Quantum Mechanics

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December 10, 2023

II. Fundamental Concepts

2.1 Kets, Bras, Operators, and Matrix Representations

2.1.1 Ket Space

Hilbert space: an extended Euclid space with: (1) vectors, (2) linear operations, (3) completeness, (4) infinite dimensions, and (5) metrizability.

Ket: a state vector defined in a complex vector space, denoted by $|\alpha\rangle$. Two kets can be added to generate a new ket:

$$|\gamma\rangle = |\alpha\rangle + |\beta\rangle . \tag{2.1}$$

A ket can be multiplied by a complex number $c \neq 0$ to generate a ket representing the same state:

$$c|\alpha\rangle = |\alpha\rangle c . \tag{2.2}$$

If $c = 0$, the resulting ket is said to be a **null ket**.

An **observable** can be represented by an **operator** and acts on a ket from the left:

$$A \cdot (|\alpha\rangle) = A|\alpha\rangle . \tag{2.3}$$

Ket space: a Hilbert space spanned by kets.

Eigenkets (eigenstates): the kets an operator applied to results in a constant times themselves:

$$A|a'\rangle = a'|a'\rangle, A|a''\rangle = a''|a''\rangle, \cdots . \tag{2.4}$$

The corresponding numbers $\{a'\}$ is called the set of **eigenvalues** of operator *A*. An arbitrary ket $|\alpha\rangle$ can be expanded by the complete set of eigenkets $\{|a'\rangle\}$:

$$|\alpha\rangle = \sum_{a'} c_{a'} |a'\rangle , \tag{2.5}$$

where $c_{a'}$ is a complex coefficient.

Eigenstate: the physical state corresponding to an eigenket.

2.1.2 Bra Space and Inner Products

Bra space: a dual correspondence of the ket space with each bra being the conjugate of the corresponding ket.

$$\begin{aligned} &|\alpha\rangle \xleftrightarrow{\text{DC}} \langle\alpha| \\ &|\alpha'\rangle, |\alpha''\rangle, \cdots \xleftrightarrow{\text{DC}} \langle\alpha'|, \langle\alpha''|, \cdots, \\ &|\alpha\rangle + |\beta\rangle \xleftrightarrow{\text{DC}} \langle\alpha| + \langle\beta| \end{aligned} \tag{2.6}$$

where DC stands for dual correspondence. Also

$$c_\alpha|\alpha\rangle + c_\beta|\beta\rangle \xleftrightarrow{\text{DC}} c_\alpha^*\langle\alpha| + c_\beta^*\langle\beta|. \tag{2.7}$$

Inner Product: the product by bra on the left and ket on the right which generates a complex number:

$$\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*. \tag{2.8}$$

Therefore, $\langle\alpha|\alpha\rangle$ is a real number, and $\langle\alpha|\alpha\rangle \geq 0$ is a .

Orthogonal kets: if

$$\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle = 0, \tag{2.9}$$

then α and β are said to be orthogonal.

Normalized ket:

$$|\tilde{\alpha}\rangle = \frac{1}{\sqrt{\langle\alpha|\alpha\rangle}}|\alpha\rangle. \tag{2.10}$$

Obviously, $\langle\tilde{\alpha}|\tilde{\alpha}\rangle = 1$, and $\sqrt{\langle\alpha|\alpha\rangle}$ is known as the norm of $|\alpha\rangle$. Physical states in quantum mechanics are normalized by default.

2.1.3 Operators

An operator acts on a ket from the left side, e.g., $X|\alpha\rangle$. For an arbitrary ket $|\alpha\rangle$, two operators are said to be equal $X = Y$ if

$$X|\alpha\rangle = Y|\alpha\rangle, \tag{2.11}$$

and *X* is a **null operator** if $X|\alpha\rangle = 0$.

Addition: commutative and associative:

$$\begin{aligned} &X + Y = Y + X \\ &X + (Y + Z) = (X + Y) + Z \end{aligned}. \tag{2.12}$$

The operators are generally (except the time-reversal operator) linear:

$$X\left(c_\alpha|\alpha\rangle + c_\beta|\beta\rangle\right) = c_\alpha X|\alpha\rangle + c_\beta X|\beta\rangle. \tag{2.13}$$

Adjoint operator: $X^\dagger$ is the adjoint operator of X if

$$X|\alpha\rangle \xleftrightarrow{\text{DC}} \langle\alpha|X^{\dagger}. \tag{2.14}$$

Hermitian operator: if

$$X = X^{\dagger}. \tag{2.15}$$

Multiplication: generally noncommutative:

$$XY \neq YX\ , \tag{2.16}$$

but associative:

$$\begin{aligned} X(YZ) &= (XY)Z = XYZ \\ X(Y|\alpha\rangle) &= (XY)|\alpha\rangle = XY|\alpha\rangle\ . \\ (\langle\beta|X)Y &= \langle\beta|(XY) = \langle\beta|XY \end{aligned} \tag{2.17}$$

Because

$$XY|\alpha\rangle = X(Y|\alpha\rangle) \xleftrightarrow{\text{DC}} (\langle\alpha|Y^{\dagger})X^{\dagger} = \langle\alpha|Y^{\dagger}X^{\dagger}, \tag{2.18}$$

we have

$$(XY)^{\dagger} = Y^{\dagger}X^{\dagger}. \tag{2.19}$$

Outer product:

$$(|\beta\rangle)\cdot(\langle\alpha|) = |\beta\rangle\langle\alpha| \tag{2.20}$$

is to be regarded as an operator. Note that $|\alpha\rangle|\beta\rangle$ is illegal if they belong to the same ket space.

The Associative Axiom of Multiplication: The associative property is *postulated* to hold as long as we are dealing with "legal" multiplications among kets, bras, and operators. For example,

$$(|\beta\rangle\langle\alpha|)\cdot|\gamma\rangle = |\beta\rangle\cdot\langle\alpha|\gamma\rangle\ . \tag{2.21}$$

If we define an operator

$$X = |\beta\rangle\langle\alpha|, \tag{2.22}$$

then

$$X^{\dagger} = |\alpha\rangle\langle\beta|. \tag{2.23}$$

Another important example is, by using Eq. (2.8), we have

$$\langle\beta|X|\alpha\rangle = \langle\alpha|X^{\dagger}|\beta\rangle^{*}. \tag{2.24}$$

For a Hermitian operator *A*, we have

$$\langle\beta|A|\alpha\rangle = \langle\alpha|A|\beta\rangle^{*}. \tag{2.25}$$

2.1.4 Base Kets

Theorem 2.1. The eigenvalues of a Hermitian operator *A* are real, and the eigenkets of *A* corresponding to different eigenvalues are orthogonal.

Proof: An eigenket $|a'\rangle$ satisfies

$$A|a'\rangle = a'|a'\rangle . \tag{2.26}$$

Because *A* is Hermitian, for another eigenket $|a''\rangle$, we also have

$$\langle a''|A = a''^{*}\langle a''| . \tag{2.27}$$

If we multiply both sides of Eq. (2.26) by $\langle a''|$, Eq. (2.27) by $|a'\rangle$, and subtract, we obtain

$$(a' - a''^{*})\langle a''|a'\rangle = 0 . \tag{2.28}$$

When $a' = a''$, we have

$$a' = a''^{*} = a'^{*} , \tag{2.29}$$

which means that the eigenvalue is real. When $a' \neq a''$, it is required that

$$\langle a''|a'\rangle = 0, \tag{2.30}$$

indicating that $|a'\rangle$ and $|a''\rangle$ are orthogonal.

The **orthonormal** condition of the eigenkets can be denoted by

$$\langle a''|a'\rangle = \delta_{a'',a'} . \tag{2.31}$$

The set of eigenkets is **complete** by construction.

Similar to the vectors in the Euclidean space, in the Hilbert space spanned by the eigenkets of *A*, an arbitrary ket $|\alpha\rangle$ can be expanded by the eigenkets serving as the **base kets** (basis set):

$$|\alpha\rangle = \sum_{a'} c_{a'}|a'\rangle . \tag{2.32}$$

Multiplying $\langle a''|$ on both sides of the above equation and utilizing Eq. (2.31), we obtain

$$c_{a'} = \langle a'|\alpha\rangle . \tag{2.33}$$

Therefore, we also have

$$|\alpha\rangle = \sum_{a'}|a'\rangle\langle a'|\alpha\rangle . \tag{2.34}$$

Because $|\alpha\rangle$ is arbitrary, from the above equation, we obtain the **completeness relation** or **closure**:

$$\sum_{a'}|a'\rangle\langle a'| = 1 . \tag{2.35}$$

The right side is usually not a number, but an **identity operator**. Define the **projection operator**

$$\Lambda_{a'} \equiv |a'\rangle\langle a'| , \tag{2.36}$$

then the completeness relation Eq. (2.35) can also be expressed as

$$\sum_{a'}\Lambda_{a'} = 1 . \tag{2.37}$$

2.1.5 Matrix Representations

For an operator *X*, by using Eq. (2.35) twice, we obtain

$$X=\sum_{a''}\sum_{a'}\left|a''\right\rangle\left\langle a''\right|X\left|a'\right\rangle\left\langle a'\right|, \tag{2.38}$$

so the operator can be represented with the basis set $\left\{a^{(i)},\quad i=1,2,\cdots,N\right\}$ by a matrix

$$X\doteq\begin{pmatrix}\left\langle a^{(1)}\right|X\left|a^{(1)}\right\rangle & \left\langle a^{(1)}\right|X\left|a^{(2)}\right\rangle & \cdots\\ \left\langle a^{(2)}\right|X\left|a^{(1)}\right\rangle & \left\langle a^{(2)}\right|X\left|a^{(2)}\right\rangle & \cdots\\ \vdots & \vdots & \ddots\end{pmatrix}. \tag{2.39}$$

In the matrix representation, the Hermitian adjoint operation Eq. (2.24) corresponds to the **complex conjugate transposed** operation

$$\left\langle a''\right|X\left|a'\right\rangle=\left\langle a'\right|X^{\dagger}\left|a''\right\rangle^{*}. \tag{2.40}$$

For a Hermitian operator *A*, we have

$$\left\langle a''\right|A\left|a'\right\rangle=\left\langle a'\right|A\left|a''\right\rangle^{*}, \tag{2.41}$$

which means that the two symmetric elements in a Hermitian matrix are conjugate to each other, and in particular the diagonal elements are real.

Given a basis set $\left\{a^{(i)},\quad i=1,2,\cdots,N\right\}$, the matrix representation of an arbitrary ket is

$$\left|\alpha\right\rangle\doteq\begin{pmatrix}\left\langle a^{(1)}\middle|\alpha\right\rangle\\ \left\langle a^{(2)}\middle|\alpha\right\rangle\\ \left\langle a^{(3)}\middle|\alpha\right\rangle\\ \vdots\end{pmatrix}, \tag{2.42}$$

and the matrix representation of the ket relation $\left|\gamma\right\rangle=X\left|\alpha\right\rangle$ can be obtained by matrix multiplication of Eq. (2.39) with Eq. (2.42) to obtain

$$\left|\gamma\right\rangle\doteq\begin{pmatrix}\left\langle a^{(1)}\middle|\gamma\right\rangle\\ \left\langle a^{(2)}\middle|\gamma\right\rangle\\ \left\langle a^{(3)}\middle|\gamma\right\rangle\\ \vdots\end{pmatrix}, \tag{2.43}$$

whose corresponding bra is

$$\begin{aligned}\left\langle\gamma\right|&\doteq\left(\left\langle\gamma\middle|a^{(1)}\right\rangle,\quad\left\langle\gamma\middle|a^{(2)}\right\rangle,\quad\left\langle\gamma\middle|a^{(3)}\right\rangle,\quad\left\langle\gamma\middle|a^{(4)}\right\rangle\right)\\&=\left(\left\langle a^{(1)}\middle|\gamma\right\rangle^{*},\quad\left\langle a^{(2)}\middle|\gamma\right\rangle^{*},\quad\left\langle a^{(3)}\middle|\gamma\right\rangle^{*},\quad\left\langle a^{(4)}\middle|\gamma\right\rangle^{*}\right)\end{aligned}. \tag{2.44}$$

The inner product is represented as

$$\langle\beta|\alpha\rangle \doteq \left(\langle a^{(1)}|\beta\rangle^*, \quad \langle a^{(2)}|\beta\rangle^*, \quad \cdots\right)\begin{pmatrix}\langle a^{(1)}|\alpha\rangle \\ \langle a^{(2)}|\alpha\rangle \\ \vdots\end{pmatrix}. \tag{2.45}$$

The outer product is represented as

$$|\beta\rangle\langle\alpha| \doteq \begin{pmatrix}\langle a^{(1)}|\beta\rangle\langle a^{(1)}|\alpha\rangle^* & \langle a^{(1)}|\beta\rangle\langle a^{(2)}|\alpha\rangle^* & \cdots \\ \langle a^{(2)}|\beta\rangle\langle a^{(1)}|\alpha\rangle^* & \langle a^{(2)}|\beta\rangle\langle a^{(2)}|\alpha\rangle^* & \cdots \\ \vdots & \vdots & \ddots\end{pmatrix}. \tag{2.46}$$

With the basis set of the eigenvalues of an observable A, the matrix representation of A is obviously diagonal:

$$A = \sum_{a'} a'\Lambda_{a'} . \tag{2.47}$$

2.2 Measurements, Observables, and Uncertainty Relations

2.2.1 Measurements

Measurement postulation: If a quantum system resides on a state $|\alpha\rangle$, which can be linearly expanded by the eigenstates of the observable A:

$$|\alpha\rangle = \sum_{a'} c_{a'}|a'\rangle = \sum_{a'}|a'\rangle\langle a'|\alpha\rangle . \tag{2.48}$$

When a measurement is performed, the system has to "collapse" to one of the eigenstate, and yields the corresponding eigenvalue. If the same measurements are repeated adequate times, all eigenstates should appear, and the appearance probability of the eigenstate $|a'\rangle$ is

$$P(|a'\rangle) = |c_{a'}|^2 = |\langle a'|\alpha\rangle|^2 . \tag{2.49}$$

Expectation value: the expectation value of A with respect to state $|\alpha\rangle$ is

$$\langle A\rangle_\alpha \equiv \langle\alpha|A|\alpha\rangle = \sum_{a'} a'P(a') . \tag{2.50}$$

Selective measurement (filtration): Applying the projection operator to a state:

$$\Lambda_{a'}|\alpha\rangle = |a'\rangle\langle a'|\alpha\rangle . \tag{2.51}$$

Commutor:

$$[A, B] \equiv AB - BA . \tag{2.52}$$

Anticommutor:

$$\{A, B\} \equiv AB + BA . \tag{2.53}$$

2.2.2 Compatible Observables

Compatible observables: If two observables *A* and *B* satisfy

$$[A,B]=0\,. \tag{2.54}$$

Degenerate: If two or more linearly independent eigenkets of *A* have the same eigenvalue, then this eigenvalue is said to be **degenerate**. As indicated below, usually another (or more) commuting observable(s) *B* can be used to label the degenerate eigenkets.

Theorem 2.2. If *A* and *B* are compatible observables, and the eigenvalues of *A* are nondegenerate, then the matrix elements $\langle a''|B|a'\rangle$ are all diagonal.

Proof: Because

$$\langle a''|[A,B]|a'\rangle=\langle a''|AB-BA|a'\rangle=(a''-a')\langle a''|B|a'\rangle=0\,, \tag{2.55}$$

$\langle a''|B|a'\rangle\neq 0$ only when $a'=a''$, which proves the assertion.

Simultaneous eigenket: According to Theorem 2.2, the matrix elements of *B* can be written as

$$|a''\rangle B|a'\rangle=\delta_{a'a''}|a'\rangle B|a'\rangle\,. \tag{2.56}$$

Using Eq. (2.38) and Eq. (2.56), we have

$$B|a'\rangle=\sum_{a''}|a''\rangle\langle a''|B|a''\rangle\langle a''|a'\rangle=\left(\langle a'|B|a'\rangle\right)|a'\rangle\,. \tag{2.57}$$

Therefore, with the basis set of the eigenvalues of *A*, the eigenvalue of *B* is represented by

$$b'\equiv\langle a'|B|a'\rangle\,, \tag{2.58}$$

and the ket $|a'\rangle$ is the **simultaneous eigenket** of *A* and *B*. To be impartial to both operators, this eigenket can be denoted as $|a',b'\rangle$, which has the property

$$\begin{aligned}A|a',b'\rangle&=a'|a',b'\rangle\\ B|a',b'\rangle&=b'|a',b'\rangle\end{aligned}\,. \tag{2.59}$$

For two compatible observables *A* and *B*, the measurement of A does not interfere the measurement of B.

2.2.3 Incompatible Observables

Incompatible observables: If *A* and *B* satisfy

$$[A,B]\neq 0\,. \tag{2.60}$$

The incompatible observables do not have a complete set of simultaneous eigenkets. To prove this assertion, let us assume that the convert to be true. Then

$$AB|a',b'\rangle=Ab'|a',b'\rangle=a'b'|a',b'\rangle \tag{2.61}$$

Likewise,

$$BA|a',b'\rangle=Ba'|a',b'\rangle=a'b'|a',b'\rangle \tag{2.62}$$

Subtract the above two equations, we obtain $[A,B]=0$, in contradiction with the given incompatible condition. Note that the compatible condition $[A,B]=0$ might be satisfied in a subspace of the ket space even if *A* and *B* are incompatible.

2.2.4 The Uncertainty Relation

Dispersion (variance, mean square deviation):

$$\left\langle (\Delta A)^2 \right\rangle = \left\langle A^2 \right\rangle - \left\langle A \right\rangle^2 , \tag{2.63}$$

where operator

$$\Delta A \equiv A - \left\langle A \right\rangle . \tag{2.64}$$

The dispersion vanishes when the state is an eigenstate of *A*.

Uncertainty relation: Let A and B be two observables, then for any state, we must have

$$\left\langle (\Delta A)^2 \right\rangle \left\langle (\Delta B)^2 \right\rangle \geq \frac{1}{4} \left| \left\langle [A,B] \right\rangle \right|^2 . \tag{2.65}$$

To prove this, we first state three lemmas.

Lemma 1. The Schwarz inequality

$$\langle \alpha | \alpha \rangle \langle \beta | \beta \rangle \geq \left| \langle \alpha | \beta \rangle \right|^2 . \tag{2.66}$$

Proof: First note

$$\left(\langle \alpha | + \lambda^* \langle \beta | \right) \cdot \left(|\alpha\rangle + \lambda |\beta\rangle \right) \geq 0 , \tag{2.67}$$

where λ can be any complex number. This inequality must hold when λ is equal to $-\langle \beta | \alpha \rangle / \langle \beta | \beta \rangle$, so we obtain Eq. (2.66).

Lemma 2. The expectation value of a Hermitian operator is purely real.

Proof: Using Eq. (2.41).

Lemma3. The expectation value of an anti-Hermitian operator, defined by $C = -C^\dagger$, is purely imaginary.

Proof: Similar to the proof of Lemma 2.

Define

$$\begin{aligned} |\alpha\rangle &= \Delta A |\gamma\rangle \\ |\beta\rangle &= \Delta B |\gamma\rangle \end{aligned} , \tag{2.68}$$

where $|\gamma\rangle$ is an arbitrary state. Put them into Eq. (2.66), considering the Hermiticity of ΔA and ΔB, we obtain

$$\left\langle (\Delta A)^2 \right\rangle \left\langle (\Delta B)^2 \right\rangle \geq \left| \langle \Delta A \Delta B \rangle \right|^2 . \tag{2.69}$$

Because $[\Delta A, \Delta B] = [A,B]$, which is anti-Hermitian:

$$\left([A,B] \right)^\dagger = \left(AB - BA \right)^\dagger = BA - AB = -[A,B] , \tag{2.70}$$

while $\{\Delta A, \Delta B\}$ is obviously Hermitian, so by using Lemma2 and Lemma 3, we have

$$\begin{aligned}\langle \Delta A \Delta B \rangle &= \left\langle \frac{1}{2}[\Delta A, \Delta B] + \frac{1}{2}\{\Delta A, \Delta B\} \right\rangle \\ &= \frac{1}{2}\langle [A, B] \rangle + \frac{1}{2}\langle \{\Delta A, \Delta B\} \rangle\end{aligned}, \tag{2.71}$$

where the first term in the right-hand side is purely imaginary, and the second term is purely real. Therefore, we have

$$|\langle \Delta A \Delta B \rangle|^2 = \frac{1}{4}|\langle [A, B] \rangle|^2 + \frac{1}{4}|\langle \{\Delta A, \Delta B\} \rangle|^2 . \tag{2.72}$$

Put the above equation into Eq. (2.69), we obtain

$$\left\langle (\Delta A)^2 \right\rangle \left\langle (\Delta B)^2 \right\rangle \geq \frac{1}{4}|\langle [A, B] \rangle|^2 + \frac{1}{4}|\langle \{\Delta A, \Delta B\} \rangle|^2 \geq \frac{1}{4}|\langle [A, B] \rangle|^2 , \tag{2.73}$$

which proves Eq. (2.65).

2.2.5 Transformation Operator and Matrix

Unitary operator: An operator *U* fulfilling

$$U^\dagger U = UU^\dagger = 1 . \tag{2.74}$$

Theorem 2.3. Given two orthonormal and complete basis sets $\{|a'\rangle\}$ and $\{|b'\rangle\}$, there exists a unitary operator *U*, which can do the **change of basis** or **change of representation** in such a way that

$$\left|b^{(1)}\right\rangle = U\left|a^{(1)}\right\rangle, \left|b^{(2)}\right\rangle = U\left|a^{(2)}\right\rangle, \cdots, \left|b^{(N)}\right\rangle = U\left|a^{(N)}\right\rangle . \tag{2.75}$$

Proof: Considering the unitary operator

$$U = \sum_k \left|b^{(k)}\right\rangle\left\langle a^{(k)}\right| , \tag{2.76}$$

we have

$$U\left|a^{(l)}\right\rangle = \left|b^{(l)}\right\rangle . \tag{2.77}$$

Furthermore, the unitarity of *U* is proved by the orthonormality of $\{|b'\rangle\}$ and the completeness of $\{|a\rangle\}$:

$$U^\dagger U = \sum_k \sum_l \left|a^{(l)}\right\rangle\left\langle b^{(l)} \middle| b^{(k)}\right\rangle\left\langle a^{(k)}\right| = \sum_k \left|a^{(k)}\right\rangle\left\langle a^{(k)}\right| = 1 . \tag{2.78}$$

$UU^\dagger = 1$ can be proved in an analogous manner.

The corresponding **transformation matrix** from $\{|a'\rangle\}$ to $\{|b'\rangle\}$ has the matrix elements

$$\left\langle a^{(k)}\right|U\left|a^{(l)}\right\rangle = \left\langle a^{(k)} \middle| b^{(l)}\right\rangle . \tag{2.79}$$

Given an arbitrary ket $|\alpha\rangle$, whose old expansion in the basis $\{|a'\rangle\}$ is

$$\left|\alpha\right\rangle = \sum_{a'}\left|a'\right\rangle\left\langle a'\middle|\alpha\right\rangle, \tag{2.80}$$

the new expansion in the set $\{|b'\rangle\}$ is

$$\left\langle b^{(k)}\middle|\alpha\right\rangle = \sum_{l}\left\langle b^{(k)}\middle|a^{(l)}\right\rangle\left\langle a^{(l)}\middle|\alpha\right\rangle = \sum_{l}\left\langle a^{(k)}\middle|U^{\dagger}\middle|a^{(l)}\right\rangle\left\langle a^{(l)}\middle|\alpha\right\rangle. \tag{2.81}$$

The relationships between the old and new matrix elements are

$$\begin{aligned}\left\langle b^{(k)}\middle|X\middle|b^{(l)}\right\rangle &= \sum_{m}\sum_{n}\left\langle b^{(k)}\middle|a^{(m)}\right\rangle\left\langle a^{(m)}\middle|X\middle|a^{(n)}\right\rangle\left\langle a^{(n)}\middle|b^{(l)}\right\rangle \\ &= \sum_{m}\sum_{n}\left\langle a^{(k)}\middle|U^{\dagger}\middle|a^{(m)}\right\rangle\left\langle a^{(m)}\middle|X\middle|a^{(n)}\right\rangle\left\langle a^{(n)}\middle|U\middle|a^{(l)}\right\rangle\end{aligned}, \tag{2.82}$$

which is the **similarity transformation** in matrix algebra:

$$X' = U^{\dagger}XU\ . \tag{2.83}$$

The **trace** of an operator X is defined as the sum of diagonal elements:

$$\mathrm{tr}\left(X\right) = \sum_{a'}\left\langle a'\middle|X\middle|a'\right\rangle, \tag{2.84}$$

which is independent of representation, as shown:

$$\begin{aligned}\sum_{a'}\left\langle a'\middle|X\middle|a'\right\rangle &= \sum_{a'}\sum_{b'}\sum_{b''}\left\langle a'\middle|b'\right\rangle\left\langle b'\middle|X\middle|b''\right\rangle\left\langle b''\middle|a'\right\rangle \\ &= \sum_{b'}\sum_{b''}\left\langle b''\middle|b'\right\rangle\left\langle b'\middle|X\middle|b''\right\rangle \\ &= \sum_{b'}\left\langle b'\middle|X\middle|b'\right\rangle\end{aligned}. \tag{2.85}$$

It is also easy to prove that

$$\begin{aligned}&\mathrm{tr}\left(XY\right) = \mathrm{tr}\left(YX\right) \\ &\mathrm{tr}\left(U^{\dagger}XU\right) = \mathrm{tr}\left(X\right) \\ &\mathrm{tr}\left(\left|a'\right\rangle\left\langle a''\right|\right) = \delta_{a'a''} \\ &\mathrm{tr}\left(\left|b'\right\rangle\left\langle a'\right|\right) = \left\langle a'\middle|b'\right\rangle\end{aligned}. \tag{2.86}$$

2.2.6 Diagonalization

If we already know the matrix elements of an operator B in a basis set $\{|a'\rangle\}$, its eigenvalue b' and eigenket $|b'\rangle$ satisfying

$$B\left|b'\right\rangle = b'\left|b'\right\rangle \tag{2.87}$$

can be obtained by following the diagonalization process.

Eq. (2.87) can be written as

$$\sum_{a'}\left\langle a''\middle|B\middle|a'\right\rangle\left\langle a'\middle|b'\right\rangle = b'\left\langle a''\middle|b'\right\rangle, \tag{2.88}$$

whose matrix notation for the lth eigenket is

$$\begin{pmatrix} B_{11} & B_{12} & B_{13} & \cdots \\ B_{21} & B_{22} & B_{23} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} C_1^{(l)} \\ C_2^l \\ \vdots \end{pmatrix} = b^{(l)} \begin{pmatrix} C_1^{(l)} \\ C_2^l \\ \vdots \end{pmatrix}, \tag{2.89}$$

where $B_{ij} = \left\langle a^{(i)} \middle| B \middle| a^{(j)} \right\rangle$ and $C_k^{(l)} = \left\langle a^{(k)} \middle| b^{(l)} \right\rangle$. $C_k^{(l)}$ have nontrivial solutions only if the characteristic equation

$$\left| B - \lambda I \right| = 0 \tag{2.90}$$

is satisfied.

Theorem 2.4. If operator U connects two sets of orthonormal basis $\{|a'\rangle\}$ and $\{|b'\rangle\}$, then UAU^{-1} is a **unitary transform** of *A*; *A* and UAU^{-1} are **unitary equivalent observables**. From

$$A\left| a^{(l)} \right\rangle = a^{(l)} \left| a^{(l)} \right\rangle, \tag{2.91}$$

we have

$$UAU^{-1}U\left| a^{(l)} \right\rangle = a^{(l)}U\left| a^{(l)} \right\rangle, \tag{2.92}$$

so

$$\left(UAU^{-1} \right)\left| b^{(l)} \right\rangle = a^{(l)} \left| b^{(l)} \right\rangle. \tag{2.93}$$

This tells us that $\{|b'\rangle\}$ are eigenkets of UAU^{-1} with *exactly the same eigenvalues* as *A*. Comparing Eq. (2.93) with

$$B\left| b^{(l)} \right\rangle = b^{(l)} \left| b^{(l)} \right\rangle, \tag{2.94}$$

we can see that *B* and UAU^{-1} are simultaneously diagonalizable.

2.3 Position, Momentum, and Wave Functions

2.3.1 Continuous Spectra

Besides observables with discrete eigenvalue spectra, there are also observables with continuous eigenvalues in quantum mechanics, e.g., position and momentum.

The eigenvalue equation in the continuous spectrum case is written as

$$\xi \left| \xi' \right\rangle = \xi' \left| \xi' \right\rangle, \tag{2.95}$$

where ξ is an operator and ξ' is a number. By replacing the Kronecker symbol by Dirac's δ -function, we have

$$\left\langle a' \middle| a'' \right\rangle = \delta_{a'a''} \rightarrow \left\langle \xi' \middle| \xi'' \right\rangle = \delta\left(\xi' - \xi'' \right), \tag{2.96}$$

$$\sum_{a'} \left| a' \right\rangle \left\langle a' \right| = 1 \rightarrow \int \mathrm{d}\xi' \left| \xi' \right\rangle \left\langle \xi' \right| = 1, \tag{2.97}$$

$$\left|\alpha\right\rangle = \sum_{a'} \left|a'\right\rangle\left\langle a'\middle|\alpha\right\rangle \to \left|\alpha\right\rangle = \int \mathrm{d}\xi' \left|\xi'\right\rangle\left\langle \xi'\middle|\alpha\right\rangle , \tag{2.98}$$

$$\sum_{a'} \left|\left\langle a'\middle|\alpha\right\rangle\right|^2 = 1 \to \int \mathrm{d}\xi' \left|\left\langle \xi'\middle|\alpha\right\rangle\right|^2 = 1 , \tag{2.99}$$

$$\left\langle\beta\middle|\alpha\right\rangle = \sum_{a'} \left\langle\beta\middle|a'\right\rangle\left\langle a'\middle|\alpha\right\rangle \to \left\langle\beta\middle|\alpha\right\rangle = \int \mathrm{d}\xi' \left\langle\beta\middle|\xi'\right\rangle\left\langle \xi'\middle|\alpha\right\rangle , \tag{2.100}$$

$$\left\langle a''\middle|A\middle|a'\right\rangle = a'\delta_{a'a''} \to \left\langle\xi''\middle|\xi\middle|\xi'\right\rangle = \xi'\delta\left(\xi''-\xi'\right) . \tag{2.101}$$

2.3.2 Position Eigenkets and Position Measurements

In one dimension, the eigenkets $\left|x'\right\rangle$ of the position operator x satisfying

$$x\left|x'\right\rangle = x'\left|x'\right\rangle \tag{2.102}$$

form a complete set, which can be used to expand an arbitrary physical state

$$\left|\alpha\right\rangle = \int_{-\infty}^{\infty} dx' \left|x'\right\rangle\left\langle x'\middle|\alpha\right\rangle . \tag{2.103}$$

The normalization condition becomes

$$\left\langle\alpha\middle|\alpha\right\rangle = 1 \Rightarrow \int_{-\infty}^{\infty} \mathrm{d}x' \left\langle\alpha\middle|x'\right\rangle\left\langle x'\middle|\alpha\right\rangle = 1 , \tag{2.104}$$

and the probability for the measurement to find the particle located within some narrow range $\left(x' - \frac{\mathrm{d}x'}{2}, x' + \frac{\mathrm{d}x'}{2}\right)$ is

$$P_\alpha\left(x'\right) = \left|\left\langle x'\middle|\alpha\right\rangle\right|^2 \mathrm{d}x' . \tag{2.105}$$

In three dimensions, the position eigenkets $\left|\mathbf{x}'\right\rangle \equiv \left|x', y', z'\right\rangle$ ($x\left|\mathbf{x}'\right\rangle = x'\left|\mathbf{x}'\right\rangle$, $y\left|\mathbf{x}'\right\rangle = y'\left|\mathbf{x}'\right\rangle$, $z\left|\mathbf{x}'\right\rangle = z'\left|\mathbf{x}'\right\rangle$) are assumed to be complete in nonrelativistic quantum mechanics, and an arbitrary state can be expanded by

$$\left|\alpha\right\rangle = \int \mathrm{d}^3x' \left|\mathbf{x}'\right\rangle\left\langle \mathbf{x}'\middle|\alpha\right\rangle . \tag{2.106}$$

Since the three components of the position vector can be measured simultaneously to arbitrary degrees of accuracy, we must have

$$[x_i, x_j] = 0 , \tag{2.107}$$

where x_1 , x_2 , and x_3 stand for *x*, *y*, and *z*, respectively.

2.3.3 Translation

Translation (spatial displacement): An operation changes a state localized around $\mathbf{x}'$ to $\mathbf{x}' + \mathrm{d}\mathbf{x}'$ with everything else unchanged, which is defined to be an infinitesimal translation by $\mathrm{d}\mathbf{x}'$, and the corresponding unitary but non-Hermitian operator is denoted as

$$\mathscr{T}\left(\mathrm{d}\mathbf{x}'\right)\left|\mathbf{x}'\right\rangle = \left|\mathbf{x}' + \mathrm{d}\mathbf{x}'\right\rangle . \tag{2.108}$$

For an arbitrary state ket $|\alpha\rangle$, the effect of infinitesimal translation

$$\begin{aligned}|\alpha\rangle \to \mathscr{T}(\mathrm{d}\mathbf{x}')|\alpha\rangle &= \mathscr{T}(\mathrm{d}\mathbf{x}')\int \mathrm{d}^3x'|\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle \\ &= \int \mathrm{d}^3x'|\mathbf{x}'+\mathrm{d}\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle = \int \mathrm{d}^3x'|\mathbf{x}'\rangle\langle\mathbf{x}'-\mathrm{d}\mathbf{x}'|\alpha\rangle\end{aligned}, \tag{2.109}$$

which shows that the wave function of the translate state $\mathscr{T}(\mathrm{d}\mathbf{x}')|\alpha\rangle$ is obtained by substituting $\mathbf{x}'-\mathrm{d}\mathbf{x}'$ for $\mathbf{x}'$ in $\langle\mathbf{x}'|\alpha\rangle$.

The following properties of the infinitesimal translation operator can be satisfied if we take

$$\mathscr{T}(\mathrm{d}\mathbf{x}') = 1 - i\mathbf{K}\cdot\mathrm{d}\mathbf{x}' \tag{2.110}$$

with **K** a Hermitian operator in three dimensions:

(1) Unitarity:

$$\mathscr{T}^\dagger(\mathrm{d}\mathbf{x}')\mathscr{T}(\mathrm{d}\mathbf{x}') = 1. \tag{2.111}$$

(2) Additivity:

$$\mathscr{T}(\mathrm{d}\mathbf{x}'')\mathscr{T}(\mathrm{d}\mathbf{x}') = \mathscr{T}(\mathrm{d}\mathbf{x}'+\mathrm{d}\mathbf{x}''). \tag{2.112}$$

(3) Invertibility:

$$\mathscr{T}(-\mathrm{d}\mathbf{x}') = \mathscr{T}^{-1}(\mathrm{d}\mathbf{x}'). \tag{2.113}$$

(4) Reducibility:

$$\lim_{\mathrm{d}\mathbf{x}'\to 0}\mathscr{T}(\mathrm{d}\mathbf{x}') = 1. \tag{2.114}$$

Operator identity:

$$[\mathbf{x}, \mathscr{T}(\mathrm{d}\mathbf{x}')] = \mathrm{d}\mathbf{x}' \tag{2.115}$$

or

$$-i\mathbf{x}\mathbf{K}\cdot\mathrm{d}\mathbf{x}' + i\mathbf{K}\cdot\mathrm{d}\mathbf{x}'\mathbf{x} = \mathrm{d}\mathbf{x}'. \tag{2.116}$$

Proof: Note that

$$\mathbf{x}\mathscr{T}(\mathrm{d}\mathbf{x}')|\mathbf{x}'\rangle = \mathbf{x}|\mathbf{x}'+\mathrm{d}\mathbf{x}'\rangle = (\mathbf{x}+\mathrm{d}\mathbf{x}')|\mathbf{x}'+\mathrm{d}\mathbf{x}'\rangle \tag{2.117}$$

and

$$\mathscr{T}(\mathrm{d}\mathbf{x}')\mathbf{x}|\mathbf{x}'\rangle = \mathbf{x}'\mathscr{T}(\mathrm{d}\mathbf{x}')|\mathbf{x}'\rangle = \mathbf{x}'|\mathbf{x}'+\mathrm{d}\mathbf{x}'\rangle; \tag{2.118}$$

hence,

$$[\mathbf{x}, \mathscr{T}(\mathrm{d}\mathbf{x}')]|\mathbf{x}'\rangle = \mathrm{d}\mathbf{x}'|\mathbf{x}'+\mathrm{d}\mathbf{x}'\rangle \simeq \mathrm{d}\mathbf{x}'|\mathbf{x}'\rangle. \tag{2.119}$$

Because $|\mathbf{x}'\rangle$ can be any position eigenket, and the position eigenkets form a complete set, we must have Eq. (2.115) to be valid.

By choosing $\mathrm{d}\mathbf{x}'$ in the direction of $\hat{\mathbf{x}}_j$ and forming the scalar product with $\hat{\mathbf{x}}_i$, we obtain

$$[x_i, K_j] = i\delta_{ij} . \tag{2.120}$$

2.3.4 Momentum as a Generator of Translation

We borrow from classical mechanics the notion that *momentum is the generator of an infinitesimal translation*. An infinitesimal translation in classical mechanics is a canonical transformation:

$$\mathbf{x}_{\text{new}} \equiv \mathbf{X} = \mathbf{x} + \mathrm{d}\mathbf{x}, \quad \mathbf{p}_{\text{new}} \equiv \mathbf{P} = \mathbf{p} \tag{2.121}$$

obtainable from the generating function

$$F(\mathbf{x}, \mathbf{P}) = \mathbf{x} \cdot \mathbf{P} + \mathbf{p} \cdot \mathrm{d}\mathbf{x} . \tag{2.122}$$

Comparing it with Eq. (2.110) and considering the de Broglie's relation

$$\frac{2\pi}{\lambda} = \frac{p}{\hbar}, \tag{2.123}$$

we may rewrite Eq. (2.110) as

$$\mathscr{T}(\mathrm{d}\mathbf{x}') = 1 - i\mathbf{p} \cdot \mathrm{d}\mathbf{x}' / \hbar , \tag{2.124}$$

where **p** is the momentum operator. The commutation relation Eq. (2.120) becomes

$$[x_i, p_j] = i\hbar\delta_{ij} , \tag{2.125}$$

which imply that x_i and p_i are incompatible observables. According to Eq. (2.65), they satisfy the **position-momentum uncertainty relation** of W. Heisenberg:

$$\left\langle (\Delta x)^2 \right\rangle \left\langle (\Delta p_x)^2 \right\rangle \geq \frac{\hbar^2}{4} . \tag{2.126}$$

For a finite translation $\Delta x'$ along the *x*-direction, we divide it into $N \to \infty$ infinitesimal translations, then

$$\mathscr{T}(\Delta \mathrm{x}'\hat{\mathbf{x}}) = \lim_{N\to\infty} \left(1 - \frac{ip_x \Delta x'}{N\hbar}\right)^N = \exp\left(-\frac{ip_x \Delta x'}{\hbar}\right). \tag{2.127}$$

Because successive translations in different directions commute, we have

$$\begin{aligned}[]
[\mathscr{T}(\Delta y'\hat{\mathbf{y}}), \mathscr{T}(\Delta x'\hat{\mathbf{x}})] &= \mathscr{T}(\Delta y'\hat{\mathbf{y}})\mathscr{T}(\Delta x'\hat{\mathbf{x}}) - \mathscr{T}(\Delta x'\hat{\mathbf{x}})\mathscr{T}(\Delta y'\hat{\mathbf{y}}) \\
&= \mathscr{T}(\Delta y'\hat{\mathbf{y}} + \Delta x'\hat{\mathbf{x}}) - \mathscr{T}(\Delta x'\hat{\mathbf{x}} + \Delta y'\hat{\mathbf{y}}) = 0
\end{aligned} . \tag{2.128}$$

On the other hand,

$$\begin{aligned}
&\left[\mathscr{T}(\Delta y'\hat{\mathbf{y}}), \mathscr{T}(\Delta x'\hat{\mathbf{x}})\right] \\
&= \left[\left(1 - \frac{ip_y \Delta y'}{\hbar} - \frac{p_y^2 (\Delta y')^2}{2\hbar^2} + \cdots\right), \left(1 - \frac{ip_x \Delta x'}{\hbar} - \frac{p_x^2 (\Delta x')^2}{2\hbar^2} + \cdots\right)\right], \\
&\simeq -\frac{(\Delta x')(\Delta y')}{\hbar^2}\left[p_y, p_x\right]
\end{aligned} \tag{2.129}$$

so

$$\left[p_x, p_y\right] = 0 , \tag{2.130}$$

or more generally

$$\left[p_i, p_j\right] = 0 , \tag{2.131}$$

which implies that p_x, p_y, and p_z are mutually compatible observables. Therefore, the translation groups in three dimensions is **Abelian**.

Let

$$|\mathbf{p}'\rangle \equiv |p'_x, p'_y, p'_z\rangle \tag{2.132}$$

be a simultaneous eigenket of p_x, p_y, and p_z, we have

$$p_x|\mathbf{p}'\rangle = p'_x|\mathbf{p}'\rangle, \quad p_y|\mathbf{p}'\rangle = p'_y|\mathbf{p}'\rangle, \quad p_z|\mathbf{p}'\rangle = p'_z|\mathbf{p}'\rangle . \tag{2.133}$$

Applying $\mathscr{T}(\mathrm{d}\mathbf{x}')$ on it, we obtain

$$\mathscr{T}(\mathrm{d}\mathbf{x}')|\mathbf{p}'\rangle = \left(1 - \frac{i\mathbf{p}\cdot \mathrm{d}\mathbf{x}'}{\hbar}\right)|\mathbf{p}'\rangle = \left(1 - \frac{i\mathbf{p}'\cdot \mathrm{d}\mathbf{x}'}{\hbar}\right)|\mathbf{p}'\rangle . \tag{2.134}$$

Therefore, consistent with $\left[\mathbf{p}, \mathscr{T}(\mathrm{d}\mathbf{x}')\right] = 0$, $|\mathbf{p}'\rangle$ is an eigenket of $\mathscr{T}(\mathrm{d}\mathbf{x}')$.

Canonical commutation relations (fundamental commutation relations):

$$\left[x_i, x_j\right] = 0, \quad \left[p_i, p_j\right] = 0, \quad \left[x_i, p_j\right] = i\hbar\delta_{ij} . \tag{2.135}$$

The quantum-mechanical commuter is analogous to the classical Poisson bracket:

$$[\ ,\ ]_{\text{classical}} \to \frac{[\ ,\ ]}{i\hbar} , \tag{2.136}$$

where the classical Poisson bracket is defined as

$$\left[A(q,p), B(q,p)\right]_{\text{classical}} = \sum_s \left(\frac{\partial A}{\partial q_s}\frac{\partial B}{\partial p_s} - \frac{\partial A}{\partial p_s}\frac{\partial B}{\partial q_s}\right). \tag{2.137}$$

Both share the same properties:

$$\begin{aligned}
&[A, A] = 0 \\
&[A, B] = -[B, A] \\
&[A, c] = 0 \\
&[A + B, C] = [A, C] + [B, C] \\
&[A, BC] = [A, B]C + B[A, C] \\
&[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0
\end{aligned} , \tag{2.138}$$

where c is a constant and the last relation is known as the **Jacobi identity**.

2.3.5 Position-Space Wave Function

In one dimension, the normalized position base kets satisfy

$$x|x'\rangle = x'|x'\rangle \tag{2.139}$$

and

$$\langle x''|x'\rangle = \delta(x'' - x') . \tag{2.140}$$

A ket representing a physical state can be expanded as

$$\left|\alpha\right\rangle = \int \mathrm{d}x' \left|x'\right\rangle\left\langle x'\middle|\alpha\right\rangle , \tag{2.141}$$

and the probability of the particle staying in a narrow interval $\mathrm{d}x'$ around x' is

$$P\left(x', \mathrm{d}x'\right) = \left|\left\langle x'\middle|\alpha\right\rangle\right|^2 \mathrm{d}x' . \tag{2.142}$$

The **wave function** is define as

$$\psi_\alpha\left(x'\right) \equiv \left\langle x'\middle|\alpha\right\rangle . \tag{2.143}$$

The probability amplitude for state $\left|\alpha\right\rangle$ to be found in state $\left|\beta\right\rangle$ independent of representations is

$$\left\langle\beta\middle|\alpha\right\rangle = \int \mathrm{d}x' \left\langle\beta\middle|x'\right\rangle\left\langle x'\middle|\alpha\right\rangle = \int \mathrm{d}x' \psi_\beta^*\left(x'\right)\psi_\alpha\left(x'\right) . \tag{2.144}$$

The **eigenfunction** of operator *A* with eigenvalue a' in the position space is

$$u_{a'}\left(x'\right) = \left\langle x'\middle|a'\right\rangle , \tag{2.145}$$

with which the wave function can be expanded as

$$\psi_\alpha\left(x'\right) = \sum_{a'}\left\langle x'\middle|a'\right\rangle\left\langle a'\middle|\alpha\right\rangle = \sum_{a'} c_{a'} u_{a'}\left(x'\right) , \tag{2.146}$$

where $c_{a'} = \left\langle a'\middle|\alpha\right\rangle$. We then have

$$\begin{aligned}\left\langle\beta\right|A\left|\alpha\right\rangle &= \int \mathrm{d}x' \int \mathrm{d}x'' \left\langle\beta\middle|x'\right\rangle\left\langle x'\right|A\left|x''\right\rangle\left\langle x''\middle|\alpha\right\rangle \\ &= \int \mathrm{d}x' \int \mathrm{d}x'' \psi_\beta^*\left(x'\right)\left\langle x'\right|A\left|x''\right\rangle\psi_\alpha\left(x''\right)\end{aligned} . \tag{2.147}$$

If $A = f\left(x\right)$, the above equation is simplified as

$$\left\langle\beta\right| f\left(x\right)\left|\alpha\right\rangle = \int \mathrm{d}x' \psi_\beta^*\left(x'\right) f\left(x'\right)\psi_\alpha\left(x'\right) . \tag{2.148}$$

2.3.6 Momentum Operator in the Position Basis

Applying Eq. (2.124) to an arbitrary ket $\left|\alpha\right\rangle$, we obtain

$$\begin{aligned}\left(1 - \frac{ip\Delta x'}{\hbar}\right)\left|\alpha\right\rangle &= \int \mathrm{d}x' \mathscr{T}\left(\Delta x'\right)\left|x'\right\rangle\left\langle x'\middle|\alpha\right\rangle \\ &= \int \mathrm{d}x' \left|x' + \Delta x'\right\rangle\left\langle x'\middle|\alpha\right\rangle \\ &= \int \mathrm{d}x' \left|x'\right\rangle\left\langle x' - \Delta x'\middle|\alpha\right\rangle \\ &= \int \mathrm{d}x' \left|x'\right\rangle\left(\left\langle x'\middle|\alpha\right\rangle - \Delta x' \frac{\partial}{\partial x'}\left\langle x'\middle|\alpha\right\rangle\right)\end{aligned} . \tag{2.149}$$

Comparison of both sides yields

$$p\left|\alpha\right\rangle = \int \mathrm{d}x' \left|x'\right\rangle\left(-i\hbar\frac{\partial}{\partial x'}\left\langle x'\middle|\alpha\right\rangle\right) , \tag{2.150}$$

which is equivalent to

$$\left\langle x'\right| p\left|\alpha\right\rangle = -i\hbar\frac{\partial}{\partial x'}\left\langle x'\middle|\alpha\right\rangle . \tag{2.151}$$

The matrix element

$$\langle x'|\, p\,|x''\rangle = -i\hbar\frac{\partial}{\partial x'}\delta\left(x'-x''\right). \tag{2.152}$$

From Eq. (2.150), we get

$$\begin{aligned}\langle\beta|\,p\,|\alpha\rangle &= \int \mathrm{d}x'\langle\beta|x'\rangle\left(-i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right)\\ &= \int \mathrm{d}x'\psi_\beta^*\left(x'\right)\left(-i\hbar\frac{\partial}{\partial x'}\right)\psi_\alpha\left(x'\right)\end{aligned}. \tag{2.153}$$

By applying Eq. (2.151) repeatedly, we also have

$$\langle x'|\,p^n\,|\alpha\rangle = \left(-i\hbar\right)^n\frac{\partial^n}{\partial x'^n}\langle x'|\alpha\rangle \tag{2.154}$$

and

$$\langle\beta|\,p^n\,|\alpha\rangle = \int \mathrm{d}x'\psi_\beta^*\left(x'\right)\left(-i\hbar\right)^n\frac{\partial^n}{\partial x'^n}\psi_\alpha\left(x'\right). \tag{2.155}$$

2.3.7 Momentum-Space Wave Function

In the one-dimensional momentum space, the base eigenkets specify

$$\begin{aligned}p|\,p'\rangle &= p'|\,p'\rangle\\ \langle p'|\,p''\rangle &= \delta\left(p'-p''\right)\end{aligned}. \tag{2.156}$$

An arbitrary state ket can be expanded as

$$|\alpha\rangle = \int \mathrm{d}p'|\,p'\rangle\langle p'|\alpha\rangle. \tag{2.157}$$

The **momentum-space wave function** is defined as

$$\phi_\alpha\left(p'\right) \equiv \langle p'|\alpha\rangle. \tag{2.158}$$

The normalization condition reads

$$\int dp'\left|\phi_\alpha\left(p'\right)\right|^2 = 1. \tag{2.159}$$

Below we derive the **transformation function** from the x-representation to the p-representation $\langle x'|\,p'\rangle$. Replacing $|\alpha\rangle$ by $|\,p'\rangle$ in Eq. (2.151), we have

$$\langle x'|\,p\,|\,p'\rangle = p'\langle x'|\,p'\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|\,p'\rangle, \tag{2.160}$$

whose solution is

$$\langle x'|\,p'\rangle = C\exp\left(\frac{ip'x'}{\hbar}\right), \tag{2.161}$$

where C is the normalization constant. To determine the value of C, first consider

$$\langle x'|x''\rangle = \int \mathrm{d}p'\langle x'|\,p'\rangle\langle p'|x''\rangle, \tag{2.162}$$

which is just

$$\delta\left(x'-x''\right) = |C|^2\int \mathrm{d}p'\exp\left[\frac{ip'\left(x'-x''\right)}{\hbar}\right] = 2\pi\hbar|C|^2\,\delta\left(x'-x''\right). \tag{2.163}$$

Choosing C to be real and positive, we determine from the above equation that $C = \frac{1}{\sqrt{2\pi\hbar}}$, so

$$\langle x' | p' \rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{ip'x'}{\hbar} \right), \tag{2.164}$$

which shows that the wave function of a momentum eigenstate is a **plane wave**. The position-space and momentum-space wave functions are related by

$$\psi_\alpha(x') = \frac{1}{\sqrt{2\pi\hbar}} \int \mathrm{d}p' \exp\left(\frac{ip'x'}{\hbar} \right) \phi_\alpha(p') \tag{2.165}$$

and

$$\phi_\alpha(p') = \frac{1}{\sqrt{2\pi\hbar}} \int \mathrm{d}x' \exp\left(\frac{-ip'x'}{\hbar} \right) \psi_\alpha(x'). \tag{2.166}$$

This pair of equations just follows the Fourier's inversion theorem.

2.3.8 Gaussian Wave Packets

The x-space wave function of a **Gaussian wave packet** is given by

$$\langle x' | \alpha \rangle = \frac{1}{\pi^{1/4} d^{1/2}} \exp\left(ikx' - \frac{x'^2}{2d^2} \right), \tag{2.167}$$

where k is the wave number, d is the width of the wave packet. The corresponding p-space wave function is given by

$$\begin{aligned} \langle p' | \alpha \rangle &= \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{\pi^{1/4} d^{1/2}} \exp\left(ikx' - \frac{x'^2}{2d^2} \right) \int_{-\infty}^{\infty} \mathrm{d}x' \exp\left(\frac{-ip'x'}{\hbar} + ikx' - \frac{x'^2}{2d^2} \right) \\ &= \sqrt{\frac{d}{\hbar\sqrt{\pi}}} \exp\left[\frac{-(p' - \hbar k)^2 d^2}{2\hbar^2} \right] \end{aligned}. \tag{2.168}$$

The position expectation value

$$\langle x \rangle = \int_{-\infty}^{\infty} \mathrm{d}x' \langle \alpha | x' \rangle x' \langle x' | \alpha \rangle = \int_{-\infty}^{\infty} \mathrm{d}x' \left| \langle x' | \alpha \rangle \right|^2 x' = 0, \tag{2.169}$$

and the position dispersion

$$\left\langle (\Delta x)^2 \right\rangle = \langle x^2 \rangle - \langle x \rangle^2 = \int_{-\infty}^{\infty} \mathrm{d}x' \left| \langle x' | \alpha \rangle \right|^2 x'^2 = \frac{d^2}{2}. \tag{2.170}$$

The momentum expectation values are

$$\begin{aligned} \langle p \rangle &= \hbar k \\ \langle p^2 \rangle &= \frac{\hbar^2}{2d^2} + \hbar^2 k^2 \end{aligned}. \tag{2.171}$$

The momentum dispersion is therefore given by

$$\left\langle (\Delta p)^2 \right\rangle = \langle p^2 \rangle - \langle p \rangle^2 = \frac{\hbar^2}{2d^2}. \tag{2.172}$$

With Eq. (2.170) and Eq. (2.172), we may verify the Heisenberg uncertainty relation

$$\left\langle (\Delta x)^2 \right\rangle \left\langle (\Delta p)^2 \right\rangle = \frac{\hbar^2}{4}. \tag{2.173}$$

Because the above is an equality relation, a Gaussian wave packet is often called a *minimum uncertainty wave packet*.

2.3.9 Generalization to Three Dimensions

The one-dimensional equations can be directly generalized to three dimensions basically by replacing the one-dimensional scalars by three-dimensional vectors:

$$\begin{aligned} \mathbf{x}|\mathbf{x}'\rangle &= \mathbf{x}'|\mathbf{x}'\rangle \\ \langle\mathbf{x}'|\mathbf{x}''\rangle &= \delta^3(\mathbf{x}'-\mathbf{x}'') \end{aligned}, \tag{2.174}$$

$$\begin{aligned} \mathbf{p}|\mathbf{p}'\rangle &= \mathbf{p}'|\mathbf{p}'\rangle \\ \langle\mathbf{p}'|\mathbf{p}''\rangle &= \delta^3(\mathbf{p}'-\mathbf{p}'') \end{aligned}, \tag{2.175}$$

$$\begin{aligned} \int \mathbf{d}^3x'|\mathbf{x}'\rangle\langle\mathbf{x}'| &= 1 \\ \int \mathbf{d}^3p'|\mathbf{p}'\rangle\langle\mathbf{p}'| &= 1 \end{aligned}, \tag{2.176}$$

$$|\alpha\rangle = \int \mathrm{d}^3x'|\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle = \int \mathrm{d}^3p'|\mathbf{p}'\rangle\langle\mathbf{p}'|\alpha\rangle, \tag{2.177}$$

$$\langle\beta|\mathbf{p}|\alpha\rangle = \int \mathbf{d}^3x'\psi_\beta^*(\mathbf{x}')(-i\hbar\nabla')\psi_\alpha(\mathbf{x}'), \tag{2.178}$$

$$\langle\mathbf{x}'|\mathbf{p}'\rangle == \frac{1}{(2\pi\hbar)^{3/2}}\exp\left(\frac{i\mathbf{p}'\cdot\mathbf{x}'}{\hbar}\right), \tag{2.179}$$

$$\psi_\alpha(\mathbf{x}') = \frac{1}{(2\pi\hbar)^{3/2}}\int \mathrm{d}^3\mathbf{p}'\exp\left(\frac{i\mathbf{p}'\cdot\mathbf{x}'}{\hbar}\right)\phi_\alpha(\mathbf{p}'), \tag{2.180}$$

$$\phi_\alpha(\mathbf{p}') = \frac{1}{(2\pi\hbar)^{3/2}}\int \mathrm{d}^3\mathbf{x}'\exp\left(\frac{-i\mathbf{p}'\cdot\mathbf{x}'}{\hbar}\right)\psi_\alpha(\mathbf{x}'). \tag{2.181}$$