m \langle u^B_m | \rho^{AB} | u^B_m\rangle | u^A_{n'}\rangle \\
&= \sum_m \langle u^A_n u^B_m | \rho^{AB} | u^A_{n'} u^B_m\rangle \\
&= \sum_m \rho^{AB}_{nm,n'm}.
\end{aligned} \tag{149}$$

From the Hermitivity of ρ^{AB}, we have $\left(\rho^{AB}_{nm,n'm'}\right)^* = \rho^{AB}_{n'm',nm}$. Hence, we find

$$\begin{aligned}
\left(\rho^A_{nn'}\right)^* &= \left(\sum_m \rho^{AB}_{nm,n'm}\right)^* = \sum_m \left(\rho^{AB}_{nm,n'm}\right)^* \\
&= \sum_m \rho^{AB}_{n'm,nm} = \rho^A_{n'n}.
\end{aligned} \tag{150}$$

Thus, ρ^A is a Hermitian operator.

<u>Normalization</u>: We can show that

$$\mathrm{Tr}\rho^A = 1. \tag{151}$$

Indeed,

$$\begin{aligned}\mathrm{Tr}\rho^A &= \sum_n \rho_{nn}^A = \sum_n \sum_m \rho_{nm,nm}^{AB} \\ &= \mathrm{Tr}\rho^{AB} = 1.\end{aligned} \tag{152}$$

Thus, the probability conservation law is valid for the reduced density operator.

<u>Average of an observable</u>: Consider an observable O^A that depends only on part A. We can show that the average of this observable is given by the formula

$$\langle O^A \rangle = \mathrm{Tr}_A \rho^A O^A = \mathrm{Tr}_A O^A \rho^A. \tag{153}$$

Indeed, by definition we have

$$\begin{aligned}\langle O^A \rangle &= \mathrm{Tr}_{AB}\rho^{AB}O^A \\ &= \mathrm{Tr}_A \mathrm{Tr}_B \rho^{AB}O^A \\ &= \mathrm{Tr}_A \left(\mathrm{Tr}_B \rho^{AB} \right) O^A \\ &= \mathrm{Tr}_A \rho^A O^A = \mathrm{Tr}_A O^A \rho^A.\end{aligned} \tag{154}$$

Another way of proving is the following:

$$\begin{aligned}\langle O^A \rangle &= \mathrm{Tr}_{AB}\rho^{AB}O^A \\ &= \sum_{nm} \langle u_{nm}^{AB} | \rho^{AB}O^A | u_{nm}^{AB} \rangle \\ &= \sum_{nm} \langle u_n^A u_m^B | \rho^{AB}O^A | u_n^A u_m^B \rangle.\end{aligned} \tag{155}$$

Since O^A does not depend on part B, it does not change any vectors in the state space of B, that is,

$$\begin{aligned}O^A | u_n^A u_m^B \rangle &\equiv O^A(| u_n^A \rangle | u_m^B \rangle) \\ &= O^A | u_n^A \rangle | u_m^B \rangle \\ &= | u_m^B \rangle O^A | u_n^A \rangle.\end{aligned} \tag{156}$$

Consequently, we have

$$\langle O^A \rangle = \sum_{nm} \langle u_n^A u_m^B | \rho^{AB} O^A | u_n^A u_m^B \rangle$$

$$= \sum_{nm} \langle u_n^A | \langle u_m^B | \rho^{AB} | u_m^B \rangle O^A | u_n^A \rangle$$

$$= \sum_{n} \langle u_n^A | \sum_{m} \{ \langle u_m^B | \rho^{AB} | u_m^B \rangle \} O^A | u_n^A \rangle \qquad (157)$$

$$= \mathrm{Tr}_A \{ \{ \mathrm{Tr}_B \rho^{AB} \} O^A \}$$

$$= \mathrm{Tr}_A \{ \rho^A O^A \} = \mathrm{Tr}_A \{ O^A \rho^A \}.$$

Thus, the average of O^A can be determined from the reduced density operator ρ^A by using the same formula as for an arbitrary quantum system. This property makes the reduced density operator ρ^A useful for describing the state of part A.

Invalidity of the Schrödinger equation: In general, the Schrödinger equation is not valid for the reduced density operator. An example is given below.

c) Spontaneous emission

Consider a two-level atom. If the atom is completely free, that is, if there is no interaction and no spontaneous emission, the evolution of the density operator ρ of the atom is governed by the generalized Schrödinger equation

$$\frac{d}{dt}\rho = \frac{1}{i\hbar}[H_0, \rho]. \qquad (158)$$

Here the Hamiltonian of the free atom is given by

$$H_0 = \hbar\omega_a |a\rangle\langle a| + \hbar\omega_b |b\rangle\langle b|. \qquad (159)$$

When spontaneous emission is included, the evolution of the density operator ρ of the atom cannot be described by the Schrödinger equation. According to the Weisskopf-Wigner theory, the reduced density operator ρ of the atom is governed by the master equation

$$\frac{d}{dt}\rho = \frac{1}{i\hbar}[H_0, \rho] - \frac{\Gamma}{2}\left(\sigma_+\sigma_-\rho - 2\sigma_-\rho\sigma_+ + \rho\sigma_+\sigma_-\right). \qquad (160)$$

Here Γ is the atomic decay rate, and $\sigma_+ = |a\rangle\langle b|$ and $\sigma_- = |b\rangle\langle a|$ are the atomic transition operators. The decay rate Γ is sometimes called the Einstein A-coefficient and is given as $\Gamma = \omega_{ab}^3 |\vec{d}|^2 /3\pi\varepsilon_0\hbar c^3$, where $\vec{d} = e|\langle a|\vec{r}|b\rangle|$ is the dipole moment of the atom and $\omega_{ab} = \omega_a - \omega_b$ is the atomic transition frequency. Equation (160) can be represented in the form

$$\dot{\rho} = \dot{\rho}_0 + \dot{\rho}_{\mathrm{decay}}, \qquad (161)$$

where

$$\dot{\rho}_0 \equiv \frac{1}{i\hbar}[H_0, \rho],$$

$$\dot{\rho}_{\text{decay}} \equiv -\frac{\Gamma}{2}\left(\sigma_+\sigma_-\rho - 2\sigma_-\rho\sigma_+ + \rho\sigma_+\sigma_-\right). \tag{162}$$

We find

$$\dot{\rho}_0 \equiv -i\left[\omega_a\left(|a\rangle\langle a|\rho - \rho|a\rangle\langle a|\right) + \omega_b\left(|b\rangle\langle b|\rho - \rho|b\rangle\langle b|\right)\right],$$

$$\dot{\rho}_{\text{decay}} \equiv -\frac{\Gamma}{2}\left(|a\rangle\langle a|\rho - 2|b\rangle\langle a|\rho|a\rangle\langle b| + \rho|a\rangle\langle a|\right). \tag{163}$$

We can easily do some exercises to show that

$$\langle a|\dot{\rho}_0|a\rangle = 0,$$
$$\langle b|\dot{\rho}_0|b\rangle = 0, \tag{164}$$
$$\langle a|\dot{\rho}_0|b\rangle = -i\omega_{ab}\rho_{ab},$$

and

$$\langle a|\dot{\rho}_{\text{decay}}|a\rangle = -\Gamma\rho_{aa},$$
$$\langle b|\dot{\rho}_{\text{decay}}|b\rangle = \Gamma\rho_{aa}, \tag{165}$$
$$\langle a|\dot{\rho}_{\text{decay}}|b\rangle = -\frac{\Gamma}{2}\rho_{ab}.$$

The equations of motion for the matrix elements of ρ can be obtained from Eq. (161):

$$\frac{d}{dt}\rho_{aa} = -\Gamma\rho_{aa},$$
$$\frac{d}{dt}\rho_{bb} = \Gamma\rho_{aa}, \tag{166}$$
$$\frac{d}{dt}\rho_{ab} = -i\omega_{ab}\rho_{ab} - \frac{\Gamma}{2}\rho_{ab}.$$

It may be noted that $\dot{\rho}_{aa} + \dot{\rho}_{bb} = 0$, that is, $\rho_{aa} + \rho_{bb} = \text{constant}$. This result is valid only in the framework of the two-level atomic model. In the case where the atom has three or more levels, the atom can decay from level a to levels other than b. In this case, the sum of the populations of levels a and b is not conserved.

The solution of Eqs. (166) is found to be

$$\rho_{aa}(t) = \rho_{aa}(0)e^{-\Gamma t},$$
$$\rho_{bb}(t) = 1 - \rho_{aa}(0)e^{-\Gamma t}, \tag{167}$$
$$\rho_{ab}(t) = \rho_{ab}(0)e^{-i\omega_{ab}t - \Gamma t/2}.$$

Thus, the upper-state population ρ_{aa} and the coherence ρ_{ab} decay exponentially with the rates Γ and $\Gamma/2$, respectively. In other words, the decay rate of ρ_{ab} is half the decay rate of ρ_{aa}.

Exercises

Exercise 1: Consider an arbitrary operator O and two arbitrary vectors $|V\rangle$ and $|U\rangle$. Show that

$$\text{Tr}\{O|V\rangle\langle U|\} = \langle U|O|V\rangle.$$

Exercise 2: Consider an arbitrary operator O and a state vector $|\psi\rangle$. Show that

$$\text{Tr}\{O|\psi\rangle\langle\psi|\} = \langle O\rangle.$$

Exercise 3: Consider an arbitrary operator O and two basis vectors $|u_n\rangle$ and $|u_m\rangle$. Show that

$$\text{Tr}\{O|u_n\rangle\langle u_m|\} = O_{mn}.$$

Exercise 4: Consider a density operator ρ and two basis vectors $|u_n\rangle$ and $|u_m\rangle$. Show that

$$\text{Tr}\{\rho|u_n\rangle\langle u_m|\} = \rho_{mn}.$$

Solutions

Exercise 1: Using the formula $\mathrm{Tr}\{|A\rangle\langle B|\} = \langle B|A\rangle$, we can show that

$$\mathrm{Tr}\{O|V\rangle\langle U|\} = \langle U|O|V\rangle.$$

Exercise 2: Use the result of exercise 1 and the definition $\langle O\rangle = \langle\psi|O|\psi\rangle$.

Exercise 3: Use the result of exercise 1 and the definition $O_{mn} = \langle u_m|O|u_n\rangle$.

Exercise 4: Use the result of exercise 1 and the definition $\rho_{mn} = \langle u_m|\rho|u_n\rangle$.

3. TWO-LEVEL ATOMS INTERACTING WITH A LIGHT FIELD

1. Atom+field interaction Hamiltonian
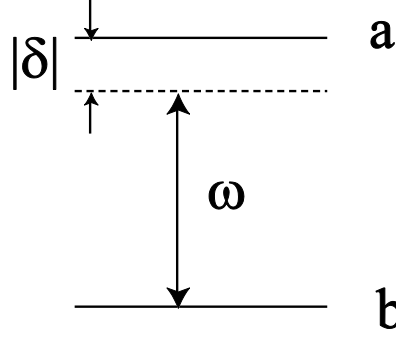
Figure 2: A two-level atom interacting with a light field.

We consider a two-level atom interacting with a light field, see Fig. 2. The total Hamiltonian of the atom in the field is given by

$$H = H_0 + H_I, \tag{168}$$

where H_0 and H_I are the free (unperturbed) and interaction parts.

The free part of the Hamiltonian is the operator for the energy of the atom when it is free and is given by

$$H_0 = \hbar\omega_a \, |a\rangle\langle a| + \hbar\omega_b \, |b\rangle\langle b|. \tag{169}$$

The projection operators $\sigma_{aa} = |a\rangle\langle a|$ and $\sigma_{bb} = |b\rangle\langle b|$ describe the populations (probabilities) of levels a and b, respectively. Indeed, we have

$$\langle\sigma_{aa}\rangle = \text{Tr}\{\rho \, |a\rangle\langle a|\} = \langle a|\rho|a\rangle = \rho_{aa} \tag{170}$$

and

$$\langle\sigma_{bb}\rangle = \text{Tr}\{\rho \, |b\rangle\langle b|\} = \langle b|\rho|b\rangle = \rho_{bb}. \tag{171}$$

Here, the diagonal matrix elements ρ_{aa} and ρ_{bb} of the density operator describe the populations of the atom in levels a and b, respectively. Note that the energy of the atom when it is free is given by

$$\begin{aligned}
\langle H_0\rangle &= \hbar\omega_a\langle|a\rangle\langle a|\rangle + \hbar\omega_b\langle|b\rangle\langle b|\rangle \\
&= \hbar\omega_a\langle\sigma_{aa}\rangle + \hbar\omega_b\langle\sigma_{bb}\rangle \\
&= \hbar\omega_a\rho_{aa} + \hbar\omega_b\rho_{bb}.
\end{aligned} \tag{172}$$

We introduce the Pauli operator $\sigma_z = |a\rangle\langle a| - |b\rangle\langle b|$, which describes the inversion of the populations of the atom. Note that $\langle \sigma_z \rangle = \rho_{aa} - \rho_{bb}$. In terms of the population inversion operator σ_z, we have

$$|a\rangle\langle a| = \frac{1}{2}(1 + \sigma_z),$$
$$|b\rangle\langle b| = \frac{1}{2}(1 - \sigma_z). \tag{173}$$

Hence, we find

$$H_0 = \frac{\hbar\omega_{ab}}{2}\sigma_z + \frac{\hbar}{2}(\omega_a + \omega_b)$$
$$= \frac{\hbar\omega_{ab}}{2}\sigma_z + \text{const}, \tag{174}$$

where $\omega_{ab} = \omega_a - \omega_b$ is the transition frequency of the atom. We can choose the middle point between ω_a and ω_b as the origin for the zero energy. This leads to $\omega_a = \omega_0/2$ and $\omega_b = -\omega_0/2$. Then, the constant is the above expression for the Hamiltonian H_0 is zero. More general, a constant in the Hamiltonian can always be neglected because it commutes with the density operator and the observables operators and consequently does not affect their time evolution.

We now describe the atom-field interaction. The interaction part of the Hamiltonian is the operator for the interaction energy between the atom and the field. We assume that the field is linearly polarized along the *x* direction. We use the dipole approximation for the interaction. Then, the interaction part of the Hamiltonian is given by

$$H_I = -\vec{d} \cdot \vec{E} = -exE$$
$$= -e(|a\rangle\langle a| x_{aa} + |b\rangle\langle b| x_{bb} + |a\rangle\langle b| x_{ab} + |b\rangle\langle a| x_{ba})E$$
$$= -e(|a\rangle\langle b| x_{ab} + |b\rangle\langle a| x_{ba})E$$
$$= -(|a\rangle\langle b| + |b\rangle\langle a|)d_x E. \tag{175}$$

Here we have used the properties $x_{aa} = x_{bb} = 0$, have introduced the notation $d_x = ex_{ab}$, which is called matrix element of the atomic dipole moment, and have assumed for simplicity that x_{ab} and consequently d_x are real parameters.

We present the electric component of the light field in the form

$$E = E_0 \cos \omega t = \frac{1}{2}\left(e^{-i\omega t} + e^{i\omega t}\right)E_0. \tag{176}$$

We introduce the Rabi frequency

$$\Omega = d_x E_0 / \hbar. \tag{177}$$

Then, we obtain

$$H_I = -\frac{\hbar}{2}(|a\rangle\langle b| + |b\rangle\langle a|)(e^{-i\omega t} + e^{i\omega t})\Omega$$
$$= -\frac{\hbar}{2}(\sigma_+ + \sigma_-)(e^{-i\omega t} + e^{i\omega t})\Omega. \tag{178}$$

Here we have introduced the upward transition operator

$$\sigma_+ = \sigma_{ab} = |a\rangle\langle b| \tag{179}$$

and the downward transition operator

$$\sigma_- = \sigma_{ba} = |b\rangle\langle a|. \tag{180}$$

We note that, for a free atom, in the Heisenberg presentation, the transition operators $\sigma_+ = |a\rangle\langle b|$ and $\sigma_- = |b\rangle\langle a|$ oscillate as $e^{i\omega_{ab}t}$ and $e^{-i\omega_{ab}t}$, respectively. Indeed, for a free atom we have $\langle\sigma_-\rangle \equiv \mathrm{Tr}\rho\sigma_- = \mathrm{Tr}\rho|b\rangle\langle a| = \langle a|\rho|b\rangle = \rho_{ab} = \rho_{ab}(0)e^{-i\omega_{ab}t}$. Therefore, the terms $\sigma_+ e^{i\omega t} = |a\rangle\langle b|e^{i\omega t}$ and $\sigma_- e^{-i\omega t} = |b\rangle\langle a|e^{-i\omega t}$ quickly vary as $e^{i(\omega_{ab}+\omega)t}$ and $e^{-i(\omega_{ab}+\omega)t}$, respectively. Meanwhile, $\sigma_+ e^{-i\omega t} = |a\rangle\langle b|e^{-i\omega t}$ and $\sigma_- e^{i\omega t} = |b\rangle\langle a|e^{i\omega t}$ slowly vary as $e^{i(\omega_{ab}-\omega)t}$ and $e^{-i(\omega_{ab}-\omega)t}$, respectively.

Let's come back to the interaction Hamiltonian (178). We neglect the fast rotating terms $|a\rangle\langle b|e^{i\omega t}$ and $|b\rangle\langle a|e^{-i\omega t}$. This approximation is called the rotating-wave approximation. The result is

$$H_I = -\frac{\hbar\Omega}{2}(\sigma_+ e^{-i\omega t} + \sigma_- e^{i\omega t})$$
$$= -\frac{\hbar\Omega}{2}(|a\rangle\langle b|e^{-i\omega t} + |b\rangle\langle a|e^{i\omega t}). \tag{181}$$

Appendix: Properties of the Pauli operators σ_+, σ_-, and σ_z:

The operators $\sigma_+ = |a\rangle\langle b|$, $\sigma_- = |b\rangle\langle a|$, and $\sigma_z = |a\rangle\langle a| - |b\rangle\langle b|$ are called the Pauli operators. The matrix forms of these operators are

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$
$$\sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{182}$$
$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The operators $\sigma_x = \sigma_+ + \sigma_-$ and $\sigma_y = -i(\sigma_+ - \sigma_-)$ together with σ_z are the original Pauli operators invented by W. Pauli to describe the spin 1/2 of an electron in the first half of the last century.

We can easily show that

$$\sigma_+^2 = \sigma_-^2 = 0,$$

$$\sigma_z^2 = 1,$$

$$\sigma_+\sigma_- = \frac{1}{2}(1+\sigma_z),$$

$$\sigma_-\sigma_+ = \frac{1}{2}(1-\sigma_z),$$

$$\sigma_z\sigma_+ = \sigma_+,$$

$$\sigma_z\sigma_- = -\sigma_-,$$

and

$$\sigma_+\sigma_z = -\sigma_+,$$

$$\sigma_-\sigma_z = \sigma_-.$$

The above relations allow us to reduce any function $f(\sigma_+,\sigma_-,\sigma_z)$ of the Pauli operators to a linear form of the type $c_+\sigma_+ + c_-\sigma_- + c_z\sigma_z$.

In particular, we find the following commutation relations:

$$[\sigma_z,\sigma_+] = 2\sigma_+,$$

$$[\sigma_z,\sigma_-] = -2\sigma_-,$$

$$[\sigma_+,\sigma_-] = \sigma_z.$$

Exercise

Consider a free two-level atom, with the Hamiltonian $H = H_0 = \dfrac{\hbar\omega_0}{2}\sigma_z$. Use the commutation relations for the Pauli operators to derive the Heisenberg equations for these operators.

Solution

The Heisenberg equation for the observable O of a quantum system with the Hamiltonian H reads

$$\frac{d}{dt}O = \frac{i}{\hbar}[H,O].$$

When we use the commutation relations $[\sigma_z,\sigma_+] = 2\sigma_+$, $[\sigma_z,\sigma_-] = -2\sigma_-$, and $[\sigma_+,\sigma_-] = \sigma_z$ and the Hamiltonian $H = H_0 = \dfrac{\hbar\omega_0}{2}\sigma_z$, we find

$$\frac{d}{dt}\sigma_z = \frac{i}{2}\omega_0[\sigma_z,\sigma_z] = 0,$$

$$\frac{d}{dt}\sigma_+ = \frac{i}{2}\omega_0[\sigma_z,\sigma_+] = i\omega_0\sigma_+,$$

$$\frac{d}{dt}\sigma_- = \frac{i}{2}\omega_0[\sigma_z,\sigma_-] = -i\omega_0\sigma_-.$$

The solutions to the above equations are $\sigma_z(t) = \sigma_z(0)$, $\sigma_+(t) = \sigma_+(0)\exp(i\omega_0 t)$, and $\sigma_-(t) = \sigma_-(0)\exp(-i\omega_0 t)$.

2. Optical Bloch equations

a) Evolution equations for the state vector of a pure state of a two-level atom

We first consider the case where the state of the atom is a pure state, described by a state vector

$$|\psi\rangle = C_a |a\rangle + C_b |b\rangle. \tag{183}$$

The state vector $|\psi\rangle$ satisfies the Schrödinger equation

$$i\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle = (H_0 + H_I)|\psi\rangle. \tag{184}$$

For the probability amplitudes C_a and C_b, we find the equations

$$\frac{d}{dt}C_a = -i\omega_a C_a + \frac{i\Omega}{2}e^{-i\omega t}C_b,$$

$$\frac{d}{dt}C_b = -i\omega_b C_b + \frac{i\Omega}{2}e^{i\omega t}C_a. \tag{185}$$

The case of exact resonance:

Let consider the case of resonance, where the frequency ω of the field coincides with the atomic transition frequency $\omega_0 = \omega_a - \omega_b$, that is, $\omega = \omega_0$. We change the fast oscillating amplitudes C_a and C_b to the slowly varying amplitudes

$$c_a = C_a e^{i\omega_a t},$$

$$c_b = C_b e^{i\omega_b t}. \tag{186}$$

Then, Eqs. (185) yield

$$\frac{d}{dt}c_a = \frac{i\Omega}{2}c_b,$$

$$\frac{d}{dt}c_b = \frac{i\Omega}{2}c_a. \tag{187}$$

The solutions for c_a and c_b can be written as

$$c_a(t) = c_a(0)\cos\left(\frac{\Omega t}{2}\right) + ic_b(0)\sin\left(\frac{\Omega t}{2}\right),$$

$$c_b(t) = c_b(0)\cos\left(\frac{\Omega t}{2}\right) + ic_a(0)\sin\left(\frac{\Omega t}{2}\right). \tag{188}$$

This solution is general with respect to the initial condition.

Example 1:

We consider the situation where the atom is initially in the ground state b, that is, $c_a(0) = 0$ and $c_b(0) = 1$. In this case, we find

$$c_a(t) = i\sin\left(\frac{\Omega t}{2}\right),$$

$$c_b(t) = \cos\left(\frac{\Omega t}{2}\right). \tag{189}$$

Hence, we have

$$C_a(t) = i\sin\left(\frac{\Omega t}{2}\right)e^{-i\omega_a t},$$

$$C_b(t) = \cos\left(\frac{\Omega t}{2}\right)e^{-i\omega_b t}. \tag{190}$$

The populations of the levels, described by the diagonal matrix elements ρ_{aa} and ρ_{bb}, are found to be

$$\rho_{aa}(t) = |C_a(t)|^2 = \sin^2\left(\frac{\Omega t}{2}\right),$$

$$\rho_{bb}(t) = |C_b(t)|^2 = \cos^2\left(\frac{\Omega t}{2}\right). \tag{191}$$

As seen, the populations oscillate in time, with the frequency Ω. Such oscillations are caused by the driving field. They are different from the optical oscillations, which occur with the frequency ω. The oscillations of the populations, caused by the driving field, are called the Rabi oscillations, and Ω is called the Rabi frequency. The Rabi oscillations mean that the atom jumps forth and back between the ground and excited states.

Meanwhile, the coherence (interference) is described by the off-diagonal matrix element

$$\begin{aligned}
\rho_{ab}(t) &= C_a(t)C_b^*(t) \\
&= i\sin\left(\frac{\Omega t}{2}\right)\cos\left(\frac{\Omega t}{2}\right)e^{-i(\omega_a - \omega_b)t} \\
&= \frac{i}{2}\sin(\Omega t)e^{-i\omega_0 t} = \frac{i}{2}\sin(\Omega t)e^{-i\omega t}.
\end{aligned} \tag{192}$$

Note that the coherence ρ_{ab} oscillates with the optical frequency $\omega_0 = \omega$, and the slowly varying envelope of the coherence oscillates with the Rabi frequency Ω. We usually have $\Omega \ll \omega$. Thus, the Rabi oscillations are usually very slow compared to the optical oscillations.

Example 2:

We consider the situation where the atom is initially in the excited state *a*, that is, $c_a(0) = 1$ and $c_b(0) = 0$. In this case, we find

$$c_a(t) = \cos\left(\frac{\Omega t}{2}\right)$$
$$c_b(t) = i\sin\left(\frac{\Omega t}{2}\right). \tag{193}$$

Hence, we have

$$C_a(t) = \cos\left(\frac{\Omega t}{2}\right)e^{-i\omega_a t},$$
$$C_b(t) = i\sin\left(\frac{\Omega t}{2}\right)e^{-i\omega_b t}. \tag{194}$$

The populations of the levels, described by the diagonal matrix elements ρ_{aa} and ρ_{bb}, are found to be

$$\rho_{aa}(t) = |C_a(t)|^2 = \cos^2\left(\frac{\Omega t}{2}\right),$$
$$\rho_{bb}(t) = |C_b(t)|^2 = \sin^2\left(\frac{\Omega t}{2}\right). \tag{195}$$

As seen, the populations oscillate in time, with the Rabi frequency Ω. Meanwhile, the coherence (interference) is

$$\rho_{ab}(t) = C_a(t)C_b^*(t)$$
$$= -i\sin\left(\frac{\Omega t}{2}\right)\cos\left(\frac{\Omega t}{2}\right)e^{-i(\omega_a - \omega_b)t} \tag{196}$$
$$= -\frac{i}{2}\sin(\Omega t)e^{-i\omega_0 t} = -\frac{i}{2}\sin(\Omega t)e^{-i\omega t}.$$

We also observe that the coherence ρ_{ab} oscillates with the optical frequency $\omega_0 = \omega$, and the slowly varying envelope of the coherence oscillates with the Rabi frequency Ω.

Example 3:

We consider the situation where the atom is initially in a linear superposition of the excited state *a* and the ground state *b*, with the probability amplitudes $c_a(0) = 1/\sqrt{2}$ and $c_b(0) = 1/\sqrt{2}$. In this case, we obtain the solution

$$c_a(t) = c_b(t) = \frac{1}{\sqrt{2}} \left[\cos\left(\frac{\Omega t}{2}\right) + i \sin\left(\frac{\Omega t}{2}\right) \right], \tag{197}$$

which leads to

$$C_a(t) = \frac{1}{\sqrt{2}} \left[\cos\left(\frac{\Omega t}{2}\right) + i \sin\left(\frac{\Omega t}{2}\right) \right] e^{-i\omega_a t},$$

$$C_b(t) = \frac{1}{\sqrt{2}} \left[\cos\left(\frac{\Omega t}{2}\right) + i \sin\left(\frac{\Omega t}{2}\right) \right] e^{-i\omega_b t}. \tag{198}$$

Hence, we find that the populations of the levels are constant in time:

$$\rho_{aa}(t) = \rho_{bb}(t) = 1/2. \tag{199}$$

We also find that the coherence is oscillating in time, with a constant envelope:

$$\rho_{ab}(t) = C_a(t) C_b^*(t) = \frac{1}{2} e^{-i(\omega_a - \omega_b)t} = \frac{1}{2} e^{-i\omega_0 t} = \frac{1}{2} e^{-i\omega t}. \tag{200}$$

b) Evolution equations for the density operator of a general quantum state of a two-level atom with no decay

We now consider the case where the state of the atom is an arbitrary state, described by a density operator ρ. The density operator ρ is governed by the Schrödinger equation

$$\frac{d}{dt}\rho = \frac{1}{i\hbar}[H, \rho]. \tag{201}$$

To obtain the evolution equations for the matrix elements of ρ, we can use Eq. (201) directly. For this purpose, we write

$$\frac{d}{dt}\rho = -i(O - O^\dagger), \tag{202}$$

where

$$O = \frac{1}{\hbar} H \rho. \tag{203}$$

In the matrix form, we have

$$\frac{d}{dt}\rho_{\alpha\beta} = -i(O_{\alpha\beta} - O^\dagger{}_{\alpha\beta}) = -i(O_{\alpha\beta} - O^*_{\beta\alpha}). \tag{204}$$

Let's calculate the matrix elements $O_{\alpha\beta}$. When we use the explicit expression for the Hamiltonian $H = H_0 + H_I$, we find

$$O = \frac{1}{\hbar} H \rho = \frac{1}{\hbar}(H_0 + H_I)\rho$$

$$= \omega_a |a\rangle\langle a| \rho + \omega_b |b\rangle\langle b| \rho - \frac{\Omega}{2}(|a\rangle\langle b| \rho e^{-i\omega t} + |b\rangle\langle a| \rho e^{i\omega t}). \tag{205}$$

We can easily show that

$$O_{aa} = \omega_a \rho_{aa} - \frac{\Omega}{2} \rho_{ba} e^{-i\omega t},$$

$$O_{bb} = \omega_b \rho_{bb} - \frac{\Omega}{2} \rho_{ab} e^{i\omega t},$$

$$O_{ab} = \omega_a \rho_{ab} - \frac{\Omega}{2} \rho_{bb} e^{-i\omega t},$$

$$O_{ba} = \omega_b \rho_{ba} - \frac{\Omega}{2} \rho_{aa} e^{i\omega t}. \tag{206}$$

When we insert the above matrix elements into Eq. (204), we obtain

$$\frac{d}{dt} \rho_{aa} = \frac{i\Omega}{2}(e^{-i\omega t} \rho_{ba} - e^{i\omega t} \rho_{ab}),$$

$$\frac{d}{dt} \rho_{bb} = -\frac{i\Omega}{2}(e^{-i\omega t} \rho_{ba} - e^{i\omega t} \rho_{ab}),$$

$$\frac{d}{dt} \rho_{ab} = -i\omega_{ab}\rho_{ab} - \frac{i\Omega}{2} e^{-i\omega t}(\rho_{aa} - \rho_{bb}). \tag{207}$$

Note that we can also derive Eqs. (207) with the use of Eqs. (185) and the definitions

$$\rho_{aa} = |C_a|^2,$$

$$\rho_{bb} = |C_b|^2,$$

$$\rho_{ab} = C_a C_b^*,$$

$$\rho_{ba} = \rho_{ab}^*. \tag{208}$$

We introduce the notation $\delta = \omega - \omega_{ab}$ for the detuning of the field. It is convenient to use new variables

$$\tilde{\rho}_{ab} = e^{i\omega t} \rho_{ab},$$

$$\tilde{\rho}_{ba} = e^{-i\omega t} \rho_{ba},$$

$$\tilde{\rho}_{aa} = \rho_{aa},$$

$$\tilde{\rho}_{bb} = \rho_{bb}. \tag{209}$$

In terms of these variables, we have

$$\frac{d}{dt}\tilde{\rho}_{aa} = \frac{i\Omega}{2}(\tilde{\rho}_{ba} - \tilde{\rho}_{ab}),$$

$$\frac{d}{dt}\tilde{\rho}_{bb} = -\frac{i\Omega}{2}(\tilde{\rho}_{ba} - \tilde{\rho}_{ab}), \tag{210}$$

$$\frac{d}{dt}\tilde{\rho}_{ab} = i\delta\tilde{\rho}_{ab} - \frac{i\Omega}{2}(\tilde{\rho}_{aa} - \tilde{\rho}_{bb}).$$

The above equations are called the optical Bloch equations for two-level atoms without decay.

Example:

We consider the situation where the atom is initially in a statistical mixture of the excited state *a* and the ground state *b*, with the weight factors $p_a = p_b = 1/2$. In this case, the matrix elements of the initial density of the atom are given by

$$\rho_{aa}(0) = \rho_{bb}(0) = 1/2,$$

$$\rho_{ab}(0) = \rho_{ba}(0) = 0. \tag{211}$$

Consequently, we have

$$\tilde{\rho}_{aa}(0) = \tilde{\rho}_{bb}(0) = 1/2,$$

$$\tilde{\rho}_{ab}(0) = \tilde{\rho}_{ba}(0) = 0. \tag{212}$$

The Bloch equations show that the above values are true for any time *t*, that is,

$$\tilde{\rho}_{aa}(t) = \tilde{\rho}_{bb}(t) = 1/2,$$

$$\tilde{\rho}_{ab}(t) = \tilde{\rho}_{ba}(t) = 0. \tag{213}$$

Note that the above solutions and the solutions for example 3 in the previous subsection give the same populations but different coherences.

Exercise

Derive Eqs. (207) from Eqs. (185). Such a derivation is valid only for the case of a pure state. However, the result is general: it coincides with that for an arbitrary state.

Solution

Equations (185) and their complex conjugates can be written as

$$\frac{d}{dt}C_a = -i\omega_a C_a + \frac{i\Omega}{2}e^{-i\omega t}C_b,$$

$$\frac{d}{dt}C_a^* = i\omega_a C_a^* - \frac{i\Omega}{2}e^{i\omega t}C_b^*,$$

$$\frac{d}{dt}C_b = -i\omega_b C_b + \frac{i\Omega}{2}e^{i\omega t}C_a,$$

$$\frac{d}{dt}C_b^* = i\omega_b C_b^* - \frac{i\Omega}{2}e^{-i\omega t}C_a^*.$$

When we use the above equations and the relations

$$\rho_{aa} = |C_a|^2,$$
$$\rho_{bb} = |C_b|^2,$$
$$\rho_{ab} = C_a C_b^*,$$
$$\rho_{ba} = \rho_{ab}^*,$$

we can easily derive Eqs. (207).

c) Evolution equations for the density operator of a system with decay

We now include the spontaneous emission of the atom into our treatment. In this case, the state of the atom is described by a reduced density operator ρ, which is governed by the master equation

$$\frac{d}{dt}\rho = \frac{1}{i\hbar}[H,\rho] + \Lambda\rho, \tag{214}$$

where the last term describes the decay and is given by

$$\Lambda\rho = -\frac{\Gamma}{2}[\sigma_+\sigma_-\rho - 2\sigma_-\rho\sigma_+ + \rho\sigma_+\sigma_-]. \tag{215}$$

We can rewrite Eq. (214) as

$$\dot{\rho} = (\dot{\rho})_{\text{coherent}} + (\dot{\rho})_{\text{decay}}, \tag{216}$$

where

$$(\dot{\rho})_{\text{coherent}} = \frac{1}{i\hbar}[H,\rho] \tag{217}$$

and

$$(\dot{\rho})_{\text{decay}} = \Lambda\rho = -\frac{\Gamma}{2}[\sigma_+\sigma_-\rho - 2\sigma_-\rho\sigma_+ + \rho\sigma_+\sigma_-]. \tag{218}$$

In the matrix form, we have

$$\dot{\rho}_{\alpha\beta} = (\dot{\rho}_{\alpha\beta})_{\text{coherent}} + (\dot{\rho}_{\alpha\beta})_{\text{decay}}. \tag{219}$$

The matrix elements $(\dot{\rho}_{\alpha\beta})_{\text{coherent}}$ are the matrix elements of the operator $(\dot{\rho})_{\text{coherent}} = \frac{1}{i\hbar}[H,\rho]$. They are given by Eqs. (207). The matrix elements $(\dot{\rho}_{\alpha\beta})_{\text{decay}}$ are the matrix elements of the operator $(\dot{\rho})_{\text{decay}} = \Lambda\rho = -\frac{\Gamma}{2}[\sigma_+\sigma_-\rho - 2\sigma_-\rho\sigma_+ + \rho\sigma_+\sigma_-]$. They are given by the expressions on the right-hand side of Eqs. (166). Indeed, we can easily show that

$$\begin{aligned}
(\dot{\rho}_{aa})_{\text{decay}} &= (\Lambda\rho)_{aa} = -\Gamma\rho_{aa}, \\
(\dot{\rho}_{bb})_{\text{decay}} &= (\Lambda\rho)_{bb} = \Gamma\rho_{aa}, \\
(\dot{\rho}_{ab})_{\text{decay}} &= (\Lambda\rho)_{ab} = -\frac{\Gamma}{2}\rho_{ab}.
\end{aligned} \quad (220)$$

To obtain the evolution equations for the matrix elements of ρ, we add to Eqs. (207) the decay terms (220). This procedure leads to

$$\begin{aligned}
\frac{d}{dt}\rho_{aa} &= -\Gamma\rho_{aa} + \frac{i\Omega}{2}(e^{-i\omega t}\rho_{ba} - e^{i\omega t}\rho_{ab}), \\
\frac{d}{dt}\rho_{bb} &= \Gamma\rho_{aa} - \frac{i\Omega}{2}(e^{-i\omega t}\rho_{ba} - e^{i\omega t}\rho_{ab}), \\
\frac{d}{dt}\rho_{ab} &= -\left(i\omega_{ab} + \frac{\Gamma}{2}\right)\rho_{ab} - \frac{i\Omega}{2}e^{-i\omega t}(\rho_{aa} - \rho_{bb}).
\end{aligned} \quad (221)$$

We introduce the notation $\delta = \omega - \omega_{ab}$ for the detuning of the field. It is convenient to use new variables

$$\begin{aligned}
\tilde{\rho}_{ab} &= e^{i\omega t}\rho_{ab}, \\
\tilde{\rho}_{ba} &= e^{-i\omega t}\rho_{ba}, \\
\tilde{\rho}_{aa} &= \rho_{aa}, \\
\tilde{\rho}_{bb} &= \rho_{bb}.
\end{aligned} \quad (222)$$

Using these variables, we obtain

$$\begin{aligned}
\frac{d}{dt}\tilde{\rho}_{aa} &= -\Gamma\tilde{\rho}_{aa} + \frac{i\Omega}{2}(\tilde{\rho}_{ba} - \tilde{\rho}_{ab}), \\
\frac{d}{dt}\tilde{\rho}_{bb} &= \Gamma\tilde{\rho}_{aa} - \frac{i\Omega}{2}(\tilde{\rho}_{ba} - \tilde{\rho}_{ab}), \\
\frac{d}{dt}\tilde{\rho}_{ab} &= \left(i\delta - \frac{\Gamma}{2}\right)\tilde{\rho}_{ab} - \frac{i\Omega}{2}(\tilde{\rho}_{aa} - \tilde{\rho}_{bb}).
\end{aligned} \quad (223)$$

The above equations are called the optical Bloch equations for two-level atoms with decay.

The above optical Bloch equations play an important role in optics. In particular, they are used to calculate the absorption spectrum of the atoms.

3. Absorption spectrum: saturation and power broadening

We introduce the population difference

$$w = \tilde{\rho}_{aa} - \tilde{\rho}_{bb} \tag{224}$$

and the optical coherence

$$\rho_c = \tilde{\rho}_{ab}. \tag{225}$$

Then, we can rewrite Eqs. (223) as

$$\frac{d}{dt} w = -\Gamma(w+1) + i\Omega(\rho_c^* - \rho_c),$$
$$\frac{d}{dt} \rho_c = \left(i\delta - \frac{\Gamma}{2} \right) \rho_c - \frac{i\Omega}{2} w. \tag{226}$$

We consider the adiabatic (steady-state) regime where

$$\frac{dw}{dt} = \frac{d\rho_c}{dt} = 0. \tag{227}$$

In this regime, Eqs. (226) yield

$$-\Gamma w + i\Omega(\rho_c^* - \rho_c) = \Gamma,$$
$$\left(i\delta - \frac{\Gamma}{2} \right) \rho_c = \frac{i\Omega}{2} w. \tag{228}$$

The solutions to the above equations are

$$w = -\frac{1}{1+s} \tag{229}$$

and

$$\rho_c = \frac{i\Omega}{2(\Gamma/2 - i\delta)(1+s)}. \tag{230}$$

Here s is the saturation parameter and is given by

$$s = \frac{\Omega^2}{2|\Gamma/2 - i\delta|^2} = \frac{\Omega^2/2}{\delta^2 + \Gamma^2/4} = \frac{s_0}{1+(2\delta/\Gamma)^2}, \tag{231}$$

where s_0 is the on-resonance saturation parameter and is defined as

$$s_0 = \frac{2\Omega^2}{\Gamma^2}. \tag{232}$$

For low saturation, $s \ll 1$, the population is mostly in the ground state ($w \cong -1$). For high saturation, $s \gg 1$, the population is almost equally distributed between the ground and excited states ($w \to 0$, i.e. $\rho_{aa}, \rho_{bb} \to 1/2$).

The parameter s_0 can be written in another form

$$s_0 = \frac{I}{I_s}. \tag{233}$$

Here

$$I = c\varepsilon_0 E_0^2 / 2 \tag{234}$$

is the intensity of the laser beam and

$$I_s = \frac{c\varepsilon_0}{2} \frac{\hbar^2 \Gamma^2}{2d_x^2} \tag{235}$$

is the so-called saturation intensity. According to the Weisskopf-Wigner theory, we have

$$\Gamma = \omega_0^3 \, |\vec{d}\,|^2 \, /3\pi\varepsilon_0 \hbar c^3 = \omega_0^3 d_x^2 / \pi\varepsilon_0 \hbar c^3. \tag{236}$$

Here we have introduced for convenience a new notation $\omega_0 = \omega_{ab} = \omega_a - \omega_b$. With the help of Eq. (236), we can show that

$$I_s = \pi hc\Gamma / \lambda_0^3 = \pi hc / \lambda_0^3 \tau, \tag{237}$$

where

$$\tau = 1/\Gamma \tag{238}$$

is the lifetime of the excited state and λ_0 is the atomic resonant wavelength.

The population of the excited state is given by

$$\rho_{aa} = \frac{1}{2}(1 + w) = \frac{s}{2(1+s)} = \frac{s_0/2}{1 + s_0 + (2\delta/\Gamma)^2}. \tag{239}$$

Since the population in the excited state decays at a rate Γ, the total scattering rate γ_{scatt} of light from the laser field is given by

$$\gamma_{\text{scatt}} = \Gamma \rho_{aa} = \frac{s_0 \Gamma / 2}{1 + s_0 + (2\delta/\Gamma)^2}. \tag{240}$$

Note that, at high intensity, γ_{scatt} saturates to $\Gamma/2$.

Equation (240) can be rewritten as

$$\gamma_{\text{scatt}} = \frac{s_0}{1 + s_0} \frac{\Gamma/2}{1 + (2\delta/\Gamma')^2}, \tag{241}$$

where

$$\Gamma' = \Gamma\sqrt{1 + s_0}. \tag{242}$$

The dependence of the scattering rate γ_{scatt} on the detuning δ is shown in Fig. 3 for several values of the saturation parameter s_0. This dependence describes the absorption spectrum. The width of the spectral profile is characterized by Γ'. Note that the width Γ' increases with increasing intensity of the field. This phenomenon is called the power broadening of the spectral profile.

The power broadening is a direct result of the fact that, for large s_0, the absorption continues to increase with increasing intensity in the wings, whereas, in the center, half of the atoms are already in the excited state. The absorption in the center is saturated, whereas in the wings it is not.
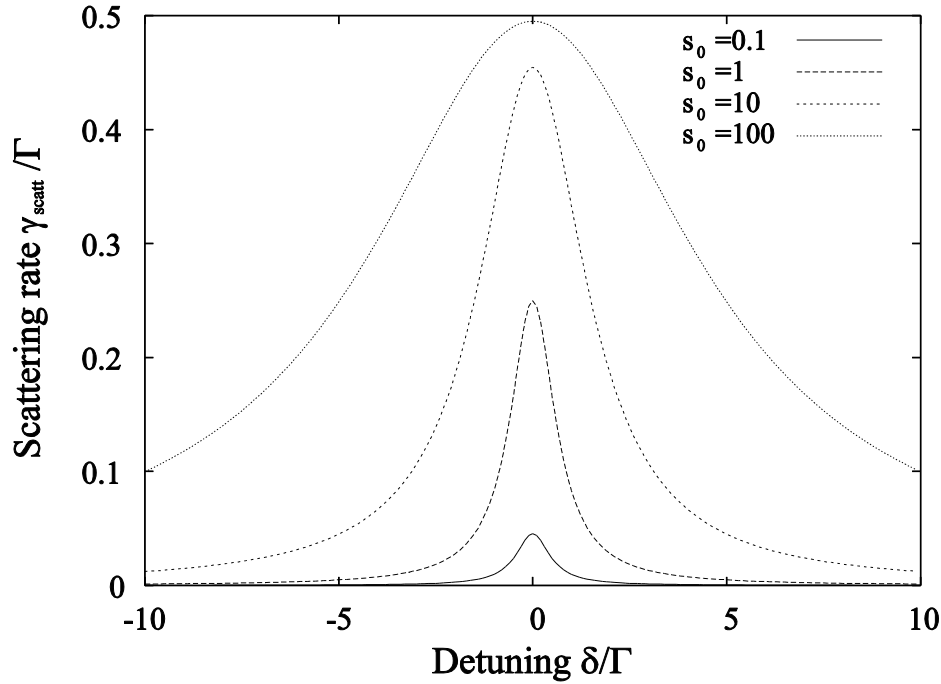
Figure 3: Scattering rate γ_{scatt} as a function of the detuning for several values of the saturation parameter s_0.

The scattering results in intensity loss when the beam travels through a sample of atoms. The amount of scattered power per unit of volume is $n\hbar\omega\gamma_{scatt}$, where n is the number density of the atoms. Thus, we have

$$\frac{dI}{dz} = -n\hbar\omega\gamma_{scatt} = -n\hbar\omega\frac{s_0\Gamma/2}{1 + s_0 + (2\delta/\Gamma)^2} = -\frac{n\hbar\omega(\Gamma/2)(I/I_s)}{1 + s_0 + (2\delta/\Gamma)^2} \tag{243}$$
$$= -n\sigma I = -\alpha I.$$

Here σ is the scattering cross section and $\alpha = n\sigma$ is the absorption coefficient. These coefficients are given by

$$\sigma = \frac{\alpha}{n} = \frac{\hbar\omega\Gamma}{2I_s} \frac{1}{1 + s_0 + (2\delta/\Gamma)^2}. \tag{244}$$

When we use the expressions $I_s = \frac{c\varepsilon_0}{2} \frac{\hbar^2\Gamma^2}{2d_x^2} = \frac{\pi hc\Gamma}{\lambda_0^3}$, we can rewrite Eq. (244) as

$$\begin{aligned}\sigma = \frac{\alpha}{n} &= \left(\frac{2\omega d_x^2}{\varepsilon_0\hbar c\Gamma}\right)\frac{1}{1 + s_0 + (2\delta/\Gamma)^2} \\ &\cong \frac{\lambda_0^2}{2\pi}\frac{1}{1 + s_0 + (2\delta/\Gamma)^2}.\end{aligned} \tag{245}$$

For low intensity, $s_0 \ll 1$, we have

$$\begin{aligned}\sigma = \frac{\alpha}{n} &= \left(\frac{2\omega d_x^2}{\varepsilon_0\hbar c\Gamma}\right)\frac{1}{1 + (2\delta/\Gamma)^2} \\ &\cong \frac{\lambda_0^2}{2\pi}\frac{1}{1 + (2\delta/\Gamma)^2}.\end{aligned} \tag{246}$$

In this regime, the absorption coefficient α is independent of the field intensity I. Therefore, the solution for the field intensity is

$$I(z) = I_0 e^{-\alpha z}. \tag{247}$$

At exact resonance ($\omega = \omega_0$), the cross section (89) reduces to

$$\sigma = \frac{\alpha}{n} = \frac{\lambda_0^2}{2\pi}. \tag{248}$$

In the case where $I \gg I_s$, the absorption coefficient α tends to zero. This does not mean the vanishing of the absorption. Indeed, in the limit

$$I \gg I_s \tag{249}$$

we have

$$\alpha I \to n\hbar\omega\Gamma/2. \tag{250}$$

Hence, Eq. (243) yields

$$\frac{dI}{dz} = -\alpha I = -n\hbar\omega(\Gamma/2). \tag{251}$$

The solution to the above equation is

$$I = I(0) - n\hbar\omega(\Gamma/2)z. \tag{252}$$

According to the above equation, the field intensity will linearly reduce with increasing propagation length. However, after the field intensity I becomes small as compared to the saturation intensity I_s, the field intensity I will exponentially decrease with increasing propagation length z.

4. Field propagation equation

We study the propagation of the field along the z direction. The one-dimensional wave equation reads

$$\left(\frac{\partial^2}{\partial z^2} - \frac{\partial^2}{c^2 \partial t^2} \right) E = \mu_0 \frac{\partial^2}{\partial t^2} P = \frac{1}{\varepsilon_0 c^2} \frac{\partial^2}{\partial t^2} P, \tag{253}$$

where P is the polarization density. We expand the field and the polarization in the forms

$$E = \frac{1}{2} \left[E_0 e^{-i(\omega t - kz)} + E_0^* e^{i(\omega t - kz)} \right],$$

$$P = \frac{1}{2} \left[P_0 e^{-i(\omega t - kz)} + P_0^* e^{i(\omega t - kz)} \right]. \tag{254}$$

Here ω and $k = \omega / c$ are the frequency and wave number of the field, respectively.

We introduce new variables

$$\zeta = z,$$

$$\tau = t - z / c. \tag{255}$$

In terms of these variables, we have

$$E = \frac{1}{2} \left(E_0 e^{-i\omega\tau} + E_0^* e^{i\omega\tau} \right),$$

$$P = \frac{1}{2} \left(P_0 e^{-i\omega\tau} + P_0^* e^{i\omega\tau} \right). \tag{256}$$

We also have

$$\frac{\partial}{\partial z} = \frac{\partial}{\partial \zeta} - \frac{\partial}{c\partial \tau},$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau}, \tag{257}$$

and, consequently,

$$\frac{\partial^2}{\partial z^2} = \frac{\partial^2}{\partial \zeta^2} - \frac{2}{c} \frac{\partial^2}{\partial \zeta \partial \tau} + \frac{\partial^2}{c^2 \partial \tau^2},$$

$$\frac{\partial^2}{\partial t^2} = \frac{\partial^2}{\partial \tau^2}. \tag{258}$$

On substituting Eqs. (256) and (258) into Eq. (253), we find

$$e^{-i\omega\tau}\left(\frac{\partial^2}{\partial\zeta^2} - \frac{2}{c}\frac{\partial^2}{\partial\zeta\partial\tau} + \frac{2i\omega}{c}\frac{\partial}{\partial\zeta}\right)E_0 + \text{c.c.}$$

$$= e^{-i\omega\tau}\frac{1}{\varepsilon_0 c^2}\left(\frac{\partial^2}{\partial\tau^2} - 2i\omega\frac{\partial}{\partial\tau} - \omega^2\right)P_0 + \text{c.c.} \tag{259}$$

The above equation will be satisfied if

$$\left(\frac{\partial^2}{\partial\zeta^2} - \frac{2}{c}\frac{\partial^2}{\partial\zeta\partial\tau} + \frac{2i\omega}{c}\frac{\partial}{\partial\zeta}\right)E_0 = \frac{1}{\varepsilon_0 c^2}\left(\frac{\partial^2}{\partial\tau^2} - 2i\omega\frac{\partial}{\partial\tau} - \omega^2\right)P_0. \tag{260}$$

We assume that the envelopes E_0 and P_0 vary slowly in space and time. When we keep only the lowest nonvanishing order on each side of Eq. (260), we obtain

$$\frac{\partial}{\partial\zeta}E_0 = \frac{i\omega}{2\varepsilon_0 c}P_0. \tag{261}$$

Since $\zeta = z$, we can rewrite Eq. (261) as

$$\frac{\partial}{\partial z}E_0 = \frac{i\omega}{2\varepsilon_0 c}P_0 = \frac{ik}{2\varepsilon_0}P_0, \tag{262}$$

keeping in mind that the partial derivative with respect to z in Eq. (262) is taken under the condition $\tau = t - z/c = \text{constant}$. Equation (262) is called the propagation equation for the field in the slowly varying envelope approximation.

5. Susceptibility, refractive index, and absorption coefficient

We have

$$P_0 = \varepsilon_0\chi E_0, \tag{263}$$

where χ is the susceptibility. We write

$$\chi = \chi' + i\chi'', \tag{264}$$

where χ' and χ'' are the real and imaginary parts of χ. Then, Eq. (262) becomes

$$\frac{\partial}{\partial z}E_0 = \frac{i\omega}{2c}(\chi' + i\chi'')E_0 = \frac{\omega}{2c}(i\chi' - \chi'')E_0. \tag{265}$$

The real part χ' determines the shift of the wave number of the field, while the imaginary part χ'' determines absorption. The refractive index of the medium is defined by

$$n_{\text{ref}} = 1 + \frac{\chi'}{2}, \tag{266}$$

while the absorption coefficient is defined by

$$\alpha = \frac{\omega}{c}\chi'' = k\chi''. \tag{267}$$

In terms of n_{ref} and α, we can rewrite Eq. (265) as

$$\frac{\partial}{\partial z}E_0 = \left[ik(n_{\text{ref}} - 1) - \frac{\alpha}{2}\right]E_0. \tag{268}$$

At low intensity, we can ignore the dependences of n_{ref} and α on the field intensity. In this case, the solution of Eq. (268) for the field envelope E_0 is

$$E_0 = Ae^{ik(n_{\text{ref}}-1)z}e^{-\alpha z/2}. \tag{269}$$

When we use the presentation $A = |A|e^{i\varphi}$ and the formula,

$$E = \frac{1}{2}\left[E_0 e^{-i(\omega t - kz)} + E_0^* e^{i(\omega t - kz)}\right], \tag{270}$$

we obtain

$$E = |A|e^{-\alpha z/2}\cos(\omega t - kn_{\text{ref}}z - \varphi). \tag{271}$$

The expression (271) explains why n_{ref} is called the refractive index and why α is called the absorption coefficient.

We now calculate χ, n_{ref}, and α. As shown in Sec. I.2.e, the polarization of a single two-level atom is $P = d_x(\rho_{ab} + \rho_{ba})$. Here, we have assumed for simplicity that d_x is a real parameter. For a medium with the atomic density n, the polarization density of the medium is given by

$$P = nd_x(\rho_{ab} + \rho_{ba}) = nd_x(\rho_c e^{-i\omega \tau} + \rho_c^* e^{i\omega \tau}). \tag{272}$$

Consequently, the envelope of the polarization density is

$$P_0 = 2nd_x\rho_c. \tag{273}$$

Inserting Eq. (230) into Eq. (273) yields

$$\begin{aligned} P_0 &= 2nd_x \frac{i\Omega}{(\Gamma - 2i\delta)(1+s)} \\ &= i\frac{2nd_x^2}{\hbar}\frac{E_0}{(\Gamma - 2i\delta)(1+s)}. \end{aligned} \tag{274}$$

Hence, we have

$$P_0 = \varepsilon_0 \chi E_0, \tag{275}$$

where the susceptibility is given by

$$\chi = \frac{P_0}{\varepsilon_0 E_0}$$

$$= i\frac{2nd_x^2}{\varepsilon_0 \hbar} \frac{1}{(\Gamma - 2i\delta)(1+s)} \tag{276}$$

$$= i\frac{2nd_x^2}{\varepsilon_0 \hbar \Gamma^2} \frac{\Gamma + 2i\delta}{1 + s_0 + (2\delta/\Gamma)^2}.$$

Then, we find

$$\chi' = -\left(\frac{4nd_x^2}{\varepsilon_0 \hbar \Gamma^2}\right)\frac{\delta}{1 + s_0 + (2\delta/\Gamma)^2} \tag{277}$$

and

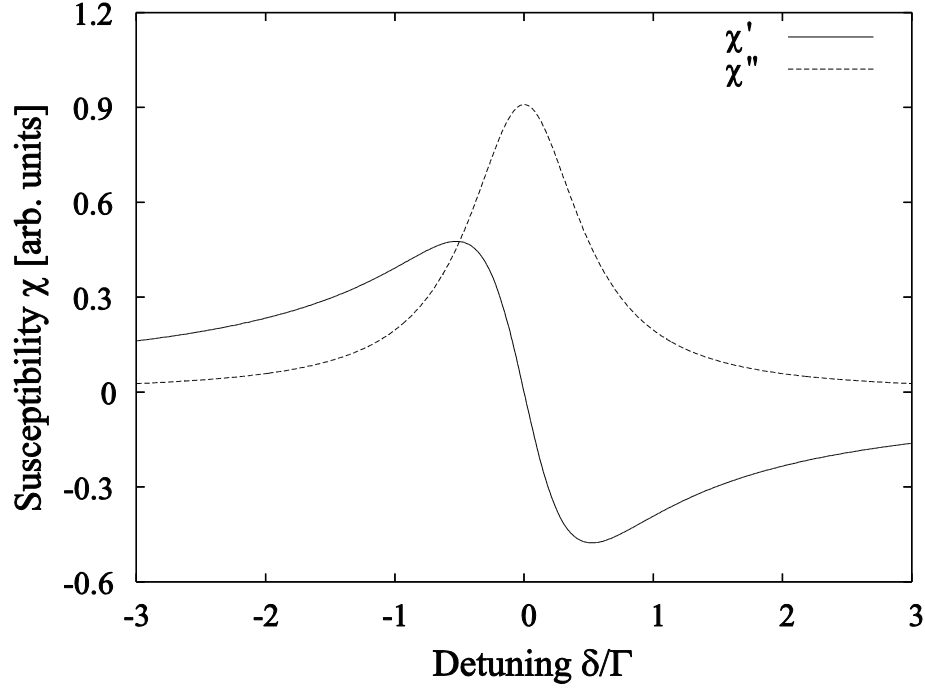$$\chi'' = \left(\frac{2nd_x^2}{\varepsilon_0 \hbar \Gamma}\right)\frac{1}{1 + s_0 + (2\delta/\Gamma)^2}. \tag{278}$$

With the help of Eqs. (266) and (267), we obtain

$$n_{\text{ref}} = 1 - \left(\frac{2nd_x^2}{\varepsilon_0 \hbar \Gamma^2}\right)\frac{\delta}{1 + s_0 + (2\delta/\Gamma)^2}$$

$$= 1 - \frac{n\lambda_0^3}{4\pi^2}\frac{\delta/\Gamma}{1 + s_0 + (2\delta/\Gamma)^2} \tag{279}$$

and

$$\alpha = \left(\frac{2n\omega d_x^2}{\varepsilon_0 \hbar c \Gamma}\right)\frac{1}{1 + s_0 + (2\delta/\Gamma)^2}$$

$$\cong \frac{n\lambda_0^2}{2\pi}\frac{1}{1 + s_0 + (2\delta/\Gamma)^2}. \tag{280}$$

Here we have used the expression $\Gamma = \omega_0^3 d_x^2 / \pi \varepsilon_0 \hbar c^3$ and the approximation $\omega \cong \omega_0$. Equation (280) is in agreement with Eq. (245). Note that n_{ref} and α depend on the field intensity via the saturation parameter s_0.

Figure 4: Real and imaginary parts of the susceptibility as functions of the normalized detuning δ/Γ **of the field for the saturation parameter** $s_0 = 0.1$.

According to Eqs. (266) and (267), the real part χ' and the imaginary part χ'' of the susceptibility determine the refractive index n_{ref} and the absorption coefficient α. We illustrate in Fig. 4 the frequency dependence of χ' and χ''. The figure shows that χ' is large in the region $\delta/\Gamma \leq 1$. However, in this region, χ'' is also large. Thus, in a medium of two-level atoms, a high refractive index is accompanied by large dispersion.