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Summary of Quantum Mechanics

Contents

Specification

The contents of this book mainly follows the discussion of R. Shankar. Some detailed sections refer to X. Ka, J.J. Sakurai and J. Zeng. The figures in this book are captured from Wikipedia and S. Brandt.

1

Basic Theory of Vector Space

It is the aim of this chapter to equip you with the necessary mathematical machinery. All the math you need is developed here, starting from some basic ideas on vectors and matrices that you are assumed to know. $\cdots$ The effort you put into this chapter will be well worth your while: not only will it prepare you for this course, but it will also unify many ideas you may have learned piecemeal.

R. Shankar

1.1 Vector Space

Definition 1.1 (Vector Space)**.** *A vector space V over field K is a collection of vectors $\{|V\rangle, |W\rangle \cdots\}$, for which there exists*

1. A definite rule for forming the vector sum, $|V\rangle + |W\rangle$;

2. A definite rule for multiplication by scalar $a, b, c \in K$, denoted $a|V\rangle$.

with the following features:

- *Addition is closure: $|W\rangle + |V\rangle = |Z\rangle \in V$;*
- *Scalar multiplication is distributive in the vectors: $a(|V\rangle + |W\rangle) = a|V\rangle + a|W\rangle$;*
- *Scalar multiplication is distributive in the scalars: $(a+b)|V\rangle = a|V\rangle + b|V\rangle$;*
- *Scalar multiplication is distributive is associative: $a(b|V\rangle) = (ab)|V\rangle$;*
- *Addition is commutative: $|V\rangle + |W\rangle = |W\rangle + |V\rangle$;*
- *Addition is associative: $|V\rangle + (|W\rangle + |Z\rangle) = (|V\rangle + |W\rangle) + |Z\rangle$;*

- *Null vector:*$|V\rangle + |0\rangle = |V\rangle$*;*
- *Inverse under addition:* $|V\rangle + |-V\rangle = |0\rangle$.

Definition 1.2. *A set of vectors* $\{|1\rangle, |2\rangle \cdots |n\rangle\}$ *is said to be* ***linearly independent*** *only if all the coefficients* $a_i = 0$ *for*

$$\sum_{i=1}^{n} a_i |i\rangle = |0\rangle \tag{1.1}$$

If a set of vectors are not linearly independent, they are ***linearly dependent****.*

Definition 1.3. *A vector space has dimension n if it can accommodate a maximum of n linear independent vectors. A set of n linearly independent vectors in a n-dimension vector space is called a* ***basis****.*

Definition 1.4. *A vector* $|V\rangle$ *in a n-dimension vector space can be uniquely expanded by a set of linear independent vectors* $\{|i\rangle\}$

$$|V\rangle = \sum_{i=1}^{n} v_i |i\rangle \tag{1.2}$$

1.2 Inner Product Space

The inner product or dot product of two column vectors $\boldsymbol{A} = (A_x, A_y, A_z)^T$ and $\boldsymbol{B} = (B_x, B_y, B_z)^T$ is defined as a scalar in terms of the sum of the product of the corresponding components:

$$\boldsymbol{A} \cdot \boldsymbol{B} = A_x B_x + A_y B_y + A_z B_z = \boldsymbol{A}^T \boldsymbol{B} \tag{1.3}$$

The inner product of the inner product between column vectors has the following features:

- $\boldsymbol{A} \cdot \boldsymbol{B} = \boldsymbol{B} \cdot \boldsymbol{A}$;
- $\boldsymbol{A} \cdot \boldsymbol{A} \leqslant 0$;
- $\boldsymbol{A} \cdot (b\boldsymbol{B} + c\boldsymbol{C}) = b\boldsymbol{A} \cdot \boldsymbol{B} + c\boldsymbol{A} \cdot \boldsymbol{C}$.

The first vector has a different role comparing to the second vector since it should be transposed to a row vector. We say that a column vector and a row vector are **dual correspondent**. To generalize the concept of inner product in vector space, we follow the reasonable definition:

Definition 1.5 (Inner Product)**.** *The denote* $\langle v|w\rangle$ *to indicate the inner product of two vectors in a vector space. The inner product should obey the following axiom:*

- $\langle V|W\rangle = \langle W|W\rangle *$
- $\langle W|W\rangle \leqslant 0$
- $\langle V|\left(a\left|W\right\rangle + b\left|Z\right\rangle\right) = \langle V|aW + bZ\rangle = a\left\langle V|W\right\rangle + c\left\langle V|Z\right\rangle$

A vector space with an inner product is called an inner ***product space****.*

In the inner product, the bra $\langle v|$ and the ket $|W\rangle$ are dual correspondent. If a scalar is multiplied on the bra vector, according to axiom 1:

$$\begin{aligned}\langle aW + bZ|V\rangle &= \langle V|aW + bZ\rangle \\ &= \left(a\left\langle V|W\right\rangle + b\left\langle V|Z\right\rangle\right)^* \\ &= a^*\left\langle V|W\right\rangle^* + b^*\left\langle V|Z\right\rangle^* \\ &= a^*\left\langle W|V\right\rangle + b^*\left\langle Z|V\right\rangle\end{aligned} \tag{1.4}$$

The following conclusion shows the antisymmetry between the bra and ket corresponding to the inner product, the inner product of a linear superposition with another vector is the corresponding superposition of inner product if the superposition occurs in the second factor, while it is the superposition with all the coefficients conjugated if the superposition occurs in the first factor.

Some other rules should be defined naturally:

Definition 1.6. *Two vectors are* ***orthogonal*** *if their inner product vanishes.(=0)*

Definition 1.7. *We refer to* $\sqrt{\langle V|V\rangle} = |V|$ *as the* ***norm*** *of the vector. A vector is* ***normalized*** *if it has a unit norm. A set of basis all of unit basis is called an* ***orthonormal basis****.*

Thus two given vector $|V\rangle = \sum_i v_i\left|i\right\rangle$ and $|W\rangle = \sum_j w_j\left|i\right\rangle$, we can naturally obtain:

$$\langle V|W\rangle = \sum_i\sum_j v_i^* w_j\left\langle i|j\right\rangle = \sum_i\sum_j v_i^* w_j\delta_{ij} \tag{1.5}$$

1.3 Linear Operators

1.3.1 Linear Operators

Definition 1.8 (Operator and Linear Operator)**.** *An operator* Ω *is a transformation from a given vector to another vector. An operator can act on both bras and kets.*

$$\Omega\left|V\right\rangle = \left|V'\right\rangle, \quad \left\langle W\right|\Omega = \left\langle W'\right| \tag{1.6}$$

An ***linear operator*** *if it obeys:*

- $\Omega a \left|V\right\rangle = a\Omega \left|V\right\rangle$
- $\Omega(a \left|V\right\rangle + b \left|W\right\rangle) = a\Omega V + b\Omega W$
- $\left\langle V\right| a\Omega = \left\langle V\right| \Omega a$
- $(\left\langle V\right| a + \left\langle W\right| b)\Omega = a \left\langle V\right| \Omega + b \left\langle W\right| \Omega$

Some special operator can be naturally given (only showing the expression of kets):

- An identity operator I
$$I \left|V\right\rangle = \left|V\right\rangle \tag{1.7}$$
- An inverse of an operator Ω if is is inversable:
$$\Omega^{-1}\Omega = \Omega\Omega^{-1} = I \tag{1.8}$$
- The commutator of two operator
$$[\Omega, \Lambda] = \Omega\Lambda - \Lambda\Omega \tag{1.9}$$
- The product of two operator
$$\Omega\Lambda \left|V\right\rangle = \Omega(\Lambda \left|V\right\rangle) = \Omega \left|\Lambda V\right\rangle \tag{1.10}$$

1.3.2 Matrix Elements of Linear Operators

We know that an operator transform a vector to another vector in a vector space with dimension n. So when a ket is regarded as a column vector, then an operator can be regarded as a $n \times n$ matrix. The elements of the matrix is

$$\Omega_{ij} = \left\langle i|\Omega|j\right\rangle \tag{1.11}$$

Then the transformation from $\left|V\right\rangle = \sum_i v_i \left|i\right\rangle$ to $\left|V'\right\rangle = \sum_j v'_j \left|j'\right\rangle$ can be written as

$$\begin{aligned} v'_i = \left\langle i|V'\right\rangle &= \left\langle i|\Omega|V\right\rangle = \left\langle i\right| \Omega(\sum_j v_j \left|j\right\rangle) \\ &= \sum_j v_j \left\langle i|\Omega|j\right\rangle \\ &= \sum_j v_j \Omega_{ij} \end{aligned} \tag{1.12}$$

1.3.3 The Adjoint of An Operator

Given a ket $|V\rangle$ and an operator Ω,

$$\Omega\,|V\rangle = |\Omega V\rangle \tag{1.13}$$

the corresponding bra is

$$\langle \Omega V| = \langle V|\,\Omega^\dagger \tag{1.14}$$

If Ω turns a $|V\rangle$ to $|V'\rangle$, then $\Omega^\dagger$ turns the $\langle V|$ into $\langle V'|$. Just as a and a^*, $|V\rangle$ and $\langle V|$ are related but distinct objects, so are Ω and $\Omega^\dagger$. The relation between Ω, and $\Omega^\dagger$, called the **adjoint** of Ω or "**omega dagger**". The matrix elements of $\Omega^\dagger$ in a certain basis

$$\Omega^\dagger_{ij} = \langle i|\Omega^\dagger|j\rangle = \langle \Omega i|j\rangle = \langle j|\Omega i\rangle^* = \langle j|\Omega|i\rangle^* = \Omega^*_{ji} \tag{1.15}$$

So in a given basis, the adjoint operation is equivalent to taking the transpose conjugate.

The adjoint of a product equals the product of the adjoint reversely

$$(\Omega\Lambda)^\dagger = \Lambda^\dagger\Omega^\dagger \tag{1.16}$$

1.3.4 Hermitian, Anti-Hermitian and Unitary

Definition 1.9. *An operator Ω is **Hermitian** if $\Omega^\dagger = \Omega$.*

Definition 1.10. *An operator Ω is **anti-Hermitian** if $\Omega^\dagger = -\Omega$.*

Definition 1.11. *An operator U is unitary if $U^\dagger U = UU^\dagger = I$.*

1.4 The Eigenvalue Problem

When a linear operator acting on a nonzero vector:

$$\Omega\,|V\rangle = |V'\rangle \tag{1.17}$$

Commonly $|V'\rangle$ will not be simply related to $|V\rangle$. However, for certain operator, the ket $|V\rangle$ is called an **eigenket** if on which its action is simply that of rescaling:

$$\Omega\,|V\rangle = \omega\,|V\rangle \tag{1.18}$$

The equation (**??**) is the eigenvalue equation of the operator Ω and $|V\rangle$ is the eigenket of Ω with an eigenvalue ω. In Quantun Mechanics, all the observables are Hermitian operators, which will be related in the next chapter. Some theorems about eigenvalue equations are given:

Theorem 1.1. *The eigenvalues of a Hermitian operator are real.*

Proof. Suppose that a Hermitian operator Ω and its orthonormal eigenket $|\omega\rangle$ corresponding to eigenvalue ω. So

$$\Omega |\omega\rangle = \omega |\omega\rangle \tag{1.19}$$

Dot both sides with $\langle\omega|$

$$\langle\omega|\Omega|\omega\rangle = \omega \tag{1.20}$$

Thus

$$\langle\omega|\Omega^\dagger|\omega\rangle = \langle\omega|\Omega|\omega\rangle = \omega^* = \omega \tag{1.21}$$

□

Theorem 1.2. *To every Hermitian operator Ω, there exists at least one basis consisting of its orthonormal eigenvectors. It is diagonal in this eigenbasis and its eigenvalue as its diagonal entries.*

Proof. pp.36. □

Theorem 1.3. *The eigenvalues of a unitary operator are complex numbers with a unit modulus.*

Theorem 1.4. *The eigenvectors of a unitary operator are mutually orthogonal. (no degeneracy.)*

Proof. Suppose that a unitary operator U and its eigenvecvtors $|u_i\rangle$ and $|u_j\rangle$ with eigenvalue u_i and u_j.

$$U |u_i\rangle = u_i |u_i\rangle , \quad U |u_j\rangle = u_j |u_j\rangle \tag{1.22}$$

Thus

$$\langle u_j|U^\dagger U|u_i\rangle = u_i u_j^* \langle u_j|u_i\rangle \tag{1.23}$$

so that

$$(1 - u_i u_j^*) \langle u_j|u_i\rangle = 0 \tag{1.24}$$

If $i = j$, then $u_i u_i^* = |u_i|^2 = 1$; If $i =\neq j$, then $\langle u_i|u_j\rangle = 0$. □

1.5 Generalization to Infinite Dimensions

When the dimension of a vector space goes to infinity, we cannot specifically describe the vectors by a column vector. However, for many variables, their eigenstate is continuous. So it is necessary to generalize the concepts to infinite dimension.

For an Hermitian operator with no degeneracy Ω

$$\Omega \left|\omega\right\rangle = \omega \left|\omega\right\rangle \tag{1.25}$$

Where ω is the eigenvalue with continuous span. For any normalized vector $|\psi\rangle$, it is reasonable to express it as the integral with respect to the eigenvalue

$$\left|\psi\right\rangle = \int \mathrm{d}\omega \left|\omega\right\rangle \left\langle\omega|\psi\right\rangle \tag{1.26}$$

The result is guarenteed by the completence of $|\omega\rangle$

$$\int \left|\omega\right\rangle \left\langle\omega\right| \mathrm{d}\omega = I \tag{1.27}$$

2

Postulates of Quantum Mechanics

In this chapter the postulates will be stated and discussed in a broad terms to bring out the essential features of quantum theory.

R.Shankar

2.1 The Postulates

The basic postulates of quantum mechanics are based on the classical counterparts. The postulates can be concluded in different ways. In this book, the postulates are divided in four different parts. The symmetry of identical particles are not included, but will be refering in the subsequent sections.

Postulated of Classical Mechanics

1. The state of a particle at any given time is **specified** by the two variables $x(t)$ and $p(t)$.
2. Every dynamical variable ω is a function of x and p: $\omega = f(x, p)$.
3. If the particle is in a state given by x and p, the measurement of the variable ω will yield a value $\omega(x, p)$. The state will remain **unaffected**.
4. The state variables change with time according to Hamilton's equation:

$$\begin{aligned} \dot{x} &= \frac{\partial H}{\partial p} \\ \dot{p} &= -\frac{\partial H}{\partial x} \end{aligned} \tag{2.1}$$

Postulates of Quantum Mechanics

1. The state of the particle is represented by a vector $|\psi(t)\rangle$ in a Hilbert space.
2. The independent variables x and p of classical mechanics are represented by Hermitian operators X and P with the following matrix elements in the eignebasis of X:

$$\langle x|X|x'\rangle = x\delta(x-x') \tag{2.2}$$

$$\langle x|P|x'\rangle = -\mathrm{i}\hbar(x-x') \tag{2.3}$$

3. If the particle is in a state $|\psi\rangle$, measurement of the variable Ω will yield one of the eignevalue ω with probability $P(\omega) \propto |\langle\omega|\psi\rangle|^2$. The stats of the system will change from $|\psi\rangle$ to $|\omega\rangle$ as a result of the measurement.
4. The state of vector $|\psi\rangle$ obeys the Schödinger equation

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle \tag{2.4}$$

2.2 Discussion of Postulates I-III

2.2.1 Possiblistic Prediction and Probability

The theory makes only possiblistic prediction for the result of a measurement of an obsevables, whose possible values are only the eigenvalues of the observables. The probability for state with eigenvalue ω_i should be the relative probability $\langle\omega_i|\psi\rangle$ divided by all the relative probability $\langle\psi|\psi\rangle$

$$P(\omega_i) = \frac{|\langle\omega_i|\psi\rangle|^2}{\langle\psi|\psi\rangle} \tag{2.5}$$

It is clear that for the orthonormal state vector $|\psi\rangle$ we have

$$P(\omega_i) = |\langle\omega_i|\psi\rangle|^2 \tag{2.6}$$

An obvious consequence is: if a state $|\psi\rangle$ is an eigenstate $|\omega_i\rangle$, then the measurement of Ω will definitely yield to ω_i instead of other values. If the state vector is a superposed state of many eigenstates, for example, the superposition of $|\omega_1\rangle$ and $|\omega_2\rangle$ with the following expression (the state vector is

orthonormal)

$$|\psi\rangle = \frac{\alpha\,|\omega_1\rangle + \beta\,|\omega_2\rangle}{(|\alpha|^2 + |\beta|^2)^{1/2}} \tag{2.7}$$

Then the measurement of Ω will yield to either ω_1 or ω_2 with probability

$$\begin{aligned} P(\omega_1) &= \langle\omega_1|\psi\rangle = \frac{|\alpha|^2}{|\alpha|^2 + |\beta|^2} \\ P(\omega_2) &= \langle\omega_2|\psi\rangle = \frac{|\beta|^2}{|\alpha|^2 + |\beta|^2} \end{aligned} \tag{2.8}$$

2.2.2 Representation in Different Basis

For two different observables Ω and Λ, we have different eigenkets and eigenvalues. So the two operators represents two different space. So in order to extract the information for an observable, we have to determine the eigenbasis of the corresponding operator and get the projection of $|\psi\rangle$ on the eigenkets. The state $|psi\rangle$ has different **representation** in different eigenbasis. For example, in the Ω basis

$$|\psi\rangle = \sum_i |\omega_i\rangle\,\langle\omega_i|\psi\rangle \tag{2.9}$$

2.2.3 Active and Passive Transformation, Change of Basis

Suppose that we have two incompatible obsevables Ω and Λ. Then the ket space can be seen as being spanned by the set of base kets of either Ω or Λ. Such that we wish to know how the two different basis are related. Suppose that the basis of Ω and Λ are separatedly $|\omega_i\rangle$ and $|\lambda_i\rangle$, then we have the following theorem

Theorem 2.1. [1] *There exists a unitary operator U such that*

$$|\omega_i\rangle = U\,|\lambda_i\rangle\,, \quad i = 1, 2\cdots n \tag{2.10}$$

or

$$|\lambda_i\rangle = U^\dagger\,|\omega_i\rangle\,, \quad i = 1, 2\cdots n \tag{2.11}$$

We have known from (**??**) that the ket $|\psi\rangle$ in Ω basis. To transform it into the basis of Λ, that is

$$|\psi\rangle = \sum_i |\lambda_i\rangle\,\langle\lambda_i|\psi\rangle \tag{2.12}$$

[1] J.J.Sakurai. Modern Quantum Mechanics. Rev. Ed., New York, Addison-Wesley. 1994. 37.

we have to obtain $\langle\lambda_i|\psi\rangle$. To accomplish our goal, we expand $\langle\lambda_i|\psi\rangle$ according to theorem **??**

$$\langle\lambda_i|\psi\rangle = \sum_j \langle\lambda_i|\omega_j\rangle \langle\omega_j|\psi\rangle = \sum_j \langle\lambda_i|U^\dagger|\lambda_j\rangle \langle\omega_j|\psi\rangle \tag{2.13}$$

So the core of the transformation between two different basis is the matrix of $U^\dagger$. We now consider the transformation of the operators. Suppose an operator A and its matrix elements in Ω basis $\langle\omega_i|A|\omega_j\rangle$ is already known. Then the matrix elements of operator A in Λ basis should be

$$\begin{aligned}\langle\lambda_i|A|\lambda_j\rangle &= \sum_k \sum_l \langle\lambda_i|\omega_k\rangle \langle\omega_k|A|\omega_l\rangle \langle\omega_l|\lambda_j\rangle \\ &= \sum_k \sum_l \langle\omega_i|U^\dagger|\omega_k\rangle \langle\omega_k|A|\omega_l\rangle \langle\omega_l|U|\omega_j\rangle\end{aligned} \tag{2.14}$$

Hence

$$A_\lambda = U_\omega^\dagger A_\omega U_\omega \tag{2.15}$$

where the subscripts represent in which basis the matrix is.

2.3 Complications

Actually, the four postulates can not solve all the problems. Some complications may easily derived from the discussion above and we must know how they are to be surmounted. Four major complications are listed below.

Complication 1: The recipe of an operator is ambiguous. In classical case, for example, $xp = px$. However, for $\omega = xp$ we don't know if $\Omega = XP$ or PX. So we have to follow certain rules to define expression of such variables to make it Hermitian. Here we introduce Bohm's rule and Weyl's rule[2]:

Definition 2.1 (Bohm's Rule)**.** *If a variable ω can be written as a polynomial of x and p in classical case and each term can be expressed in terms of $f(x)g(x)$, then the operator of this term is defined as*

$$\frac{1}{2}[f(X)g(P) + g(P)f(X)] \tag{2.16}$$

Definition 2.2 (Weyl's Rule)**.** *To expand the variable with an expression of Fourier integral in classical case*

$$\Omega(x,p) = \int_{-\infty}^{\infty} \mathrm{d}\xi \int_{-\infty}^{\infty} \omega(\xi,\eta)\mathrm{e}^{\mathrm{i}\xi x + \mathrm{i}\eta p}\mathrm{d}\eta \tag{2.17}$$

[2]Ka X. Advanced Quantum Mechanics (2nd ed). Beijing : Higher Education Press, 2001.8

Substitute (x, p) with (X, P) we obtain the expression of the operator

$$\Omega(X,P) = \int_{-\infty}^{\infty} \mathrm{d}\xi \int_{-\infty}^{\infty} \omega(\xi,\eta) \mathrm{e}^{\mathrm{i}\xi X + \mathrm{i}\eta P} \mathrm{d}\eta \tag{2.18}$$

Complication 2: The operator Ω is degenerate. For example $\omega_1 = \omega_2 = \omega$, we select some orthogonal basis $|\omega_1\rangle$ and $|\omega_2\rangle$ in the eigenspace with eigenvalue ω, then

$$P(\omega) = |\langle\omega_1|\psi\rangle|^2 + |\langle\omega|\omega\rangle_2 \psi|^2 \tag{2.19}$$

Complication 3: The eigenvalue spectrum of Ω is continuous. In this case an state vector can be expanded as

$$|\psi\rangle = \int |\omega\rangle \langle\omega|\psi\rangle \, \mathrm{d}\omega \tag{2.20}$$

We expect $\langle\omega|\psi\rangle = \psi(\omega)$ to be a smooth function, which is called **wave function in the ω space**.

Complication 4: The quantum varaible has no classical counterpart. For example, spin.

2.4 Expectation Value and Uncertainty

In classical cases, the expectation of a variables at any moment is specified if the dynamic equation is determined. In quantum theory, the expectation of a variable Ω yield to different values with different probability. The probability can predicted statistically by testing a considerable number of measurements. The expectation value is the mean value defined in statistics:

$$\langle\Omega\rangle = \sum_i P(\omega_i)\omega_i = \sum_i \langle\psi|\omega_i\rangle \langle\omega_i|\psi\rangle \omega_i = \sum_i \langle\psi|\Omega|\omega_i\rangle \langle\omega_i|\psi\rangle = \langle\psi|\Omega|\psi\rangle \tag{2.21}$$

Then **standard deviation** can be naturally defined to give the fluctuation of measurement around the mean value:

$$\Delta\Omega = \left\langle (\Omega - \langle\Omega\rangle)^2 \right\rangle^{1/2} \tag{2.22}$$

2.5 Ensembles and The Density Operator

The following discussion is mainly based on J.J.Sakurai.[3]

[3] J.J.Sakurai. Modern Quantum Mechanics. Rev. Ed., New York, Addison-Wesley. 1994. 176-177.

A pure ensemble is a system in which every member selected randomly is in the state $|i\rangle$. A mixed ensemble, in contrast, is a system in which some members with relative populations w_i can be characterized by $|i\rangle$, while some others with relative population w_j can be characterized by $|j\rangle$, and so on. We have to emphasize that the state $|i\rangle$, $|j\rangle$ need not to be orthognal and its sum need not to coincide the dimensionality of the ket space.

If we take a measurement on a mixed ensemble of some observable Ω, the question we are longing to solve is the average value of Ω when a considerable amount of measurements are taken. We thus introduce the **ensemble average** which is defined by

$$\bar{\Omega} = \sum_i w_i \langle i|\Omega|i\rangle = \sum_i \sum_{\omega_j} w_i |\langle \omega_j|i\rangle|^2 \omega_j \tag{2.23}$$

To transform (**??**) into another basis $\{|\lambda_j\rangle\}$

$$\begin{aligned} \bar{\Omega} &= \sum_i w_i \sum_{\lambda_k}\sum_{\lambda_l} \langle i|\lambda_k\rangle \ \langle\lambda_k|\Omega|\lambda_l\rangle \langle\lambda_l|i\rangle \\ &= \sum_{\lambda_k}\sum_{\lambda_l}(\sum_i w_i \langle\lambda_l|i\rangle \langle i|\lambda_k\rangle) \langle\lambda_k|\Omega|\lambda_l\rangle \end{aligned} \tag{2.24}$$

we define **the density operator** ρ by

$$\rho = \sum_i w_i |i\rangle \langle i| \tag{2.25}$$

Thus the **density matrix** is

$$\langle\lambda_l|\rho|\lambda_k\rangle = \sum_i w_i \langle\lambda_l|i\rangle \langle i|\lambda_k\rangle \tag{2.26}$$

so that

$$\begin{aligned} \bar{\Omega} &= \sum_{\lambda_l}\sum_{\lambda_k} \langle\lambda_l|\rho|\lambda_k\rangle) \langle\lambda_k|\Omega|\lambda_l\rangle \\ &= \sum_{\lambda_l}\sum_{\lambda_k} \langle\lambda_l|\rho|\Omega\rangle \lambda_l \\ &= \mathrm{tr}\{\rho\Omega\} \end{aligned} \tag{2.27}$$

Due to that the trace is independent of representation (the trace is the same value in different basis), we can use whatever useful basis if we want. Obviously we obtain

$$\mathrm{tr}\{\rho\} = 1 \tag{2.28}$$

3

Classical 1-D Problems

3.1 Free Particle

The simplest problem is the problem of the free particle. The free particle is not influenced by the potential. The Schödinger equation is

$$\mathrm{i}\hbar\left|\dot{\psi}\right\rangle = H\left|\psi\right\rangle = \frac{P^2}{2m}\left|\psi\right\rangle \tag{3.1}$$

The statiionary state are the solutions of the form

$$\left|\psi\right\rangle = \left|E\right\rangle \mathrm{e}^{-\mathrm{i}Et/\hbar} \tag{3.2}$$

so

$$H\left|E\right\rangle = \frac{P^2}{2m}\left|E\right\rangle = E\left|E\right\rangle \tag{3.3}$$

It is obvious that any eigenstate of P is also the eigenstate of P^2. So for an eigenstate $\left|p\right\rangle$ of P, we have

$$\frac{P^2}{2m}\left|p\right\rangle = E\left|p\right\rangle \tag{3.4}$$

If we rewrite

$$p = \sigma\sqrt{2mE} \tag{3.5}$$

then the eigenstate of E can be written as

$$\left|E,\sigma\right\rangle = \left|p = \sigma\sqrt{2mE}\right\rangle \tag{3.6}$$

Thus we find that to the energy eigenvalue E there corresponds a degenerate two-dimensional eigenspace, spanned by the above vectors. Physically it shows that the particle goes either left or right with momentum $|p|$ has the unique energy E.

3.2 The Particle in a Box

For a potential

$$V(x) = \begin{cases} 0, |x| \leqslant L/2 \\ \infty, |x| \geqslant L/2 \end{cases} \tag{3.7}$$

The eigenvalue equation writes in X basis

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi + \frac{2m}{\hbar^2}[E - V]\psi = 0 \tag{3.8}$$

That the potential diverges to infinity shows the particle cannot exist in the region $|x| \geqslant L/2$, where the wave function must vanish. The particle must be confined in the region $|x| \leqslant L/2$. So

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi + \frac{2mE}{\hbar^2}\psi = 0 \tag{3.9}$$

which is solved by

$$\psi = A\mathrm{e}^{-\mathrm{i}kx} + B\mathrm{e}^{\mathrm{i}kx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}} \tag{3.10}$$

It is obvious to ensure that

$$\psi(-L/2) = \psi(L/2) = 0 \tag{3.11}$$

so that

$$k = \frac{n\pi}{L}, \quad n \in \mathbb{Z} \tag{3.12}$$

which means the energy eigenvalue is

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2\pi^2\hbar^2}{2\pi L^2} \tag{3.13}$$

and the corresponding orthonormal wave function

$$\psi(x) = \begin{cases} \sqrt{\dfrac{2}{L}}\cos\Big(\dfrac{n\pi}{L}x\Big), & n = \text{odd number} \\ \sqrt{\dfrac{2}{L}}\sin\Big(\dfrac{n\pi}{L}x\Big), & n = \text{even number} \end{cases} \tag{3.14}$$

3.3 The Continuity Equation for Probability

The Schrödinger equation

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \tag{3.15}$$

and its conjugate

$$-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\psi^* = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^* \tag{3.16}$$

Notice that $H = -\dfrac{\hbar^2}{2m}\nabla^2 + V$ has to be Hermitian, which means that the potential is a real function. So $V = V^*$. Multiplying the first equation with ψ^* and the second one with ψ, and taking their difference, we obtain

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}(\psi\psi^*) = -\frac{\hbar^2}{2m}(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*) = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}\cdot(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*) \tag{3.17}$$

We already now that the **probability density** is

$$P = \int \psi^*(\boldsymbol{r},t)\psi(\boldsymbol{r},t)\mathrm{d}^3\boldsymbol{r} \tag{3.18}$$

and we define the **probability current density** by

$$\boldsymbol{j} = \frac{\hbar}{2m\mathrm{i}}(\psi^*\boldsymbol{\nabla}\psi - \psi\boldsymbol{\nabla}\psi^*) \tag{3.19}$$

So equation (**??**) can be rewrited as

$$\frac{\mathrm{d}P}{\mathrm{d}t} = -\boldsymbol{\nabla}\cdot\boldsymbol{j} \tag{3.20}$$

Globally we obtain

$$\int\frac{\mathrm{d}P}{\mathrm{d}t}\mathrm{d}^3\boldsymbol{r} = -\int\boldsymbol{\nabla}\cdot\boldsymbol{j}\mathrm{d}^3\boldsymbol{r} = -\int_S \boldsymbol{j}\cdot\mathrm{d}\boldsymbol{S} \tag{3.21}$$

which physically means that the probability density of finding a particle in a region is changing by a rate of the probability current density flowing through the bound surface of the region.

3.4 1-D Problems in Scattering

Consider the potential barrier

$$V(x) = \begin{cases} V_0, & 0 < x < a \\ 0, & x > a,\ x < 0 \end{cases} \tag{3.22}$$

Imagine a particle with energy E is shot from the left of the potential barrier. In classical situation, the particle will not pass through the barrier if $E < V_0$, however, in the quantum counterpart, the particle will have probability to pass through the barrier. We now consider the case $E < V_0$.

When the particle is located outside the barrier, the steady state Schrödinger equation writes

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi + \frac{2mE}{\hbar^2}\psi = 0 \tag{3.23}$$

Since there are both reflected wave and the incident wave on the left side of the barrier, the steady state of the wave function can be expanded by the two solutions of (**??**)(Here the incident wave function is normalized)

$$\psi_L(x) = \mathrm{e}^{\mathrm{i}kx} + R\mathrm{e}^{-\mathrm{i}kx} \tag{3.24}$$

where $k = \sqrt{2mE}/\hbar$ and the first term indicates the incident wave and the second term indicates the reflected wave. Similarly, the transmitted wave on the right side can be written as

$$\psi_R(x) = S\mathrm{e}^{\mathrm{i}kx} \tag{3.25}$$

In the barrier, we just simply replace E by $E - V_0$ in (**??**)

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi - \frac{2m(V_0 - E)}{\hbar^2}\psi = 0 \tag{3.26}$$

Thus the wave function inside the barrier writes

$$\psi_B(x) = A\mathrm{e}^{k'x} + B\mathrm{e}^{-k'x} \tag{3.27}$$

where $k' = \sqrt{2m(V_0 - E)}/\hbar$

Due to the continuity of the wave function at the boundaries of the barrier, we have to ensure the continuity of the wave function and the derivative of the wave function. So at $x = 0$ we obtain

$$1 + R = A + B \tag{3.28}$$

$$\mathrm{i}k(1 - R) = k'(A - B) \tag{3.29}$$

at $x = a$, similarly

$$A\mathrm{e}^{k'a} + B\mathrm{e}^{-k'a} = S\mathrm{e}^{\mathrm{i}ka} \tag{3.30}$$

$$k'A\mathrm{e}^{k'a} - k'B\mathrm{e}^{-k'a} = \mathrm{i}kS\mathrm{e}^{\mathrm{i}ka} \tag{3.31}$$

Thus we can derive

$$A = \frac{1}{2}[(1 + \frac{\mathrm{i}k}{k'}) + R(1 - \frac{\mathrm{i}k}{k'})] \tag{3.32}$$

$$B = \frac{1}{2}[(1 - \frac{\mathrm{i}k}{k'}) + R(1 + \frac{\mathrm{i}k}{k'})] \tag{3.33}$$

$$R = \frac{(k^2 + k'^2)^2 \sinh^2 k'a}{(k^2 + k'^2)^2 \sinh^2 k'a + 4k^2k'^2} \tag{3.34}$$

$$S = \frac{4k^2k'^2}{(k^2 + k'^2)^2 \sinh^2 k'a + 4k^2k'^2} \tag{3.35}$$

It is easy to find that the reflectance coefficient and the transmittance coefficient satisfy

$$|R|^2 + |S|^2 = 1 \tag{3.36}$$

3.5 δ Potential

We now consider a δ-potential barrier with the following form

$$V(x) = \gamma\delta(x), \quad \gamma > 0 \tag{3.37}$$

So the Schrödinger equation writes

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi + \frac{2m}{\hbar^2}[E - \gamma\delta(x)]\psi = 0 \tag{3.38}$$

Integrate both sides of equation (**??**) in the region $(-\epsilon, \epsilon)$, where ϵ is an infinitesimal value. When $\epsilon \to 0$, we have

$$\psi'(0^+) - \psi'(0^-) = \frac{2m\gamma}{\hbar^2}\psi(0) \tag{3.39}$$

That is the boundary condition of delta potential since the continuity of derivative of wave function is not satisfied in this case. Following the discussion in the above section, we can easily have

$$|S|^2 = \frac{1}{1 + m\gamma^2/2\hbar^2 E} \tag{3.40}$$

$$|R|^2 = \frac{m\gamma^2/2\hbar^2 E}{1 + m\gamma^2/2\hbar^2 E} \tag{3.41}$$

and obviously

$$|R|^2 + |S|^2 = 1 \tag{3.42}$$

4

Periodic Potential and Floquet Theory

4.1 Periodic Potential

We study the motion of particles in periodic potential with following expression

$$V(\boldsymbol{x}+\boldsymbol{a}) = V(\boldsymbol{x}) \tag{4.1}$$

where $\boldsymbol{a}$ is a constant vector representing the potential field has a translational invariance.

4.2 Basic Floquet Theory

Floquet theory is aimed to solve linear differential equation with periodicity of the following form

$$\dot{\boldsymbol{x}} = \boldsymbol{A}(t)\boldsymbol{x} \tag{4.2}$$

where $\boldsymbol{x}$ is a $n-$dimension column vector and $\boldsymbol{A}$ is a $n \times n$ matrix. If equation (**??**) has n solutions $\boldsymbol{x}_1, \boldsymbol{x}_2 \cdots \boldsymbol{x}_n$, then we call the following $n \times n$ matrix a **fundamental matrix**

$$\boldsymbol{X}(t) = (\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots \boldsymbol{x}_2) \tag{4.3}$$

It is easy to prove that any fundamental matrix multplied by a constant non-singular matrix is still a fundamental matrix. Such that

$$\boldsymbol{Y}(t) = \boldsymbol{X}(t)\boldsymbol{B} \tag{4.4}$$

is a fundamental matrix. We define the Wronskian $W(t)$ of $\boldsymbol{X}(t)$ be the determinant of $\boldsymbol{X}(t)$. We find that

$$W(t) = W(t_0)\exp\left\{\int_{t_0}^{t} \boldsymbol{A}(\tau)\mathrm{d}\tau\right\} \tag{4.5}$$

Based on the above discussion, we introduce two theorems:

Theorem 4.1. *If $\boldsymbol{A}(t)$ has a period T, which means $\boldsymbol{A}(t+T) = \boldsymbol{A}(t)$. If $\boldsymbol{X}(t)$ is a fundamental matrix of equation (??), then so is $\boldsymbol{X}(t+T)$ and there exists a constant non-singular matrix $\boldsymbol{B}$*

1. $\boldsymbol{X}(t+T) = \boldsymbol{X}(t)\boldsymbol{B}$
2. $\det\{\boldsymbol{B}\} = \exp\left\{\int_0^T \boldsymbol{A}(\tau)\mathrm{d}\tau\right\}$

Proof. It is easy to see that

$$\dot{\boldsymbol{X}}(t+T) = \boldsymbol{A}(t+T)\boldsymbol{X}(t+T) = \boldsymbol{A}(t)\boldsymbol{X}(t+T) \tag{4.6}$$

so $\boldsymbol{X}(t+T)$ is a fundamental matrix.

1. Let $\boldsymbol{B} = \boldsymbol{X}^{-1}(t)\boldsymbol{X}(t+T)$, so that $\boldsymbol{X}(t+T) = \boldsymbol{X}(t)\boldsymbol{B}$. To ensure the uniqueness of the solutions, we have to make $\boldsymbol{B}$ a time-independent matrix. Since $\boldsymbol{B}$ is time-independent, we can calculate it by forcing $t = 0$, so that $\boldsymbol{B} = \boldsymbol{X}^{-1}(0)\boldsymbol{X}(T)$.

2. We see that

$$\begin{aligned} W(t+T) &= W(t_0)\exp\left\{\int_{t_0}^{t+T} \boldsymbol{A}(\tau)\mathrm{d}\tau\right\} \\ &= W(t_0)\exp\left\{\int_{t_0}^{t} \boldsymbol{A}(\tau)\mathrm{d}\tau + \int_{t}^{t+T} \boldsymbol{A}(\tau)\mathrm{d}\tau\right\} \\ &= W(t_0)\exp\left\{\int_{t_0}^{t} \boldsymbol{A}(\tau)\mathrm{d}\tau\right\}\exp\left\{\int_{t}^{t+T} \boldsymbol{A}(\tau)\mathrm{d}\tau\right\} \\ &= W(t)\exp\left\{\int_{0}^{T} \boldsymbol{A}(\tau)\mathrm{d}\tau\right\} \end{aligned} \tag{4.7}$$

Since

$$W(t+T) = \det\{\boldsymbol{X}(t+T)\} = \det\{\boldsymbol{X}(t)\boldsymbol{B}\} = W(t)\det\{\boldsymbol{B}\} \tag{4.8}$$

So

$$\det\{\boldsymbol{B}\} = \exp\left\{\int_0^T \boldsymbol{A}(\tau)\mathrm{d}\tau\right\} \tag{4.9}$$

□

We introduce the **characteristic multiplier** of the fundamental matrix. The eigenvalues $\rho_1, \rho_2 \cdots \rho_n$ of $\boldsymbol{B}$ are called the characteristic multipliers for $\boldsymbol{X}$ and the corresponding Floquet exponents are complex numbers $\mu_1, \mu_2 \cdots \mu_n$ with the following expression

$$\rho_i = \mathrm{e}^{\mu_i T}, \mu_i \in \mathbb{C}, i = 1, 2, \cdots n \tag{4.10}$$

Theorem 4.2. *Let ρ be a characteristic multiplier and let μ be the corresponding characteristic exponent. Then there exists a solution $\boldsymbol{x}(t)$ of $\dot{\boldsymbol{x}} = \boldsymbol{A}(t)\boldsymbol{x}$ such that*

1. $\boldsymbol{x}(t+T) = \rho\boldsymbol{x}(t)$
2. $\boldsymbol{x}(t) = \mathrm{e}^{\mu t}\boldsymbol{p}(t)$, *where $\boldsymbol{p}(t)$ is a periodic function with period T.*

Proof. The proof follows two steps

1. Let $\boldsymbol{b}$ be a eigenvector of $\boldsymbol{B}$ and $\boldsymbol{x}(t) = \boldsymbol{X}(t)\boldsymbol{b}$, so that
$$\boldsymbol{x}(t+T) = \boldsymbol{X}(t+T)\boldsymbol{b} = \boldsymbol{X}(t)\boldsymbol{B}\boldsymbol{b} = \rho\boldsymbol{X}(t)\boldsymbol{b} = \rho\boldsymbol{x}(t) \tag{4.11}$$
2. Let $\boldsymbol{p}(t) = \boldsymbol{x}(t)\mathrm{e}^{-\mu t}$, we now prove that it is periodic matrix
$$\boldsymbol{p}(t+T) = \boldsymbol{x}(t+T)\mathrm{e}^{-\mu(t+T)} = \mathrm{e}^{\mu T}\boldsymbol{x}(t)\mathrm{e}^{-\mu(t+T)} = \boldsymbol{x}(t)\mathrm{e}^{-\mu t} = \boldsymbol{p}(t) \tag{4.12}$$
So $\boldsymbol{p}(t)$ is a T-period matrix. Thus $\boldsymbol{x}(t) = \mathrm{e}^{\mu T}\boldsymbol{p}(t)$.

□

4.3 Schrödinger Equation with Periodic Potential

A 1-D Schrödinger Equation with Periodic Potential shows

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi = \frac{2m}{\hbar}[E - V(x)]\psi = A(x)\psi \tag{4.13}$$

where $A(x)$ is a periodic function with the same period a as the potential function. We now let $x_1 = \psi, x_2 = \psi'$, so the above eqaution turns into a matrix equation

$$\frac{\mathrm{d}}{\mathrm{d}x}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ A(x) & 0 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \tag{4.14}$$

Due to (**??**), if we obtain a fundamental matrix

$$\begin{pmatrix} x_1^{(1)}(t) & x_1^{(2)}(t) \\ x_2^{(1)}(t) & x_2^{(2)}(t) \end{pmatrix} \tag{4.15}$$

Then there existsa constant matrix $\boldsymbol{B}$ so that

$$\begin{aligned} \begin{pmatrix} x_1^{(1)}(x+a) & x_1^{(2)}(x+a) \\ x_2^{(1)}(x+a) & x_2^{(2)}(x+a) \end{pmatrix} &= \begin{pmatrix} x_1^{(1)}(x) & x_1^{(2)}(x) \\ x_2^{(1)}(x) & x_2^{(2)}(x) \end{pmatrix}\boldsymbol{B} \\ &= \begin{pmatrix} x_1^{(1)}(x) & x_1^{(2)}(x) \\ x_2^{(1)}(x) & x_2^{(2)}(x) \end{pmatrix}\begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \end{aligned} \tag{4.16}$$

Equation (**??**) show that the wavefunction at $x + a$ can be expanded as combination of two independent wavefunction at x.

4.4 Bloch Theorem

We now introduce Bloch theorem.

Theorem 4.3. *The wavefunction for a particle in a periodic potential field with period* $\boldsymbol{a}$ *can be writen in the form of*

$$\psi(\boldsymbol{r}) = \mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{r}} u(\boldsymbol{r}) \tag{4.17}$$

where $u(\boldsymbol{r})$ *has the same period* $\boldsymbol{a}$*.*

Proof. See proof of theorem **??** □

Bloch theorem shows that the wave function of a particle in a periodic potential can be also a periodic function, simultaneously with the same period as the potential. We notify that the Bloch wave vector $\boldsymbol{K}$, which represents the propagation of the particle, is not unique and so is $u(\boldsymbol{r})$. Replacing $\boldsymbol{K}$ by $\boldsymbol{K} + \boldsymbol{G}$, where $\boldsymbol{G}$ is a arbitrary reciprocal lattice vector $\boldsymbol{G}$ obeying

$$\boldsymbol{G} \cdot \boldsymbol{r} = 2\pi N, N \in \mathbb{Z} \tag{4.18}$$

we have

$$\mathrm{e}^{\mathrm{i}(\boldsymbol{K}+\boldsymbol{G})\cdot\boldsymbol{r}} = \mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{r}} \mathrm{e}^{\mathrm{i}2\pi N} = \mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{r}} \tag{4.19}$$

5

The Harmonic Oscillators

A harmonic oscillator is a classic model which has specific solution in classical situations. Any system fluctuated around the equilibrium point by a small amplitude can be described by the Harmonic Oscillator. In the classical situation, the Hamiltonian for the HO is

$$H = T + V = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \tag{5.1}$$

Any Hamiltonian of such form is called a Harmonic Oscillator Hamiltonian.

5.1 Quantization of Harmonic Oscillator (Coordinate Basis)

In quantum mechanics, the Hamiltonian operator is

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2 \tag{5.2}$$

The eigenvalue equation of H cames naturally (in energy basis)

$$H\,|E\rangle = (\frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2)\,|E\rangle = E\,|E\rangle \tag{5.3}$$

We project the equation (**??**) onto coordinate basis. Thus $X \to x, P \to -\mathrm{i}\hbar\dfrac{\mathrm{d}}{\mathrm{d}x}, |E\rangle \to \langle x|E\rangle = \psi_E(x)$. So that

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi + \frac{2m}{\hbar^2}(E - \frac{1}{2}m\omega x^2)\psi = 0 \tag{5.4}$$

The solution of equation (**??**) and corresponding eigenvalue spectrum can be solved in a routine method:

$$E_n = (n + 1/2)\hbar\omega, \quad n = 0, 1, 2\cdots \tag{5.5}$$

$$\psi_E(x) = \psi_n(x) = (\frac{m\omega}{\pi\hbar 2^{2n}(n!)^2})^{1/4} \exp\left\{(-\frac{m\omega x^2}{2\hbar})\right\} H_n[(\frac{m\omega}{\hbar})^{1/2}x] \tag{5.6}$$

Where $H_n(x)$ is called Hermite polynomial with n order defined by:

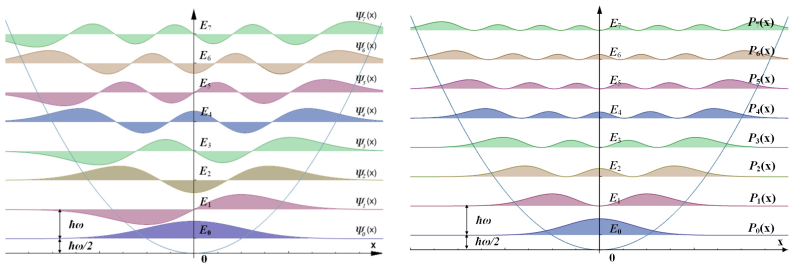
$$H_n(x) = (-1)^n \mathrm{e}^{x^2} \frac{\mathrm{d}^n}{\mathrm{d}x^2}(\mathrm{e}^{-x^2}) \tag{5.7}$$

Hermite polynomials obeys the following recursion relations:

$$H_n'(x) = 2nH_{n-1}(x) \tag{5.8}$$

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \tag{5.9}$$

From the equation (**??**) we can discover that the energy is quantized, or in another perspective, the energy spectrum is discrete. The following figure **??** shows the wave function in coordinate basis and the probability density with respect to different energy.



(a) The wave function of Harmonic Oscillator.

(b) The corresponding probability density

FIGURE 5.1
(a) Wavefunction representations for the first eight bound eigenstates, n = 0 to 7. The horizontal axis shows the position x. Note: The graphs are not normalized, and the signs of some of the functions differ from those given in the text. (b) Corresponding probability density $|\psi(x)|^2$.

5.2 In Energy Basis and "Ladder Operator" Method

We introduce the **lowering operator**

$$a = (\frac{m\omega}{2\hbar})^{1/2} X + \mathrm{i}(\frac{1}{2m\omega\hbar})^{1/2} P \tag{5.10}$$

and its adjoint, the **raising operator**

$$a^\dagger = (\frac{m\omega}{2\hbar})^{1/2} X - \mathrm{i}(\frac{1}{2m\omega\hbar})^{1/2} P \tag{5.11}$$

They satisfy the commutation relation

$$[a, a^\dagger] = 1 \tag{5.12}$$

and it is easy to verify that

$$H = (aa^\dagger + 1/2)\hbar\omega \tag{5.13}$$

Define a new operator $\hat{H}$

$$\hat{H} = \frac{H}{\hbar\omega} = (aa^\dagger + 1/2) \tag{5.14}$$

whose eigenvalues ϵ measured energy in units of $\hbar\omega$. So the problem turns into solving the eigenvalue problem of $\hat{H}$

$$\hat{H}\,|\epsilon\rangle = \epsilon\,|\epsilon\rangle \tag{5.15}$$

It is also easy to verify that

$$[a, \hat{H}] = [a, aa^\dagger + 1/2] = [a, aa^\dagger] = a \tag{5.16}$$

and

$$[a^\dagger, \hat{H}] = -a^\dagger \tag{5.17}$$

So

$$\begin{aligned} \hat{H}a\,|\epsilon\rangle &= (a\hat{H} - [a, \hat{H}])\,|\epsilon\rangle \\ &= (a\hat{H} - a)\,|\epsilon\rangle \\ &= (\epsilon - 1)a\,|\epsilon\rangle \end{aligned} \tag{5.18}$$

Equation (**??**) shows that $a\,|\epsilon\rangle$ is a eigenstate with eigenvalue of $\epsilon - 1$. Similarly we can get the similar relation of $a^\dagger$

$$\begin{aligned} \hat{H}a^\dagger\,|\epsilon\rangle &= (a^\dagger\hat{H} - [a^\dagger, \hat{H}])\,|\epsilon\rangle \\ &= (a^\dagger\hat{H} + a^\dagger)\,|\epsilon\rangle \\ &= (\epsilon - 1)a^\dagger\,|\epsilon\rangle \end{aligned} \tag{5.19}$$

which shows that $a^\dagger\,|\epsilon\rangle$ is a eigenstate with eigenvalue of $\epsilon + 1$. The lowering and the raising operator decreases and increases the quanta of the energy by 1 respectively. So from a certain eigenvalue ϵ, we can get all the other eigenvalues $\epsilon_1, \epsilon_2 \cdots$ by lowering and raising operators. However, there exists a minimum energy of harmonic oscillator, so the eigenvalue cannot be decreased to $-\infty$. So for the lowest energy ϵ_0

$$a\,|\epsilon_0\rangle = 0 \tag{5.20}$$

so that

$$aa^\dagger |\epsilon_0\rangle = (\hat{H} - 1/2) |\epsilon_0\rangle = 0 \tag{5.21}$$

so

$$\epsilon_0 = 1/2 \tag{5.22}$$

so

$$E_n = (n + 1/2)\hbar\omega, n = 0, 1, 2 \cdots \tag{5.23}$$

Our next step is to solve the eigenstate of a and $a^\dagger$. From (**??**) we know that

$$a |n\rangle = C_n |n-1\rangle \tag{5.24}$$

The adjoint of the eqaution cames

$$\langle a|^\dagger = C_n^* \langle n-1| \tag{5.25}$$

so

$$\begin{aligned} \langle n|a^\dagger a|n\rangle &= C_n^* C_n \langle n-1|n-1\rangle \\ \langle n|\hat{H} - 1/2|n\rangle &= C_n^* C_n \\ \langle n|n|n\rangle &= C_n^* C_n \\ |C_n|^2 &= n \end{aligned} \tag{5.26}$$

which means $C_n = \sqrt{n}\mathrm{e}^{\mathrm{i}\theta}$. If we choose $\theta = 0$, then

$$a |n\rangle = \sqrt{n} |n-1\rangle \tag{5.27}$$

Similarly

$$a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \tag{5.28}$$

Here are some useful conclusions:

- Any eigenstate $|n\rangle$ can derived from the zero state acted by raising operator.

$$|n\rangle = \frac{(a^\dagger)^n}{(n!)^{1/2}} |0\rangle \tag{5.29}$$

  or from another eigenstate $|m\rangle$ with eigenvalue $m < n$.

$$|n\rangle = \frac{(a^\dagger)^{n-m}}{(n!)^{1/2}/(m!)^{1/2}} |m\rangle \tag{5.30}$$

- The matrix of X operator and P operator

$$\begin{aligned} \langle n|X|n\rangle &= (\frac{\hbar}{2m\omega})^{1/2} \langle n|a + a^\dagger|n\rangle \\ &= (\frac{\hbar}{2m\omega})^{1/2} \langle n|a|n\rangle + (\frac{\hbar}{2m\omega})^{1/2} \langle n|a^\dagger|n\rangle \\ &= (\frac{\hbar}{2m\omega})^{1/2} \sqrt{n} \langle n|n-1\rangle + (\frac{\hbar}{2m\omega})^{1/2} \sqrt{n+1} \langle n|n+1\rangle \\ &= (\frac{\hbar}{2m\omega})^{1/2} \sqrt{n}\delta_{n,n-1} + (\frac{\hbar}{2m\omega})^{1/2} \sqrt{n+1}\delta_{n,n+1} \end{aligned} \tag{5.31}$$

$$\begin{aligned}\langle n|P|n\rangle &= \mathrm{i}(\frac{m\omega\hbar}{2})^{1/2}\langle n|a^\dagger - a|n\rangle \\ &= \mathrm{i}(\frac{m\omega\hbar}{2})^{1/2}\sqrt{n+1}\delta_{n,n+1} - \mathrm{i}(\frac{m\omega\hbar}{2})^{1/2}\sqrt{n}\delta_{n,n-1}\end{aligned} \tag{5.32}$$

5.3 Passage from the Energy Basis to the Coordinate Basis

We already know that

$$a\,|0\rangle = 0 \tag{5.33}$$

we project ket onto X basis

$$a \to (\frac{m\omega}{2\hbar})^{1/2}X + i(\frac{1}{2m\omega\hbar})^{1/2}P = (\frac{m\omega}{2\hbar})^{1/2}x + (\frac{\hbar}{2m\omega})^{1/2}\frac{\mathrm{d}}{\mathrm{d}x} \tag{5.34}$$

$$|0\rangle \to \langle x|0\rangle = \psi_0(x) \tag{5.35}$$

In terms of $y = (m\omega/\hbar)^{1/2}x$,

$$a = \frac{1}{\sqrt{2}}(y + \frac{\mathrm{d}}{\mathrm{d}y}) \tag{5.36}$$

and

$$a^\dagger = \frac{1}{\sqrt{2}}(y - \frac{\mathrm{d}}{\mathrm{d}y}) \tag{5.37}$$

Then equation (**??**) turns into

$$(y + \frac{\mathrm{d}}{\mathrm{d}y})\psi_0(y) = 0 \tag{5.38}$$

so the normalized solution is

$$\psi_0(y) = (\frac{m\omega}{\pi\hbar})^{1/4}\exp\{-y^2\} \tag{5.39}$$

Due to the equation (**??**) and (**??**)

$$\begin{aligned}\psi_n(x) = \frac{(a^\dagger)^n}{(n!)^{1/2}}\psi_0(x) = (\frac{m\omega}{\pi\hbar(n!)^2})^{1/4}[\frac{1}{\sqrt{2}}(y - \frac{\mathrm{d}}{\mathrm{d}y})]^n\exp\{-y^2\} \\ (\frac{m\omega}{\pi\hbar 2^{2n}(n!)^2})^{1/4}\exp\left\{(-\frac{m\omega x^2}{2\hbar})\right\}H_n[(\frac{m\omega}{\hbar})^{1/2}x]\end{aligned} \tag{5.40}$$

6

Systems With N Degrees of Freedom

6.1 Direct Sum Space

V and W are two vector spaces over field K. The dimensionality of V and W are n_1 and n_2. We simply almagalmate one vector $|V\rangle$ from V and another one $|W\rangle$ from W to form a new vector

$$|V\rangle \oplus |W\rangle \tag{6.1}$$

called the **direct sum** of $|V\rangle$ and $|W\rangle$. It is easy to verify that all the direct sum vectors forms a vector space, which is the **direct sum** of vector space V and W, denoted by

$$V \oplus W \tag{6.2}$$

with the following definition of addition and scalar multiplication

- Addition: $(|V_1\rangle \oplus |W_1\rangle) + (|V_2\rangle \oplus |W_2\rangle) = (|V_1\rangle + |V_2\rangle) \oplus (|W_1\rangle + |W_2\rangle)$
- Scalar multiplication: $(|V\rangle \oplus |W\rangle)a = |V\rangle\, a \oplus |W\rangle\, a, a \in K$

Furthermore, the inner product of the direct sum space is defined by the sum of the inner prodcut of the corresponding components

$$(\langle V_1| \oplus \langle W_1|)(|V_2\rangle \oplus |W_2\rangle) = \langle V_1|V_2\rangle + \langle W_1|W_2\rangle \tag{6.3}$$

Assume that $\Omega_1, \Omega_2 \cdots$ and $\Lambda_1, \Lambda_2 \cdots$ are respectively the operators on space V and W. We care about the sum and product of the operator in the direct sum space. A fine definition is given

$$(\Omega \oplus \Lambda)(|V\rangle \oplus |W\rangle) = (\Omega\,|V\rangle) \oplus (\Lambda\,|W\rangle) \tag{6.4}$$

and

- Addition of operators: $(\Omega_1 \oplus \Lambda_1) + (\Omega_2 \oplus \Lambda_2) = (\Omega_1 + \Omega_2) \oplus (\Lambda_1 + \Lambda_2)$
- Product of operators: $(\Omega_1 \oplus \Lambda_1)(\Omega_2 \oplus \Lambda_2) = (\Omega_1\Omega_2) \oplus (\Lambda_1\Lambda_2)$

Another obvious result is: The dimensionality of the direct sum space $V \oplus W$ equals the sum of the dimensionality of V and W.

$$\dim V \oplus W = \dim V + \dim W \tag{6.5}$$

6.2 Direct Product Space

We follow the assumptions in section **??** and define the direct product

$$|V\rangle \otimes |W\rangle \tag{6.6}$$

and the **direct product space** formed by the direct product vectors

$$V \otimes W \tag{6.7}$$

We have to first define the basis in this new space. Let $|v_i\rangle, i = 1, 2 \cdots n_1$ and $|w_j\rangle, j = 1, 2 \cdots n_2$ be the basis separatedly in the space V and W. Then the new basis in the direct product space is defined by

$$|v_i\rangle \oplus |w_j\rangle, i = 1, 2 \cdots n_1, j = 1, 2 \cdots n_2 \tag{6.8}$$

So for any vector $|V\rangle = \sum_{i=1}^{n_1} v_i |v_i\rangle$ and $|W\rangle = \sum_{j=1}^{n_2} w_j |w_j\rangle$, we naturally have

$$|V\rangle \otimes |W\rangle = (\sum_{i=1}^{n_1} v_i |v_i\rangle) \otimes (\sum_{j=1}^{n_2} w_j |w_j\rangle) = \sum_{i=1}^{n_1}\sum_{j=1}^{n_2} v_i w_j |v_i\rangle \otimes |w_j\rangle \tag{6.9}$$

So there exists the addition and multiplication:

- Addition: $|V_1\rangle \otimes |W_1\rangle + |V_2\rangle \otimes |W_2\rangle = (|V_1\rangle + |V_2\rangle) \otimes (|W_1\rangle + |W_2\rangle)$
- Scalar multiplication: $(|V\rangle \otimes |W\rangle)a = (|V\rangle a) \otimes |W\rangle = |V\rangle \otimes (|W\rangle a)$

and the operator in the direct product space

$$(\Omega \otimes \Lambda)(|V\rangle \otimes |W\rangle) = (\Omega |V\rangle) \otimes (\Lambda |W\rangle) \tag{6.10}$$

and the sum and product of the operators

- Addition of operators: $(\Omega_1 \otimes \Lambda_1) + (\Omega_2 \otimes \Lambda_2) = (\Omega_1 + \Omega_2) \otimes (\Lambda_1 + \Lambda_2)$
- Product of operatora: $(\Omega_1 \otimes \Lambda_1)(\Omega_2 \otimes \Lambda_2) = (\Omega_1\Omega_2) \otimes (\Lambda_1\Lambda_2)$

The dimensionality of the direct product space $V \otimes W$ is the product of the dimensionality of V and W

$$\dim V \otimes W = \dim V \dim W \tag{6.11}$$

6.3 The Two-Particle Hilbert Space

We start with the case $N = 2$, which means a two-particle system. In the space of the two-particle system, evert state vector is with respect of the variables of

the two particles, for example, the momentum eigenket $|p_1 p_2\rangle$ consists of both the eigenstates of particle 1 and 2. More generally, we can use the simultaneous eigenkets $|\omega_1\omega_2\rangle$ of two commuting operators $\Omega_1(X_1, P_1)$ and $\Omega_2(X_2, P_2)$ to define the Ω basis[1]. We denote the **two-particle Hilbert space** by $V_{1\otimes 2}$ spanned by any of these basis. $V_{1\otimes 2}$ is a direct product space of V_1 and V_2. $V_i, i = 1, 2$ is the Hilebert space of particle 1 formed by specific complete basis. So

$$|\omega_1\omega_2\rangle = |\omega_1\rangle \otimes |\omega_2\rangle \tag{6.12}$$

A rule of denotation in the following discussion: we use superscript $(1), (2)$ to represent numbers of the vector space and subscript $1, 2$ to represent the corresponding particle numbers. According the discussion in section **??** we can obtain

$$X_1^{(1)\otimes(2)} = X_1^{(1)} \otimes I^{(2)}, \quad X_2^{(1)\otimes(2)} = I^{(2)} \otimes X_2^{(1)} \tag{6.13}$$

and similarly the momentum operator

$$P_1^{(1)\otimes(2)} = P_1^{(1)} \otimes I^{(2)}, \quad P_2^{(1)\otimes(2)} = I^{(2)} \otimes P_2^{(1)} \tag{6.14}$$

It is naturally to understand because the operator on particle 1 is unaffected on particle 2. More generally

$$(\Omega_1^{(1)} \otimes \Lambda_2^{(2)})\,|\omega_1\rangle \otimes |\omega_2\rangle = \left|\Omega_1^{(1)}\omega_1\right\rangle \otimes \left|\Lambda_2^{(2)}\omega_2\right\rangle \tag{6.15}$$

6.4 Evolution of Two-Particle State Vector

The state vector$|\psi\rangle$ is an element in $V_{(1)\otimes(2)}$ and it evolved in time according to Schrödinger equation

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\,|\psi\rangle = [\frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2} + V(X_1, X_2)]\,|\psi\rangle\,^2 \tag{6.17}$$

There are two classes of problems according to whether the potential operator V is separable or not.

- Class A: $V(X_1, X_2) = V_1(X_1) + V_2(X_2)$. So that

$$H = H_1 + H_2 = \frac{P_1^2}{2m_1} + V_1(X_1) + \frac{P_2^2}{2m_2} + V_2(X_2) \tag{6.18}$$

- Class B: $V(X_1, X_2) \neq V_1(X_1) + V_2(X_2)$

[1] Here we use the subscript 1 and 2 to indicate the particles.

[2] Notice that the entire expasion should be

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\,|\psi\rangle = [\frac{(P_1^{(1)} \otimes I^{(2)})^2}{2m_1} + \frac{(I^{(1)} \otimes P_2^{(2)})^2}{2m_2} + V(X_1^{(1)\otimes(2)}, X_2^{(1)\otimes(2)})]\,|\psi\rangle \tag{6.17}$$

6.4.1 Class A: Separable Hamiltonians

For stationary state

$$|\psi(t)\rangle = |E\rangle \, \mathrm{e}^{-\mathrm{i}Ht/\hbar} \tag{6.19}$$

and the Schrödinger equation becomes

$$H\,|E\rangle = [H_1 + H_2]\,|E\rangle = E\,|E\rangle \tag{6.20}$$

Since $[H_1, H_2] = 0$, we can find their simultaneous eigenstates $|E_1\rangle \otimes |E_2\rangle = |E_1 E_2\rangle$, where

$$H_1^{(1)}\,|E_1\rangle = E_1\,|E_1\rangle\,, \quad H_2^{(2)}\,|E_2\rangle = E_2\,|E_2\rangle \tag{6.21}$$

and

$$H\,|E\rangle = (H_1+H_2)\,|E_1\rangle\otimes|E_2\rangle = (H_1\,|E_1\rangle)\otimes(H_2\,|E_2\rangle) = (E_1+E_2)\,|E_1\rangle\otimes|E_2\rangle \tag{6.22}$$

so that

$$E = E_1 + E_2 \tag{6.23}$$

So

$$|\psi(t)\rangle = |E_1\rangle \, \mathrm{e}^{-\mathrm{i}E_1 t/\hbar} \otimes |E_2\rangle \, \mathrm{e}^{-miE_2 t/\hbar} \tag{6.24}$$

By projecting the state vector on coordinate basis, we have

$$\begin{aligned} \psi_E(x_1, x_2, t) &= \langle x_1 x_2 | \psi(t)\rangle = \langle x_1 x_2 | E_1\rangle \, \mathrm{e}^{-\mathrm{i}E_1 t/\hbar} \, \langle x_1 x_2 | E_2\rangle \, \mathrm{e}^{-\mathrm{i}E_2 t/\hbar} \\ &= \psi_{E_1}(x_1)\mathrm{e}^{-\mathrm{i}E_1 t/\hbar}\psi_{E_2}(x_2)\mathrm{e}^{-\mathrm{i}E_2 t/\hbar} \end{aligned} \tag{6.25}$$

6.4.2 Class B: Two Interacting Particles

By employing the centre mass coordinate

$$x_{CM} = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} \tag{6.26}$$

and

$$x = x_1 - x_2 \tag{6.27}$$

we can obtain

$$\psi(x_{CM}, x) = \frac{\mathrm{e}^{\mathrm{i}p_{CM}\cdot x_{CM}/\hbar}}{(2\pi\hbar)^{1/2}} \psi_{E_{\mathrm{rel}}}(x) \tag{6.28}$$

where

$$E = \frac{p_{CM}^2}{2M} + E_{\mathrm{rel}} = \frac{p_{CM}^2}{2M} + \frac{p}{2\mu} + V(x) \tag{6.29}$$

where

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \tag{6.30}$$

is the reduced mass.

6.5 Identical Particles

6.5.1 Two Particle Systems - Symmetric and Antisymmetric States

The state vector representing that a variable ω is measured to be ω_1 on particle 1 and ω_2 on particle 2 should be

$$|\psi\rangle = |\omega_1\omega_2\rangle \tag{6.31}$$

If the two particles are **distinguishable**, then $|\omega_2\omega_1\rangle$, which means that particle 1 is on the state ω_2 and particle 2 is on the state ω_2, is a different state vector from $|\omega_1\omega_2\rangle$. However, if the two particles are **identical particles**, then $|\omega_1\omega_2\rangle$ must be the rescale of $|\omega_1\omega_2\rangle$.

$$|\omega_1\omega_2\rangle = a\,|\omega_2\omega_1\rangle \tag{6.32}$$

Let $|\psi(\omega_1,\omega_2)\rangle = b\,|\omega_1\omega_2\rangle + c\,|\omega_2\omega_1\rangle$. From (**??**), it is easy to verify that

$$a = \sigma 1 \tag{6.33}$$

So there are two possible state vectors

- Symmetric state vector: $|\omega_1\omega_2, S\rangle = |\omega_1\omega_2\rangle + |\omega_2\omega_1\rangle$
- Antisymmetric state vector: $|\omega_1\omega_2, A\rangle = |\omega_1\omega_2\rangle - |\omega_2\omega_1\rangle$

6.5.2 Bosons and Fermions, Pauli's Exclusion Principle

The experiment results show that some particles such as the pion, photon, and graviton are always found in symmetic states and they are called **bosons**. And particles like electrons, protons and neutrons are always found in antisymmetric states and thay are called **fermions.**

For a two-fermion state, let $\omega_1 = \omega_2 = \omega$, then

$$|\omega_1\omega_2, A\rangle = |\omega\omega\rangle - |\omega\omega\rangle = 0 \tag{6.34}$$

This is the Pauli exclusion principle: **Two identical fermions cannot be in the same quantum state**.

6.6 Bosonic and Fermionic Hilbert Space

We call V_S the Hilbert space of symmetric state vectors and V_A the Hilbert space of antisymmetric state vectors.

In V_S (V_A is similar. The discussion is ignored here), any state vectors corresponding to the eigenbasis of Ω operator with discrete eigenvalue can be expressed as

$$|\omega_1\omega_2, S\rangle = C\,|\omega_1\omega_2\rangle + C\,|\omega_2\omega_1\rangle \tag{6.35}$$

To normalize the state vector we should have the constraint that

$$1 = \langle\omega_1\omega_2, S|\omega_2\omega_2, S\rangle = |C|^2(\langle\omega_1\omega_2|\omega_1\omega_2\rangle + \langle\omega_2\omega_1|\omega_2\omega_1\rangle) = 2|C|^2 \tag{6.36}$$

we can choose $C = 1/\sqrt{2}$, so that the normalized state vector is

$$|\omega_1\omega_2, S\rangle = \frac{1}{\sqrt{2}}[|\omega_1\omega_2\rangle + |\omega_2\omega_1\rangle] \tag{6.37}$$

Notice that equation (**??**) is only true when $\omega_1 \neq \omega_2$. When $\omega_1 = \omega_2 = \omega$, the state vector $|\omega\omega\rangle$ is itself a normalized state vector. So in this case we choose

$$|\omega\omega, S\rangle = |\omega\omega\rangle \tag{6.38}$$

If the operator Ω has continuous eigenvalue spectrum, we have to take the projection of $|\psi_S\rangle$ on the normalized eigenket. Hence, it is convenient to define the wave function as

$$\psi_S(\omega_1, \omega_2) = \frac{1}{\sqrt{2}}\,\langle\omega_1\omega_2, S|\psi_S\rangle \tag{6.39}$$

6.7 System of N Identical Particles

7

Symmetries and Their Consequences

7.1 Translational Invariance

A state vector $|\psi\rangle$ under a **infinitesimal translation** transfigure into a translated state $|\psi_\epsilon\rangle$, such that the expectation value of X increased by a infinitesimal value ϵ and keeps the momentum conserved (we will discuss specifically later)

$$\langle\psi_\epsilon|X|\psi_\epsilon\rangle = \langle\psi|X|\psi\rangle + \epsilon \tag{7.1}$$

$$\langle\psi_\epsilon|P|\psi_\epsilon\rangle = \langle\psi|P|\psi\rangle \tag{7.2}$$

In terms of $T(\epsilon)$, the translational operator

$$|\psi_\epsilon\rangle = T(\epsilon)\,|\psi\rangle \tag{7.3}$$

So equation (**??**) and (**??**) turns into

$$\langle\psi|T^\dagger XT|\psi\rangle = \langle\psi|X|\psi\rangle + \epsilon \tag{7.4}$$

$$\langle\psi|T^\dagger PT|\psi\rangle = \langle\psi|P|\psi\rangle \tag{7.5}$$

This is called the **active transformation picture**. Physically it corresponds to moving a particle to the right by a infinitesimal displacement ϵ. Furthermore

$$T^\dagger XT = X + \epsilon I \tag{7.6}$$

$$T^\dagger PT = P \tag{7.7}$$

This is called the **passive transformation picture**. Physically it corresponds to moving the environment to the left by a infinitesimal displacement ϵ. The two pictures are equivalent in describing the same fact.

To specify the translational invariance, we have to first stress the requirements of the translation operator. One important fact is that the X basis is not unique: **A given X basis $|x\rangle$ can be changed to another basis $|\tilde{x}\rangle$ by multiplying a phase factor, which doesn't change the norm and the orthogonality of the basis.** Due to this fact, the state vector under tranlation should be expressed by

$$T(\epsilon)\,|x\rangle = \mathrm{e}^{\mathrm{i}\epsilon g(x)/\hbar}\,|x+\epsilon\rangle \tag{7.8}$$

where $g(x)$ is a funtion of x. The equation is reasonable by enforcing $\epsilon \to 0, T(\epsilon)\,|x\rangle \to |x\rangle$.So

$$\langle X\rangle \to \langle X\rangle + \epsilon \tag{7.9}$$

$$\langle P\rangle \to \langle P\rangle + \epsilon\,\langle g'(X)\rangle \tag{7.10}$$

To ensure that the momentum is conserved, $g'(X)$ should vanish, which means that $g(x)$ is a constant (can be chosen to be 0). So we can say that

$$T(\epsilon)\,|x\rangle = |x+\epsilon\rangle \tag{7.11}$$

A obvious result is

$$\langle x|T(\epsilon)|\psi\rangle = \psi(x-\epsilon)^1 \tag{7.12}$$

Expand the operator $T(\epsilon)$ to order ϵ

$$T(\epsilon) = I - \frac{\mathrm{i}\epsilon}{\hbar}G \tag{7.13}$$

where G is called the **generator of translations**. Expand both sides of equation (**??**) to the order of ϵ

$$\langle x|I|\psi\rangle - \frac{\mathrm{i}\epsilon}{\hbar}\,\langle x|G|\psi\rangle = \psi(x) - \frac{\mathrm{d}\psi}{\mathrm{d}x}\epsilon \tag{7.14}$$

So

$$G = -\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x} = P \tag{7.15}$$

Such that

$$T(\epsilon) = I - \frac{\mathrm{i}\epsilon}{\hbar}P \tag{7.16}$$

It shows that the momentum is the generator of translation, which matches the classical picture. Thus the momentum conservation leads to the translational invariance

$$\begin{aligned}\langle\psi_\epsilon|H|\psi_\epsilon\rangle =\ & \langle\psi|T^\dagger HT|\psi\rangle =\ \langle\psi|(I+\frac{\mathrm{i}\epsilon}{\hbar}P)H(I-\frac{\mathrm{i}\epsilon}{\hbar}P)|\psi\rangle \\ =\ & \langle\psi|H|\psi\rangle + \frac{\mathrm{i}\epsilon}{\hbar}\,\langle\psi|[P,H]|\psi\rangle + O(\epsilon^2) = 0\end{aligned} \tag{7.17}$$

Where the second term yielding to Ehrenfest theorem vanishes

$$\langle\psi|[P.H]|\psi\rangle = \mathrm{i}\hbar\frac{\mathrm{d}P}{\mathrm{d}t} = 0 \tag{7.18}$$

[1] Proof: $x' = x+\epsilon$

$$\begin{aligned}\langle x|T(\epsilon)|\psi\rangle &= \langle x|\,T(\epsilon)\int_{-\infty}^{\infty}|x\rangle\,\langle x|\psi\rangle\,\mathrm{d}x = \langle x|\int_{-\infty}^{\infty}|x+\epsilon\rangle\,\langle x|\psi\rangle\,\mathrm{d}x \\ &= \langle x|\int_{-\infty}^{\infty}|x'\rangle\,\langle x'-\epsilon|\psi\rangle\,\mathrm{d}x' = \langle x-\epsilon|\psi\rangle = \psi(x-\epsilon)\end{aligned}$$

The above discussion is under the active tranformation picture. The totally same consequence can be also derived from the passive tranformation picture.

For a finite translation a, it is easy to derive the similar operator by integrating the infinitesimal translation

$$T(a) = \lim_{N\to\infty}(T(a/N))^N = \mathrm{e}^{-\mathrm{i}aP/\hbar} \tag{7.19}$$

Obvious we have

$$T(a)T(b) = T(a+b) \tag{7.20}$$

For tranlation in 3 dimension, the operator should be in terms of the vector momentum operator

$$\boldsymbol{P} = P_x\hat{\boldsymbol{e_x}} + P_y\hat{\boldsymbol{e_y}} + P_z\hat{\boldsymbol{e_z}} \tag{7.21}$$

Hence a finite translation $\boldsymbol{a}$ represents

$$T(\boldsymbol{a}) = \mathrm{e}^{-\mathrm{i}\boldsymbol{a}\cdot\boldsymbol{P}/\hbar} \tag{7.22}$$

7.2 Parity Invariance

The parity operator, corresponding to the reflection of the state of the particle through the origin, is defined by, in anology with the classical case

$$\Pi\,|x\rangle = |-x\rangle \tag{7.23}$$

$$\Pi\,|p\rangle = |-p\rangle \tag{7.24}$$

Here are some features of Π operator

- $\Pi^{-1} = \Pi = \Pi^\dagger$ (Π is Hermitian and Unitary)
- The eigenvalues of Π are only $\sigma 1$
- $\langle x|\Pi|\psi\rangle = \psi(-x)$

Obviously the action of Π on the operators

$$\Pi^\dagger X\Pi = -X \tag{7.25}$$

$$\Pi^\dagger P\Pi = -P \tag{7.26}$$

And we say that $H(X,P)$ is **parity invariant** if

$$\Pi^\dagger H\Pi = H(-X,-P) = H \tag{7.27}$$

8

Rotational Invariance and Angular Momentum

8.1 Rotation in Two Dimensions

Classically, a rotation by an angle $\phi_0 \hat{\boldsymbol{e_z}}$ along z axis is descirbed by

$$\begin{aligned} \tilde{x} &= \cos\phi_0 x - \sin\phi_0 y \\ \tilde{y} &= \sin\phi_0 x + \cos\phi_0 y \end{aligned} \tag{8.1}$$

$$\begin{aligned} \tilde{p_x} &= \cos\phi_0 p_x - \sin\phi_0 p_y \\ \tilde{p_y} &= \sin\phi_0 p_x + \cos\phi_0 p_y \end{aligned} \tag{8.2}$$

The operator that rotates the two dimension vectors is denoted by $R(\phi_0 \hat{\boldsymbol{e_z}})$. Correspondingly, a rotation operator in quantum mechanics

$$|\psi\rangle \to |\psi_R\rangle = U[R(\psi_0 \hat{\boldsymbol{e_z}})] \tag{8.3}$$

should also have the similar effect:

$$\begin{aligned} \langle X\rangle_R &= \cos\phi_0 \langle X\rangle - \sin\phi_0 \langle Y\rangle \\ \langle Y\rangle_R &= \sin\phi_0 \langle X\rangle + \cos\phi_0 \langle Y\rangle \end{aligned} \tag{8.4}$$

$$\begin{aligned} \langle P_x\rangle_R &= \cos\phi_0 \langle P_x\rangle - \sin\phi_0 \langle P_y\rangle \\ \langle P_y\rangle_R &= \sin\phi_0 \langle P_x\rangle + \cos\phi_0 \langle P_y\rangle \end{aligned} \tag{8.5}$$

where

$$\langle X\rangle_R = \langle\psi_R|X|\psi_R\rangle\,, \quad \langle X\rangle = \langle\psi|X|\psi\rangle \tag{8.6}$$

In anology with the translational operator, we obtain

$$U[R(\phi \hat{\boldsymbol{e_z}})]\,|x,y\rangle = |\cos\phi_0 x - \sin\phi_0 y, \sin\phi_0 x + \cos\phi_0 y\rangle \tag{8.7}$$

8.1.1 The Infinitesimal Rotation and Derivation of L_z

We previse that the generator of infinitesimal rotation, in anology with the generator of infinitesimal translation, is L_z, the angular momentum along z axis. So for a infinitesimal rotation $\phi_0 = \epsilon$, we obtain

$$U[R(\epsilon\hat{\boldsymbol{e}_z})] = I - \frac{\mathrm{i}\epsilon L_z}{\hbar} \tag{8.8}$$

since $\cos\epsilon \sim 1$ and $\sin\epsilon \sim \epsilon$, we obtain

$$U[R]\,|x,y\rangle = |x - y\epsilon, x\epsilon + y\rangle \tag{8.9}$$

and we can prove that for any state ψ we have

$$\langle x,y|I - \frac{\mathrm{i}\epsilon L_z}{\hbar}|\psi\rangle = \phi(x + y\epsilon, y - x\epsilon) \tag{8.10}$$

Expanding both sides to the order of ϵ, we have

$$\langle x,y|L_z|\psi\rangle = [x(-\mathrm{i}\hbar\frac{\partial}{\partial y}) - y(-\mathrm{i}\hbar\frac{\partial}{\partial x})]\psi(x,y) \tag{8.11}$$

Thus under the coordinate basis we have the explicit construction of L_z

$$L_z = x(-\mathrm{i}\hbar\frac{\partial}{\partial y}) - y(-\mathrm{i}\hbar\frac{\partial}{\partial x}) = XP_y - YP_x \tag{8.12}$$

It is also useful by changing the coordinates to polar coordinates, so

$$L_z = -\mathrm{i}\hbar\frac{\partial}{\partial\phi} \tag{8.13}$$

8.1.2 Finite Rotation

The finite rotation is thus easy to obtain by integrating the equation (**??**)

$$U[R(\phi_0\hat{\boldsymbol{e}_z})] = \lim_{N\to\infty}(I - \frac{\mathrm{i}\phi_0}{\hbar N}L_z)^N = \mathrm{e}^{-\mathrm{i}\phi_0 L_z/\hbar} \tag{8.14}$$

8.2 The Eigenvalue Problem of L_z

The eigenvalue equation of L_z writes

$$L_z\,|l_z\rangle = l_z\,|l_z\rangle \tag{8.15}$$

In the polar coordinate basis we have

$$-\mathrm{i}\hbar\frac{\partial}{\partial\phi}\psi(\rho,\phi) = l_z\psi(\rho,\phi) \tag{8.16}$$

It is obvious that

$$\psi(\rho,\phi) = R(\rho)\mathrm{e}^{\mathrm{i}l_z\phi/\hbar} = R(\rho)\Phi(\phi) \tag{8.17}$$

To acquire the eigenvalue l_z of $\Phi(\phi)$, the eigenfunction should obey the periodic boundary condition

$$\Phi(0) = \Phi(2\pi) \tag{8.18}$$

which means that a rotation by the angle 2π will keep the invariance of the state. Such that the eigenvalue l_z should be the integral multiple of $\hbar$

$$l_z = m\hbar, \quad m = 1, 2, \cdots \tag{8.19}$$

Obviously the normalized eigenfunction writes

$$\Phi_m(\phi) = \frac{1}{(2\pi)^{1/2}} \mathrm{e}^{\mathrm{i}m\phi} \tag{8.20}$$

8.3 Angular Momentum in Three Dimensions

The angular momentum operators around x and y axes can be derived from equation (**??**)

$$L_x = YP_z - ZP_y \tag{8.21}$$

$$L_y = ZP_x - XP_z \tag{8.22}$$

We introduce the **total angular momentum operator**

$$L^2 = L_x^2 + L_y^2 + L_z^2 \tag{8.23}$$

or in terms of a vector operator

$$\boldsymbol{L} = L_x\hat{\boldsymbol{e_x}} + L_y\hat{\boldsymbol{e_y}} + L_z\hat{\boldsymbol{e_z}} \tag{8.24}$$

Some important results about L^2 and L_i are listed:

- $[L_i, L_j] = \mathrm{i}\hbar\epsilon_{ijk}L_k$, where ϵ_{ijk} are the components of an antisymmetric tensor of rank 3, with the following properties

  1. $\epsilon_{123} = 1$.
  2. They change sign when any two indices are exchanged. Consequently they are zero if any two indices are equal.

- $[L^2, L_i] = 0$

After introducing the concept of total angular momentum, we can thus consider a rotation around any spatial direction. A finite rotation $\boldsymbol{\theta} = \theta_x\hat{\boldsymbol{e_x}} + \theta_y\hat{\boldsymbol{e_y}} + \theta_z\hat{\boldsymbol{e_z}}$ [1]around along a vector with all the components in three

[1]The implication of the denotation $\theta_i\hat{\boldsymbol{e_i}}$ means that the vector rotates around $\hat{\boldsymbol{e_i}}$ by an angle θ_i.

dimension Cartesian coordinate can be decomposed to three separate rotation respectively along x ,y and z axes. So

$$\begin{aligned} U[R(\boldsymbol{\theta})] &= U[R(\theta_x \hat{\boldsymbol{e_x}})] \cdot U[R(\theta_y \hat{\boldsymbol{e_y}})] \cdot U[R(\theta_z \hat{\boldsymbol{e_z}})] \\ &= \mathrm{e}^{-\mathrm{i}\theta_x L_x/\hbar} \mathrm{e}^{-\mathrm{i}\theta_y L_y/\hbar} \mathrm{e}^{-\mathrm{i}\theta_z L_z/\hbar} \\ &= \mathrm{e}^{-\mathrm{i}\boldsymbol{\theta}\cdot\boldsymbol{L}/\hbar} \end{aligned} \tag{8.25}$$

8.4 The Eigenvalue Problem of L^2 and L_z, The "Ladder Method" of Angular Momentum

We have already known that $[L^2, L_z] = 0$, which means that they have simlultaneous eigenstate, denoted by $|\alpha\beta\rangle$, where α and β are separatedly the eigenvalues of L^2 and L_z. Such that

$$L^2 |\alpha\beta\rangle = \alpha |\alpha\beta\rangle \tag{8.26}$$

.

$$L_z |\alpha\beta\rangle = \beta |\alpha\beta\rangle \tag{8.27}$$

We now define **raising and lowering operators of angular momentum**

$$L_\pm = L_x \pm \mathrm{i} L_y \tag{8.28}$$

which satisfy

$$[L_z, L_\pm] = \pm\hbar L_\pm \tag{8.29}$$

It is not easy to verify that

$$[L^2, L_\pm] = 0, \quad [L_z, L_\pm] = \pm\hbar L_\pm \tag{8.30}$$

It shows that the raising/lowering operator raise/lower the eigenvalue of L_z by $\hbar$. Actually

$$\begin{aligned} L_z(L_+ |\alpha\beta\rangle) &= (L_+ L_z + [L_z, L_+]) |\alpha\beta\rangle \\ &= (L_+\beta + \hbar L_+) |\alpha\beta\rangle \\ &= (\beta + \hbar)(L_+ |\alpha\beta\rangle) \end{aligned} \tag{8.31}$$

and

$$L^2 L_+ |\alpha\beta\rangle = L + L^2 |\alpha\beta\rangle = \alpha L_+ |\alpha\beta\rangle \tag{8.32}$$

so

$$L_+ |\alpha\beta\rangle = C_+ |\alpha, \beta + \hbar\rangle \tag{8.33}$$

where C_+ is a constant with respect to α and β. Similarly we obtain that

$$L_- |\alpha\beta\rangle = C_- |\alpha, \beta - \hbar\rangle \tag{8.34}$$

In harmonic oscillators, the eigenvalue of energy can be raised to infinite since there is not bound for the energy levels. However, the eigenvalue of L_z, β, cannot be infinitely raised. A clear explanation is that $L_z^2 \leqslant L^2$ must be satisfied, which means that any components of angular momentum cannot overtake its total angular momentum. Such that

$$\alpha \leqslant \beta^2 \tag{8.35}$$

which means that β is bounded by α, so there exists a maximum of $\beta_{\max}$ and an eigenstate $|\alpha\beta_{\max}\rangle$ that cannot be raised. Simultaneously, a $\beta_{\min}$ and an eigenstate $|\alpha\beta_{\min}\rangle$ that cannot be lowered.

$$L_+ |\alpha\beta_{\max}\rangle = 0, \quad L_- |\alpha\beta_{\min}\rangle = 0 \tag{8.36}$$

so

$$\begin{aligned} L_- L_+ |\alpha\beta_{\max}\rangle &= (L^2 - L_z^2 - \hbar L_z) |\alpha\beta_{\max}\rangle \\ &= (\alpha - \beta_{\max}^2 - \hbar\beta_{\max}) |\alpha\beta_{\max}\rangle = 0 \end{aligned} \tag{8.37}$$

so

$$\alpha = \beta_{\max}(\beta_{\max} + \hbar) \tag{8.38}$$

Similarly

$$\alpha = \beta_{\min}(\beta_{\min} - \hbar) \tag{8.39}$$

So choose $\beta_{\max} = -\beta_{\min} = l\hbar$, rewrite β by $m\hbar$, so[2]

$$-l < m < l, \quad \alpha = l(l+1)\hbar^2 \tag{8.40}$$

Hence

$$\begin{aligned} L^2 |lm\rangle &= l(l+1)\hbar^2 |lm\rangle, l = 0, 1, 2 \cdots \\ L_z |lm\rangle &= m\hbar |lm\rangle, m = -l, -l+1, \cdots, l-1, l \end{aligned} \tag{8.41}$$

Thus the constants C_+ and C_- can be derived

$$C_+ = \hbar\sqrt{(l-m)(l+m+1)}, \quad C_- = \hbar\sqrt{(l+m)(l-m+1)} \tag{8.42}$$

So the matrices elements of L_x and L_y in angular momentum basis writes

$$\begin{aligned} \langle l'm'|L_x|lm\rangle &= \langle l'm'|\frac{L_+ + L_-}{2}|lm\rangle \\ &= \frac{\hbar}{2}[\delta_{ll'}\delta_{m,m+1}\sqrt{(l-m)(l+m+1)} + \delta_{ll'}\delta_{m,m+1}\sqrt{(L+m)(l-m+1)}] \\ \langle l'm'|L_y|lm\rangle &= \langle l'm'|\frac{L_+ - L_-}{2}|lm\rangle \\ &= \frac{\hbar}{2}[\delta_{ll'}\delta_{m,m+1}\sqrt{(l-m)(l+m+1)} - \delta_{ll'}\delta_{m,m+1}\sqrt{(L+m)(l-m+1)}] \end{aligned} \tag{8.43}$$

[2]A deeper discussion including the total angular momentum $\boldsymbol{J}$ is related in [pp.326]. Here we simply take $\boldsymbol{J} = \boldsymbol{L}$ and the spin is not considered.

8.5 Angular Momentum Eigenfunctions in Coordinate Basis

From the topmost state $|ll\rangle$ we have

$$L_+ |ll\rangle = 0 \tag{8.44}$$

The raising operator L_+ in spherical coordinate writes

$$L_\sigma = \sigma\hbar \mathrm{e}^{\sigma \mathrm{i}\phi}(\frac{\partial}{\partial\theta}\sigma \mathrm{i}\cot\theta\frac{\partial}{\partial\phi}) \tag{8.45}$$

So for the eigenfunction $\psi_l^l(r,\theta,\phi)$ corresponding to $|ll\rangle$ we obtain

$$\hbar \mathrm{e}^{\mathrm{i}\phi}(\frac{\partial}{\partial\theta} + \mathrm{i}\cot\theta\frac{\partial}{\partial\phi})\psi_l^l(r,\theta,\phi) = 0 \tag{8.46}$$

so in the absence of radial function we get

$$Y_l^l(\theta,\phi) = (-1)^l\sqrt{\frac{2l+1}{4\pi}}\frac{1}{2^l l!}(\sin\theta)^l \mathrm{e}^{\mathrm{i}l\phi} \tag{8.47}$$

To obtain Y_l^m by using the lowering operator for $l-m$ times and Rodrigues formula[3]

$$\begin{aligned} Y_l^m &= (-1)^l\sqrt{\frac{2l+1}{4\pi}}\frac{1}{2^l l!}\sqrt{\frac{(l+m)!}{(l-m)!}}(\sin\theta)^{-m}\mathrm{e}^{\mathrm{i}m\phi}\frac{\mathrm{d}^{l-m}(\sin\theta)^{2l}}{\mathrm{d}(\cos\theta)^{l-m}} \\ &= (-1)^m\sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)\mathrm{e}^{\mathrm{i}m\phi} \end{aligned} \tag{8.50}$$

The eigenfunction (**??**) is called the **spherical harmonics**.

[3]Rodrigues formula: for $l > 0$ and $0 \leqslant m \leqslant l$, the derivation of Associated Legendre Polynomials

$$P_l^m(\cos\theta) = (-1)^m\frac{1}{2^l l!}(\sin\theta)^m\frac{\mathrm{d}^{l+m}(\sin\theta)^{2l}}{\mathrm{d}(\cos\theta)^{l+m}} \tag{8.48}$$

and

$$\frac{\mathrm{d}^{l-m}(\sin\theta)^{2l}}{\mathrm{d}(\cos\theta)^{l-m}} = (-1)^m\frac{(l-m)!}{(l+m)!}(\sin\theta)^{2m}\frac{\mathrm{d}^{l+m}(\sin\theta)^{2l}}{\mathrm{d}(\cos\theta)^{l+m}} \tag{8.49}$$

9

Charged Particles In Electromagnetic Field

9.1 Introduction

9.1.1 Classical Case

In classical case, the motion equation of a charged particle with charge q and mass m in a uniform electromagnetic field $(\boldsymbol{E}, \boldsymbol{B})$ can be written as

$$m\ddot{\boldsymbol{r}} = q\boldsymbol{E} + q\dot{\boldsymbol{r}} \times \boldsymbol{B} \tag{9.1}$$

By introducing the vector potential $\boldsymbol{A}$ and scalar potential ϕ, we substitute $(\boldsymbol{E}, \boldsymbol{B})$ by (in Gauss Unit)

$$\boldsymbol{E} = -\boldsymbol{\nabla}\phi - \frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t} \tag{9.2}$$

$$\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A} \tag{9.3}$$

Such that (**??**) writes

$$m\ddot{\boldsymbol{r}} = -q(\boldsymbol{\nabla}\phi + \frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t}) + q\dot{\boldsymbol{r}} \times (\boldsymbol{\nabla} \times \boldsymbol{A}) \tag{9.4}$$

By defining the Hamiltonian

$$H = \frac{1}{2m}(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A})^2 + q\phi \tag{9.5}$$

and utilizing the corresponding canonical equation, we can derive equation (**??**). Where $\boldsymbol{p}$ is the canonical momentum defined by Hamiltonian canonical equation and $\boldsymbol{\pi} = \boldsymbol{p} - \frac{q}{c}\boldsymbol{A} = m\dot{\boldsymbol{r}}$ is the mechanical momentum.

9.1.2 In Quantum Mechanics

We can naturally obtain the Schrödinger equation by preserving the form of the Hamiltonian

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\left|\alpha\right\rangle = H\left|\alpha\right\rangle = [\frac{1}{2m}(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A})^2 + q\phi]\left|\alpha\right\rangle \tag{9.6}$$

Project the eigenket on x-basis we have

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi_\alpha(\boldsymbol{x}) = [\frac{1}{2m}(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A})^2 + q\phi]\psi_\alpha(\boldsymbol{x}) \tag{9.7}$$

Before specifying the solution of equation (**??**), we first have to emphasize the gauge transformation. Since the electromagnetic field $(\boldsymbol{E}, \boldsymbol{B})$ stay the same as $(\boldsymbol{A}, \phi)$ undergo a gauge transformation, we guess that the wavefunction should have a similar gauge invariance, so do the probability of measurement. The fact is that the wavefunction will only be multiplied by a factor with module of 1 if $(\boldsymbol{A}, \phi)$ get a gauge trasnformation.

Proposition 9.1. *If ψ_α is a solution of* (**??**) *and we make a gauge transformation*

$$\boldsymbol{A} \to \boldsymbol{A} + \boldsymbol{\nabla}\Lambda \tag{9.8}$$

$$\phi \to \phi - \frac{\partial\Lambda}{\partial t} \tag{9.9}$$

then the solution becomes $\mathrm{e}^{\mathrm{i}q\Lambda/\hbar c}\psi_\alpha$

Though the wavefunction is multiplied by a factor $\mathrm{e}^{\mathrm{i}q\Lambda/\hbar c}$, the conservation of probability density $\rho = \psi\psi^*$ and probability flux density $\boldsymbol{j}$ hold still. Therefore, the wavefunction has a gauge invariance.

9.2 An Electron in A Uniform Magnetic Field, Landau Levels

9.2.1 Classical Case

We now discuss the problem of an electron travelling in a uniform magnetic field. Suppose that the magnetic field $\boldsymbol{B} = B\hat{\boldsymbol{e_z}}$ points along z-direction. In classical case, the solution is simple by giving the initial condition: the particle will undergo a circular motion in xy-plane the moves by constant speed along z-direction. The circular frequency is

$$\omega = \frac{eB}{mc} \tag{9.10}$$

9.2.2 Quantum Mechanics; Landau levels in Landau Gauge

To solve the problem in quantum mechanics, we first need to specify the vector potential. In this subsection we discuss the gauge originated by Laudau. Since the magnetic field is along z-direction, the components of the vector potential can always be written as

$$A_x = -By,\ A_y = A_z = 0 \tag{9.11}$$

Obviously, it satisfies Coulomb gauge $\boldsymbol{\nabla} \cdot \boldsymbol{A} = 0$. So the Hamiltonian writes

$$H = \frac{1}{2m}(\boldsymbol{p} + \frac{e}{c}\boldsymbol{A})^2 = \frac{1}{2m}[(p_x - \frac{e}{c}By)^2 + p_y^2] + \frac{1}{2m}p_z^2 = H_{xy} + H_z \quad (9.12)$$

We find that $[p_z, H] = 0$, which indicats that p_z and H have simultaneous eigenstates. Therefore, the wavefunction can be written in the form of the product of a plane wave along z-direction and an eignefunction of H_{xy}:

$$\psi_E(\boldsymbol{x}) = \psi(x, y)\mathrm{e}^{\mathrm{i}k_z z} \quad (9.13)$$

where

$$p_z \mathrm{e}^{\mathrm{i}k_z z} = E_z \mathrm{e}^{\mathrm{i}k_z z} = \hbar k_z \mathrm{e}^{\mathrm{i}k_z z} \quad (9.14)$$

So

$$E_{xy} = E - \frac{\hbar^2 k_z^2}{2m} \quad (9.15)$$

Similarly we find $[p_x, H_{xy}] = 0$ and we have

$$\psi(x, y) = \phi(y)\mathrm{e}^{\mathrm{i}k_x x} \quad (9.16)$$

Thus the operator p_x can be substituted by the eigenvalues $p_x = \hbar k_x$. Finally we obtain the equation of $\phi(y)$

$$\frac{1}{2m}[(\hbar k_x - \frac{e}{c}By)^2 + p_y^2]\phi(y) = E_{xy}\phi(y) \quad (9.17)$$

Define $y_0 = \dfrac{c\hbar k_x}{eB}$ and $\omega_c = \dfrac{eB}{mc}$, then we have

$$[\frac{p_y^2}{2m} + \frac{1}{2}m\omega_c^2(y - y_0)^2]\phi(y) = E_{xy}\phi(y) \quad (9.18)$$

The form of the above equation is totally the same as the eigenequation of harmonica oscillators. So the energy levels are determined.

$$E_{xy} = E_n = (n + 1/2)\hbar\omega_c \quad (9.19)$$

$$E = E_{xy} + E_z = (n + 1/2)\hbar\omega_c + \frac{\hbar^2 k_z^2}{2m} \quad (9.20)$$

(**??**) shows the famous Landau levels.

We concern about the degree of degeneracy(DOD) of the system. The degeneracy is with respect to the equilibrium point y_0, or, k_x. If the area we focus is infinitely big, then k_x can be taken as any values. So the DOD is infinite. Otherwise, if the area is bounded, for example, by a rectangular with sides L_x and L_y, then k_x must satisfy the periodic boundary condition

$$\mathrm{e}^{\mathrm{i}k_x(L_x + x)} = \mathrm{e}^{\mathrm{i}k_x x} \quad (9.21)$$

so

$$k_x = \frac{2\pi}{L_x} n_x, n_x \in \mathbb{Z} \tag{9.22}$$

So k_x is discrete, and so is y_0. Due to thay L_y is limited, so the number of y_0 that can be at most contained in $[0, L_y]$ is the DOD, which is

$$N = L_y/(\frac{y_0}{n_x}) = \frac{L_x}{2c\hbar\pi/eBL_x} = \frac{BL_xL_y}{hc/e} = \frac{\Phi_B}{hc/e} \tag{9.23}$$

where Φ_B is the magnetic flux through the area and hc/e is the quantized magnetic flux.

9.2.3 Landau levels in Symmetric Gauge

The symmetric gauge is another gauge used to describe $\boldsymbol{A}$

$$A_x = -\frac{1}{2}By,\ A_y = \frac{1}{2}Bx,\ A_z = 0 \tag{9.24}$$

Define $\omega_L = \frac{1}{2}\omega_c$, then the xy-Hamiltonian can be written as

$$H_{xy} = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{1}{2}m\omega_L^2(x^2 + y^2) + \omega_L L_z \tag{9.25}$$

The following works to solve the equation are trivial.

9.2.4 Landau Levels by Raising And Lowering Operators

We now introduce a more simple method to solve Landau levels. We have known that the Hamiltonian of xy-plane is

$$H_{xy} = \frac{1}{2m}(\pi_x^2 + \pi_y^2) \tag{9.26}$$

An important result giving the commutative relationship of mechanical momentum is

$$[\pi_i, \pi_j] = \mathrm{i}\hbar\frac{q}{c}\epsilon_{ijk}B_k \tag{9.27}$$

So we define the raising and lowering operators in anology of harmonic oscillator

$$a = (\frac{c}{2\hbar Be})^{1/2}(\pi_x + \mathrm{i}\pi_y) \tag{9.28}$$

$$a^\dagger = (\frac{c}{2\hbar Be})^{1/2}(\pi_x - \mathrm{i}\pi_y) \tag{9.29}$$

Their commutation

$$[a, a^\dagger] = \frac{c}{2\hbar Be}[\pi_x + \mathrm{i}\pi_y, \pi_x - \mathrm{i}\pi_y] = \frac{c}{2\hbar Be}(-2\mathrm{i})[\pi_x, \pi_y] = 1 \tag{9.30}$$

And the Hamiltonian becomes

$$H_{xy} = (aa^\dagger + 1/2)\hbar\omega_c \tag{9.31}$$

So the energy levels write

$$E_n = (n + 1/2)\hbar\omega_c \tag{9.32}$$

10

The Hydrogen Atom

10.1 The Eigenvalue Problem

The hydrogen atom is one of the most classical problem in quantum mechanics and it can be well expained by the two-body model. Since the Coulomb potential between the electron and the nuclei is proportional to the reciprocal of r

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r} \tag{10.1}$$

So the Schrödinger equation in spherical coordinate writes

$$\begin{aligned} &-\frac{\hbar^2}{2\mu}[\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}]\psi(r,\theta,\phi) \\ &+\frac{e^2}{4\pi\epsilon_0 r} = E\psi(r,\theta,\phi) \end{aligned} \tag{10.2}$$

Due to that the system is spherical symmetric, the wave functions take the forms of

$$\psi(r,\theta,\phi) = R(r)Y_l^m(\theta,\phi) = \frac{\chi(r)}{r}Y_l^m(\theta,\phi) \tag{10.3}$$

so $\chi(r)$ obeys

$$\frac{\mathrm{d}^2\chi(r)}{\mathrm{d}r^2} + \frac{2\mu}{\hbar^2}[E + \frac{e^2}{4\pi\epsilon_0 r} - \frac{l(l+1)\hbar^2}{2\mu r^2}]\chi(r) = 0 \tag{10.4}$$

We next factor out the asymptotic behaviour of $\chi(r)$

$$\chi(r) \sim_{r\to 0} r^{l+1}, \quad \chi(r) \sim_{r\to\infty} \mathrm{e}^{-\sqrt{-2\mu E/\hbar^2}r} = \mathrm{e}^{-\beta r} \tag{10.5}$$

and the auxiliary function v defined by

$$\chi(r) = \mathrm{e}^{-\beta r}v(r) = \mathrm{e}^{-\rho}v(\rho) \tag{10.6}$$

such that $v(r)$ obeys

$$\frac{\mathrm{d}^2}{\mathrm{d}\rho 2}v(\rho) - 2\frac{\mathrm{d}v(\rho)}{\mathrm{d}\rho} + [\frac{e^2\lambda}{\rho} - \frac{l(l+1)}{\rho^2}]v(\rho) = 0 \tag{10.7}$$

where

$$\lambda = \sqrt{-2m/\hbar^2 E} \tag{10.8}$$

According to the behaviour near $\rho = 0$ we have

$$v = \rho^{l+1} \sum_{k=0}^{\infty} C_k \rho^k \tag{10.9}$$

whose coefficients C_k satisfy

$$\frac{C_{k+1}}{C_k} = \frac{-e^2\lambda + 2(k+l+1)}{(k+l+2)(k+l+1) - l(l+1)} \sim_{k\to\infty} \frac{2}{k} \tag{10.10}$$

To prohibit the divergence of the function at $\rho = \infty$ we must make the series terminate at a certain k. This will happen if

$$e^2\lambda = e^2\sqrt{-2m/\hbar^2 E} = 2(k+l+1) \tag{10.11}$$

So

$$E = -\frac{me^4}{2\hbar^2(k+l+1)^2} = -\frac{me^4}{2\hbar^2 n^2} \tag{10.12}$$

where

$$n = k + l + 1 = 1, 2, 3 \cdots \tag{10.13}$$

is called the **principal quantum number**. For a certain n, l can take the values from 0 to n-1 to keep the same energy. For each l, similarly, m has $2l+1$ selections. So obviously the degeneracy for each n is

$$\sum_{l=0}^{n-1}(2l+1) = n^2 \tag{10.14}$$

10.2 The Wave Functions

The orthonormal radial function takes the form of

$$R_{nl}(r) = \sqrt{(\frac{2}{na_0})^3 \frac{(n-l-1)!}{2n(n+l)!}} \mathrm{e}^{-r/na_0} (\frac{r}{na_0}^{\ l}) L_{n-l-1}^{2l+1}(\frac{2r}{na_0}) \tag{10.15}$$

where

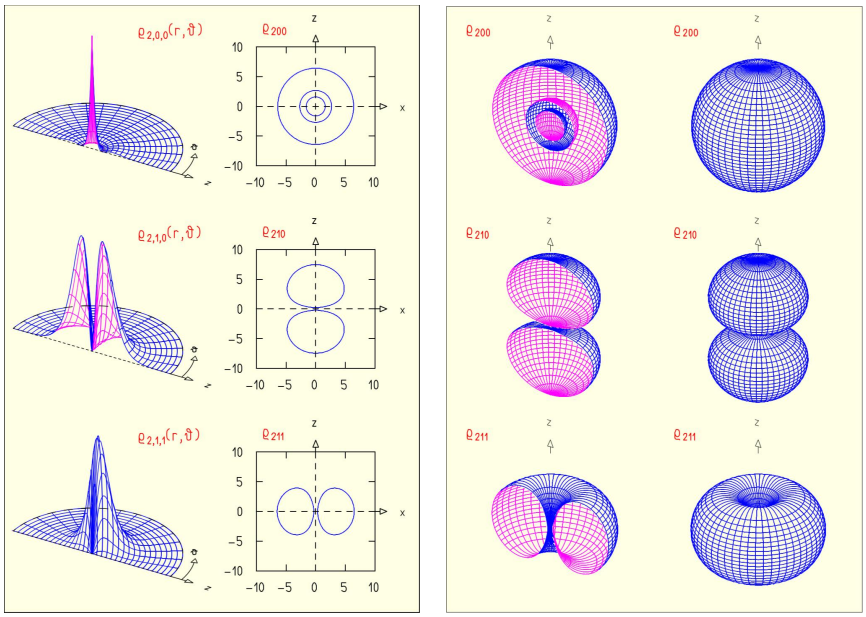
$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^4} \tag{10.16}$$

is called the **reduced Bohr radius**. L_p^k is called the **associated Laguerre polynomial**. For integer k and p

$$\begin{aligned} L_p^0(x) &= \frac{\mathrm{e}^x}{n!}(\frac{\mathrm{d}^p}{\mathrm{d}x^p})(\mathrm{e}^{-x}x^p) \\ L_p^k(x) &= (-1)^k(\frac{\mathrm{d}^p}{\mathrm{d}x^p})L_{p+k}^0 \end{aligned} \tag{10.17}$$

The intact wave function is

$$\psi(r,\theta,\phi) = R_{nl}(r)Y_l^m(\theta,\phi)$$
$$\sqrt{(\frac{2}{na_0})^3\frac{(n-l-1)!}{2n(n+l)!}}\mathrm{e}^{-r/na_0}(\frac{r}{na_0}^{\ l})L_{n-l-1}^{2l+1}(\frac{2r}{na_0})Y_l^m(\theta,\phi) \tag{10.18}$$



(a) Spatial probability density and its contour lines

(b) Contour surface of spatial probability density

FIGURE 10.1
(a) Left: Spatial probability density ρ_{2lm} for an electron in the hydrogen atom shown over a half-plane bounded by the z axis. Different scales are used in the three plots. Right: Contour lines $\rho_{2lm} = 0.002$ in the x, z plane. Numbers are in units of the Bohr radius. (b)Contour surface of spatial probability density of $\psi_{2lm} = 0.002$ in full space (right) and in the half-space $x > 0$ (left). [1]

[1] S. Brandt, H. D. Dahmen. The Picture Book of Quantum Mechanics, 4th ed., Springer, New York, 2012. 274-275.

11

Spin

11.1 The Stern Gerlach Experiment

The Stern-Gerlach experiment was first conducted by Otto Stern and Walter Gerlach in 1922. The experiment demonstrates that the particle has an intrinsic angular momentum, which takes quantized values.

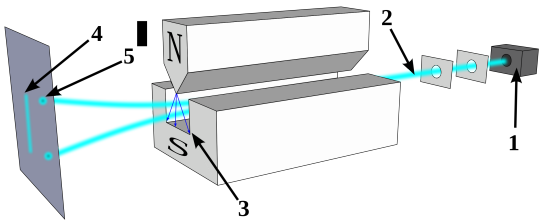


FIGURE 11.1
Stern–Gerlach experiment: Silver atoms travelling through an inhomogeneous magnetic field, and being deflected up or down depending on their spin; (1) furnace, (2) beam of silver atoms, (3) inhomogeneous magnetic field, (4) classically expected result, (5) observed result. Picture source: Wikipedia, Stern-Gerlach experiment.

In the experiment, the silver atoms are emitted from the furnace and shot on the screen after being experienced the interaction of magnetic field. The silver atom consists of a nucleus and 47 electrons, in which only the intrinsic angular momentum of the outmost electron is considered. The combination of the inside 46 electrons forms a spherical electron cloud which owning no net angular momentum. Such that the net angular momentum of the atom equals

the angular momentum of the outmost electron.[1] The magnetic momentum of the atom is thus

$$\boldsymbol{\mu} = \frac{e}{m_e c}\boldsymbol{S} \tag{11.1}$$

where $\boldsymbol{S}$ is the electron spin. The vertical component (z-component in our discussion) of the magnetic force of the atom in the magnetic field is proportional to gradient of the potential energy, ehich takes the form of

$$\boldsymbol{F}_z = -\boldsymbol{\nabla}(-\boldsymbol{\mu}\cdot\boldsymbol{B}) = \mu\boldsymbol{\nabla}B = \mu\frac{\partial B_z}{\partial z}\hat{\boldsymbol{e}_z} \tag{11.2}$$

Classically, the magnetic momentum is continuous, which means that the image on the screen would be a continuous bundle of beams. However, the observed result are two separate lines on the screen, which indicates that the electron intrinsic angular momentum takes the quantized values.

11.2 Representation of Spin, Pauli Matrices and Spin Space

We assume that the components of operator S obeys

$$[S_i, S_j] = \mathrm{i}\hbar\epsilon_{ijk}S_z \tag{11.3}$$

The Hilbert space of spin V_s of a single elctron is a two-dimension space, since S^2 and S_z can be chosen as a complete set of commutative operators. So the eigenvector can be provided by

$$|s, m_s\rangle\,, \quad s = 1/2, m_s = \sigma 1/2 \tag{11.4}$$

Such that in S_z basis, the two eigenkets write

$$|1/2, 1/2\rangle \longrightarrow \begin{pmatrix}1\\0\end{pmatrix}, \quad |1/2, -1/2\rangle \longrightarrow \begin{pmatrix}0\\1\end{pmatrix} \tag{11.5}$$

So any ket $|\chi\rangle$ in V_s can be represented in S_z basis as

$$|\chi\rangle = \alpha\,|1/2, 1/2\rangle + \beta\,|1/2, -1/2\rangle \longrightarrow \begin{pmatrix}\alpha\\\beta\end{pmatrix} \tag{11.6}$$

We introduce **Pauli Matrices** to represent the relationship of spin. Pauli Matrices $\boldsymbol{\sigma}$, which are named after Wolfgang Pauli, are defined by

$$\sigma_x = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix},\ \sigma_y = \begin{pmatrix}0 & -\mathrm{i}\\\mathrm{i} & 0\end{pmatrix},\ \sigma_z = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix} \tag{11.7}$$

[1] J.J.Sakurai. Modern Quantum Mechanics. Rev. Ed., New York, Addison-Wesley. 1994. 2-3.

So that the total spin is

$$\boldsymbol{S} = \frac{\hbar}{2}\boldsymbol{\sigma} = \frac{\hbar}{2}(\sigma_x \hat{\boldsymbol{e_x}} + \sigma_y \hat{\boldsymbol{e_y}} + \sigma_z \hat{\boldsymbol{e_z}}) \tag{11.8}$$

Here are some important properties of Pauli matrices

1. The commutation and anti-commutation relations

$$[\sigma_i, \sigma_j] = 2\mathrm{i}\epsilon_{ijk}\sigma_k, \quad [\sigma_i, \sigma_j]_+ = 2\delta_{ij} \tag{11.9}$$

   Or in a combined equation

$$\sigma_i\sigma_j = \mathrm{i}\epsilon_{ijk}\sigma_k + \delta_{ij}I \tag{11.10}$$

2. The square of any Pauli matrix equals I

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I \tag{11.11}$$

3. Pauli matrices are traceless

$$\mathrm{tr}(\sigma_i) = 0 \tag{11.12}$$

4. For any spatial direction unit vector $\hat{\boldsymbol{n}}$

$$(\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma})^2 = I \tag{11.13}$$

5. For any vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ that commute with σ

$$(\boldsymbol{a} \cdot \boldsymbol{\sigma})(\boldsymbol{b} \cdot \boldsymbol{\sigma}) = \boldsymbol{a} \cdot \boldsymbol{b}I + \mathrm{i}(\boldsymbol{a} \times \boldsymbol{b}) \cdot \boldsymbol{\sigma}^2 \tag{11.15}$$

6. The exponential of a Pauli matrix

$$\mathrm{e}^{\mathrm{i}a\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}} = I\cos(a) + \mathrm{i}\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}\sin(a)^3 \tag{11.17}$$

[2]Proof:

$$a_i\sigma_i b_j\sigma_j = a_i b_j \sigma_i\sigma_j = a_i b_j(\mathrm{i}\epsilon_{ijk}\sigma_k + \delta_{ij}I) = a_i b_i I + \mathrm{i}(\boldsymbol{a} \times \boldsymbol{b})_k\sigma_k \tag{11.15}$$

[3]Proof: Due to $(\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma})^2 = I$, so

$$\begin{aligned}
\mathrm{e}^{\mathrm{i}a\hat{\boldsymbol{n}}\cdot\boldsymbol{\sigma}} &= \sum_{k=0}^{\infty} \frac{\mathrm{i}^k a^k}{k!}(\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma})^k = \sum_{p=0}^{\infty} \frac{(-1)^p a^{2p}}{(2p)!}(\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma})^{2p} + \mathrm{i}\sum_{q=0}^{\infty} \frac{(-1)^q a^{2q+1}}{(2q+1)!}(\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma})^{2q+1} \\
&= I\sum_{p=0}^{\infty} \frac{(-1)^p a^{2p}}{(2p)!} + \mathrm{i}(\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma})\sum_{q=0}^{\infty} \frac{(-1)^q a^{2q+1}}{(2q+1)!} \\
&= I\cos(a) + \mathrm{i}\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}\sin(a)
\end{aligned} \tag{11.17}$$

One of some interests is the projection of the spin on some arbitary direction. We consider a unit vector $\hat{\boldsymbol{n}}$ in the (θ, ϕ), which writes

$$\hat{\boldsymbol{n}} = \sin\theta\cos\phi\hat{\boldsymbol{e_x}} + \sin\theta\cos\phi\hat{\boldsymbol{e_y}} + \cos\theta\hat{\boldsymbol{e_z}} \tag{11.18}$$

and the projection of the spin operator on $\hat{\boldsymbol{n}}$ is thus (in S_z basis)

$$\begin{aligned}\boldsymbol{S}\cdot\hat{\boldsymbol{n}} &= \frac{\hbar}{2}(\sigma_x\sin\theta\cos\phi + \sigma_y\sin\theta\cos\phi + \sigma_z\cos\theta) \\ &= \frac{\hbar}{2}\begin{pmatrix}\cos\theta & \sin\theta\mathrm{e}^{-\mathrm{i}\phi} \\ \sin\theta\mathrm{e}^{\mathrm{i}\phi} & -\cos\theta\end{pmatrix}\end{aligned} \tag{11.19}$$

It is easy to solve the eigenproblem of (**??**) and we find two eigen states

$$|\hat{n}\uparrow\rangle = |\chi_1\rangle = \begin{pmatrix}\cos(\theta/2)\mathrm{e}^{-\mathrm{i}\phi/2} \\ \sin(\theta/2)\mathrm{e}^{\mathrm{i}\phi/2}\end{pmatrix} \tag{11.20}$$

$$|\hat{n}\downarrow\rangle = |\chi_2\rangle = \begin{pmatrix}-\sin(\theta/2)\mathrm{e}^{-\mathrm{i}\phi/2} \\ \cos(\theta/2)\mathrm{e}^{\mathrm{i}\phi/2}\end{pmatrix} \tag{11.21}$$

and we can verify that

$$\langle\chi_1|\boldsymbol{S}|\chi_2\rangle = \frac{\hbar}{2}\hat{\boldsymbol{n}} \tag{11.22}$$

Equation (**??**) shows that the expectation value of the spin is invariant in any direction.

11.3 System of Two Spin-1/2 Particles

The Hilbert space of the system of two spin-1/2 particle is the direct product of the space of both particles

$$V_{1\otimes 2} = V_1 \otimes V_2 \tag{11.23}$$

Such that the eigenkets in the space writes

$$|s_1m_1, s_2m_2\rangle = |s_1m_1\rangle \otimes |s_2m_2\rangle\,, \quad s_1 = s_2 = 1/2,\ m_{1,2} = \pm 1/2 \tag{11.24}$$

It is obvious that the space has a dimensionality of four. The eigenbasis can be naturally chosen as

$$\begin{aligned}|\uparrow\uparrow\rangle &\longrightarrow s_1 = s_2 = 1/2,\ m_1 = 1/2,\ m_2 = 1/2 \\ |\uparrow\downarrow\rangle &\longrightarrow s_1 = s_2 = 1/2,\ m_1 = 1/2,\ m_2 = -1/2 \\ |\downarrow\uparrow\rangle &\longrightarrow s_1 = s_2 = 1/2,\ m_1 = -1/2,\ m_2 = 1/2 \\ |\downarrow\downarrow\rangle &\longrightarrow s_1 = s_2 = 1/2,\ m_1 = -1/2,\ m_2 = -1/2\end{aligned} \tag{11.25}$$

We consider the total spin operator

$$\boldsymbol{S} = \boldsymbol{S_1} + \boldsymbol{S_2} \tag{11.26}$$

by the sum of the spins of the separate particles. And its z-component

$$S_z = S_{1z} + S_{2z} \tag{11.27}$$

Our goal next is to find the eigenvalues and the eigenvectors of S^2 and S_z. It is easy to verify that all the four eigenkets in equation (**??**) are eigenvectors of S_z.

$$\begin{aligned} S_z\,|\uparrow\uparrow\rangle &= \hbar\,|\uparrow\uparrow\rangle \\ S_z\,|\uparrow\downarrow\rangle &= 0 \\ S_z\,|\downarrow\uparrow\rangle &= 0 \\ S_z\,|\downarrow\downarrow\rangle &= |\downarrow\downarrow\rangle \end{aligned} \tag{11.28}$$

Also $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ are eigenvectors of S^2 while $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ are not. However, the following combinations are

$$\begin{aligned} |\chi_{10}\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |\chi_{00}\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \end{aligned} \tag{11.29}$$

Thus the eigenbasis in total spin space can be written as

$$\begin{aligned} |\chi_{11}\rangle &= |\uparrow\uparrow\rangle \\ |\chi_{1,-1}\rangle &= |\downarrow\downarrow\rangle \\ |\chi_{10}\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |\chi_{00}\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \end{aligned} \tag{11.30}$$

The three spin-1 states are called the **triplets** and the spin-0 states is called the **singlets**. An interesting result is: the first two states in (**??**) can be written as the direct product of the states of the two particles, that

$$|\chi_{11}\rangle = |\uparrow\rangle_1 \otimes |\uparrow\rangle_2 \tag{11.31}$$

$$|\chi_{11}\rangle = |\downarrow\rangle_1 \otimes |\downarrow\rangle_2 \tag{11.32}$$

We call them **separable states**. While the last two states in (**??**) can not be written as the direct product of two independent states. We call them **entangled states**. We should emphasize that the entangled states cannot become separable in any basis.

12

Time-Independent Perturbation Theory

12.1 Formalism of Non-degenerate System

Time-independent perturbation theory is an approximation method to solve the kinds of problem: the eigenvalue of H^0 is known, and we want to know the eigenvalue of $H = H^0 + H^1$, where H^1 is a small perturbation compared to H.We assume that

$$H^0 \left|n^0\right\rangle = E_n^0 \left|n^0\right\rangle \tag{12.1}$$

where $\left|n^0\right\rangle$ is the eigenket of H^0 corresponding to the eigenvalue E_n^0. And we assume that the eigenkets and the eigenvalues of H can be expanded in a **petturbation series**

$$\begin{aligned} |n\rangle &= \left|n^0\right\rangle + \left|n^1\right\rangle + \left|n^2\right\rangle + \cdots \\ E_n &= E_n^0 + E_n^1 + E_n^2 + \cdots \end{aligned} \tag{12.2}$$

Our goal is to find the explicit expression of $\left|n^k\right\rangle$ and E_n^k. The eigenvalue equation writes

$$\begin{aligned} &(H^0 + H^1)(\left|n^0\right\rangle + \left|n^1\right\rangle + \left|n^2\right\rangle + \cdots) \\ &= (E_n^0 + E_n^1 + E_n^2 + \cdots)(\left|n^0\right\rangle + \left|n^1\right\rangle + \left|n^2\right\rangle + \cdots) \end{aligned} \tag{12.3}$$

The zeroth-order terms of equation (**??**) satisfy

$$H^0 \left|n^0\right\rangle = E_n^0 \left|n^0\right\rangle \tag{12.4}$$

The first-order terms of equation (**??**) satisfy

$$H^0 \left|n^1\right\rangle + H^1 \left|n^0\right\rangle = E_n^0 \left|n^1\right\rangle + E_n^1 \left|n^0\right\rangle \tag{12.5}$$

Notice that $\left\langle n^0\right| H^0 = \left\langle n^0\right| E_n^0$ and $\left\langle n^0|n^0\right\rangle = 1$, we dot both sides with $\left\langle n^0\right|$ to obtain

$$E_n^1 = \left\langle n^0|H^1|n^0\right\rangle \tag{12.6}$$

which is the expectation value of the perturbation Hamiltonian under the basis of the unperturbated eigenkets. If we dot both sides of equation (**??**) by $\left\langle m^0\right|$ where $m \neq n$, we have

$$\left\langle m^0|n^1\right\rangle = \frac{\left\langle m^0|H^1|n^0\right\rangle}{E_n^0 - E_m^0} \tag{12.7}$$

such that

$$\left|n^1\right\rangle = \sum_{m,m\neq n} \frac{\left|m^0\right\rangle \left\langle m^0\right|H^1\left|n^0\right\rangle}{E_n^0 - E_m^0} \tag{12.8}$$

The second-order terms of equation (**??**) satisfy

$$H^0\left|n^2\right\rangle + H^1\left|n^1\right\rangle = E_n^0\left|n^2\right\rangle + E_n^1\left|n^1\right\rangle + E_n^2\left|n^0\right\rangle \tag{12.9}$$

Dot both sides with $\left\langle n^0\right|$ we obtain

$$\begin{aligned} E_n^2 &= \left\langle n^0\right|H^1\left|n^1\right\rangle \\ &= \sum_{m,m\neq n} \frac{\left\langle n^0\right|H^1\left|m^0\right\rangle \left\langle m^0\right|H^1\left|n^0\right\rangle}{E_n^0 - E_m^0} \\ &= \sum_{m,m\neq n} \frac{\left|\left\langle m^0\right|H^1\left|n^0\right\rangle\right|^2}{E_n^0 - E_m^0} \end{aligned} \tag{12.10}$$

Until now we get the first-order term and the second order term of the energy eigenvalue and the corresponding approximation of eigenkets

$$\begin{aligned} \left|n\right\rangle &\approx \left|n^0\right\rangle + \left|n^1\right\rangle \\ &= \left|n^0\right\rangle + \sum_{m,m\neq n} \frac{\left|m^0\right\rangle \left\langle m^0\right|H^1\left|n^0\right\rangle}{E_n^0 - E_m^0} \end{aligned} \tag{12.11}$$

12.2 The Harmonic Oscillators in Uniform Electric Field

We now consider a harmonic oscillator with mass m and charge q subjected in an external uniform electric field ϵ. So the Hamiltonian can be expressed as

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2 - q\epsilon X = H^0 + H^1 \tag{12.12}$$

where $H^0 = \dfrac{P^2}{2m} + \dfrac{1}{2}m\omega^2 X^2$ is the Hamiltonian of unperturbated harmonic oscillator and $H^1 = -q\epsilon X$ is the perturbation caused by electric force. We now want to determine the eigenvalue E_n of H. According to the discussion in the last section, the zeroth-term is the energy of the unperturbated harmonic oscillator

$$E^0 = (n + 1/2)\hbar\omega \tag{12.13}$$

and the first-order term is the expectation value of H_1 under the energy basis of H^0

$$\begin{aligned} E^1 &= \langle n^0|H^1|n^0\rangle = -q\epsilon\langle n^0|X|n^0\rangle \\ &= -q\epsilon\sqrt{\frac{\hbar}{2m\omega}}\langle n^0|a^\dagger + a|n^0\rangle \\ &= -q\epsilon\sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n+1}\langle n^0|(n+1)^0\rangle + \sqrt{n}\langle n^0|(n+1)^0\rangle) \\ &= 0 \end{aligned} \tag{12.14}$$

and the second-order term is

$$\begin{aligned} E_n^2 &= \sum_{m,m\neq n}\frac{|\langle m^0|H^1|n^0\rangle|^2}{E_n^0 - E_m^0} \\ &= q^2\epsilon^2\frac{\hbar}{2m\omega}\sum_{m,m\neq n}\frac{|\langle m^0|a^\dagger + a|n^0\rangle|^2}{E_n^0 - E_m^0} \\ &= q^2\epsilon^2\frac{\hbar}{2m\omega}\sum_{m,m\neq n}\frac{|\sqrt{n+1}\delta_{m,n+1} + \sqrt{n}\delta_{m,n-1}|^2}{(n+1/2)\hbar\omega - (m+1/2)\hbar\omega} \\ &= q^2\epsilon^2\frac{\hbar}{2m\omega}(\frac{n+1}{-\hbar\omega} + \frac{n}{\hbar\omega}) \\ &= -\frac{q^2\epsilon^2\hbar}{2m\omega} \end{aligned} \tag{12.15}$$

So the energy eigenvalue of H is

$$\begin{aligned} E_n &= E_n^0 + E_n^1 + E_n^2 \\ &= (n+1/2)\hbar\omega - \frac{q^2\epsilon^2\hbar}{2m\omega} \end{aligned} \tag{12.16}$$

and the corresponding eigentstates

$$|n\rangle = |n^0\rangle + \frac{q\epsilon}{\hbar\omega}\sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n+1}\,|(n+1)^0\rangle - \sqrt{n}\,|(n-1)^0\rangle) \tag{12.17}$$

An approximation of the energy and eigenstates of the harmonic oscillators in E-field is given in the above discussion, since the electric potential energy is regarded as a pertubation compared to the original Hamiltonian. The strict solution to this problem is based on Schrödinger's equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi + (\frac{1}{2}m\omega^2X^2 - q\epsilon X)\psi = E\psi \tag{12.18}$$

Let

$$\xi = \sqrt{\frac{m\omega}{\hbar}}x,\ \xi_0 = \frac{e\epsilon}{\omega}\sqrt{m\hbar\omega},\ \eta = \xi - \xi_0,\ \lambda = \frac{2E}{\hbar\omega} + \xi_0^2 \tag{12.19}$$

Then equation (**??**) turns into

$$\frac{\mathrm{d}^2}{\mathrm{d}\eta^2}\psi - \eta^2\psi + \lambda\psi = 0 \tag{12.20}$$

The eigenvalue of the above equation can only be chosen $\lambda = 2n+1, n \in \mathbb{N}$, such that the energy takes the values of

$$E_n = (n+1/2)\hbar\omega - \frac{q^2\epsilon^2\hbar}{2m\omega} \tag{12.21}$$

and the corresponding eigenfunction

$$\psi_n(x) = (\frac{m\omega}{\pi\hbar 2^{2n}(n!)^2})^{1/4}\exp\left\{-\frac{1}{2}\alpha^2(x-x_0)^2\right\}H_n(\alpha(x-x_0)), \quad x_0 = \frac{q\epsilon}{m\omega^2} \tag{12.22}$$

12.3 Degenerate Perturbation Theory

The discussions in this section and the next section are mainly based on J. Zeng[1]. Assume that the system is at energy E_n^0 without perturbation. The degree of degeneracy is f_n. In the case of this degenerate system, the zeroth wavefunction cannot be determined first, but can be expressed in terms of the expansion of

$$\left|n^0\right\rangle = \sum_{\nu=1}^{f_n}\left|(n\nu)^0\right\rangle\left\langle(n\nu)^0\middle|n^0\right\rangle = \sum_{\nu=1}^{f_n}\left|(n\nu)^0\right\rangle\alpha_\nu \tag{12.23}$$

Substitute $\left|n^0\right\rangle$ in equation (**??**) by the above equation we can obtain

$$(H^0 - E_n^0)\left|n^1\right\rangle = (E_n^1 - H^1)\sum_{\nu=1}^{f_n}\left|(n\nu)^0\right\rangle\alpha_\nu \tag{12.24}$$

Dot both sides by $\left|(n\nu')^0\right\rangle$, we have

$$\sum_\nu(\left\langle(n\nu')^0\middle|H^1\middle|(n\nu)^0\right\rangle - E_n^1\delta_{\nu',\nu})\alpha_\nu = 0 \tag{12.25}$$

The prerequisite to obtain a non-zero solutions of α_ν is to ensure

$$\det\left(\left\langle(n\nu')^0\middle|H^1\middle|(n\nu)^0\right\rangle - E_n^1\delta_{\nu',\nu}\right) = 0 \tag{12.26}$$

[1] J. Zeng, Quantum Mechanics. Vol 1. 5th Ed., Beijing, Science Press. 2013. 372.

12.4 Stark Effect in Hydrogen

In this section we discuss the Stark effect in the $n = 2$ level of hydrogen. A hydrogen is subjected into an electric field $\boldsymbol{E}$ along z direction. The perturbation Hamiltonian is thus

$$H^1 = e\boldsymbol{r} \cdot \boldsymbol{E} = eZE \tag{12.27}$$

According to Selection rule we obtain the only nonzero matrix elements of H^1 are

$$\langle 210|H^1|200\rangle = \langle 200|H^1|210\rangle = -3e^2Ea \tag{12.28}$$

Due to (**??**) we have the energy

$$E^1 = \pm 3e^2Ea, 0, 0 \tag{12.29}$$

13

Time-Dependent Perturbation Theory

13.1 First-Order Perturbation Theory

In thIs chapter we consider the perturbative solutions with Hamiltonian

$$H(t) = H^0 + H^1(t) \tag{13.1}$$

where H^0 is the time-independent part whose eigenvalue problem has been solved and H^1 is the time-dependent perturbation.

We suppose that at $t = 0$ the system is at the state $\left|i^0\right\rangle$. Since the eigenbasis of H^0 is complete, we can always write

$$|\psi(t)\rangle = \sum_n c_n(t) \left|n^0\right\rangle \mathrm{e}^{-\mathrm{i}E_n^0 t/\hbar} \tag{13.2}$$

where $\left|n^0\right\rangle$ is the eigenvectors of H^0 and the exponential term is the time evolution operator. Since the motion of the state follows Schrödinger equation, we have

$$\begin{aligned}
\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle &= \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}(\sum_n c_n(t)\left|n^0\right\rangle \mathrm{e}^{-\mathrm{i}E_n^0 t/\hbar}) \\
&= \mathrm{i}\hbar\sum_n \dot{c}_n(t)\left|n^0\right\rangle \mathrm{e}^{-\mathrm{i}E_n^0 t/\hbar} + \mathrm{i}\hbar\sum_n c_n(t)\left|n^0\right\rangle(-\mathrm{i}E_n^0/\hbar)\mathrm{e}^{-\mathrm{i}E_n^0 t/\hbar} \\
&= E_n^0\sum_n c_n(t)\left|n^0\right\rangle \mathrm{e}^{-\mathrm{i}E_n^0 t/\hbar} + \sum_n c_n(t)H^1\left|n^0\right\rangle \mathrm{e}^{-\mathrm{i}E_n^0 t/\hbar}
\end{aligned} \tag{13.3}$$

Thus

$$\mathrm{i}\hbar\sum_n \dot{c}_n(t)\left|n^0\right\rangle \mathrm{e}^{-\mathrm{i}E_n^0 t/\hbar} = \sum_n c_n(t)H^1\left|n^0\right\rangle \mathrm{e}^{-\mathrm{i}E_n^0 t/\hbar} \tag{13.4}$$

Dot both sides by $\left|j^0\right\rangle$ we obtain

$$\mathrm{i}\hbar\dot{c}_j(t)\mathrm{e}^{-\mathrm{i}E_j^0 t/\hbar} = \sum_n c_n(t)\mathrm{e}^{-\mathrm{i}E_n^0 t/\hbar}\left\langle j^0\right|H^1\left|n^0\right\rangle \tag{13.5}$$

Or in another form

$$\mathrm{i}\hbar\dot{c}_j = \sum_n \mathrm{e}^{\mathrm{i}\omega_{jn}t}\left\langle j^0\right|H^1\left|n^0\right\rangle c_n, \quad \omega_{ji} = \frac{E_j^0 - E_n^0}{\hbar} \tag{13.6}$$

Consider that the perturbation is so small compared to the time-independent part, we use the first-oder approximation

$$c_i(t) \approx 1, \quad c_{n\neq i} \approx 0 \tag{13.7}$$

So equation (**??**) turns to

$$\mathrm{i}\hbar\dot{c}_j = \mathrm{e}^{\mathrm{i}\omega_{ji}t} \left\langle j^0 \middle| H^1 \middle| i^0 \right\rangle \tag{13.8}$$

The solution to which, with the right initial condition, is

$$c_j(t) = \delta_{ji} + \frac{1}{\mathrm{i}\hbar} \int_0^t \mathrm{e}^{\mathrm{i}\omega_{ji}\tau} \left\langle j^0 \middle| H^1(\tau) \middle| i^0 \right\rangle \mathrm{d}\tau \tag{13.9}$$

So

$$|c_j(t)|^2 = |\delta_{ji} + \frac{1}{\mathrm{i}\hbar} \int_0^t \mathrm{e}^{\mathrm{i}\omega_{ji}\tau} \left\langle j^0 \middle| H^1(\tau) \middle| i^0 \right\rangle \mathrm{d}\tau|^2 \tag{13.10}$$

where $|c_j(t)|^2$ is the probability that the system is in the state $\left|j^0\right\rangle$ at time t since the initial state is $\left|i^0\right\rangle$, which is conventionally called **transition probability** and sometimes writes as $|c_{ji}(t)\rangle$.

13.2 An Excited Hydrogen Atom

We consider a hydrogen atom which is in the ground state. The atom is excited by a pulsed electric field with the following form

$$E(t) = E_0\delta(t) \tag{13.11}$$

We now aim to know the probability of the hydrogen atom transiting to any excited state. First, we let the orientation of the electric field be z direction, thus the perturbation Hamiltonian writes

$$H' = eE_0z\delta(t) \tag{13.12}$$

We directly give the expression of the wave function

$$\psi(\boldsymbol{r}, t) = \sum_n \sum_l \sum_m \psi_{nlm}(\boldsymbol{r}) C_{nlm}(t) \mathrm{e}^{-\mathrm{i}E_nt/\hbar} \tag{13.13}$$

and the initial condition

$$\psi(\boldsymbol{r}, t) = \psi_{100}(\boldsymbol{r}) \tag{13.14}$$

According to equation (**??**). Let $(n, l, m) \neq (1, 0, 0)$ and we have

$$\begin{aligned} c_{nlm}(t) &= \frac{1}{\mathrm{i}\hbar} \int_0^t \mathrm{e}^{\mathrm{i}(E_n - E_1)t/\hbar} \langle nlm|H'(\tau)|100\rangle \, \mathrm{d}\tau \\ &= \frac{eE_0}{\mathrm{i}\hbar} \int_0^t \mathrm{e}^{\mathrm{i}(E_n - E_1)t/\hbar} \langle nlm|z|100\rangle \, \delta(t)\mathrm{d}\tau \\ &= \frac{eE_0}{\mathrm{i}\hbar} \langle nlm|z|100\rangle \end{aligned} \tag{13.15}$$

So the corresponding probability

$$P_{nlm} = |\frac{eE_0}{\mathrm{i}\hbar} \langle nlm|z|100\rangle|^2 = (\frac{eE_0}{\hbar})^2 |\langle nlm|z|100\rangle|^2 \tag{13.16}$$

Due to the selection rules we know that the final state should be $(n, l, m) = (n, 1, 0)$. And the total probabilty that the atom leaves the ground state is

$$\begin{aligned} P_{\text{exc}} &= \sum_{(n,l)\neq(1,0)} P_{nl0} = \sum_{n,l}(P_{nl0} - P_{100}) \\ &= (\frac{eE_0}{\hbar})^2(\sum_{n,l} |\langle nl0|z|100\rangle|^2 - |\langle 100|z|100\rangle|^2) \\ &= (\frac{eE_0}{\hbar})^2 |\sum_{n,l} \langle nl0|z|100\rangle|^2 \\ &= (\frac{eE_0}{\hbar})^2 \sum_{n,l} \langle 100|z|nl0\rangle \langle nl0|z|100\rangle \\ &= (\frac{eE_0}{\hbar})^2 \langle 100|z^2|100\rangle \end{aligned} \tag{13.17}$$

The wave function of the hydrogen atom in the ground state is

$$\psi_{100}(\boldsymbol{r}) = R_{100}(r)Y_0^0(\theta,\phi) = \frac{2}{a_0^{3/2}}\mathrm{e}^{-r/a_0}Y_0^0 \tag{13.18}$$

So

$$\begin{aligned} \langle 100|z^2|100\rangle &= \frac{1}{3}\langle 100|r^2|100\rangle \\ &= \frac{1}{3}\int_0^\infty R_{100}^* r^2 R_{100} r^2 \mathrm{d}r \\ &= \frac{1}{3}\frac{4}{a_0^3}\int_0^\infty \mathrm{e}^{-2r/a_0} r^4 \mathrm{d}r = a_0^2 \end{aligned} \tag{13.19}$$

Consequently, the probability theta the atom stays in the ground state and jumps to an excited state are respectively given

$$P_{\text{exc}} = (\frac{eE_0}{\hbar})^2 \langle 100|z^2|100\rangle = (\frac{eE_0 a_0}{\hbar})^2 \tag{13.20}$$

$$P_{\text{ground}} = 1 - (\frac{eE_0 a_0}{\hbar})^2 \tag{13.21}$$

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