Quantum Mechanics I

TanXG lecture notes on theoratical physics

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Introduction

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Contents

Chapter 1

Mathematics Foundation

The first chapter gives a rather brief introduction to the main mathematical concepts and methods needed in these introductory lecture notes of Quantum Mechanics, including Hilbert space, operators, unitary transformation and unitary opators. This chapter provides the basic mathematical langurage of these lecture notes.

Then I'd like to show the references that I prefer while writing this chapter:

- The PPTs of Prof.Yeo Ye in NUS, which is the BEST references that I've met for learning quantum mechanics up to now. I leart all the Dirac notations from his PPTs.
- David Tong's lecture notes on Quantum Mechanics. Please always trust Dr.Tong.
- *Basic principles of quantum mechanics*, written by Prof.Ying Zhang from Xi'an Jiaotong university. The advantage of this textbook is that it has rich content, while the disadvantage is that it has lots of typos and fail to illustrate some of the concepts very naturally and clearly.
- *Mathematcs for Quantum Mechanics*, written by John David Jackson, who is rather famous for his textbook *Classical Electrodynamics*. This is a kind of mini hand book about the Mathematcs for Quantum Mechanics, which is worth trying. And it also sparks me for the proof of the properties of Hermitian operators, especially for the usage of Schmidt process.

Alright, time to begin our adventure!

1.1 Hilbert space

1.1.1 Hilbert space

We have been very familiar with $\mathbb{R}^3$, the 3-dimensional Euclidean space that we live in. In this space, we define a stuff named vector to help us deal with the dynamics of the particles in the framework of Newtonian mechanics.

The story is rather similar in the context of quantum mechanics, where we also use vectors to describe the dynamics of a quantum particle. But the vectors aren't living in the Euclidean space; they live in *Hilbert space*.

What is Hilbert Space?

First of all, Hilbert space is a kind of linear space whose elements are generally called vectors. And importantly, it's defined on the complex number field. We denote Hilbert space as $\mathcal{H}$. And we generally denote the vectors in Hilbert space as $|\psi\rangle$, which is called *Dirac right vector*, or more formally, *Dirac ket*. The notation and the name of $|\psi\rangle$ are patents of physicists[1].

What's more, $\mathcal{H}$ defines a kind of inner product among its vectors, say $|\psi\rangle$ and $|psi\rangle$ which is denoted as $\langle\phi|\psi\rangle$. For this notation, you can view it as that you put $\langle\phi|$ and $|\psi\rangle$ shoulder by shoulder. Here, $\langle\phi|$ is called *Dirac left vector* or *Dirac bra*. Mathematically, we say $\langle\phi|$ resides in the dual space of $\mathcal{H}$ instead of $\mathcal{H}$ itself.

Furthermore, $\mathcal{H}$ is a complete space, which means that you can find a set of complete basis, say $|e_1\rangle, |e_2\rangle, \cdots, |e_n\rangle$. Here, "complete basis" means that you can formulate any vector $|\psi\rangle$ as

$$|\psi\rangle = \sum_i \psi_i |e_i\rangle \tag{1.1}$$

where generally $\psi_i \in \mathbb{C}$. If the basis are all orthonormal, then we can easily specify the coefficients by

$$\psi_i = \langle e_i|\psi\rangle \tag{1.2}$$

[1] Nonetheless, sometimes for clarity, we will throw away the Dirac notations and just use ψ to denote the vector, or the matrix that we will mention below. Dirac bracket in most circumstances can be a good teacher, while sometimes it can't. Anyway, clarity instead of rigid consistancy is what we really want to have.

Matrix Rrepresentation of Vectors

Armed with completeness, we can denote $|\psi\rangle$ in a way that you like and familiar with by using matrix:

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix} \tag{1.3}$$

However, this kind of notation sometimes can be troublesome since it hides the information of basis behind it. Thus we should always keep in mind which basis we've choosen to describe the vectors in $\mathcal{H}$. Nonetheless, we still embrace the matrix notation since it's elegant, it's familiar, and it can help us better understand why we say that "quantum mechanics is really a theory of linear algebra".

Although we've asked matrixes for help, it's not necessary. The inner product is independent of the basis, and the effect of matrixes is just to make the abstract thing more concrete.

1.1.2 Hilbert Space vs Euclidean Space

It seems like $\mathcal{H}$ is very similar to $\mathbb{R}^3$: they both define a kind of inner product, which is also very important in Newtonian mechanics. And both of them are complete. But there are still some essential differences between them.

First of all, there are some subtleties in the inner product in $\mathcal{H}$. Let's calculate the module of the vector $|\psi\rangle$ using the matrix notation. Maybe you would like to say that the module of $|\psi\rangle$ is[2]

$$\langle\psi|\psi\rangle = \begin{pmatrix} \psi_1 & \psi_2 & \dots & \psi_n \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix} = \sum_i \psi_i^2$$

But remember that generally $\psi_i \in \mathbb{C}$, that's to say $\langle\psi|\psi\rangle$ is also generally complex. But for some reasons[3] we want the module of $|\psi\rangle$ to be real. Thus, we define $\langle\psi|\psi\rangle$ as

$$\langle\psi|\psi\rangle = \psi_1^*\psi_1 + \psi_2^*\psi_2 + \cdots + \psi_n^*\psi_n = \sum_i |\psi_i|^2 \tag{1.4}$$

[2]In these lecture notes, we don't impose the Einstein's summation convention, because the summation isn't frequnt in quantum mechanics.

[3]Maybe in order to being compatible with the physical magnitudes which are real numbers

The conjugation saves us. Equation (1.4) just implies that the bra $\langle\psi|$ meets that

$$\langle\psi| = \begin{pmatrix} \psi_1^* & \psi_2^* & \dots & \psi_3^* \end{pmatrix} \tag{1.5}$$

In the matrix notation, we say that $\langle\psi|$ is the conjugate transpose of $|\psi\rangle$. Sometimes $\langle\psi|$ is also called the adjoint matrix of $|\psi\rangle$.If we throw away the Dirac brackets and just denote vector(matrix) as ψ, then its adjoint matrix is denoted as $\psi^\dagger$. By using the matrix notation, we can also define that the inner product has the property of

$$\langle\psi_1|\psi_2\rangle = \langle\psi_2|\psi_1\rangle^* \tag{1.6}$$

Equation (1.6) is also different from the case in Euclidean space where $\boldsymbol{A}\cdot\boldsymbol{B} = \boldsymbol{B}\cdot\boldsymbol{A}$ holds, simply because in classical mechanics we don't need to worry about complex numbers, while in quantum mechanics we do have to. Actually, complex numbers are intrinsic for quantum mechanics, which can be reflected by the fundamental equation — Schrödinger equation. We'll meet it in next chapter.

The difference is also reflected in the matrix notation above, where all the matrixes can have either finite dimensions or even INFINITE dimensions, which is of courese hard to believe in Newtonian mechanics. Nonetheless, for our purpose of quantum machanics, we should ask the module (1.4) of any vector, no matter what dimensions it has, is finite. Only then can the vectors in Hilbert space represente the right and meaningful microscopic states for quantum particles.

And then, the formula in (1.1) implies that we defaultly view $\mathcal{H}$ as a discrete space. But it's not always the case, and $\mathcal{H}$ can be a continuous space, which means that we can modify (1.1) into an integral. We'll see both the continuous case and the discrete case as we proceed in quantum mechanics.

Anyway, Hilbert space isn't a patent of physics and quantum mechanics. Physicists just borrow it from mathematicians because it turns out that we need $\mathcal{H}$ as a mathematical framework as well as a structure to describe the microscopic world.

1.2 Operators

1.2.1 Operators

Mathematically and generally speaking, an *operator* $\hat{O}$ is a kind of map

$$\hat{O} : |\psi\rangle \to |\phi\rangle \tag{1.7}$$

which transfers a vector $|\psi\rangle$ into another $|\phi\rangle$, both of which live in the same Hilbert space[4]. If the operator satisfies

$$\hat{O}(\alpha|\psi_1\rangle + \beta|\psi_2\rangle) = \alpha|\phi_1\rangle + \beta|\phi_2\rangle \tag{1.8}$$

Then it's a linear operator. We'll only focus on the linear operators in these lecture notes.

1.2.2 Eigenvalue problem

In classical mechanics, eigenvalue problem plays an important role in many problems, such as the tiny vibration system. In quantum mechanics, eigenvalue problem is even much more important, and is written directly into the fundamental postulates of quantum mechanics which we'll meet in the future. For now, I will just provide a brief and general introduction of the eigenvalue problem.

Last subsection we mentioned that an operator $\hat{O}$ transfer a vector $|\psi\rangle$ into another one $|\phi\rangle$. If the result $|\phi\rangle$ is nothing but simply multiply $|\psi\rangle$ by a complex constant, i.e.

$$\hat{O}|\psi\rangle = \lambda|\psi\rangle \ , \ \lambda \in \mathbb{C} \tag{1.9}$$

then (1.9) is called the eigen equation of the operator $\hat{O}$, with $|\psi\rangle$ called the eigenvector or, in quantum mechanics, eigenstate of $\hat{O}$.λ is the eigenvalue corresponding to the eigenstate $|\psi\rangle$.

1.2.3 Hermitian Operators

Hermitian opators are the key roles in our stroy.

Firstly, I need to introduce what is adjoint operator. The adjoint operator of $\hat{O}$ is denoted as $\hat{O}^\dagger$, which is defined to satisfy that

$$\langle\psi_1|\hat{O}\psi_2\rangle = \langle\hat{O}^\dagger\psi_1|\psi_2\rangle \tag{1.10}$$

Then the definition of a Hermitian Operator is quite simple. Hermitian Operators are

[4] And therefore share the same basis.

defined as the opators which satisfy

$$\hat{O}^\dagger = \hat{O}$$

which is also mathematically called self-adjoint.

Properties of Hermitian Operators

The mathematical properties of the Hermitian operators can be fancy and important.
Property 1: The eigenvalues of a Hermitian operator must be real numbers.
Proof: It's easy to figure out that

$$\langle\psi|\hat{O}\psi\rangle = \langle\hat{O}^\dagger\psi|\psi\rangle = \langle\hat{O}\psi|\psi\rangle$$

and

$$\langle\psi|\hat{O}\psi\rangle = \lambda\langle\psi|\psi\rangle$$

$$\langle\hat{O}\psi|\psi\rangle = \lambda^*\langle\psi|\psi\rangle$$

Thus

$$(\lambda - \lambda^*)\langle\psi|\psi\rangle = 0$$

Generally the eigen vector $|\psi\rangle \neq 0$, or that will be meaningless. So $\langle\psi|\psi\rangle \neq 0$, and we ultimately get that $\lambda = \lambda^*$ which simply means that λ is real.

Property 2: You can always find a set of ortho-normal eigenvectors for a Hermitian operator.
Proof: Suppose that $|\psi_i\rangle$ and $|\psi_j\rangle$ satisfy that

$$\hat{O}|\psi_i\rangle = \lambda_i|\psi_i\rangle$$

$$\hat{O}|\psi_j\rangle = \lambda_j|\psi_j\rangle$$

If $|\psi_i\rangle$ is not a normalized vector, don't worry, $\frac{|\psi_i\rangle}{\langle\psi_i|\psi_i\rangle}$ will be, so we can just simply assume that all the vector below is normalized. Then, the similar trick can be played

$$\langle\psi_i|\hat{O}\psi_j\rangle = \langle\hat{O}\psi_i|\psi_j\rangle$$

so

$$(\lambda_i^* - \lambda_j)\langle\psi_i|\psi_j\rangle = (\lambda_i - \lambda_j)\langle\psi_i|\psi_j\rangle = 0$$

If there's no degeneracy, then $\lambda_i \neq \lambda_j$, so we get

$$\langle\psi_i|\psi_j\rangle = \delta_{ij} = \begin{cases} 0\ , & i \neq j \\ 1\ , & i = j \end{cases}$$

If $\lambda_i = \lambda_j = \lambda$, i.e. there exists degeneracy, then the $\langle\psi_i|\psi_j\rangle$ can't automatically be δ_{ij}. Nonetheless, we can impose the *Schmidt process*.

If $\langle\psi_i|\psi_j\rangle \neq \delta_{ij}$, everything is OK. However, assume that $\langle\psi_i|\psi_j\rangle \neq \delta_{ij}$, then we generally make up a new vector $|\psi_k\rangle = |\psi_i\rangle + \alpha|\psi_j\rangle$, which obviously also satisfy that $\hat{O}|\psi_k\rangle = \lambda|\psi_k\rangle$. Then we REQUEST that $\langle\psi_i|\psi_k\rangle = \delta_{ik}$ which can be true as long as

$$\langle\psi_i|\psi_k\rangle = \langle\psi_i|\psi_i\rangle + \alpha\langle\psi_i|\psi_j\rangle = \delta_{ik}$$

i.e. as long as we request $\alpha = \frac{\delta_{ik}-1}{\langle\psi_i|\psi_j\rangle}$, then the $|\psi_i\rangle$ and $|\psi_k\rangle$ are what we want.

All in all, a set of orthonormal eigenvectors can always be found whether there exists degeneracy or not.

Property 3: The eigenvectors of a Hermitian consist of a complete set of basis, which means we can write any vector by the form of

$$|\psi\rangle = \sum_i \langle\alpha_i|\psi\rangle|\alpha_i\rangle \tag{1.11}$$

where $\langle\alpha_i|\psi\rangle$ is a number. We won't show precisely mathematical justifications for this, but property 3 can be practiclely useful and can be physically meaningful. We'll be convinced by this in next Chapter.

What's more, the equation above reveals another useful formula. Since

$$|\psi\rangle = \sum_i |\alpha_i\rangle\langle\alpha_i|\psi\rangle = I|\psi\rangle$$

thus we can identify that

$$\sum_i |\alpha_i\rangle\langle\alpha_i| = I \tag{1.12}$$

which turns out to be very useful as we proceed. This formula in some places are called the completeness of basis, although I don't no why it has this name.

Operators in general formulism

By considering the mathematical properties above, we can find a general formulism for an operator.

Suppose that $\hat{O}$ has eigenvectors $|\phi_i\rangle$, with eigenvalues λ_i. Then $\hat{O}$ can be represented by $|\phi_i\rangle$ as

$$\hat{O} = \sum_i \lambda_i|\phi_i\rangle\langle\phi_i| \tag{1.13}$$

This is reasonable, because we just need to confirm that

$$\hat{O}|\phi_j\rangle = \sum_i \lambda_i |\phi_i\rangle\langle\phi_i|\phi_j\rangle = \sum_i \lambda_i |\phi_i\rangle\delta_{ij} = \lambda_j|\phi_j\rangle$$

which is just the eigen equation.

1.2.4 Operators under Matrix Representation

Finally, we can consider how to represent an operator by using matrix.

Suppose we've chosen a series of basis $\{\hat{e}_i\}$, and we can denote the eigenvector of $\hat{O}$ as a column matrix

$$|\phi_i\rangle = \begin{pmatrix} \phi_1^i \\ \phi_2^i \\ \vdots \\ \phi_n^i \end{pmatrix}$$

Then according to (1.13), the operator oughts to be a $n \times n$ matrix, whose components can be identified as

$$O_{ij} = \langle e_i|\hat{O}e_j\rangle = \sum_m \lambda_m \langle e_i|\phi_m\rangle\langle\phi_m|e_j\rangle \tag{1.14}$$

Armed with this kind of notation, we can still figure out that

$$O^\dagger_{ij} = \langle e_i|\hat{O}^\dagger e_j\rangle = \langle \hat{O}e_i|e_j\rangle = \langle e_j|\hat{O}e_i\rangle^* = O^*_{ji} \tag{1.15}$$

which is just to say: the matrix $\hat{O}^\dagger$ is the conjugate of the transpose of matrix $\hat{O}$.

1.2.5 Commutator

Last but not least, I want to briefly introduce an important notation between operators, which can be seen frequently in quantum mechanics — the *commutator*. The commutator of two operators $\hat{A}$ and $\hat{B}$ are defined as

$$[\hat{A}, \hat{B}] := \hat{A}\hat{B} - \hat{B}\hat{A} \tag{1.16}$$

which is also an operator. We say that $\hat{A}$ and $\hat{B}$ are commutative if $[\hat{A}, \hat{B}] = 0$.

Then comes to a very useful therom: *the commutative operators have same series of eigenvectors.* Let's have a brief proof about this therom. Suppose that $\hat{B}|b_i\rangle = b_i|b_i\rangle$. Then, on the one hand, we have $\hat{A}\hat{B}|b_i\rangle = b_i\hat{A}|b_i\rangle$, on the other hand we also have $\hat{A}\hat{B}|b_i\rangle = \hat{B}\hat{A}|b_i\rangle$. Therefore $\hat{B}(\hat{A}|b_i\rangle) = b_i(\hat{A}|b_i\rangle)$. Compare this equation with the eigen equation of $\hat{B}$, we get that $\hat{A}|b_i\rangle = \lambda|b_i\rangle$, $\lambda \in \mathbb{C}$, which means that $|b_i\rangle$ is the eigenvector of $\hat{A}$ too.

1.3 Unitary Transformation

1.3.1 Unitary transformation

Unitary transformation is the transformation among the basis of the Hilbert space.

Suppose now we have two Hermitian operators $\hat{A}$ and $\hat{B}$, with eigenvectors $|a_i\rangle$ and $|b_i\rangle$.

$$\hat{A}|a_i\rangle = a_i|a_i\rangle$$

$$\hat{B}|b_i\rangle = b_i|b_i\rangle$$

Now that both $|a_i\rangle$ and $|b_i\rangle$ are complete, of course we can use $|b_i\rangle$ to expand $|a_i\rangle$.

$$|a_i\rangle = \sum_j \langle b_j|a_i\rangle|b_j\rangle \tag{1.17}$$

The equation above implies that we've chosen $|b_i\rangle$ as a kind of basis, and meanwhile view $|a_i\rangle$ as a normal vector in Hilbert space. It also tells us that

$$\sum_j |b_j\rangle\langle b_j| = I \tag{1.18}$$

which is obvious because both $|a_i\rangle$ and $|b_i\rangle$ can be a series of basis of $\mathcal{H}$.

(1.17) can be viewed as a transformation between different basis of $\mathcal{H}$. We call this kind of transformation as *unitary transformation*[5].

1.3.2 Properties of Unitary Transformation

This subsection might be fussy, so I want to firstly tell you what I want to say in the end. My purpose is to illustrate that: thanks to the unitary transformation, the mathematical forms of all the things we meet are independent of the choice of basis.

[5]The origin of this name is reasonable, which refers to the unitary transformation in $\mathbb{R}^n$ but with a subtle difference. Actually the coefficient $\langle b_j|a_i\rangle$ can be seen as a component of a matrix

$$U_{ij} = \langle b_j|a_i\rangle$$

Then we calculate that

$$\begin{aligned}\sum_j U_{ij}U^*_{kj} &= \sum_j \langle b_j|a_i\rangle\langle a_k|b_j\rangle \\ &= \langle a_k|\sum_j |b_j\rangle\langle b_j||a_i\rangle \\ &= \langle a_k|a_i\rangle \\ &= \delta_{ik}\end{aligned}$$

which is equivalent to

$$\hat{U}\hat{U}^\dagger = I \tag{1.19}$$

The equation above oughts to be viewed as the definition of unitary matrix in complex zone, which is similar to the definition in real zone.

The first property of Unitary transformation is that it keeps the inner product. Suppose that

$$|\psi\rangle = \sum_i \psi_i |a_i\rangle = \sum_{i,j} \psi_i \langle b_j|a_i\rangle |b_j\rangle$$

$$|\phi\rangle = \sum_m \phi_m |a_m\rangle = \sum_{m,n} \phi_m \langle b_n|a_m\rangle |b_n\rangle$$

Above we simply use $|b_i\rangle$ as basis to represent these two vectors. Then the inner product

$$\begin{aligned}
\langle\phi|\psi\rangle &= \sum_{i,j,m,n} \phi_m^* \psi_i \langle a_m|b_n\rangle\langle b_j|a_i\rangle\langle b_n|b_j\rangle \\
&= \sum_{i,j,m,n} \phi_m^* \psi_i \langle a_m|b_n\rangle\langle b_j|a_i\rangle\delta_{nj} \\
&= \sum_{i,m} \phi_m^* \psi_i \langle a_m| \sum_j |b_j\rangle\langle b_j||a_i\rangle \\
&= \sum_{i,m} \phi_m^* \psi_i \langle a_m|a_i\rangle \\
&= \sum_{i,m} \phi_m^* \psi_i \delta_{im} \\
&= \sum_i \phi_i^* \psi_i
\end{aligned}$$

which turns out to be equivalent to calculate under the original basis of $|a_i\rangle$.

Secondly, let's consider the general form of operator under unitary transformation

$$\hat{A} = \sum_i a_i |a_i\rangle\langle a_i| = \sum_{i,m,n} a_i \langle b_m|a_i\rangle\langle a_i|b_n\rangle |b_m\rangle\langle b_n|$$

then we can confirm that the eigen equation still holds

$$\begin{aligned}
\hat{A}|a_k\rangle &= \sum_{i,j,m,n} a_k \langle b_m|a_i\rangle\langle a_i|b_n\rangle |b_m\rangle\langle b_n|\langle b_j|a_k\rangle|b_j\rangle \\
&= \sum_{i,j,m} a_k \langle b_m|a_i\rangle\langle a_i|b_j\rangle\langle b_j|a_k\rangle|b_m\rangle \\
&= \sum_{j,m} a_k \delta_{mj} \langle b_j|a_k\rangle|b_m\rangle \\
&= \sum_m a_k \langle b_m|a_k\rangle|b_m\rangle \\
&= a_k|a_k\rangle
\end{aligned}$$

Finally, let's talk about the commutative relation under unitary transformation. Sup-

pose that

$$\begin{cases} \hat{A} = \sum_i a_i |a_i\rangle\langle a_i| = \sum_{i,m,n} a_i \langle b_m|a_i\rangle\langle a_i|b_n\rangle |b_m\rangle\langle b_n| \\ \hat{B} = \sum_i b_i |b_i\rangle\langle b_i| \end{cases}$$

Thus, the commutator

$$\begin{aligned} [\hat{A}, \hat{B}] &= \hat{A}\hat{B} - \hat{B}\hat{A} \\ &= \sum_{i,j,m,n} a_i b_j \langle b_m|a_i\rangle\langle a_i|b_n\rangle |b_m\rangle\langle b_n|b_j\rangle\langle b_j| - \sum_{i,j,m,n} a_i b_j \langle b_m|a_i\rangle\langle a_i|b_n\rangle |b_j\rangle\langle b_j|b_m\rangle\langle b_n| \\ &= \sum_{i,j,m} a_i b_j \langle b_m|a_i\rangle\langle a_i|b_j\rangle |b_m\rangle\langle b_j| - \sum_{i,j,n} a_i b_j \langle b_j|a_i\rangle\langle a_i|b_n\rangle |b_j\rangle\langle b_n| \\ &= \sum_{i,j,m} a_i b_j \langle a_i|b_j\rangle |b_m\rangle\langle b_m|a_i\rangle\langle b_j| - \sum_{i,j,n} a_i b_j \langle b_j|a_i\rangle |b_j\rangle\langle a_i|b_n\rangle\langle b_n| \\ &= \sum_{i,j} a_i b_j |a_i\rangle\langle a_i|b_j\rangle\langle b_j| - \sum_{i,j} a_i b_j |b_j\rangle\langle b_j|a_i\rangle\langle a_i| \end{aligned}$$

In the process above, we frequently utilize the kind of fomula like (1.18). The equation above also gives the most general form of a commutator.

All the things above seems kind of fussy and obvious, because there's nothing changed for vectors and operators and we just use another basis, that's all! However, I have to say, the mathematical essence of why you can just change basis and keep any other things still is that this kind of transformation is unitary.

1.4 Unitary Operators

1.4.1 Unitary Operator

Besides the unitary transformation, there's another one unitary thing — unitary operator, which is defined to satisfy

$$\hat{U}\hat{U}^\dagger = I \tag{1.20}$$

Just like other operators, $\hat{U}$ transfer a vector $|\psi\rangle$ into another one $\hat{U}|\psi\rangle$, but keeps the basis unchanged[6].

1.4.2 Properties of Unitary Operators

First of all, like the unitary transformation, $\hat{U}$ keeps the inner product. Suppose that

$$|\phi'\rangle = \hat{U}|\phi\rangle$$

$$|\psi'\rangle = \hat{U}|\psi\rangle$$

Thus

$$\langle\phi'|\psi'\rangle = \langle\phi|\hat{U}^\dagger\hat{U}|\psi\rangle = \langle\phi|\psi\rangle \tag{1.21}$$

Secondly, it also keeps the relation that

$$\sum |\alpha'\rangle\langle\alpha'| = U\left(\sum |\alpha\rangle\langle\alpha|\right)U^\dagger = UU^\dagger = I \tag{1.22}$$

Thirdly we consider operators operated by unitary operator. Suppose that

$$\hat{O}|\psi\rangle = |\phi\rangle$$

then we multiply $\hat{U}$ on each side, and get

$$\hat{U}\hat{O}|\psi\rangle = (\hat{U}\hat{O}\hat{U}^\dagger)\hat{U}\psi\rangle = \hat{U}|\phi\rangle$$

i.e.

$$\hat{O}'|\psi'\rangle = |\phi'\rangle$$

where

$$\hat{O}' = \hat{U}\hat{O}\hat{U}^\dagger \tag{1.23}$$

which should be viewed as the new operator under the operation of $\hat{U}$. This kind of form can be very good. Firstly, it's easy to confirm that $\hat{O}'$ has the same eigenvalue as $\hat{O}$.

[6] While the unitary transformation changes the basis and, therefore, the components, but keeps the vector unchanged.

What's more, this form also keeps the commutative relation. Suppose that

$$[\hat{A}, \hat{B}] = \hat{C}$$

then we can get that

$$\begin{aligned}
[\hat{A}', \hat{B}'] &= \hat{A}'\hat{B}' - \hat{B}'\hat{A}' \\
&= \hat{U}(\hat{A}\hat{U}^\dagger\hat{U}\hat{B} - \hat{B}\hat{U}^\dagger\hat{U}\hat{A})\hat{U}^\dagger \\
&= \hat{U}[\hat{A}, \hat{B}]\hat{U}^\dagger \\
&= \hat{U}\hat{C}\hat{U}^\dagger \\
&= \hat{C}'
\end{aligned}$$

Chapter 2

Wave Mechanics

The initial theories of quantum mechanics built in 1925 and 1926 consists of Heisenberg's ***matrix mechanics*** and Schrödinger's ***wave mechanics***. Later, the forms of wave mechanics are mostly used and the textbooks even always refer wave mechanics as quantum mechanics itself. In this chapter, we will learn the basis of Schrödinger's wave mechanics, and we also refer the wave mechanics as "quantum mechanics" in our contents.

Figure 2.1: Austrian physicist Erwin Schrödinger (1887-1961), who put forward wave mechanics in 1926.

2.1 Postulates of Quantum Mechanics

Last chapter we have equipped ourselves with the mathematical foundations, which can be viewed as the language of quantum mechanics. This chapter, we will know how to deal with these mathematical concept and to construct the rules of microscopic world.

2.1.1 Quantum States and Schrödinger Equation

In classical mechanics, we can use a the point in the phase space to label a state of motion of a system. However, because of the wave-particle duality of the quantum particles, the concept of trajectory is meaningless. Therefore, we can't use the same method to label a state in quantum world.

In quantum world, we use the vector in Hilbert space $|\psi\rangle$ to label a *quantum state*. The $|\psi\rangle$ can envolve with time thus should be viewed as a function of time t $|\psi(t)\rangle$.

The time evolving of $|\psi\rangle$ is govened by the *Schrödinger equation*

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle \tag{2.1}$$

which should be treated as the fundamental equation in quantum mechanics. Above $\hat{H}$ is the Hamiltonian operator. This form of the Schrödinger equation is very abstract: we don't know the exact form of the Hamiltonian operator and we can't even do any calculations. That's because we don't choose the *representation* yet now. Only with both the equation and the representation can we do calculations. We will illustrate this in next section.

2.1.2 Superposition

In classical mechanics, of courese a system can't be in different states simultaneously. But in quantum mechanics that can be true! This is the *principle of superposition*.

Suppose both $|\psi_1\rangle$ and $|\psi_2\rangle$ can be the quantum states of a particle, then the state $|\psi\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle$ can also be a quantum state of the system, which is called the state of superposition.

2.1.3 Observables

Observables such as position, momentum, energy and angular momentum are important in both classical and quantum mechanics since they are the bridges of theory and experiments. Among these observables, the position and momentum are basic, and the other observables can be represented as a function of them.

In quantum mechanics, every observable corresponds to a Hermitian operator. Now we use A to denote the observable and use $\hat{A}$ to denote the corresponding operator.

In classical mechanics, the position and momentum are basic things, and they consist of the coordinates of the phase space. Every other observable like energy(Hamiltonian) and angular momentum can be seen as a function of position and momentum. In quantum mechanics, there exists no phase space, and the observables are replaced by the corresponding Hermitian operators. But the position operator and the momentum operator are still basic. In quantum mechanics, if you want to find the forms of the other observables, what you need to do is to first represent them by using x and p using the classical relationship, then you just replace x and p by their operators $\hat{x}$ and $\hat{p}$ and you will reach the answers. By using this kind of progrem, you don't need to worry about the Hermitian of the new operator since the $\hat{x}$ and $\hat{p}$ are both Hermitian.

In the Hilbert space $\mathcal{H}$, suppose the orthonormal eigenvectors of $\hat{A}$ are $|a_i\rangle$ with the eigenvalue a_i. In quantum mechanics, we say $|a_i\rangle$ as the *eigenstate* of the observable $\hat{A}$, and a_i as the *eigenvalue* of $\hat{A}$.

We have known that the eigenvectors of a Hermitian operator can be the basis of $\mathcal{H}$. That is to say, any quantum state of the system $|\psi\rangle$ in the $\mathcal{H}$ can be expanded by the $|a_i\rangle$ as

$$|\psi\rangle = \sum_i c_i |a_i\rangle \tag{2.2}$$

where the complex coefficient $c_i = \langle a_i|\psi\rangle$. This should also be viewed as a kind of superposition.

Measurements and Collapse

The postulate of quantum mechanics tells us that: if you now measure the magnitude of the observable A, the state $|\psi\rangle$ will immediately collapse into one of the eigenstate $|a_i\rangle$, then the result of the measurement is the corresponding eigenvalue a_i.

The problem is that: which eigenstate $|a_i\rangle$ will the system collapse into? Well, this is a game of probability. We can only say that the probability that the $|\psi\rangle$ collapse into $|a_i\rangle$ equals to

$$|c_i|^2 = |\langle\psi|a_i\rangle|^2 \tag{2.3}$$

Obviously we should have that $\sum_i |c_i|^2 = 1$, thus we have the nomalization of the quantum state as

$$\begin{aligned}\langle\psi|\psi\rangle &= \left(\sum_i c_i^* \langle a_i|\right)\left(\sum_j c_j |a_j\rangle\right) \\ &= \sum_{i,j} c_i^* c_j \langle a_i|a_j\rangle\end{aligned}$$

$$
\begin{aligned}
&= \sum_{i,j} c_i^* c_j \delta_{ij} \\
&= \sum_i |c_i|^2 \\
&= 1
\end{aligned} \tag{2.4}
$$

Always keep in mind that $|a_i\rangle$ are orthonormal vectors.

What's more, according to the property of Hermitian operator, we can figure out that if two observables, say $\hat{A}$ and $\hat{B}$, are commutative, they can share the same set of quantum states. Thus one can measure the magnitudes of both $\hat{A}$ and $\hat{B}$ simultaneously. And neither the order of measurements nor the repeated measurements will affect the results obtained.

What if $\hat{A}$ and $\hat{B}$ are not commutative? This will directly lead to the uncertenty principle of the measurements, which will be shown in next chapter.

Average

Now imagine you have a great number of identical systems in the same state $|\psi\rangle$. Then we take measurement for A on these systems one by one and find the average of A. Of course the average is

$$\langle A \rangle = \sum_i |c_i|^2 a_i \tag{2.5}$$

which can also be represented as $\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle$ since we have that

$$
\begin{aligned}
\langle \psi | \hat{A} | \psi \rangle &= \sum_{i,j} c_i^* c_j \langle a_i | \hat{A} | a_j \rangle \\
&= \sum_{i,j} c_i^* c_j \langle a_i | a_j | a_j \rangle \\
&= \sum_i |c_i|^2 a_i
\end{aligned} \tag{2.6}
$$

2.2 Representation Transformation

2.2.1 Representation

Last section we said that any quantum state $|\psi\rangle$ in $\mathcal{H}$ can be represented as

$$|\psi\rangle = \sum_i \langle a_i|\psi\rangle |a_i\rangle \tag{2.7}$$

where $|a_i\rangle$ is the eigenstate of $\hat{A}$. Above we simply expand $|\psi\rangle$ by the basis of $\mathcal{H}$.

Now let's have a look at the coefficient $\langle a_i|\psi\rangle$, which can be seen as a function of both t and a. The quantum state $|\psi\rangle$ is very abstract, and before we say that we can't do calculation with the quantum state $|\psi\rangle$. But now we can calculate the $\langle a_i|\psi\rangle$ since it is also a function of a, especially when a is a continuous variable. We call the $\langle a_i|\psi\rangle$ the *wavefunction* under the *representation of* A. That's to say, ***only by choosing a representation for the rather abstract quantum state*** $|\psi\rangle$ ***and get the wavefunction can we do the calculations***.

Typical representations are representation of position, momentum and energy. Let's talk about them then. Suppose the eigenstate of $\hat{x}$, $\hat{p}$ and $\hat{H}$ are $|x\rangle$, $|p\rangle$ and $|E\rangle$ respectively, which satisfy that

$$\begin{cases} \hat{x}|x\rangle = x|x\rangle \\ \hat{p}|p\rangle = p|p\rangle \\ \hat{H}|E\rangle = E|E\rangle \end{cases} \tag{2.8}$$

and

$$\begin{cases} \int |x\rangle\langle x|dx = I \\ \int |p\rangle\langle p|dp = I \\ \sum |E\rangle\langle E| = I \end{cases} \tag{2.9}$$

where for $|x\rangle$ and $|p\rangle$ we use integral instead of summation, because the eigenvalues of $\hat{x}$ and $\hat{p}$ are continuous.

Representation of Position

Firstly let's talk about the position representation, which is mostly used in quantum mechanics, because it have more vivid physical significance. We can represent $|\psi\rangle$ by $|x\rangle$ as

$$|\psi\rangle = I|\psi\rangle = \int \langle x|\psi\rangle |x\rangle dx \tag{2.10}$$

We further denote $\langle x|\psi\rangle = \psi(x,t)$, which is called the wave function (under position representation).

According to (2.3), we can know the physical significance of $|\psi(x,t)|^2 dx$ as the proba-

bility to find the quantum particle in the interval $(x, x+dx)$ at time t. Thus the $|\psi(x,t)|^2$ is the *probability density*. Of course we have the normalization of the wavefunction as

$$\int |\psi(x,t)|^2 dx = \int \langle\psi|x\rangle\langle x|\psi\rangle dx = \langle\psi|I|\psi\rangle = 1 \tag{2.11}$$

Furthermore, there is a funny question: what's the $\langle x|x'\rangle$? Have a look at

$$\psi(x,t) = \langle x|\psi\rangle = \langle x|I|\psi\rangle = \int \langle x|x'\rangle\langle x'|\psi\rangle dx' = \int \psi(x',t)\langle x|x'\rangle dx'$$

Considering the property of the delta function, we can identify that

$$\langle x'|x\rangle = \delta(x'-x) = \delta(x-x') \tag{2.12}$$

Representation of Momentum

Then let's talk about the momentum representation. We can represent $|\psi\rangle$ by $|p\rangle$ as

$$|\psi\rangle = \int \langle p|\psi\rangle|p\rangle dp = \int \phi(p,t)|p\rangle dp \tag{2.13}$$

where $\phi(p,t)$ is the wavefunction in the momentum representation, and $|\phi(p,t)|^2$ is the probability density to find the momentum of the system in the interval $(p, p+dp)$ at time t.

Similarly we have that

$$\langle p|p'\rangle = \delta(p-p') \tag{2.14}$$

Representation of Energy

Lastly let's talk about the energy representation. We can represent $|\psi\rangle$ by $|E\rangle$ as

$$|\psi\rangle = \sum \langle E|\psi\rangle|E\rangle = \sum \zeta_E(t)|E\rangle \tag{2.15}$$

where $\zeta_E(t)$ is the wavefunction in the energy representation, and $|\zeta_E(t)|^2$ is the probability density to find the energy of the system is E at time t.

Similarly we have that

$$\langle E'|E\rangle = \delta_{EE'} \tag{2.16}$$

.

2.2.2 Representation Transformation of Wavefunctions

Now let's consider the representation transformation of the wavefunction.

We can connect the wavefunctions under position and momentum by

$$\psi(x,t) = \langle x|\psi\rangle = \langle x|I|\psi\rangle = \int \langle x|p\rangle\langle p|\psi\rangle dp = \int \phi(p,t)\langle x|p\rangle dp$$

we should view this equation as the representation transformation of wavefunction from the momentum representation to the position representation. Furthermore, link this with the inverse Fourier transformation [1]

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int \phi(p,t) e^{i\frac{p}{\hbar}x} dp$$

we can confirm that

$$\langle x|p\rangle = u_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}px} \tag{2.17}$$

which is the wavefunction of the momentum eigenstate under position representation. Further, we can write $\psi(x,t)$ as

$$\psi(x,t) = \int \phi(p,t) u_p(x) dp$$

i.e. the $\psi(x,t)$ can be seen as the continuous superposition of the momentum eigenfunction $u_p(x)$, with the coefficient $\phi(p,t)$.

However, I have to say, the concrete form of $\langle x|p\rangle$ might be mathematically arbitrary. Why it isn't $\langle x|p\rangle = \frac{1}{\sqrt{2\pi}} e^{ipx}$? Why we need a $\hbar$ here? ***Well, it turns out that you need to view (2.17) as a postulate!*** By doing so, the argument below might be easier.

Armed with $\langle x|p\rangle$, we can know that

$$\langle p|x\rangle = u_x(p) = \langle x|p\rangle^* = \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}px} \tag{2.18}$$

which is the wavefunction of the position eigenstate under momentum representation.

Finally Let's think about the wave function in position and energy representations. We have that

$$\psi(x,t) = \langle x|\psi\rangle = \langle x|I|\psi\rangle = \sum \langle x|E\rangle\langle E|\psi\rangle = \sum u_E(x)\zeta_E(t) \tag{2.19}$$

where $u_E(x) = \langle x|E\rangle$ is the energy eigenstate under position representation. We should

[1] Where the initial transformation is that

$$\phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int \psi(x,t) e^{-i\frac{p}{\hbar}x} dx$$

You don't need to worry the $\hbar$ in the coefficient $\frac{1}{\sqrt{2\pi\hbar}}$, since you substitute the inverse transformation into the fomula of transformation, you will still find that you've got the right answer!

view the equation above as the representation transformation of wavefunction from the energy representation to the position representation. It also reveals that the $\psi(x,t)$ can be seen as the superposition of the energy eigenfunctions $u_E(x)$, with the coefficient $\zeta_E(t)$. To find the concrete forms of $u_E(x)$, we need to solve the time-independent Schrödinger equation in position representation.

2.2.3 Operators Under Different Representations

Just now we said that operators are maps from one state $|\psi\rangle$ to another $|\phi\rangle$. Now we choose the representation of A to represent the abstract quantum state, and there ought to have corresponding maps from wave function $\langle a|\psi\rangle$ to $\langle a|\phi\rangle$, which is the operator under this certain representation. Most of time we'll use the same notations for operators and operators under certain representations and it won't lead to misunderstanding. But during our deduction below, we will denote the operator $\hat{A}$ under certain representation as A_{op} to distinguish.

Below it turns out that the essential relation to be used is that

$$\langle a|\,\hat{A}\,|\psi\rangle = A_{\text{op}}\,\langle a|\psi\rangle \tag{2.20}$$

Under Position Representation

Firstly let's look at the most important case, which is the operators under the position representation. Let's see the position operator first. Obviously in this context we can calculate that

$$\begin{aligned}
\langle x|\hat{x}|\psi\rangle &= \int \langle x|\hat{x}|x'\rangle\langle x'|\psi\rangle dx' \\
&= \int x'\langle x|x'\rangle\langle x'|\psi\rangle dx' \\
&= \int x'\langle x|\psi\rangle\delta(x-x')dx' \\
&= x\langle x|\psi\rangle \\
&= \hat{x}_{\text{op}}\langle x|\psi\rangle
\end{aligned}$$

Thus we can identify that in position representation we have

$$x_{\text{op}} = x \tag{2.21}$$

Opps... Seems to have a more simple way to deduce here

$$\langle x|\hat{x}|p\rangle = \left(\hat{x}^\dagger|x\rangle\right)^\dagger|p\rangle = \left(\hat{x}|x\rangle\right)^\dagger|p\rangle = (x|x\rangle)^\dagger|p\rangle = x\langle x|p\rangle = x_{\text{op}}\langle x|p\rangle$$

So we can also get $x_{\text{op}} = x$. What's more, we can also easily get that $y_{\text{op}} = y$ and $z_{\text{op}} = z$. Thus $\boldsymbol{r}_{\text{op}} = \boldsymbol{r}$.

Then let's consider the momentum operator. Obviously in this context we have

$$\begin{aligned}
\langle x|\hat{p}|\psi\rangle &= \int \langle x|p\rangle\langle p|\hat{p}|\psi\rangle dp \\
&= \int \langle x|p\rangle p\langle p|\psi\rangle dp \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int p e^{\frac{i}{\hbar}px}\phi(p,t)dp \\
&= -i\hbar\frac{\partial}{\partial x}\left[\frac{1}{\sqrt{2\pi\hbar}}\int \phi(p,t)e^{\frac{i}{\hbar}px}dp\right] \\
&= -i\hbar\frac{\partial}{\partial x}\langle x|\psi\rangle \\
&= \hat{p}_{\text{op}}\langle x|\psi\rangle
\end{aligned}$$

Or more simply $\langle x|\hat{p}|p\rangle = \langle x|p|p\rangle = p\langle x|p\rangle = p_{\text{op}}\langle x|p\rangle$, and considering that $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}px}$, we can identify that

$$p_{\text{op}} = -i\hbar\frac{\partial}{\partial x} \tag{2.22}$$

Above we implicitly play in 1-dimension. For the 3-dimension, it's easy to generalize that

$$\boldsymbol{p}_{\text{op}} = -i\hbar\nabla \tag{2.23}$$

Furthermore, the Hamiltonian operator is

$$H_{\text{op}} = \frac{p_{\text{op}}^2}{2m} + V(x_{\text{op}}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) \tag{2.24}$$

Now, armed with H_{op}, we can get the Schrödinger equation under position representation. Initially we have

$$\langle x|i\hbar\frac{\partial}{\partial t}|\psi\rangle = \langle x|\hat{H}|\psi\rangle$$

so

$$i\hbar\frac{\partial}{\partial t}\langle x|\psi\rangle = H_{\text{op}}\langle x|\psi\rangle$$

i.e.

$$i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{r},t) + V(\boldsymbol{r})\psi(\boldsymbol{r},t) \tag{2.25}$$

which is the time-dependent Schrödinger equation. The eigen equation of H_{op} is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{r},t) + V(\boldsymbol{r})\psi(\boldsymbol{r},t) = E\psi(\boldsymbol{r},t) \tag{2.26}$$

which is also called the time-independent Schrödinger equation, from where we can get $\langle x|E\rangle = u_E(x)$.

Under Momentum Representation

Then let's quickly find the form of x_{op}, p_{op} and H_{op} in the momentum representation. Firstly it's easy to find that in this context

$$\langle p|\hat{p}|x\rangle = p\langle p|x\rangle = p_{\text{op}}\langle p|x\rangle$$

Thus we have

$$p_{\text{op}} = p \tag{2.27}$$

And we can find that

$$\langle p|\hat{x}|x\rangle = x\langle p|x\rangle = x_{\text{op}}\langle p|x\rangle$$

Considering that $\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{-\frac{i}{\hbar}px}$, we can identify that

$$x_{\text{op}} = i\hbar\frac{\partial}{\partial p} \tag{2.28}$$

Hence, the Hamiltonian becomes

$$H_{\text{op}} = \frac{p^2}{2m} + V\left(i\hbar\frac{\partial}{\partial p}\right) \tag{2.29}$$

2.3 Time Evolution of Quantum States

2.3.1 Schrödinger Picture

In wave mechanics, we utilize the *Schrödinger picture* of the time evolution. That is the operators are determined and the quantum states $|\psi\rangle$ will evolves with time. We call it the Schrödinger picture is to distinguish it from the Heisenberg picture, which will be discussed in the next chapter.

2.3.2 Time Evolution Operator

The time evolution of the quantum state $|\psi\rangle$ is governed by the Schrödinger equation. To understand this, let's do some analysis. It's easy to know that

$$|\psi(t+dt)\rangle = |\psi(t)\rangle + \frac{\partial}{\partial t}|\psi(t)\rangle dt + o(dt)$$

According to the Schrödinger equation we can get that

$$\frac{\partial}{\partial t}|\psi(t)\rangle = -i\frac{\hat{H}}{\hbar}|\psi\rangle$$

Thus we have

$$|\psi(t+dt)\rangle = \left(1 - i\frac{\hat{H}}{\hbar}dt\right)|\psi(t)\rangle + o(dt) \approx \left(1 - i\frac{\hat{H}}{\hbar}dt\right)|\psi(t)\rangle$$

We further define an operator

$$\hat{U}(dt) = 1 - i\frac{\hat{H}}{\hbar}dt \tag{2.30}$$

which is called the *infiniesimal time evolution operator*. Attention, here strictly the "1" oughts to be the unit operator instead of a number.

It's easy to check that $\hat{U}$ is unitary, since

$$\hat{U}^\dagger(dt)\hat{U}(dt) = \left(1 + i\frac{\hat{H}^\dagger}{\hbar}dt\right)\left(1 - i\frac{\hat{H}}{\hbar}dt\right) = 1 + i\frac{\hat{H}^\dagger}{\hbar}dt - i\frac{\hat{H}}{\hbar}dt + \frac{\hat{H}^2}{\hbar^2}dt^2 = 1 \tag{2.31}$$

where we reasonably ignore the dt^2 term. What's more, the $\hat{U}(dt)$ also has a property that

$$\hat{U}(dt_1)\hat{U}(dt_2) = \left(1 - i\frac{\hat{H}}{\hbar}dt_1\right)\left(1 - i\frac{\hat{H}}{\hbar}dt_2\right) = 1 - i\frac{\hat{H}}{\hbar}(dt_1 + dt_2) = \hat{U}(dt_1 + dt_2) \tag{2.32}$$

Armed with $\hat{U}(dt)$, we can write that

$$|\psi(dt)\rangle = \hat{U}(dt)|\psi(0)\rangle$$

And go ahead to find that

$$|\psi(t)\rangle = |\psi(Ndt)\rangle = \hat{U}(Ndt)|\psi(0)\rangle = \left(1 - i\frac{\hat{H}}{\hbar}\frac{t}{N}\right)^N |\psi(0)\rangle$$

If you know $\lim_{N\to\infty}\left(1+\frac{a}{N}\right)^N = e^a$, then you can convince yourself that when N is large we have

$$|\psi(t)\rangle = e^{-i\frac{\hat{H}}{\hbar}t}|\psi(0)\rangle = \hat{U}(t)|\psi(0)\rangle$$

where we've got the *finite time evolution operator*

$$\hat{U}(t) = e^{-i\frac{\hat{H}}{\hbar}t} \tag{2.33}$$

which obviously satisfies that $\hat{U}^\dagger\hat{U} = 1$ and $\hat{U}(t_1)\hat{U}(t_2) = \hat{U}(t_1+t_2)$.

The unitarity of $\hat{U}$ is important, since it ensures that once the quantum state $|\psi\rangle$ is normalized at $t = 0$, then it will keep normalized in the future. What's more, the unitarity also ensures that the property $\Sigma\,|\alpha\rangle\,\langle\alpha| = 1$ of basis $|\alpha\rangle$ is always valid no matter when.

2.3.3 Time Evolution of a General Quantum State

Now let's find a more explicitly formula for the time evolution of any general quantum state $|\psi\rangle$. We can approach this by expanding $|\psi\rangle$ by the eigenstate of $\hat{H}$ as

$$|\psi(0)\rangle = \sum_n \langle E_n(0)|\psi(0)\rangle |E_n(0)\rangle = \sum_n c_n|E_n(0)\rangle$$

Since, for the eigenstate of energy, we have that

$$\hat{U}(t)|E\rangle = e^{-i\frac{\hat{H}}{\hbar}t}|E\rangle = \sum \frac{\left(-\frac{i}{\hbar}t\right)^n}{n!}\hat{H}^n|E\rangle = \sum \frac{\left(-\frac{i}{\hbar}t\right)^n}{n!}E^n|E\rangle = e^{-i\frac{E}{\hbar}t}|E\rangle$$

So we can get

$$|\psi(t)\rangle = \sum_n c_n\hat{U}(t)|E_n(0)\rangle = \sum_n c_n e^{-i\frac{E_n}{\hbar}t}|E_n(0)\rangle \tag{2.34}$$

Further choosing the position representation gives us that

$$\psi(x,t) = \sum_n c_n u_{E_n}(x,0)e^{-i\frac{E_n}{\hbar}t} \tag{2.35}$$

where the coefficients satisfy that

$$c_n = \langle \psi(0)|E_n(0)\rangle = \int \langle \psi(0)|x\rangle\langle x|E_n(0)\rangle dx = \int \psi^*(x,0)u_{E_n}(x,0)dx \tag{2.36}$$

and the $u_{E_n}(x,0)$ is the eigenfunction with eigenvalue E_n of the time independent Schrödinger equation.

Chapter 3

Matrix Mechanics

In this chapter we'd like to introduce the matrix mechanics, which was built by Heisenberg, Born and Jordan mainly in 1925. The matrix mechanics was also the most initial format of quantum mechanics.

However, the contents in this chapter may not be precisely what it was like in 1925, and there will be lots of morden things. Thus it will be better to say that the content in this chapter is *the matrix form of quantum mechanics* instead of the matrix mechanics in 1925.

Figure 3.1: Werner Heisenberg(1901-1976), Max Born(1882-1970) and Pascual Jordan(1902-1980), farthers of matrix mechanics

What's different?

Now let's have a brief discuss about the differences between wave mechanics and matrix mechanics.

We still have the concept and the same meaning of qunatum state $|\psi\rangle$ and operator $\hat{A}$, but being opposite to the Schrödinger picture, in matrix mechanics the state is determined and the operators are envolving with time. This is called the Heisenberg picture. In matrix mechanics, the time evolution of operators are governed by the Heisenberg equation, which can be seen as the dual equation of the Schrödinger equation.

Besides, all the things are similar to what it like in wave mechanics, such as the significance of representations, measurements, collapse, average and so on. And we can happlily utilize the Dirac notation in matrix mechanics too.

3.1 Canonical Quantization