PHYS 5340: Quantum Mechanics I

Richard S. Camuccio

Department of Physics and Astronomy

University of Texas Rio Grande Valley

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Contents

1 Bras, Kets, and Operators

Hilbert Space is an infinite dimensional complex vector space. In quantum mechanics, a *physical state* is represented by a *state vector* (e.g. an atom with definite spin orientation).

Dirac notation: A state vector α is in a complex vector space, denoted as $|\alpha\rangle$, and referred to as a 'state ket'. The skate ket contains complete information about the physical state.

Addition:

$$|\alpha\rangle + |\beta\rangle = |\gamma\rangle \tag{1.1}$$

Multiplication:

$$c|\alpha\rangle = |\alpha\rangle c \tag{1.2}$$

In the case of Equation (1.2), c is a complex number. If $c = 0$, the result is called *null ket*.

An *observable* in quantum mechanics is represented by an *operator* A (e.g. position, momentum, spin, ...)

$$A \cdot (|\alpha\rangle) = A|\alpha\rangle \tag{1.3}$$

If

$$A|a'\rangle = a'|a'\rangle,\ A|a''\rangle = a''|a''\rangle,\ \cdots, \tag{1.4}$$

where a', a'', $\cdots$, are numbers, then $|a'\rangle$, $|a''\rangle$, ... are called *eigenkets* of operator A and a', a'', ..., are called *eigenvalues* of A. The whole set of eigenvalues are denoted by $\{a'\}$. The physical state corresponding to an eigenket is called an *eigenstate*.

For example, consider a spin $\frac{1}{2}$ system,

$$S_z|S_z;+\rangle = \frac{\hbar}{2}|S_z;-\rangle \tag{1.5a}$$
$$S_z|S_z;-\rangle = -\frac{\hbar}{2}|S_z;-\rangle \tag{1.5b}$$

where S_z is the operator, $|S_z;+\rangle$ is the eigenket, and $-\frac{\hbar}{2}$ is the eigenvalue (using the case of Equation (1.5b) as an example).

We can write Equation (1.5), this time in the context of the x-direction, more compactly as

$$S_x|S_x;\pm\rangle = \pm\frac{\hbar}{2}|S_x;\pm\rangle \tag{1.6}$$

If an N-dimensional vector space is spanned by N eigenkets of observable A, then we can write them as a linear combination of a sum of complex coefficients acting on the eigenkets:

$$|\alpha\rangle = \sum_{a'} c_{a'}|a'\rangle \tag{1.7}$$

where $c_{a'},\ c_{a''},\ \cdots,\ c_{a^{(N)}}$ are complex coefficients and $\sum_{a'}|a'\rangle \implies |a'\rangle+|a''\rangle+,\ \cdots,\ |a^{(N)}\rangle$.

The *bra space* is a vector space dual to the ket space. Corresponding to every ket $|\alpha\rangle$, $\exists\ \langle\alpha|$ in dual space.

The dual correspondence between the bra and ket spaces carries with it similar properties:

$$|\alpha\rangle \leftrightarrow \langle\alpha| \tag{1.8a}$$
$$|a'\rangle,\ |a''\rangle,\ \cdots \leftrightarrow \langle a'|,\ \langle a''|,\ \cdots \tag{1.8b}$$
$$|\alpha\rangle + |\beta\rangle \leftrightarrow \langle\alpha| + \langle\beta| \tag{1.8c}$$

Note, however, that

$$c_\alpha|\alpha\rangle + c_\beta|\beta\rangle \leftrightarrow c_\alpha^*\langle\alpha| + c_\beta^*\langle\beta| \tag{1.9}$$

We define the inner product as

$$\langle\beta|\alpha\rangle \equiv (\langle\beta|)\cdot(|\alpha\rangle) \tag{1.10}$$

We also state some fundamental properties of the dual correspondence:

$$\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^* \tag{1.11a}$$

$$\langle\alpha|\alpha\rangle \geq 0 \tag{1.11b}$$

$$\langle\alpha|\beta\rangle = 0 \tag{1.11c}$$

$$|\tilde{\alpha}\rangle = \left(\frac{1}{\sqrt{\langle\alpha|\alpha\rangle}}\right)|\alpha\rangle \tag{1.11d}$$

$$\langle\tilde{\alpha}|\tilde{\alpha}\rangle = 1 \tag{1.11e}$$

Equation (1.11a) is the definition of the complex conjugate. The equality in Equation (1.11b) holds only for null kets. If two kets $|\alpha\rangle$ and $|\beta\rangle$ are orthogonal, then Equation (1.11c) is satisfied. If $|\alpha\rangle$ is not a null ket, we can construct a normalized ket $|\tilde{\alpha}\rangle$, also called the norm of $|\alpha\rangle$, such that Equation (1.11d) holds.

Let there be operators $X,\ Y,\ \cdots$, such that:

$$X = Y \implies X|\alpha\rangle = Y|\alpha\rangle \tag{1.12}$$

If $X|\alpha\rangle = 0$, this implies that X is a null operator.

The operators X and Y satisfy the commutative property of addition:

$$X + Y = Y + X \tag{1.13}$$

They satisfy the associative property as well:

$$X + (Y + Z) = (X + Y) + Z \tag{1.14}$$

The operator X is a linear operator:

$$X(c_\alpha|\alpha\rangle + c_\beta|\beta\rangle) = c_\alpha X|\alpha\rangle + c_\beta X|\beta\rangle \tag{1.15}$$

Note the following:

$$X|\alpha\rangle \leftrightarrow \langle\alpha|X^\dagger \tag{1.16}$$

where $X^\dagger$ is the adjoint of X. X is considered Hermitian if

$$X = X^\dagger \tag{1.17}$$

Multiplication of operators is not commutative:

$$XY \neq YX \tag{1.18}$$

Multiplication is associative:

$$X(YZ) = (XY)Z = XYZ \tag{1.19}$$

$$X(Y|\alpha\rangle) = (XY)|\alpha\rangle = XY|\alpha\rangle \tag{1.20a}$$

$$(\langle\beta|X)Y = \langle\beta|(XY) = \langle\beta|XY \tag{1.20b}$$

Note that:

$$(XY)^\dagger = Y^\dagger X^\dagger \tag{1.21}$$

Proof of Equation (1.21)

$$XY|\alpha\rangle = X(Y|\alpha\rangle) \leftrightarrow ((\langle\alpha\ Y^\dagger)X^\dagger = \langle\alpha|Y^\dagger X^\dagger \tag{1.22}$$

The *outer product* is defined as:

$$|\beta\rangle\langle\alpha| \tag{1.23}$$

The Associative Axiom

Let

$$(|\beta\rangle\langle\alpha|) \cdot |\gamma\rangle = |\beta\rangle \cdot (\langle\alpha|\gamma\rangle) \tag{1.24}$$

where $(\langle\alpha|\gamma\rangle)$ is a number. Therefore, $|\beta\rangle\langle\alpha|$ acts as an operator. So, if

$$X = |\beta\rangle \implies X^\dagger = |\alpha\rangle\langle\beta| \tag{1.25}$$

Again,

$$(\langle\beta| \cdot (X|\alpha\rangle) = (\langle\beta|X) \cdot (|\alpha\rangle) \tag{1.26}$$

We write this in a compact form as

$$\langle\beta|X|\alpha\rangle \tag{1.27}$$

for both the right- and left-hand sides.

$$\Longrightarrow \langle\beta|X|\alpha\rangle = \langle\beta|\cdot(X|\alpha\rangle) = \left(\langle\alpha|X^\dagger)\cdot|\beta\rangle\right)^* = \langle\alpha|X^\dagger|\beta\rangle^* \tag{1.28}$$

For a Hermitian operator X,

$$\langle\beta|X|\alpha\rangle = \langle\alpha|X|\beta\rangle^* \tag{1.29}$$

Base Kets and Matrix Representation

Theorem Let A be a Hermitian operator. The eigenvalues of a Hermitian operator A are real. The eigenkets of A corresponding to different eigenvalues are orthogonal.

Proof

Start with

$$A|\alpha'\rangle = a'|a'\rangle \tag{1.30}$$

A is Hermitian, so

$$\langle\alpha''|A = \alpha''^*\langle\alpha''| \tag{1.31}$$

where $\alpha', \alpha'', \cdots$ are eigenvalues of A.

From Equation (1.30), $\langle\alpha''|A|\alpha'\rangle = \langle\alpha''|\alpha'|\alpha'\rangle$

$$\Longrightarrow (\alpha' - \alpha''^*)\langle\alpha''|\alpha'\rangle = 0 \tag{1.32}$$

Now, Equation (1.32) implies that $\alpha' = \alpha''^*$ which, assuming $\alpha' = \alpha''$, further implies that $\alpha' = \alpha'^*$ (where $|\alpha'\rangle$ is not a null ket).

Thus, α' is real. QED.

Now, let $\alpha' \neq \alpha''$. Therefore, from Equation (1.32), $(\alpha' - \alpha'')\langle\alpha''|\alpha'\rangle = 0$, which implies that $\langle\alpha''|\alpha'\rangle = 0$. Therefore, the eigenkets of A corresponding to different eigenvalues are orthogonal.

It is convenient to normalize $|\alpha'\rangle$ so that $\{|\alpha'\rangle\}$ form an orthonormal set:

$$\langle\alpha''|\alpha'\rangle = \delta_{\alpha'\alpha''} \tag{1.33}$$

2 Eigenkets as Base Kets

Given that normalized eigenkets of A form a complete orthonormal set, an arbitrary ket can be expanded in terms of eigenkets of A.

$$|\alpha\rangle = \sum_{a'} c_{a'} |a'\rangle \tag{2.1}$$

This implies that $\langle a''|\alpha\rangle = \sum_{a'} c_{a'} \langle a''|a'\rangle$, where

$$c_{a'} = \langle a'|\alpha\rangle \tag{2.2}$$

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \tag{2.3}$$

$$\sum_{a'} |a'\rangle\langle a'| = 1 \tag{2.4}$$

Equation (2.4) is the completeness, or closure, property, and 1 is the identity operator.

Now, $\langle\alpha|\alpha\rangle = \langle\alpha| \cdot \Big(\sum_{a'} |a'\rangle\langle a'| \Big) \cdot |\alpha\rangle$

$$= \sum_{a'} |\langle a'|\alpha\rangle|^2 \tag{2.5}$$

$$\sum_{a'} |c_{a'}|^2 = \sum_{a'} |\langle a'|\alpha\rangle|^2 = 1 \tag{2.6}$$

Equation (2.6) assumes that $|\alpha\rangle$ is normalized. Also, $\Lambda_{a'} = |a'\rangle\langle a'|$ is called the *projection operator*.

Matrix Representation

Let us write an operator X such that

$$X = \sum_{a''} \sum_{a'} |a''\rangle\langle a''|X|a'\rangle\langle a'| \tag{2.7}$$

There are N^2 ($N \rightarrow$ is the dimensionality of the ket space) terms of the form $\langle a''|X|a'\rangle$.

We may arrange them into an $N \times N$ matrix such as $\langle a''|X|a'\rangle$, where $\langle a''|$ represents a row matrix, $|a'\rangle$ represents a column matrix, and X is represented as

$$X = \begin{bmatrix} \langle a^{(1)}|X|a^{(1)}\rangle & \langle a^{(1)}|X|a^{(2)}\rangle & \dots \\ \langle a^{(2)}|X|a^{(1)}\rangle & \langle a^{(2)}|X|a^{(2)}\rangle & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} \tag{2.8}$$

Again,

$$\langle a''|X|a'\rangle = \langle a'|X^\dagger|a''\rangle \tag{2.9}$$

Note: Equation (2.9) involves a Hermitian adjoint operation $\equiv$ complex conjugate transposed.

If we have an operator B which is Hermitian, then

$$\langle a''|B|a'\rangle = \langle a'|X|a''\rangle^* \tag{2.10}$$

Let $Z = XY$. Then we have

$$\langle a''|Z|a'\rangle = \langle a''|XY|a'\rangle = \sum_{a'''} \langle a''|X|a'''\rangle\langle a'''|Y|a'\rangle \tag{2.11}$$

which satisfies the rule of matrix multiplication.

Let us now consider

$$|\gamma\rangle = X|\alpha\rangle. \tag{2.12}$$

This immediately leads to the implication that

$$\langle a'|\gamma\rangle = \langle a'|X|\alpha\rangle = \sum_{a''}\langle a'|X|a''\rangle\langle a''|\alpha\rangle \tag{2.13}$$

Equation (2.13) is akin to matrix multiplication rule with column matrices

$$|\alpha\rangle = \begin{bmatrix}\langle a^{(1)}|\alpha\rangle \\ \langle a^{(2)}|\alpha\rangle \\ \vdots\end{bmatrix},\ |\gamma\rangle = \begin{bmatrix}\langle a^{(1)}|\gamma\rangle \\ \langle a^{(2)}|\gamma\rangle \\ \vdots\end{bmatrix} \tag{2.14}$$

Likewise,

$$\langle\gamma| = \langle\alpha|X \tag{2.15}$$

which gives us

$$\langle\gamma|a'\rangle = \sum_{a''}\langle\alpha|a''\rangle\langle a''|X|a'\rangle \tag{2.16}$$

The bra vector is represented by a row matrix

$$\langle\gamma| = \begin{bmatrix}\langle\gamma|a^{(1)}\rangle & \langle\gamma|a^{(2)}\rangle & \dots\end{bmatrix} = \begin{bmatrix}\langle a^{(1)}|\gamma\rangle^* & \langle a^{(2)}|\gamma\rangle^* & \dots\end{bmatrix} \tag{2.17}$$

Therefore, the inner product can be written as a multiplication of a row matrix and a column matrix.

$$\langle\beta|\alpha\rangle = \sum_{a'}\langle\beta|a'\rangle\langle a'|\alpha\rangle = \begin{bmatrix}\langle a^{(1)}|\beta\rangle^* & \langle a^{(2)}|\beta\rangle^* & \dots\end{bmatrix}\begin{bmatrix}\langle a^{(1)}|\alpha\rangle \\ \langle a^{(2)}|\alpha\rangle \\ \vdots\end{bmatrix} \tag{2.18}$$

The matrix representation of A becomes simple if the eigenkets of A are used as base kets:

$$A = \sum_{a''}\sum_{a'} |a''\rangle\langle a''|A|a'\rangle\langle a'| \tag{2.19}$$

But the square matrix $\langle a''|A|a'\rangle$ is diagonal:

$$\langle a''|A|a'\rangle = \langle a'|A|a'\rangle\delta_{a'a''} = a'\delta_{a'a''} \tag{2.20}$$

Therefore,

$$A = \sum_{a'} a'|a'\rangle\langle a'| = \sum_{a'} a'\Lambda_{a'} \tag{2.21}$$

For example, consider a spin $\frac{1}{2}$ system, where we let the base kets be $|S_z;\pm\rangle \equiv |\pm\rangle$. The simplest operator spanned by $|\pm\rangle$ is the identity operator:

$$1 = |+\rangle\langle+| + |-\rangle\langle-| \tag{2.22}$$

From Equation (2.21) we can write

$$S_z = \left(\frac{\hbar}{2}\right)\left[\Big(|+\rangle\langle+|\Big) + \Big(|-\rangle\langle-|\Big)\right] \tag{2.23}$$

We have the eigenvalue relation

$$S_z|\pm\rangle = \pm\left(\frac{\hbar}{2}\right)|\pm\rangle \tag{2.24}$$

Let us now look at the other components:

$$S_+ \equiv \hbar|+\rangle\langle-|, \quad S_- \equiv \hbar|-\rangle\langle+| \tag{2.25}$$

Both S_+ and S_- are non-Hermitian. Interpretation: S_+ acts on $|-\rangle$ to turn it into $\hbar|+\rangle$ by raising the spin component by one unit of $\hbar$. S_+ acting on $|+\rangle$ returns a null ket.

Matrix representations:

$$|+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |-\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{2.26}$$

$$S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad S_+ = \hbar\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad S_- = \hbar\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \tag{2.27}$$

Measurements, Observables, and Uncertainty Relations

"A measurement always causes the system to jump into an eigenstate of the dynamical variable that is being measured." — Dirac

Before measurement:

$$|\alpha\rangle = \sum_{a'} c_{a'}|a'\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \tag{2.28}$$

After measurement:

$$|\alpha\rangle \to |a'\rangle \tag{2.29}$$

Measurement causes a change of state. However, if the state is an eigenstate, it remains unchanged.

We postulate that the probability of jumping into some particular state $|a'\rangle$ is

$$|\langle a'|\alpha\rangle|^2 \tag{2.30}$$

A collection of identically prepared systems all in the same state (e.g. $|\alpha\rangle$) are a *pure ensemble*. Equation (2.30) is one of the fundamental postulates of quantum mechanics. We define the *expectation value* of A taken with respect to state $|\alpha\rangle$ as

$$\langle A \rangle = \langle \alpha | A | \alpha \rangle \tag{2.31}$$

$$\langle A \rangle = \sum_{a'} \sum_{a''} \langle \alpha | a'' \rangle \langle a'' | A | a' \rangle \langle a' | \alpha \rangle = \sum_{a'} a' |\langle a' | \alpha \rangle|^2 \tag{2.32}$$

3 Commutators, Uncertainty Relation, and Change of Basis

The commutator and anti-commutator of two observables A and B are defined, respectively, as

$$[A, B] = AB - BA \tag{3.1a}$$

$$\{A, B\} = AB + BA \tag{3.1b}$$

If $[A, B] = 0$, then A and B are compatible (and vice versa). If two or more linearly independent eigenkets of A have the same eigenvalue, the eigenvalues of the two eigenkets are said to be *degenerate*.

Theorem Suppose A and B are compatible observables and eigenvalues of A are non-degenerate. Then the matrix elements $\langle a''|B|a'\rangle$ are all diagonal.

Proof

$$\langle a''|[A, B]|a'\rangle = \langle a''|AB - BA|a'\rangle = (a'' - a')\langle a''|B|a'\rangle = 0 \tag{3.2}$$

Therefore, if $a'' \neq a'$, then $\langle a''|B|a'\rangle = 0$. QED.

We can write $\langle a''|B|a'\rangle = \delta_{a'a''}\langle a'|B|a'\rangle$. Now remember that matrix elements of A are already diagonal if $\{|a'\rangle\}$ are base kets. Therefore, both A and B can be represented by diagonal matrices with the same set of base kets.

$$B = \sum_{a''} |a''\rangle\langle a''|B|a''\rangle\langle a''| \tag{3.3}$$

Therefore,

$$B|a'\rangle = \sum_{a''} |a''\rangle\langle a''|B|a''\rangle\langle a''|a'\rangle = \Big(\langle a'|B|a'\rangle\Big) \cdot |a'\rangle \tag{3.4}$$

Equation (3.4) is the eigenvalue equation of B with eigenvalue b', where

$$b' = \langle a'|B|a'\rangle \tag{3.5}$$

The ket $|a'\rangle$ is the simultaneous eigenket of A and B. Let $|a', b'\rangle$ be the notation for a simultaneous eigenket of A and B with eigenvalues a' and b', respectively.

Properties:

$$A|a', b'\rangle = a'|a', b'\rangle \tag{3.6a}$$

$$B|a', b'\rangle = b'|a', b'\rangle \tag{3.6b}$$

Uncertainty Relation

Let us define an operator ΔA as

$$\Delta A = A - \langle A\rangle \tag{3.7}$$

The dispersion is thus defined as

$$\langle(\Delta A)^2\rangle = \langle(A^2 - 2A\langle A\rangle + \langle A\rangle^2)\rangle = \langle A^2\rangle - \langle A\rangle^2 \tag{3.8}$$

<u>Theorem</u> If A and B are two observables, the following must hold true:

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[A, B]\rangle|^2 \tag{3.9}$$

<u>Proof</u>

Lemma 1. The Schwarz Inequality is

$$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2 \tag{3.10}$$

To show that the Schwarz Inequality is true, we note that

$$(\langle\alpha| + \lambda^*\langle\beta|)\cdot(|\alpha\rangle + \lambda|\beta\rangle) \geq 0 \tag{3.11}$$

where λ is any complex number. By setting $\lambda = -\frac{\langle\beta|\alpha\rangle}{\langle\beta|\beta\rangle}$, we get

$$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle - |\langle\alpha|\beta\rangle|^2 \geq 0 \tag{3.12}$$

which is the Schwarz Inequality written in Equation (3.10).

Lemma 2. The expectation value of a Hermitian operator is real. Hint: Use the fact that $\langle a''|B|a'\rangle = \langle a'|B|a''\rangle^*$.

Lemma 3. The expectation value of an anti-Hermitian operator is purely imaginary. Hint: Remember that $C = -C^\dagger$ for an anti-Hermitian operator.

Now let

$$|\alpha\rangle = \Delta A|\rangle \tag{3.13a}$$

$$|\beta\rangle = \Delta B|\rangle \tag{3.13b}$$

where we have used blank kets to represent any arbitrary ket. From Lemma 1 we have

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq |\langle\Delta A\Delta B\rangle|^2 \tag{3.14}$$

where we note that ΔA and ΔB are Hermitian. By looking at the RHS of Equation (3.14), we take note that $\Delta A\Delta B$ can be expressed as

$$\Delta A\Delta B = \frac{1}{2}[\Delta A, \Delta B] + \frac{1}{2}\{\Delta A, \Delta B\} \tag{3.15}$$

Then, we take note that $[\Delta A, \Delta B] = [A, B]$ is anti-Hermitian. As such we have

$$([A, B])^\dagger = (AB - BA)^\dagger = BA - AB = -[A, B] \tag{3.16}$$

However, $\{\Delta A, \Delta B\}$ is Hermitian. Therefore, using Lemmas 2 and 3, we get

$$\langle \Delta A, \Delta B \rangle = \frac{1}{2}\langle [A, B] \rangle + \frac{1}{2}\langle \{\Delta A, \Delta B\} \rangle \tag{3.17}$$

where the first term on the RHS is imaginary and the second term on the RHS is real. The RHS of Equation (3.14) is now

$$|\langle \Delta A \Delta B \rangle|^2 = \frac{1}{4}|\langle [A, B] \rangle|^2 + \frac{1}{4}|\langle \{\Delta A, \Delta B\} \rangle|^2 \tag{3.18}$$

QED.

Change of Basis

Let there be two incompatible operators A and B. The ket space can be spanned either by $\{|a'\rangle\}$ or by $\{|b'\rangle\}$. This is known as *change of basis* or *representation.* We can construct a transformation operator that connects an old orthonormal set $\{|a'\rangle\}$ to a new one $\{|b'\rangle\}$.

Theorem Given two sets of base kets both satisfying orthonormality and completeness, $\exists$ a unitary operator U such that

$$|b'\rangle = U|a'\rangle; \quad |b''\rangle = U|a''\rangle \tag{3.19}$$

where

$$U^\dagger U = 1, \quad UU^\dagger = 1 \tag{3.20}$$

Proof

Let

$$U = \sum_k |b^{(k)}\rangle\langle a^{(k)}| \tag{3.21}$$

$$\implies U|a^{(l)}\rangle = |b^{(l)}\rangle \tag{3.22}$$

Furthermore,

$$U^\dagger U = \sum_k \sum_l |a^{(l)}\rangle\langle b^{(l)}|b^{(k)}\rangle\langle a^{(k)}| = \sum_k |a^{(k)}\rangle\langle a^{(k)}| = 1 \tag{3.23}$$

4 Transformation Matrix, Diagonalization, and Physical Observables

What is the representation of U in $\{|a'\rangle\}$? The transformation matrix can be written as

$$\langle a^{(k)}|U|a^{(l)}\rangle = \langle a^{(k)}|b^{(l)}\rangle \tag{4.1}$$

where we have used the U-transformation to arrive at a new set of basis vectors. Now,

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \tag{4.2}$$

$$\langle b^{(k)}|\alpha\rangle = \sum_l \langle b^{(k)}|a^{(l)}\rangle\langle a^{(l)}|\alpha\rangle = \sum_l \langle a^{(k)}|U^\dagger|a^{(l)}\rangle\langle a^{(l)}|\alpha\rangle \tag{4.3}$$

In Equation (4.3), $\langle b^{(k)}|\alpha\rangle$ is the column matrix in the new basis $\{|b'\rangle\}$ and $\langle a^{(l)}|\alpha\rangle$ is the column matrix in the old basis $\{|a'\rangle\}$. The matrix representation of $U^\dagger$ is $\sum_l \langle a^{(k)}|U^\dagger|a^{(l)}\rangle$.

The relation between old matrix element and new matrix element is

$$\begin{aligned}\langle b^{(k)}|X|b^{(l)}\rangle &= \sum_m \sum_n \langle b^{(k)}|a^{(m)}\rangle\langle a^{(m)}|X|a^{(n)}\rangle\langle a^{(n)}|b^{(l)}\rangle \\ &= \sum_m \sum n \langle a^{(k)}|U^\dagger|a^{(m)}\rangle\langle a^{(m)}|X|a^{(n)}\rangle\langle a^{(n)}|U|a^{(l)}\rangle\end{aligned} \tag{4.4}$$

which is the formula for a *similarity transformation*: $X' = U^\dagger X U$.

The trace of an operator is defined as

$$tr(X) = \sum_{a'} \langle a'|X|a'\rangle \tag{4.5}$$

<u>Theorem</u> Trace is independent of representation.

<u>Proof</u>

$$\begin{aligned}\sum_{a'}\langle a'|X|a'\rangle &= \sum_{a'}\sum_{b'}\sum_{b''}\langle a'|b'\rangle\langle b'|X|b''\rangle\langle b''|a'\rangle \\ &= \sum_{b'}\sum_{b''}\langle b''|b'\rangle\langle b'|X|b''\rangle \\ &= \sum_{b'}\langle b'|X|b'\rangle\end{aligned} \tag{4.6}$$

Some properties of the trace:

$$tr(XY) = tr(YX) \tag{4.7a}$$

$$tr(U^{\dagger}XU) = tr(X) \tag{4.7b}$$

$$tr\Big(|a'\rangle\langle a''|\Big) = \delta_{a'a''} \tag{4.7c}$$

$$tr\Big(|b'\rangle\langle a'|\Big) = \langle a'|b'\rangle \tag{4.7d}$$

Diagonalization

Let $\{|a'\rangle\}$ be known. How to obtain b' and $|b'\rangle$ similarity transformation?

$$B|b'\rangle = b'|b'\rangle \tag{4.8}$$

$$\Longrightarrow \sum_{a'}\langle a''|B|a'\rangle\langle a'|b'\rangle = b'\langle a''|b'\rangle \tag{4.9}$$

If

$$B_{ij} = \langle a^{(i)}|B|a^{(j)}\rangle \tag{4.10a}$$

$$C_k^{(l)} = \langle a^{(k)}|b^{(l)}\rangle \tag{4.10b}$$

$$\begin{bmatrix} B_{11} & B_{12} & \dots \\ B_{21} & B_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix}\begin{bmatrix} C_1^{(l)} \\ C_2^{(l)} \\ \vdots \end{bmatrix} = b^{(l)}\begin{bmatrix} C_1^{(l)} \\ C_2^{(l)} \\ \vdots \end{bmatrix} \tag{4.11}$$

where $i, j, k \;\rightarrow\; 1, \ldots, N$.

Non-trivial solution results in the characteristic equation

$$\det(B - \lambda 1) = 0 \tag{4.12}$$

Comparing $C_k^{(l)}$ in Equation (4.10) with $\langle a^{(k)}|U|a^{(l)}\rangle = \langle a^{(k)}|b^{(l)}\rangle$, we find that the $C_k^{(l)}$s are elements of the unitary matrix that changes basis $\{|a'\rangle\} \rightarrow \{|b'\rangle\}$. Remember that the Hermiticity of B is important.

<u>Theorem</u> Consider two sets of orthonormal bases $\{|a'\rangle\}$ and $\{|b'\rangle\}$. Let there be a unitary operator U that acts on $\{|a'\rangle\}$ such that $\{|a'\rangle\} \rightarrow \{|b'\rangle\}$. Knowing U, we may construct a *unitary transform* of A, UAU^{-1}. A and UAU^{-1} are called *unitary equivalent observables.*

<u>Proof</u>

$$A|a^{(l)}\rangle = a^{(l)}|a^{(l)}\rangle \tag{4.13}$$

$$\Longrightarrow \; UAU^{-1}U|a^{(l)}\rangle = a^{(l)}U|a^{(l)}\rangle \tag{4.14}$$

$$\Longrightarrow \; (UAU^{-1})|b^{(l)}\rangle = a^{(l)}|b^{(l)}\rangle \tag{4.15}$$

Therefore, $|b'\rangle$s are eigenkets of UAU^-1 with exactly the same eigenvalues as A. Unitary equivalent observables have identical spectra.

Now,

$$B|b^{(l)}\rangle = b^{(l)}|b^{(l)}\rangle \tag{4.16}$$

B and UAU^{-1} are simultaneously diagonalizable.

Question Is UAU^{-1} the same as B itself?

Answer

Yes, sometimes. For example, consider $S_x \to US_z$. S_x and S_z have the same set of eigenvalues $\pm\frac{\hbar}{2}$.

Position, Momentum, and Translation

In quantum mechanics, we have observables with continuous spectra (e.g. $p_x : -\infty \to +\infty$).

The eigenvalue equation, for instance, becomes

$$\xi|\xi'\rangle = \xi'|\xi'\rangle \tag{4.17}$$

Also,

$$\langle a'|a''\rangle = \delta_{a'a''} \;\to\; \langle \xi'|\xi''\rangle = \delta(\xi' - \xi'') \tag{4.18a}$$

$$\sum_{a'} |a'\rangle\langle a'| = 1 \;\to\; \int d\xi' |\xi'\rangle\langle\xi'| = 1 \tag{4.18b}$$

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \;\to\; \int d\xi' |\xi'\rangle\langle\xi'|\alpha\rangle \tag{4.18c}$$

$$\sum_{a'} |\langle a'|\alpha\rangle|^2 = 1 \;\to\; \int d\xi' |\langle\xi'|\alpha|^2 = 1 \tag{4.18d}$$

$$\langle\beta|\alpha\rangle = \sum a'\langle\beta|a'\rangle\langle a'|\alpha\rangle \;\to\; \langle\beta|\alpha\rangle = \int d\xi' \langle\beta|\xi'\rangle\langle\xi'|\alpha\rangle \tag{4.18e}$$

$$\langle a''|A|a'\rangle = a'\delta_{a'a''} \;\to\; \langle\xi''|\xi|\xi'\rangle = \xi'\delta(\xi'' - \xi') \tag{4.18f}$$

Now, let eigenkets of the position operator x satisfy

$$x|x'\rangle = x'|x'\rangle \tag{4.19}$$

For any arbitrary state ket $|\alpha\rangle$, we have

$$|\alpha\rangle = \int_{-\infty}^{+\infty} dx' |x'\rangle\langle x'|\alpha\rangle \tag{4.20}$$

When $|\alpha\rangle$ is normalized,

$$\langle\alpha|\alpha\rangle = \int_{-\infty}^{+\infty} dx' \langle\alpha|x'\rangle\langle x'|\alpha\rangle = 1 \tag{4.21}$$

Note: The same can be easily extended to three dimensions.

In general,

$$[x_i, x_j] = 0 \tag{4.22}$$

All three components of the position vector can be measured simultaneously with arbitrary degrees of accuracy.

Two results to note:

(i) The infinitesimal translation operator:

$$T(d\bar{x}') = 1 - \frac{i\bar{p} \cdot d\bar{x}'}{\hbar} \tag{4.23a}$$

$$[x_i, p_j] = i\hbar\delta_{ij} \tag{4.23b}$$

It is impossible to find simultaneous eigenkets of x and p_x (or y and p_y; z and p_z).

(ii) Position-momentum uncertainty (Heisenberg's uncertainty relation):

$$\langle(\Delta x)^2\rangle\langle(\Delta p_x)^2\rangle \geq \frac{\hbar^2}{4} \tag{4.24}$$

$$[p_i, p_j] = 0 \tag{4.25}$$

Translatin in different directions commute (the translation in 3-D is an Abelian group, therefore the generators for the transformation, i.e. p_is, commute).

$$[x_i, x_j] = 0 \tag{4.26a}$$

$$[p_i, p_j] = 0 \tag{4.26b}$$

$$[x_i, p_j] = i\hbar\delta_{ij} \tag{4.26c}$$

Canonical Commutation Relations

$$[A, A] = 0 \tag{4.27a}$$

$$[A, B] = -[B, A] \tag{4.27b}$$

$$[A, c] = 0 \tag{4.27c}$$

$$[A + B, C] = [A, C] + [B, C] \tag{4.27d}$$

$$[A, BC] = [A, B]C + B[A, C] \tag{4.27e}$$

$$[A[B, C]] + [B, [C, A]] + [C, [A, B]] = 0 \tag{4.27f}$$

where c is a number in Equation (4.27c), and Equation (4.27f) is known as the Jacobi identity.

Position Space Wave Function

$$x|x'\rangle = x'|x'\rangle \tag{4.28}$$

$$\langle x''|x'\rangle = \delta(x'' - x') \tag{4.29}$$

$$|\alpha\rangle = \int dx'|x'\rangle\langle x'|\alpha\rangle \tag{4.30}$$

$|\langle x'|\alpha\rangle|^2 \;\rightarrow\;$ probability that the particle is found in $x' \pm dx'$.

The wave function for state $|\alpha\rangle$ is

$$\langle x'|\alpha\rangle = \psi_\alpha(x') \tag{4.31}$$

We interpret the inner product $\langle\beta|\alpha\rangle$ to be the overlap between two wave functions. In other words, it is the probability amplitude for the state $|\alpha\rangle$ to be found in the state $|\beta\rangle$. We can write it as

$$\langle\beta|\alpha\rangle = \int dx' \langle\beta|x'\rangle\langle x'|\alpha\rangle = \int dx' \psi_\beta^*(x')\psi_\alpha(x') \tag{4.32}$$

Again,

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \tag{4.33}$$

$$\Longrightarrow\;\; \langle x'|\alpha\rangle = \sum_{a'} \langle x'|a'\rangle\langle a'|\alpha\rangle \tag{4.34}$$

$$\Longrightarrow\;\; \psi_\alpha(x') = \sum_{a'} c_{a'} u_{a'}(x') \tag{4.35}$$

where $u_{a'}(x') = \langle x'|a'\rangle$ is the eigenfunction of the operator A with eigenvalue a'.

Also,

$$\langle\beta|A|\alpha\rangle = \int dx' \int dx'' \langle\beta|x'\rangle\langle x'|A|x''\rangle\langle x''|\alpha\rangle = \int dx' \int dx'' \psi_\beta^*(x')\langle x'|A|x''\rangle\psi_\alpha(x') \tag{4.36}$$

For example, let $A = x^2$.

$$\Longrightarrow\;\; \langle x'|x^2|x''\rangle = (\langle x'|) \cdot ({x''}^2|x'') = {x'}^2\delta(x'-x'') \tag{4.37}$$

$$\implies \langle\beta|x^2|\alpha\rangle = \int dx'\langle\beta|x'\rangle {x'}^2\langle x'|\alpha\rangle = \int dx'\psi_\beta^*(x'){x'}^2\psi_\alpha(x') \tag{4.38}$$

In general, for any operator $f(x)$ and number $f(x')$,

$$\langle\beta|f(x)|\alpha\rangle = \int dx'\psi_\beta^*(x')f(x')\psi_\alpha(x') \tag{4.39}$$

Momentum Operator in Position Basis

Recall that $\left(1 - \frac{ip\Delta x'}{\hbar}\right) \rightarrow T(\Delta x')$.

$$\begin{aligned} T(\Delta x')|\alpha\rangle &= \int dx' T(\Delta x')|x'\rangle\langle x'|\alpha\rangle \\ &= \int dx'|x'+\Delta x'\rangle\langle x'|\alpha\rangle \\ &= \int dx'|x'\rangle\langle x'-\Delta x'|\alpha\rangle \\ &= \int dx'|x'\rangle\Big(\langle x'|\alpha\rangle - \Delta x'\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\Big) \end{aligned} \tag{4.40}$$

Comparing the LHS and RHS yields

$$p|\alpha\rangle = \int dx'|x'\rangle\Big(-i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\Big) \tag{4.41}$$

$$\langle x'|p|\alpha\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle \tag{4.42}$$

Matrix element p in x-representation:

$$\langle x'|p|x''\rangle = -i\hbar\frac{\partial}{\partial x'}\delta(x'-x'') \tag{4.43}$$

References