

Review of Quantum Mechanics

Jhih-Sheng Wu

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Quantum mechanics is a modern mathematical theory used to describe the quantum phenomena. Although many scientists think it is not the ultimate theory, it is the most accurate theory today that describes the experiments. Quantum mechanics is formulated under the postulates, which are made by the scientists to explain the experiments. In classical mechanics, a physical system consists of physical quantities which have definite values. For examples, the position x and the momentum p of a particle at any given time t are assumed to be some numbers. On the contrary, a physical system in quantum mechanics is described by a state $|\psi\rangle$. The notation $|\psi\rangle$ is called a ket. In a closed system, the state $|\psi\rangle$ contains all the information of the systems. The exotic part of quantum mechanics is that even $|\psi\rangle$ is complete, the outcome of observed quantities are still probabilistic.

1 Wavefunction

Let's use the wavefunction to elaborate the nature of probability. The wavefunction of a particle is obtained by writing $|\psi\rangle$ in the x basis $|x\rangle$,

$$\psi(x) \equiv \langle x|\psi\rangle. \quad (1)$$

For a given wavefunction $\psi(x)$, the probability to find the particle to be at x is $|\psi(x)|^2 dx$. Since the total probability is one, the normalization of a state requires that

$$\int |\psi(x)|^2 dx = 1. \quad (2)$$

The average position $\langle x \rangle$ (expectation value) of the particle is

$$\langle x \rangle = \int x |\psi(x)|^2 dx. \quad (3)$$

With the definitions, the well known Schrödinger's equation reads

$$i\hbar \frac{\partial}{\partial t} \psi = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + V(x)\psi. \quad (4)$$

The representation of a state $|\psi\rangle$ is not unique. For example, we can use the momentum basis $|p\rangle$ to write $|\psi\rangle$,

$$\phi(p) \equiv \langle p|\psi\rangle, \quad (5)$$

and

$$\int |\phi(p)|^2 dp = 1. \quad (6)$$

Eq. (4), the Schrödinger's equation, is only one example of the Hamiltonian. In quantum mechanics (or classical mechanics), a Hamiltonian is roughly speaking the total energy of a system. Thus, the Schrödinger's equation only describes the kinetic energy and the potential energy of an electron. If we want to describe the other energies, we need to use the other Hamiltonians. This will be elaborated in Postulate 2.

Example 1: Plane Wave

Let $|p\rangle$ be the eigenstate of the momentum operator \hat{p} such that

$$\hat{p}|p\rangle = p|p\rangle.$$

The state $|p\rangle$ has a well-defined momentum p . A plane wave is indeed the projection of $|p\rangle$ onto the x basis.

$$\langle x|p\rangle = e^{i\frac{px}{\hbar}}.$$

If instead, we project the state $|p\rangle$ onto the p basis,

$$\langle p'|p\rangle = \delta(p - p').$$

That is, a plane wave in the p space is a delta function. This relation is analogous to the Fourier transform of a single frequency signal $e^{i\omega t}$ is a delta function.

2 Dirac Notations

In quantum mechanics, the Bra-Ket notations are convenient tools. Any states are written as kets $|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, \dots$. You can think a ket as a column vector. However, the representation of a column vector depends on the bases. For example, in the position basis, a ket can be defined as:

$$|\psi\rangle = \begin{pmatrix} \psi(x_1) \\ \psi(x_2) \\ \vdots \\ \psi(x_N) \end{pmatrix}. \quad (7)$$

whereas in the momentum basis

$$|\psi\rangle = \begin{pmatrix} \phi(p_1) \\ \phi(p_2) \\ \vdots \\ \phi(p_N) \end{pmatrix}. \quad (8)$$

The role of a bra is similar to row vectors in linear algebra. **A bra is defined as the hermitian conjugate of a ket.** For examples, in the position basis, a bra can be defined as:

$$\langle\psi| = (\psi^*(x_1) \quad \psi^*(x_2) \quad \dots \quad \psi^*(x_N)). \quad (9)$$

whereas in the momentum basis

$$\langle\psi| = (\phi^*(p_1) \quad \phi^*(p_2) \quad \dots \quad \phi^*(p_N)). \quad (10)$$

The inner product of two states $|\psi\rangle$ and $|\phi\rangle$ is

$$\langle\psi|\phi\rangle, \quad (11)$$

which is a complex number. The inner product $\langle\psi_i|\psi_i\rangle$ is the probability to find the particle in the i th state. The outer product of two states $|\psi\rangle$ and $|\phi\rangle$ is

$$|\phi\rangle\langle\psi| \quad (12)$$

which is a matrix.

Note 1: Continuous and discrete variables

A state $|\psi\rangle$ can be a finite or an infinite column vector. This will depend on which basis we express the state in. For example, the state of an electron ψ in the x basis is an infinite vector, and in the spin basis, it is a 2-component vector. Here, x is the continuous variable, and spin is the discrete variable. In the cases of light, the photon number is a discrete variable, and the amplitude of the electric field is a continuous variable. More specifically, a state $|\psi\rangle$ is fully categorized by all its commutable observables. For example, an electron is fully described by x and spin. Its Hamiltonian is block-diagonalized, where each block has a spin value.

Exercise 1: Calculation of bras and kets

Let

$$|a\rangle = \begin{pmatrix} 1 \\ 2i \\ 3 \end{pmatrix} \quad (13)$$

$$|b\rangle = \begin{pmatrix} i \\ 0 \\ 2 \end{pmatrix} \quad (14)$$

1. What are $\langle a|$ and $\langle b|$?
2. Calculate $\langle a|a\rangle$, $\langle b|b\rangle$, $\langle a|b\rangle$ and $\langle b|a\rangle$?
3. Calculate $|a\rangle\langle b|$ and $|b\rangle\langle a|$. Are they complex conjugate of each other?

If $|\psi\rangle$ is to describe a single particle, the normalization of a state requires the inner product

$$\langle\psi|\psi\rangle = 1 \quad (15)$$

or in a specific basis

$$\sum_i |\psi_i|^2 = 1, \quad (16)$$

and for a continuous variable like x ,

$$\int dx |\psi(x)|^2 = 1. \quad (17)$$

In the position basis, the position is a operator \hat{x} (a matrix).

$$\hat{x} = \begin{pmatrix} x_1 & 0 & 0 & 0 \\ 0 & x_2 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & x_N \end{pmatrix} \quad (18)$$

As it should be, the operator \hat{x} is a diagonal matrix in the position basis. In the Dirac's notation, the expectation value of x is

$$\langle x \rangle = \langle \psi | \hat{x} | \psi \rangle \quad (19)$$

$$= \sum_i x_i |\psi_i|^2 \quad (20)$$

$$= \int x |\psi(x)|^2 dx. \quad (21)$$

3 Postulates of Quantum Mechanics

Postulate 1: State Vector

A physical system is completely described by a **complex** state vector $|\psi\rangle$ in the Hilbert space. The Hilbert space is a vector space constructed by all the state vectors $|\psi\rangle$ whose inner products are finite.

The state vector $|\psi\rangle$ contains all the information. The state vector can be written as a sum of other (basis) vectors.

$$|\psi\rangle = \sum_i \alpha_i |\psi_i\rangle \quad (22)$$

The probability to find the system in the i th state is $|\alpha_i|^2$. The simplest example is the qubit,

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle. \quad (23)$$

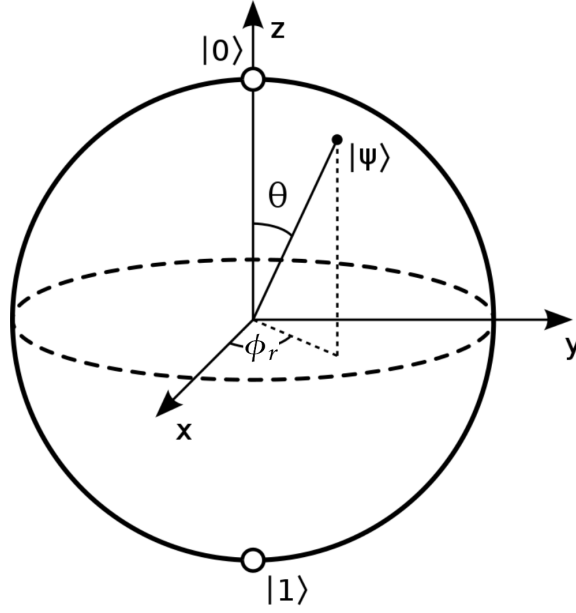


Figure 1: Bloch sphere.

Without losing the generality, the qubit can be written as ($|\alpha|^2 + |\beta|^2 = 1$)

$$|\psi\rangle = e^{i\phi_g} \left(\cos \frac{\theta}{2} |0\rangle + \sin \frac{\theta}{2} e^{i\phi_r} |1\rangle \right), \quad (24)$$

where ϕ_g is the global phase, and ϕ_r is the relative phase between the $|0\rangle$ and $|1\rangle$ states. Without comparing with another qubit, the phase ψ_g does not have much meaning. The degrees of freedoms of a qubit are given by θ and ϕ_r , which correspond to a surface of a sphere. The space of a qubit is called the Bloch sphere.

Postulate 2: Temporal Evolution

The evolution of a closed quantum state is described by the unitary transformation.

The state $|\psi(t')\rangle$ is related to the state $|\psi(t)\rangle$ by

$$|\psi(t')\rangle = \hat{U}(t, t') |\psi(t)\rangle, \quad (25)$$

where $U(t, t')$ is a unitary operator (a matrix), $U^\dagger U = \mathbb{1}$.¹

The postulate comes from the conservation of total probabilities,

$$\langle \psi(t') | \psi(t') \rangle = \langle \psi(t) | \psi(t) \rangle = 1 \quad (26)$$

The unitary operator can be written as

¹For the sake of simplicity, I won't use a hat for an operator all the time unless there will be confusion.

$$U(t, t') = e^{-i\frac{\mathcal{H}}{\hbar}(t'-t)}, \quad (27)$$

where \mathcal{H} has to be hermitian, $\mathcal{H} = \mathcal{H}^\dagger$, to make $U(t', t)$ unitary.

Exercise 2: Exponential Function of Matrices

Show that the operator defined by Eq. (27) is unitary. Use the following facts,

- The matrix exponential of a matrix M is defined $e^M = \mathbb{1} + M + \frac{M^2}{2!} + \dots$
- $e^A e^B = e^{A+B}$ if $[A, B] \equiv AB - BA = 0$. This can be proved by using the above definition. This equation is a special case of the [Baker-Campbell-Hausdorff formula](#), which reads

$$e^X e^Y = e^Z$$

$$Z = X + Y + \frac{1}{2}[X, Y] + \frac{1}{12}[X, [X, Y]] - \frac{1}{12}[Y, [X, Y]] + \dots,$$

- $\mathcal{H} = \mathcal{H}^\dagger$

The evolution of a state is then given by

$$|\psi(t')\rangle = e^{-i\frac{\mathcal{H}}{\hbar}(t'-t)}|\psi(t)\rangle, \quad (28)$$

or more generally, if $\mathcal{H}(t)$ is time-dependent,

$$|\psi(t')\rangle = e^{-i\int_t^{t'} \frac{\mathcal{H}(\tau)d\tau}{\hbar}}|\psi(t)\rangle. \quad (29)$$

Equation (29) is simply a consequence of the unitary evolution. By differentiating Eq. (29), one can obtain the general form of the Schrödinger's equation,

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \mathcal{H}|\psi\rangle. \quad (30)$$

The operator \mathcal{H} is called the “**Hamiltonian**” of the system. The Hamiltonian, coming from the classical mechanics, typically is the total energy of the system. For example, for a particle, the Hamiltonian $\mathcal{H} = \frac{p^2}{2m} + V(x)$. The case of a particle is only one of the examples. If the systems are discrete and finite (energy levels), the Hamiltonian is a finite-dimensional matrix. For example, classically, the energy of a magnetic moment $\boldsymbol{\mu}$ in a magnetic field \mathbf{B} is $E = -\boldsymbol{\mu} \cdot \mathbf{B}$. The magnetic moment $\boldsymbol{\mu}$ is related to the angular momentum \mathbf{L} by $\boldsymbol{\mu} = \gamma \mathbf{L}$, where γ is the gyromagnetic ratio. Quantumly the Hamiltonian is $\mathcal{H} = -\boldsymbol{\mu} \cdot \mathbf{B}$, and the angular momentum \mathbf{L} becomes an operator. In quantum mechanics, the angular momentum operators do not commute, and they satisfy the relation,

$$[L_i, L_j] = i\epsilon_{ijk}\hbar L_k. \quad (31)$$

In the case of an electron, the angular momentum operator is $\sigma = (\sigma_x, \sigma_y, \sigma_z)$, where σ_i are the Pauli matrices (2 by 2 matrices). Hence, the dimension of the Hamiltonian is two.

Let's consider a system with N levels of the energies E_1, E_2, \dots, E_N . The energy eigenstates, $|E_i\rangle$, satisfy

$$\mathcal{H}|E_i\rangle = E_i|E_i\rangle. \quad (32)$$

The Hamiltonian in the energy bases $|E_i\rangle$ is diagonal

$$\mathcal{H} = \begin{pmatrix} E_1 & 0 & 0 & 0 \\ 0 & E_2 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & E_N \end{pmatrix}. \quad (33)$$

The solution of the time-dependent Schrödinger's equation (Eq. (30)) is

$$|\psi(t)\rangle = \sum_i \alpha_i e^{-i\frac{E_i}{\hbar}t} |E_i\rangle, \quad (34)$$

where α_i are the coefficients of the initial state in terms of $|E_i\rangle$.

Postulate 3: Measurement

Quantum measurement (collapse). A measurement makes a system $|\psi\rangle$ collapse randomly into some state $|\psi_i\rangle$. The possible outcome states $|\psi_i\rangle$ depend on the measurements. For example, if we measure the position of a particle, the outcome states are $|x\rangle$ with $-\infty < x < \infty$. A measurement is described by a set of operators $\{M_m\}$, where m denotes all the possible outcome states. After a measurement, the state becomes

$$\frac{M_m|\psi\rangle}{\sqrt{\langle\psi|M_m^\dagger M_m|\psi\rangle}} \quad (35)$$

with the probability

$$p(m) = \langle\psi|M_m^\dagger M_m|\psi\rangle. \quad (36)$$

The completeness theorem requires that

$$\sum_m M_m^\dagger M_m = \mathbb{1}. \quad (37)$$

For example, the measurement operators on a qubit are

$$M_0 = |0\rangle\langle 0| \quad (38)$$

$$M_1 = |1\rangle\langle 1| \quad (39)$$

Exercise 3: Qubit Measurement

The initial qubit state is $\frac{1}{2}|0\rangle + \frac{\sqrt{3}}{2}|1\rangle$.

1. What are the two possible states after a measurement of $\{M_0, M_1\}$?
2. What are the probabilities to be the above two states, respectively?

Heisenberg uncertainty principle

Postulate 4: Hermiticity

Any physical observables are Hermitian operators. For example, in the position basis, the position and momentum operators are

$$\hat{x} = x \quad (40)$$

$$\hat{p} = -i\hbar \frac{\partial}{\partial x} \quad (41)$$

Let \hat{A} be the physical observable operator. The expectation value of \hat{A} of a state $|\psi\rangle$ is

$$\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle. \quad (42)$$

The state $|p\rangle$ is the eigenvector of the momentum operator \hat{p} ,

$$\hat{p}|p\rangle = p|p\rangle, \quad (43)$$

and for the position operator \hat{x} ,

$$\hat{x}|x\rangle = x|x\rangle. \quad (44)$$

Note that the eigenvectors of a Hermitian operator form a complete set of bases of the space.

The eigenvectors $|A_i\rangle$ of A forms a complete set of bases of the state space. The eigenstates are orthogonal and normal,

$$\langle A_j | A_i \rangle = \delta_{ij}. \quad (45)$$

That is, any state $|\psi\rangle$ can be written as

$$|\psi\rangle = \sum_i \alpha_i |A_i\rangle. \quad (46)$$

The completeness implies that the identity $\mathbb{1}$ is,

$$\mathbb{1} = \sum_i |A_i\rangle\langle A_i| \quad (47)$$

The standard deviation of A is $\sigma(A)$,

$$\sigma(A) \equiv \sqrt{\langle A^2 \rangle - \langle A \rangle^2}. \quad (48)$$

Two operators A and B are compatible if their commutator $[A, B] \equiv AB - BA = 0$. Otherwise, they are incompatible. If

$$[A, B] = c \quad (49)$$

and c is a number, the general uncertainty principle reads

$$\sigma(A)\sigma(B) \geq \frac{|\langle \psi | [A, B] | \psi \rangle|}{2} = \frac{|c|}{2}. \quad (50)$$

Exercise 4: Uncertainty Principle

Prove the Heisenberg uncertainty principle, Eq. (50). Hint: use the Cauchy-Schwarz inequality.

$$\langle \psi | \psi \rangle \langle \phi | \phi \rangle \geq |\langle \psi | \phi \rangle|^2, \quad (51)$$

where $|\psi\rangle$ and $|\phi\rangle$ are two states.

The most classical example of the uncertainty principle is about x and p ,

$$[x, p] = i\hbar. \quad (52)$$

The uncertainty principle reads

$$\sigma(x)\sigma(p) \geq \frac{\hbar}{2}. \quad (53)$$

4 Quantum Dynamics: Schrödinger, Interaction, Heisenberg Pictures

The state $|\psi\rangle$ of a physical system contains all the informations, but is not the direct observable. We do not directly see or measure the state $|\psi\rangle$, but rather we measure the physical quantities

such position, momentum, and so on. These physical quantities are the expectations of the observable operators (such as \hat{x} and \hat{p}). For example, when we measure the position of a state, the averaged outcome is

$$x(t) = \langle \psi(t) | \hat{x} | \psi(t) \rangle.$$

This outcome is called the observable.

More generally, let's consider a physical observable operator \hat{A} , and its expectation is

$$A(t) = \langle \psi(t) | \hat{A} | \psi(t) \rangle \quad (54)$$

The number $A(t)$ is what we measured in the experiment. To obtain the evolution of $A(t)$ belongs to the subject of quantum dynamics. In quantum dynamics, there are three main pictures to solve the problems.

4.1 Schrödinger Picture

Consider that the observable operator A is static and the states $|\psi(t)\rangle$ is evolving.

$$|\psi(t)\rangle \equiv |\psi(t)\rangle_S = e^{-\frac{i\mathcal{H}t}{\hbar}} |\psi(0)\rangle \quad (55)$$

The expectation value in this picture is

$$\langle A(t) \rangle = \langle \psi(t) | A | \psi(t) \rangle \quad (56)$$

4.2 Heisenberg Picture

Consider that the observable operator $A(t)$ is dynamic and the states $|\psi(t)\rangle$ is static.

$$A_h \equiv A(t) = e^{\frac{i\mathcal{H}t}{\hbar}} A e^{-\frac{i\mathcal{H}t}{\hbar}}, \quad (57)$$

and the expectation value is

$$\langle A(t) \rangle = \langle \psi(0) | A_h | \psi(0) \rangle. \quad (58)$$

The evolution of A_h follows the Heisenberg's equation,

$$i\hbar \frac{\partial A_h}{\partial t} = [A_h, \mathcal{H}]. \quad (59)$$

Exercise 5: Proof of the Heisenberg's equation

Let $U(t) = e^{-\frac{i\mathcal{H}t}{\hbar}}$ so that $A_h = U^\dagger A U$. Differentiating A_h with respect to t gives

$$\frac{\partial A_h}{\partial t} = \frac{\partial U^\dagger}{\partial t} A U + U^\dagger A \frac{\partial U}{\partial t} \quad (60)$$

First, show that the derivative of $U(t)$ is

$$i\hbar \frac{\partial}{\partial t} U(t) = \mathcal{H}U(t). \quad (61)$$

Use the two above equations to prove the Heisenberg's equation.

Example 2: Harmonic Oscillator in Heisenberg Picture

The Hamiltonian of a harmonic oscillator is

$$\mathcal{H} = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}.$$

In this case, the position operator in the Heisenberg Picture is

$$\hat{x}_h = e^{\frac{i\mathcal{H}t}{\hbar}} \hat{x} e^{-\frac{i\mathcal{H}t}{\hbar}}.$$

At $t = 0$, $\hat{x}_h(0) = \hat{x}(0)$. The operator $\hat{x}_h(t)$ at a later time, can be obtained by

$$i\hbar \frac{\partial \hat{x}_h}{\partial t} = [\hat{x}_h, \mathcal{H}].$$

You can show that

$$\frac{\partial \hat{x}_h}{\partial t} = -m\omega^2 \hat{x}_h.$$

4.3 Interaction Picture

When the Hamiltonian includes two terms: one is the original Hamiltonian \mathcal{H}_0 and the interaction with the external system $V(t)$, it is convenient to use the interaction picture, where both the states and the operator are evolving. The total Hamiltonian is $\mathcal{H} = \mathcal{H}_0 + V(t)$. The state $|\psi\rangle_I$ is

$$|\psi\rangle_I = e^{i\frac{\mathcal{H}_0 t}{\hbar}} |\psi(t)\rangle_S, \quad (62)$$

and the operator A_I is

$$A_I = e^{i\frac{\mathcal{H}_0 t}{\hbar}} A e^{-i\frac{\mathcal{H}_0 t}{\hbar}}, \quad (63)$$

The Schrödinger equation becomes

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle_I = V_I(t) |\psi\rangle_I, \quad (64)$$

$$V_I(t) \equiv e^{i\frac{\mathcal{H}_0 t}{\hbar}} V(t) e^{-i\frac{\mathcal{H}_0 t}{\hbar}}. \quad (65)$$

Note that the solution to Eq. (64) is not $|\psi(t)\rangle_I = e^{-i\frac{V_I}{\hbar}t} |\psi(0)\rangle_I$ because the $V_I(t)$ is time-dependent. The solution to Eq. (64) is

$$|\psi(t)\rangle_I = U_I(t, t_0) |\psi(t_0)\rangle_I \quad (66)$$

$$U_I(t, t_0) = \mathbb{1} - \frac{i}{\hbar} \int_{t_0}^t V_I(t') U_I(t', t_0) dt' \quad (67)$$

The Heisenberg's equation becomes

$$i\hbar \frac{\partial A_I}{\partial t} = [A_I, \mathcal{H}_0]. \quad (68)$$

5 Harmonic Oscillators

The Hamiltonian of a simple harmonic oscillator is

$$\mathcal{H} = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}, \quad (69)$$

where $\omega = \sqrt{k/m}$ and k is the spring constant. We define the creation operator a^\dagger and the annihilation operator a ,

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{ip}{m\omega} \right), \quad (70)$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(x - \frac{ip}{m\omega} \right). \quad (71)$$

Exercise 6: Commutation Relation

Show that

$$[a, a^\dagger] = 1. \quad (72)$$

Use the relation $[x, p] = i\hbar$.

The Hamiltonian is rewritten as

$$\mathcal{H} = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) \quad (73)$$

$$= \hbar\omega \left(N + \frac{1}{2} \right) \quad (74)$$

where $N = a^\dagger a$ is the number operator. The eigenvector of N is $|n\rangle$

$$N|n\rangle = n|n\rangle, \quad (75)$$

where n is the eigenvalue. The number states are orthonormal

$$\langle m|n\rangle = \delta_{mn}. \quad (76)$$

Important identities are

$$[N, a] = -a, \quad (77)$$

$$[N, a^\dagger] = a^\dagger, \quad (78)$$

As a result, we have

$$N a^\dagger |n\rangle = (a^\dagger N + a^\dagger) |n\rangle = (n+1) a^\dagger |n\rangle, \quad (79)$$

$$N a |n\rangle = (a N - a) |n\rangle = (n-1) a |n\rangle, \quad (80)$$

These equations imply that

$$a |n\rangle = c_- |n-1\rangle, \quad (81)$$

$$a^\dagger |n\rangle = c_+ |n+1\rangle, \quad (82)$$

The constants c_- and c_+ can be fixed by noting that

$$\langle n|a^* a|n\rangle = n = |c_-|^2, \quad (83)$$

$$\langle n|a a^*|n\rangle = n+1 = |c_+|^2. \quad (84)$$

Taking c_- and c_+ to be positive by convention, $c_- = \sqrt{n}$ and $c_+ = \sqrt{n+1}$. We have the important relations which explain the names, creation and annihilation,

$$a |n\rangle = \sqrt{n} |n-1\rangle, \quad (85)$$

$$a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle. \quad (86)$$

Note 2: Representation in the number basis

The number n is the number of the energy quanta. The smallest number of n is $n = 0$. The physical meaning of $|n\rangle$ is a state containing n energy quanta. Thus, $|n\rangle$ is called the **number state**. The energy of a harmonic oscillator is

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad (87)$$

The $\frac{1}{2}\hbar\omega$ is interpreted as the vacuum energy since it exists even when $n = 0$. Applying a creation operator on the $|n\rangle$, the state $|n\rangle$ becomes $\sqrt{n+1}|n+1\rangle$, that is, the a^\dagger will create one single quantum to the original state. Similarly, the a will annihilate one energy quantum from the system. We can also prove that

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle. \quad (88)$$

The position operator x and momentum operator p can be expressed as

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \quad (89)$$

$$p = i\sqrt{\frac{m\omega\hbar}{2}}(-a + a^\dagger) \quad (90)$$

5.1 Number States in the Position Bases

As the familiar wave function $\psi(x)$, we can express the $|n\rangle$ in the x bases. The wavefunctions are $\psi_n(x) \equiv \langle x|n\rangle$. Let's solve the ground states first $\psi_0(x)$. We start with

$$a|0\rangle = 0 \quad (91)$$

$$\Rightarrow \langle x|a|0\rangle = 0 \quad (92)$$

$$\Rightarrow \sqrt{\frac{m\omega}{2\hbar}} \left\langle x \left| x + \frac{ip}{m\omega} \right| 0 \right\rangle = 0 \quad (93)$$

$$\Rightarrow \left(x + \frac{\hbar}{m\omega} \frac{\partial}{\partial x} \right) \psi_0(x) = 0 \quad (94)$$

$$\Rightarrow \psi_0(x) = \frac{1}{\pi^{1/4} \sqrt{x_0}} e^{-\frac{1}{2} \left(\frac{x}{x_0} \right)^2}, \quad (95)$$

where $x_0 = \sqrt{\frac{\hbar}{m\omega}}$

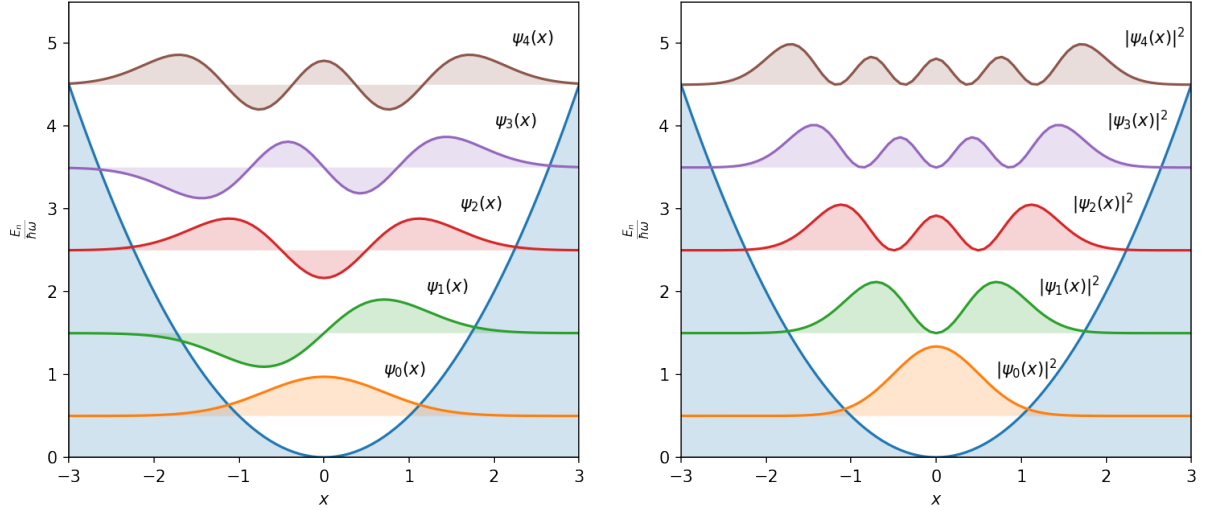


Figure 2: Wavefunction $\psi_n(x)$.

Exercise 7: Uncertainty of the ground state

Show that for the ground state $\psi_0(x)$, the uncertainty relation has a equal sign, that is, the state has the minimum uncertainty,

$$\sigma(x)\sigma(p) = \frac{\hbar}{2}. \quad (96)$$

Using Eqs. (88) and (95), we obtain the expression for $\psi_n(x)$,

$$\psi_n(x) = \left(\frac{1}{\pi^{1/4} \sqrt{2^n n! x_0^{n+1/2}}} \right) \left(x - x_0^2 \frac{\partial}{\partial x} \right)^n e^{-\frac{1}{2} \left(\frac{x}{x_0} \right)^2}. \quad (97)$$

5.2 Dynamics of a Harmonic Oscillator

The Heisenberg's Equations of a and $a^\dagger(t)$ are

$$i\hbar \frac{da^\dagger}{dt} = [a^\dagger, H] = -\hbar\omega a^\dagger, \quad (98)$$

$$i\hbar \frac{da}{dt} = [a, H] = \hbar\omega a, \quad (99)$$

$$(100)$$

whose solutions are

$$a(t) = a(0)e^{-i\omega t}, \quad (101)$$

$$a^\dagger(t) = a^\dagger(0)e^{i\omega t}. \quad (102)$$

In terms of x and p , Eqs. (101) and (102) read

$$a(t) = x(t) + \frac{ip(t)}{m\omega} = \left(x(0) + \frac{ip(0)}{m\omega} \right) e^{-i\omega t}, \quad (103)$$

$$a^\dagger(t) = x(t) - \frac{ip(t)}{m\omega} = \left(x(0) - \frac{ip(0)}{m\omega} \right) e^{i\omega t}. \quad (104)$$

Solving the equations for $x(t)$ and $p(t)$, we have

$$x(t) = x(0) \cos \omega t + \frac{p(0)}{m\omega} \sin \omega t, \quad (105)$$

$$p(t) = -m\omega x(0) \sin \omega t + p(0) \cos \omega t. \quad (106)$$

Note 3: Heisenberg picture of x and p of a harmonic oscillator

Equations (105) and (106) are exactly the same as the equations of motion derived from the classical mechanics. In contrast, $x(0)$ and $p(0)$ are operators. If we take the number state $|n\rangle$, the expectation value $\langle n|x(t)|n\rangle$ vanishes. We will not observe an expectation value $\langle x(t) \rangle$ obeying the classical motion. It turns out that the state mostly close to a classical state is the coherent state $|\lambda\rangle$, which is the eigenvector of the annihilation operator a ,

$$a|\lambda\rangle = \lambda|\lambda\rangle. \quad (107)$$

We will talk more about the coherent states later.

6 Coherence and Decoherence at a Glance

Coherence refers to many meanings in different circumstances. We consider its usages in the context of physics. Roughly speaking, coherence means that two (or more than two) states (waves, particles) have a well-defined correlation as time t or positions x change.

6.1 Two Waves

For instance, there are two waves with the complex amplitudes $\psi_1(x, t)$ and $\psi_2(x, t)$, respectively. In terms of the absolute amplitudes A and phases ϕ , they can be written as $\psi_1(x, t) = A_1(x, t) \exp(i\phi_1(x, t))$ and $\psi_2(x, t) = A_2(x, t) \exp(i\phi_2(x, t))$. Coherence means that the difference between their phases $\phi_1 - \phi_2$ is constant as t or x changes. In the two-slit experiments, coherent light source is required to produce interference patterns. In this definition, two plane waves $\exp(ik_1x - \omega_1t + \phi_1)$ and $\exp(ik_2x - \omega_2t + \phi_2)$ are coherent if $k_1 = k_2$ and $\omega_1 = \omega_2$. The

reason for the same frequencies or the same wavenumber is as following. When we measure the interference, frequently we collect the data for a long time over many periods . The interference signal is the time-average of the product $\psi_1^*(t)\psi_2(t)$. $|\psi_1(t)|^2$ and $|\psi_2(t)|^2$ are the background intensity. The time-averaged interference is

$$I_{\text{interference}} = \lim_{T \rightarrow \infty} \frac{\int_0^T 2\text{Re}[\psi_1^*(t)\psi_2(t)]}{T}. \quad (108)$$

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

Another question is that are any two waves fully coherent if they have the same frequencies. The answer is not necessary. Why? It is because the phases ϕ_1 and ϕ_2 can fluctuate. The coherence implies that $\delta = \phi_1 - \phi_2$ is a constant as time t and position x changes. In practical situations, as the waves propagate, the environment provides noises to the phases. As a result, the time-average becomes smaller. This process is called “**decoherence**” Typically, a system gradually loses its coherence as t increases or traveled length x increases.

6.2 Many Waves and Ensemble

A more realistic system consists of many waves (states, particles)²,

$$\psi(x, t) = \psi_1(x, t) + \psi_2(x, t) + \psi_3(x, t) + \dots \quad (109)$$

The interference involves all the cross-product terms $\psi_1^*(t)\psi_2(t)$, $\psi_2^*(t)\psi_3(t)$, $\psi_3^*(t)\psi_4(t)$, and so on. To deal with a system containing a large number of waves (particles), it is more convenient to use a statistical tool than listing all the states. The idea is to use probabilities to describe distributions of states. Such a tool in quantum mechanics is called the density operator or matrix. Basically, a density matrix contains the information of the probability in each state.

7 Density Operator Formulation

Let's introduce the concepts of an ensemble.

Note 4: Ensemble

An ensemble is a statistical tool to describe a system of many particles. An ensemble consists of a large number (ideally, infinite) of virtual copies of a particle. Each copy represents a possible state that a particle can be in. A specific ensemble is specified

²We use the terms “particle”, “waves”, and “states” interchangeably.

by assigning the probability in each state. For example, a photon state $|\text{photon}\rangle$ is decomposed as

$$|\text{photon}\rangle = \alpha|L\rangle + \beta|R\rangle, \quad (110)$$

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

$$p_L + p_R = 1. \quad (111)$$

The probabilities p_L and p_R specify the ensemble where there are infinite particles, and each has the probability p_L (p_R) in the state $|L\rangle$ ($|R\rangle$).

However, we can not use the following expression to describe an ensemble,

~~$$|\text{ensemble}\rangle = p_L|L\rangle + p_R|R\rangle, \quad (112)$$~~

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

$$\hat{\rho} = p_L|L\rangle\langle L| + p_R|R\rangle\langle R|. \quad (113)$$

7.1 Density Operators

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

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \quad (114)$$

$$\sum_i p_i = 1, \quad (115)$$

$$0 \leq p_i \leq 1, \quad (116)$$

where $|\psi_i\rangle$ are the basis states, and p_i is the probability to find a particle in the i th state. Most times, $|\psi_i\rangle$ are chosen to be orthonormal vectors. In the definition by Eq. (114), the density matrix is a diagonal matrix. In general, a density matrix can have nonzero off-diagonal elements in another basis. Consider a new set of orthonormal basis vectors $|a_i\rangle$, obtained by the unitary transformation

$$|a_i\rangle = \sum_j U_{ij} |\psi_j\rangle. \quad (117)$$

where $U^\dagger U = \mathbb{1}$. The matrix element U_{ij} can be obtained explicitly by multiplying $\langle\psi_j|$ on the both sides of Eq. (117),

$$U_{ij} = \langle\psi_j|a_i\rangle. \quad (118)$$

The inverse transforms are

$$|\psi_i\rangle = \sum_j U_{ij}^\dagger |a_j\rangle, \quad (119)$$

$$\langle\psi_i| = \sum_{j'} U_{j'i} \langle a_{j'}|. \quad (120)$$

In the new basis,

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle \langle\psi_i| \quad (121)$$

$$= \sum_i p_i \left(\sum_j U_{ij}^\dagger |a_j\rangle \right) \left(\sum_{j'} U_{j'i} \langle a_{j'}| \right) \quad (122)$$

$$= \sum_{j,j'} \left(\sum_i p_i U_{ij}^\dagger U_{j'i} \right) |a_j\rangle \langle a_{j'}| \quad (123)$$

$$\equiv \sum_{j,j'} \rho_{jj'} |a_j\rangle \langle a_{j'}|, \quad (124)$$

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

$$\rho_{jj'} = \sum_i U_{j'i} p_i U_{ij}^\dagger \quad (125)$$

$$= (UPU^\dagger)^T, \quad (126)$$

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

Example 3: Two-Level System

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

$$\rho = 0|L\rangle\langle L| + 1|R\rangle\langle R|, \quad (127)$$

or in the matrix form

$$\rho = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \quad (128)$$

Keep in mind that the matrix in Eq. (128) is written in the basis vector defined by

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv |L\rangle, \quad (129)$$

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv |R\rangle. \quad (130)$$

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

$$|L\rangle = \frac{1}{\sqrt{2}} (|X\rangle - i|Y\rangle), \quad (131)$$

$$|R\rangle = \frac{1}{\sqrt{2}} (|X\rangle + i|Y\rangle). \quad (132)$$

The unitary transformation is

$$\begin{pmatrix} |L\rangle \\ |R\rangle \end{pmatrix} = U^\dagger \begin{pmatrix} |X\rangle \\ |Y\rangle \end{pmatrix}, \quad (133)$$

where

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

$$U = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{pmatrix}. \quad (135)$$

In the new bases, using Eq. (126) the density matrix is

$$\hat{\rho} = \left[\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \right]^T \quad (136)$$

$$= \begin{pmatrix} \frac{1}{2} & \frac{-i}{2} \\ \frac{i}{2} & \frac{1}{2} \end{pmatrix}. \quad (137)$$

Note that the matrix in Eq. (137) is written in the new basis (see Eq. (124)). For this matrix, the column vectors $(1, 0)^T$ and $(0, 1)^T$ represent the new basis vectors $|a_1\rangle$ and $|a_2\rangle$, which in this case are

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv |X\rangle, \quad (138)$$

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv |Y\rangle. \quad (139)$$

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

Exercise 8: Density Matrix

Consider an ensemble of the density matrix

$$\rho = \frac{1}{4}|L\rangle\langle L| + \frac{3}{4}|R\rangle\langle R|. \quad (140)$$

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

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

$$\langle A \rangle = \sum_i p_i \langle \psi_i | A | \psi_i \rangle \quad (141)$$

$$= \sum_{i,j} p_i \langle \psi_i | \psi_j \rangle \langle \psi_j | A | \psi_i \rangle \quad (142)$$

$$= \sum_j \langle \psi_j | A \underbrace{\sum_i |\psi_i\rangle p_i \langle \psi_i|}_{\text{This term is } A\rho} | \psi_j \rangle \quad (143)$$

$$= \sum_j \langle \psi_j | A \rho | \psi_j \rangle \quad (144)$$

$$= \text{Tr}(A\rho). \quad (145)$$

Although we derive the ensemble average Eq. (145) in the $|\psi_i\rangle$ bases, the trace of a matrix is independent of the bases. Thus, Eq. (145) is valid in any basis. This basis-free property is the advantage of using a trace. One direct application is when $A = \mathbb{1}$,

$$\text{Tr}(\rho) = \sum_i p_i = 1, \quad (146)$$

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

Exercise 9: Properties of Density Matrix

Some important properties of density matrix are listed below:

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

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

Note 5: Pure and Mixed Ensemble

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

$$\text{Tr}(\rho^2) = 1, \quad (147)$$

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

$$\text{Tr}(\rho^2) < 1. \quad (148)$$

One particle state is always a pure ensemble. One common mistake is to be confused by the superposition of one particle and the mixed ensemble.³ Consider a one-particle state (qubit) composed of the superposition of $|0\rangle$ and $|1\rangle$.

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle. \quad (149)$$

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

$$\rho = |\psi\rangle\langle\psi| \quad (150)$$

$$= (\alpha|0\rangle + \beta|1\rangle)(\alpha^*\langle 0| + \beta^*\langle 1|) \quad (151)$$

$$= |\alpha|^2|0\rangle\langle 0| + |\beta|^2|1\rangle\langle 1| + \alpha\beta^*|0\rangle\langle 1| + \alpha^*\beta|1\rangle\langle 0| \quad (152)$$

$$= \begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{pmatrix}, \quad (153)$$

where

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv |0\rangle, \quad (154)$$

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv |1\rangle. \quad (155)$$

It is possible to find the bases where ρ is diagonal, since ρ is a hermitian matrix. The off-diagonal elements in Eq. (153) describe the correlations between the states $|0\rangle$ and $|1\rangle$. An example of a mixed ensemble of qubits is

$$\rho = |\alpha|^2|0\rangle\langle 0| + |\beta|^2|1\rangle\langle 1| \quad (156)$$

$$= \begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix}, \quad (157)$$

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

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

$$\rho_{\text{MR}} = \frac{1}{N} \sum_{i=1}^N |\psi_i\rangle\langle\psi_i| \quad (158)$$

$$= \frac{1}{N} \mathbb{1}_{N \times N}, \quad (159)$$

where $\mathbb{1}_{N \times N}$ is the N -by- N identity. The off-diagonal elements of the ensemble ρ_{MR} are always zero, i.e., there is not any correlation between the basis states. It can be shown that an entangled system must be in a mixed ensemble. The extent of entanglement of an ensemble is somewhat related to von Neumann entropy.

Exercise 10: Pure Ensemble

Which density matrices are pure ensembles?

(a)

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

(b)

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

(c)

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

(d)

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

³In many places, mixed states are called instead of mixed ensemble, although the latter is properer.

7.2 Dynamics of Density Operators

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

$$\rho(t) = \sum_i p_i |\psi_i(t)\rangle\langle\psi_i(t)|, \quad (160)$$

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

$$i\hbar \frac{\partial}{\partial t} |\psi_i(t)\rangle = \mathcal{H} |\psi_i(t)\rangle, \quad (161)$$

$$-i\hbar \frac{\partial}{\partial t} \langle\psi_i(t)| = \langle\psi_i(t)| \mathcal{H}. \quad (162)$$

Using Eqs. (160), (161) and (162), we obtain

$$\frac{\partial \rho(t)}{\partial t} = \frac{i}{\hbar} [\rho(t), \mathcal{H}]. \quad (163)$$

This equation is known as the von Neumann equation or quantum Liouville equation. Equation (163) describes a closed system where $\text{Tr}(\rho^2)$ is a constant in time. This means that the coherence of the system is not changed. How could a system have dissipation and decoherence? When a system is open to the environment, the interaction between the system and the environment leads to dissipation and decoherence. The idea is to write $\mathcal{H} = \mathcal{H}_{\text{sys}} + \mathcal{H}_{\text{env}}$ and to derive a equation only about the reduced density matrix

$$\frac{\partial \rho(t)_{\text{sys}}}{\partial t} = \frac{i}{\hbar} [\rho(t)_{\text{sys}}, \mathcal{H}_{\text{sys}}] + \text{environment terms}, \quad (164)$$

where the reduced density matrix is obtained by the partial trace

$$\rho(t)_{\text{sys}} = \text{Tr}_{\text{env}}(\rho(t)). \quad (165)$$

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

Exercise 11: Quantum Liouville Equation

Derive the von Neumann equation, Eq. (163). The first step is to differentiate Eq. (160).

Example 4: Dynamics of a Two Level System

Let the unperturbed Hamiltonian be

$$\mathcal{H} = \begin{pmatrix} E_c & 0 \\ 0 & E_v \end{pmatrix}, \quad (166)$$

and write the density matrix in this basis

$$\rho = \begin{pmatrix} \rho_{cc} & \rho_{cv} \\ \rho_{vc} & \rho_{vv} \end{pmatrix}. \quad (167)$$

Using the von Neumann equation, Eq. (163), we can obtain four first-order differential equations. Two of them are redundant because $\rho_{cc} + \rho_{vv} = 1$ and $\rho_{cv} = \rho_{vc}^*$. We need only two equations

$$\frac{\partial}{\partial t} \rho_{cc} = 0, \quad (168)$$

$$\frac{\partial}{\partial t} \rho_{cv} = \frac{i}{\hbar} \rho_{cv} (E_v - E_c), \quad (169)$$

with the solutions

$$\rho_{cc}(t) = \rho_{cc}(0), \quad (170)$$

$$\rho_{vv}(t) = \rho_{vv}(0), \quad (171)$$

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

$$(173)$$

with $\omega_{cv} = \frac{E_c - E_v}{\hbar}$. The populations ρ_{cc} and ρ_{vv} are unchanged in an unperturbed system. The off-diagonal element ρ_{cv} has a constant amplitude and a linearly-growing phase in time. This means that the coherence of the system is unchanged. In a realistic situation, the system will be dephased. A phenomenological way to add the dephasing is to add $-\gamma\rho_{cv}$ in Eq. (169),

$$\frac{\partial}{\partial t} \rho_{cv} = \frac{i}{\hbar} \rho_{cv} (E_v - E_c) - \gamma \rho_{cv}, \quad (174)$$

with the solution

$$\rho_{cv}(t) = \rho_{cv}(0) e^{-i\omega_{cv}t - \gamma t}, \quad (175)$$

$$(176)$$

and γ is called the dephasing rate. The time $T_2 = \frac{1}{\gamma}$ is the characteristic time of dephasing. If the system is open, the probability of the top level ρ_{cc} can decay. This can be described as

$$\frac{\partial}{\partial t} \rho_{cc} = -\gamma_r \rho_{cc}, \quad (177)$$

where γ_r is the relaxation rate. The time $T_1 = \frac{1}{\gamma_r}$ is the characteristic time of relaxation.

Exercise 12: Quantum Liouville Equation

Derive Eqs. (168) and (169).

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