Notes on Quantum Mechanics

Richard Camuccio
Department of Physics and Astronomy
University of Texas Rio Grande Valley

11 March 2019

These notes are collected and printed from lectures given by Soma Mukherjee and Soumya Mohanty during the Spring 2019 semester at the University of Texas Rio Grande Valley. Also included are notes taken from J. J. Sakurai's *Modern Quantum Mechanics* (Revised Edition), D. J. Griffiths' *Introduction to Quantum Mechanics* (2nd edition), and E. Merzbacher's *Quantum Mechanics*. As you will surely note, I am constantly adding and revising material in these notes. My hope is that eventually they will be intelligible. I appreciate feedback on these notes.

Contents

1 Kets, Bras, and Operators

The state of a system classically is defined by a vector in a vector space. In classical mechanics, we assume that any act of measurement does not affect the system being measured. In principle, one could measure the position and momentum of a particle simultaneously to an infinite precision. Quantum mechanics tells us that, in reality, we cannot access the state of a system directly. We can only make measurements of quantities which we represent as operators on a state.

In quantum mechanics, we consider the state of a system to be represented by a vector in a vector space. In general, this vector space is infinite, but we must tread carefully with the subtle mathematical reasoning.

Given a finite, N-dimensional vector space V, then, for any vector $\vec{v} \in V$, we have

$$\vec{v} = \sum_{k=1}^{N} \alpha_k \vec{e}_k \tag{1}$$

Suppose we generalize this finite-dimensional vector space to an infinite-dimensional vector space. Then, we have

$$\vec{v} = \sum_{k=1}^{\infty} \alpha_k \vec{e}_k \tag{2}$$

But this is a problem. We could possibly produce a divergent set or produce a member outside of the set (since taking an infinite sum need not be in the set e.g. sum of rational numbers $\longrightarrow$ irrational numbers). How do we counter that? We say that the vector space is a Hilbert space. Then every convergent sum yields a vector in the space. This property guarantees us a basis. Therefore,

$$\vec{v} = \sum_{k=1}^{\infty} \alpha_k \vec{e}_k \tag{3}$$

is valid given that V is a Hilbert space. Then every convergent sum belongs to V.

We usually indicate a finite numbers of dimensions, N, of the vector space under consideration. For many physical systems the dimension of the state space is denumerably infinite. Consider, for example, the denumerably-infinite dimensions of a harmonic oscillator with infinite, yet discrete energy levels. The results that follow consider finite spaces, although they extend to cases with denumerably infinite dimensions as well.

1.1 Ket Space

In quantum mechanics, a *physical state* is represented by a *state vector* (e.g. an atom with definite spin orientation) in an infinite-dimensional complex vector space, or *Hilbert space*. A Hilbert space is specifically the case of continuous spectra (position, momentum), where the number of alternatives is nondenumerably infinite.

Dirac notation: A state vector $|\alpha\rangle$ is in a complex vector space and is referred to as a 'state ket'. The state ket contains complete information about the physical state and everything we are allowed to ask about the system is contained within it.

Two kets obey addition

$$|\alpha\rangle + |\beta\rangle = |\gamma\rangle \tag{4}$$

where the sum $|\gamma\rangle$ is just another state ket. We can also multiply the ket by a complex number c such that

$$c|\alpha\rangle = |\alpha\rangle c \tag{5}$$

(where it makes no difference if c is on the right or left side). If $c = 0$, the result is called *null ket* $|0\rangle$.

Postulate One of the physics postulates is that $|\alpha\rangle$ and $c|\alpha\rangle$ (with $c \neq 0$) represent the same physical state. Only the direction in the vector space is significant (mathematically-speaking we are dealing with rays and not vectors).

An *observable* in quantum mechanics is represented by an *operator* A (e.g. position, momentum, or spin components) and which acts on a ket from the left,

$$A \cdot (|\alpha\rangle) = A|\alpha\rangle \tag{6}$$

which is yet another ket. In general, $A|\alpha\rangle$ is not a constant A times $|\alpha\rangle$. There are special kets, called *eigenkets* of operator A, denoted by

$$|a'\rangle,\ |a''\rangle,\ \cdots \tag{7}$$

and have the particular property that

$$\begin{aligned} A|a'\rangle &= a'|a'\rangle, \\ A|a''\rangle &= a''|a''\rangle, \\ &\cdots, \end{aligned} \tag{8}$$

where $a',\ a'',\ \cdots$, are numbers called the *eigenvalues* of A. The whole set of eigenvalues are denoted by $\{a'\}$ and can be expanded with notation either like $\{a', a'', a''', \cdots\}$ or $\{a^{(1)}, a^{(2)}, a^{(3)}, \cdots\}$. The physical state corresponding to an eigenket is called an *eigenstate*.

Example Consider a spin $\frac{1}{2}$ system, which is the simplest case of an eigenstate. The eigenvalue-eigenket relation is expressed as

$$S_z|S_z;\pm\rangle = \pm\frac{\hbar}{2}|S_z;\pm\rangle \tag{9}$$

where S_z is an operator, $|S_z;\pm\rangle$ are the eigenkets, and $\pm\frac{\hbar}{2}$ are eigenvalues. We can consider eigenkets of S_x and S_y as well:

$$S_x|S_x;\pm\rangle = \pm\frac{\hbar}{2}|S_x;\pm\rangle \tag{10}$$

$$S_y|S_y;\pm\rangle = \pm\frac{\hbar}{2}|S_y;\pm\rangle \tag{11}$$

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:

$$|\alpha\rangle = \sum_{a'} c_{a'}|a'\rangle \tag{12}$$

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 orthogonality of eigenkets must first be proven, before proving the uniqueness of such an expansion.

1.2 Bra Space and Inner Products

The *bra space* is a vector space dual to the ket space. We postulate that, corresponding to every ket $|\alpha\rangle$, $\exists\ \langle\alpha|$ in a dual, or bra, space. The bra space is spanned by eigenbras $\{\langle a'|\}$, which correspond to the eigenkets $\{|a'\rangle\}$. There is a dual correspondence between the bra and ket spaces:

$$|\alpha\rangle \longleftrightarrow \langle\alpha| \tag{13a}$$

$$|a'\rangle,\ |a''\rangle,\ \cdots \longleftrightarrow \langle a'|,\ \langle a''|,\ \cdots \tag{13b}$$

$$|\alpha\rangle + |\beta\rangle \longleftrightarrow \langle\alpha| + \langle\beta| \tag{13c}$$

We can roughly conceive of the bra space as a kind of mirror image of the ket space. We postulate that the bra dual to $c|\alpha\rangle$ is $c^*\langle\alpha|$. In general, we have the dual correspondence

$$c_\alpha|\alpha\rangle + c_\beta|\beta\rangle \longleftrightarrow c_\alpha^*\langle\alpha| + c_\beta^*\langle\beta| \tag{14}$$

We define the inner product of a bra and ket. The product is a bra standing on the left and a ket standing on the right, for example

$$\langle\beta|\alpha\rangle \equiv (\langle\beta|) \cdot (|\alpha\rangle) \tag{15}$$

where the product of the bra and the ket forms a "bra(c)ket" and is, in general, a complex number. In forming an inner product, we always take one vector from the bra space and one vector from the ket space.

We also state some fundamental properties of the dual correspondence. First, we note that $\langle\beta|\alpha\rangle$ and $\langle\alpha|\beta\rangle$ are complex conjugates of each other

$$\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^* \tag{16}$$

We must make a distinction between $\langle\beta|\alpha\rangle$ and $\langle\alpha|\beta\rangle$. The inner product is analogous to the scalar product $\vec{a}\cdot\vec{b}$ in three-dimensional Euclidean space, except for the need of the distinction since $\vec{a}\cdot\vec{b} = \vec{b}\cdot\vec{a}$ in real vector space.

Letting $\langle\beta| \longrightarrow \langle\alpha|$, we deduce that $\langle\alpha|\alpha\rangle$ must be a real number:

$$\langle\alpha|\alpha\rangle = \langle\alpha|\alpha\rangle^* \tag{17}$$

The second postulate on inner products is

$$\langle\alpha|\alpha\rangle \geq 0 \tag{18}$$

where the equality sign holds only if $|\alpha\rangle$ is a null ket. The postulate is sometimes known as the postulate of *positive definite metric*. From a physicist's point of view, this postulate is essential for the probabilistic interpretation of quantum mechanics. Attempts to abandon this postulate have led to physical theories with "indefinite metric."

Two kets are *orthogonal* if

$$\langle\alpha|\beta\rangle = 0 \tag{19}$$

and also

$$\langle\beta|\alpha\rangle = 0 \tag{20}$$

Given a ket which is not a null ket, we can form a *normalized ket* $|\tilde{\alpha}\rangle$, where

$$|\tilde{\alpha}\rangle = \left(\frac{1}{\sqrt{\langle\alpha|\alpha\rangle}}\right)|\alpha\rangle \tag{21}$$

with the property

$$\langle\tilde{\alpha}|\tilde{\alpha}\rangle = 1 \tag{22}$$

In general, $\sqrt{\langle\alpha|\alpha\rangle}$ is known as the *norm* of $|\alpha\rangle$, which is analogous to the magnitude of vector $\sqrt{\vec{a}\cdot\vec{a}} = |\vec{a}|$ in Euclidean vector space. By postulating that $|\alpha\rangle$ and $c|\alpha\rangle$ represent the same physical state, we might as well require that the kets we use for physical states be normalized in the sense of $\langle\tilde{\alpha}|\tilde{\alpha}\rangle$. For eigenkets of observables with continuous spectra, different normalization conventions are used.

1.3 Operators

Physical observables are represented by operators that act on kets. An operator X acts on a ket $|\alpha\rangle$ from the left side resulting in another ket:

$$X \cdot (|\alpha\rangle) = X|\alpha\rangle \tag{23}$$

Let there be *equal* operators X and Yjaj such that:

$$X = Y \implies X|\alpha\rangle = Y|\alpha\rangle \tag{24}$$

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

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

$$X + Y = Y + X \tag{25}$$

They satisfy the associative property as well:

$$X + (Y + Z) = (X + Y) + Z \tag{26}$$

The operator X is a linear operator:

$$X(c_\alpha|\alpha\rangle + c_\beta|\beta\rangle) = c_\alpha X|\alpha\rangle + c_\beta X|\beta\rangle \tag{27}$$

Note the following:

$$X|\alpha\rangle \leftrightarrow \langle\alpha|X^\dagger \tag{28}$$

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

$$X = X^\dagger \tag{29}$$

Multiplication of operators is not commutative:

$$XY \neq YX \tag{30}$$

Multiplication is associative:

$$X(YZ) = (XY)Z = XYZ \tag{31}$$

$$X(Y|\alpha\rangle) = (XY)|\alpha\rangle = XY|\alpha\rangle \tag{32a}$$

$$(\langle\beta|X)Y = \langle\beta|(XY) = \langle\beta|XY \tag{32b}$$

Note that:

$$(XY)^\dagger = Y^\dagger X^\dagger \tag{33}$$

Proof of Equation (33)

$$XY|\alpha\rangle = X(Y|\alpha\rangle) \leftrightarrow (\langle\alpha\ Y^\dagger)X^\dagger = \langle\alpha|Y^\dagger X^\dagger \tag{34}$$

The *outer product* is defined as:

$$|\beta\rangle\langle\alpha| \tag{35}$$

1.4 The Associative Axiom

Let

$$(|\beta\rangle\langle\alpha|)\cdot|\gamma\rangle = |\beta\rangle\cdot(\langle\alpha|\gamma\rangle) \tag{36}$$

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

$$X = |\beta\rangle \implies X^\dagger = |\alpha\rangle\langle\beta| \tag{37}$$

Again,

$$(\langle\beta|\cdot(X|\alpha\rangle) = (\langle\beta|X)\cdot(|\alpha\rangle) \tag{38}$$

We write this in a compact form as

$$\langle\beta|X|\alpha\rangle \tag{39}$$

for both the right- and left-hand sides.

$$\implies \langle\beta|X|\alpha\rangle = \langle\beta|\cdot(X|\alpha\rangle) = (\langle\alpha|X^\dagger)\cdot|\beta\rangle^* = \langle\alpha|X^\dagger|\beta\rangle^* \tag{40}$$

For a Hermitian operator X,

$$\langle\beta|X|\alpha\rangle = \langle\alpha|X|\beta\rangle^* \tag{41}$$

1.5 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

$$A|\alpha'\rangle = a'|a'\rangle \tag{42}$$

A is Hermitian, so

$$\langle\alpha''|A = \alpha''^{*}\langle\alpha''| \tag{43}$$

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

From Equation (42), $\langle\alpha''|A|\alpha'\rangle = \langle\alpha''|\alpha'|\alpha'\rangle$

$$\implies (\alpha' - \alpha''^{*})\langle\alpha''|\alpha'\rangle = 0 \tag{44}$$

Now, Equation (44) 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 (44), $(\alpha' - \alpha'')\langle\alpha''|\alpha'\rangle = 0$, 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:

$$\langle\alpha''|\alpha'\rangle = \delta_{\alpha'\alpha''} \tag{45}$$

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.

$$|\alpha\rangle = \sum_{a'} c_{a'} |a'\rangle \tag{46}$$

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

$$c_{a'} = \langle a'|\alpha\rangle \tag{47}$$

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \tag{48}$$

$$\sum_{a'} |a'\rangle\langle a'| = 1 \tag{49}$$

Equation (49) is the completeness, or closure, property, and 1 is the identity operator.

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

$$= \sum_{a'} |\langle a'|\alpha\rangle|^2 \tag{50}$$

$$\sum_{a'} |c_{a'}|^2 = \sum_{a'} |\langle a'|\alpha\rangle|^2 = 1 \tag{51}$$

Equation (51) assumes that $|\alpha\rangle$ is normalized. Also, $\Lambda_{a'} = |a'\rangle\langle a'|$ is called the *projection operator*.

2.1 Matrix Representation

Let us write an operator X such that

$$X = \sum_{a''} \sum_{a'} |a''\rangle\langle a''|X|a'\rangle\langle a'| \tag{52}$$

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

$$X = \begin{bmatrix} \langle a^{(1)}|X|a^{(1)}\rangle & \langle a^{(1)}|X|a^{(2)}\rangle & \dots \\ \langle a^{(2)}|X|a^{(1)}\rangle & \langle a^{(2)}|X|a^{(2)}\rangle & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} \tag{53}$$

Again,

$$\langle a''|X|a'\rangle = \langle a'|X^{\dagger}|a''\rangle \tag{54}$$

Note: Equation (54) involves a Hermitian adjoint operation $\equiv$ complex conjugate transposed.

If we have an operator B which is Hermitian, then

$$\langle a''|B|a'\rangle = \langle a'|X|a''\rangle^{*} \tag{55}$$

Let $Z = XY$. Then we have

$$\langle a''|Z|a'\rangle = \langle a''|XY|a'\rangle = \sum_{a'''}\langle a''|X|a'''\rangle\langle a'''|Y|a'\rangle \tag{56}$$

which satisfies the rule of matrix multiplication.

Let us now consider

$$|\gamma\rangle = X|\alpha\rangle. \tag{57}$$

This immediately leads to the implication that

$$\langle a'|\gamma\rangle = \langle a'|X|\alpha\rangle = \sum_{a''}\langle a'|X|a''\rangle\langle a''|\alpha\rangle \tag{58}$$

Equation (58) is akin to matrix multiplication rule with column matrices

$$|\alpha\rangle = \begin{bmatrix} \langle a^{(1)}|\alpha\rangle \\ \langle a^{(2)}|\alpha\rangle \\ \vdots \end{bmatrix}, |\gamma\rangle = \begin{bmatrix} \langle a^{(1)}|\gamma\rangle \\ \langle a^{(2)}|\gamma\rangle \\ \vdots \end{bmatrix} \tag{59}$$

Likewise,

$$\langle\gamma| = \langle\alpha|X \tag{60}$$

which gives us

$$\langle\gamma|a'\rangle = \sum_{a''}\langle\alpha|a''\rangle\langle a''|X|a'\rangle \tag{61}$$

The bra vector is represented by a row matrix

$$\langle\gamma| = \begin{bmatrix}\langle\gamma|a^{(1)}\rangle & \langle\gamma|a^{(2)}\rangle & \dots\end{bmatrix} = \begin{bmatrix}\langle a^{(1)}|\gamma\rangle^* & \langle a^{(2)}|\gamma\rangle^* & \dots\end{bmatrix} \tag{62}$$

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

$$\langle\beta|\alpha\rangle = \sum_{a'}\langle\beta|a'\rangle\langle a'|\alpha\rangle = \begin{bmatrix}\langle a^{(1)}|\beta\rangle^* & \langle a^{(2)}|\beta\rangle^* & \dots\end{bmatrix}\begin{bmatrix}\langle a^{(1)}|\alpha\rangle \\ \langle a^{(2)}|\alpha\rangle \\ \vdots\end{bmatrix} \tag{63}$$

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

$$A = \sum_{a''}\sum_{a'}|a''\rangle\langle a''|A|a'\rangle\langle a'| \tag{64}$$

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

$$\langle a''|A|a'\rangle = \langle a'|A|a'\rangle\delta_{a'a''} = a'\delta_{a'a''} \tag{65}$$

Therefore,

$$A = \sum_{a'} a'|a'\rangle\langle a'| = \sum_{a'} a'\Lambda_{a'} \tag{66}$$

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:

$$1 = |+\rangle\langle+| + |-\rangle\langle-| \tag{67}$$

From Equation (66) we can write

$$S_z = \left(\frac{\hbar}{2}\right)\left[\Big(|+\rangle\langle+|\Big) + \Big(|-\rangle\langle-|\Big)\right] \tag{68}$$

We have the eigenvalue relation

$$S_z|\pm\rangle = \pm\left(\frac{\hbar}{2}\right)|\pm\rangle \tag{69}$$

Let us now look at the other components:

$$S_+ \equiv \hbar|+\rangle\langle-|, \quad S_- \equiv \hbar|-\rangle\langle+| \tag{70}$$

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:

$$|+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |-\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{71}$$

$$S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad S_+ = \hbar\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad S_- = \hbar\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \tag{72}$$

2.2 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:

$$|\alpha\rangle = \sum_{a'} c_{a'}|a'\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \tag{73}$$

After measurement:

$$|\alpha\rangle \rightarrow |a'\rangle \tag{74}$$

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

$$|\langle a'|\alpha\rangle|^2 \tag{75}$$

A collection of identically prepared systems all in the same state (e.g. $|\alpha\rangle$) are a *pure ensemble*. Equation (75) is one of the fundamental postulates of quantum mechanics. We define the *expectation value* of A taken with respect to state $|\alpha\rangle$ as

$$\langle A\rangle = \langle\alpha|A|\alpha\rangle \tag{76}$$

$$\langle A\rangle = \sum_{a'}\sum_{a''}\langle\alpha|a''\rangle\langle a''|A|a'\rangle\langle a'|\alpha\rangle = \sum_{a'} a'|\langle a'|\alpha\rangle|^2 \tag{77}$$

3 Commutators, Uncertainty Relation, and Change of Basis

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

$$[A, B] = AB - BA \tag{78a}$$

$$\{A, B\} = AB + BA \tag{78b}$$

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*.

<u>Theorem</u> 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.

<u>Proof</u>

$$\langle a''|[A, B]|a'\rangle = \langle a''|AB - BA|a'\rangle = (a'' - a')\langle a''|B|a'\rangle = 0 \tag{79}$$

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.

$$B = \sum_{a''} |a''\rangle\langle a''|B|a''\rangle\langle a''| \tag{80}$$

Therefore,

$$B|a'\rangle = \sum_{a''} |a''\rangle\langle a''|B|a''\rangle\langle a''|a'\rangle = \Big(\langle a'|B|a'\rangle\Big) \cdot |a'\rangle \tag{81}$$

Equation (81) is the eigenvalue equation of B with eigenvalue b', where

$$b' = \langle a'|B|a'\rangle \tag{82}$$

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:

$$A|a', b'\rangle = a'|a', b'\rangle \tag{83a}$$

$$B|a', b'\rangle = b'|a', b'\rangle \tag{83b}$$

3.1 Uncertainty Relation

Let us define an operator ΔA as

$$\Delta A = A - \langle A \rangle \tag{84}$$

The dispersion is thus defined as

$$\langle (\Delta A)^2 \rangle = \langle (A^2 - 2A\langle A \rangle + \langle A \rangle^2) \rangle = \langle A^2 \rangle - \langle A \rangle^2 \tag{85}$$

Theorem If A and B are two observables, the following must hold true:

$$\langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq \frac{1}{4} |\langle [A, B] \rangle|^2 \tag{86}$$

Proof

Lemma 1. The Schwarz Inequality is

$$\langle \alpha|\alpha \rangle \langle \beta|\beta \rangle \geq |\langle \alpha|\beta \rangle|^2 \tag{87}$$

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

$$(\langle \alpha| + \lambda^* \langle \beta|) \cdot (|\alpha\rangle + \lambda|\beta\rangle) \geq 0 \tag{88}$$

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

$$\langle \alpha|\alpha \rangle \langle \beta|\beta \rangle - |\langle \alpha|\beta \rangle|^2 \geq 0 \tag{89}$$

which is the Schwarz Inequality written in Equation (87).

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

$$|\alpha\rangle = \Delta A|\rangle \tag{90a}$$

$$|\beta\rangle = \Delta B|\rangle \tag{90b}$$

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

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq |\langle \Delta A \Delta B\rangle|^2 \tag{91}$$

where we note that ΔA and ΔB are Hermitian. By looking at the RHS of Equation (91), we take note that $\Delta A \Delta B$ can be expressed as

$$\Delta A \Delta B = \frac{1}{2}[\Delta A, \Delta B] + \frac{1}{2}\{\Delta A, \Delta B\} \tag{92}$$

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

$$([A, B])^\dagger = (AB - BA)^\dagger = BA - AB = -[A, B] \tag{93}$$

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

$$\langle \Delta A, \Delta B\rangle = \frac{1}{2}\langle [A, B]\rangle + \frac{1}{2}\langle\{\Delta A, \Delta B\}\rangle \tag{94}$$

where the first term on the RHS is imaginary and the second term on the RHS is real. The RHS of Equation (91) is now

$$|\langle \Delta A \Delta B\rangle|^2 = \frac{1}{4}|\langle [A, B]\rangle|^2 + \frac{1}{4}|\langle\{\Delta A, \Delta B\}\rangle|^2 \tag{95}$$

QED.

3.2 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

$$|b'\rangle = U|a'\rangle; \quad |b''\rangle = U|a''\rangle \tag{96}$$

where

$$U^\dagger U = 1, \quad UU^\dagger = 1 \tag{97}$$

Proof

Let

$$U = \sum_k |b^{(k)}\rangle\langle a^{(k)}| \tag{98}$$

$$\implies U|a^{(l)}\rangle = |b^{(l)}\rangle \tag{99}$$

Furthermore,

$$U^\dagger U = \sum_k \sum_l |a^{(l)}\rangle\langle b^{(l)}|b^{(k)}\rangle\langle a^{(k)}| = \sum_k |a^{(k)}\rangle\langle a^{(k)}| = 1 \tag{100}$$

4 Transformation Matrix, Diagonalization, and Physical Observables

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

$$\langle a^{(k)}|U|a^{(l)}\rangle = \langle a^{(k)}|b^{(l)}\rangle \tag{101}$$

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

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \tag{102}$$

$$\langle b^{(k)}|\alpha\rangle = \sum_l \langle b^{(k)}|a^{(l)}\rangle\langle a^{(l)}|\alpha\rangle = \sum_l \langle a^{(k)}|U^\dagger|a^{(l)}\rangle\langle a^{(l)}|\alpha\rangle \tag{103}$$

In Equation (103), $\langle b^{(k)}|\alpha\rangle$ 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

$$\begin{aligned}\langle b^{(k)}|X|b^{(l)}\rangle &= \sum_m \sum_n \langle b^{(k)}|a^{(m)}\rangle\langle a^{(m)}|X|a^{(n)}\rangle\langle a^{(n)}|b^{(l)}\rangle \\ &= \sum_m \sum n \langle a^{(k)}|U^\dagger|a^{(m)}\rangle\langle a^{(m)}|X|a^{(n)}\rangle\langle a^{(n)}|U|a^{(l)}\rangle\end{aligned} \tag{104}$$

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

The trace of an operator is defined as

$$tr(X) = \sum_{a'} \langle a'|X|a'\rangle \tag{105}$$

Theorem Trace is independent of representation.

Proof

$$\begin{aligned}\sum_{a'} \langle a'|X|a'\rangle &= \sum_{a'}\sum_{b'}\sum_{b''} \langle a'|b'\rangle\langle b'|X|b''\rangle\langle b''|a'\rangle \\ &= \sum_{b'}\sum_{b''} \langle b''|b'\rangle\langle b'|X|b''\rangle \\ &= \sum_{b'} \langle b'|X|b'\rangle\end{aligned} \tag{106}$$

Some properties of the trace:

$$tr(XY) = tr(YX) \tag{107a}$$
$$tr(U^\dagger XU) = tr(X) \tag{107b}$$
$$tr\Big(|a'\rangle\langle a''|\Big) = \delta_{a'a''} \tag{107c}$$
$$tr\Big(|b'\rangle\langle a'|\Big) = \langle a'|b'\rangle \tag{107d}$$

4.1 Diagonalization

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

$$B|b'\rangle = b'|b'\rangle \tag{108}$$

$$\implies \sum_{a'} \langle a''|B|a'\rangle\langle a'|b'\rangle = b'\langle a''|b'\rangle \tag{109}$$

If

$$B_{ij} = \langle a^{(i)}|B|a^{(j)}\rangle \tag{110a}$$
$$C_k^{(l)} = \langle a^{(k)}|b^{(l)}\rangle \tag{110b}$$

$$\begin{bmatrix} B_{11} & B_{12} & \dots \\ B_{21} & B_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} C_1^{(l)} \\ C_2^{(l)} \\ \vdots \end{bmatrix} = b^{(l)} \begin{bmatrix} C_1^{(l)} \\ C_2^{(l)} \\ \vdots \end{bmatrix} \tag{111}$$

where $i, j, k \ \rightarrow \ 1, \dots, N$.

Non-trivial solution results in the characteristic equation

$$\det(B - \lambda 1) = 0 \tag{112}$$

Comparing $C_k^{(l)}$ in Equation (110) 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.

Theorem 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 $\{|a'\rangle\} \to \{|b'\rangle\}$. Knowing U, we may construct a *unitary transform* of A, UAU^{-1}. A and UAU^{-1} are called *unitary equivalent observables.*

Proof

$$A|a^{(l)}\rangle = a^{(l)}|a^{(l)}\rangle \tag{113}$$

$$\implies UAU^{-1}U|a^{(l)}\rangle = a^{(l)}U|a^{(l)}\rangle \tag{114}$$

$$\implies (UAU^{-1})|b^{(l)}\rangle = a^{(l)}|b^{(l)}\rangle \tag{115}$$

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

Now,

$$B|b^{(l)}\rangle = b^{(l)}|b^{(l)}\rangle \tag{116}$$

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 $\pm\frac{\hbar}{2}$.

4.2 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

$$\xi|\xi'\rangle = \xi'|\xi'\rangle \tag{117}$$

Also,

$$\langle a'|a''\rangle = \delta_{a'a''} \;\rightarrow\; \langle \xi'|\xi''\rangle = \delta(\xi' - \xi'') \tag{118a}$$

$$\sum_{a'} |a'\rangle\langle a'| = 1 \;\rightarrow\; \int d\xi' |\xi'\rangle\langle \xi'| = 1 \tag{118b}$$

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \;\rightarrow\; \int d\xi' |\xi'\rangle\langle \xi'|\alpha\rangle \tag{118c}$$

$$\sum_{a'} |\langle a'|\alpha\rangle|^2 = 1 \;\rightarrow\; \int d\xi' |\langle \xi'|\alpha|^2 = 1 \tag{118d}$$

$$\langle \beta|\alpha\rangle = \sum a' \langle \beta|a'\rangle\langle a'|\alpha\rangle \;\rightarrow\; \langle \beta|\alpha\rangle = \int d\xi' \langle \beta|\xi'\rangle\langle \xi'|\alpha\rangle \tag{118e}$$

$$\langle a''|A|a'\rangle = a'\delta_{a'a''} \;\rightarrow\; \langle \xi''|\xi|\xi'\rangle = \xi'\delta(\xi'' - \xi') \tag{118f}$$

Now, let eigenkets of the position operator x satisfy

$$x|x'\rangle = x'|x'\rangle \tag{119}$$

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

$$|\alpha\rangle = \int_{-\infty}^{+\infty} dx' |x'\rangle\langle x'|\alpha\rangle \tag{120}$$

When $|\alpha\rangle$ is normalized,

$$\langle \alpha|\alpha\rangle = \int_{-\infty}^{+\infty} dx' \langle \alpha|x'\rangle\langle x'|\alpha\rangle = 1 \tag{121}$$

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

In general,

$$[x_i, x_j] = 0 \tag{122}$$

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:

$$T(d\bar{x}') = 1 - \frac{i\bar{p}\cdot d\bar{x}'}{\hbar} \tag{123a}$$

$$[x_i, p_j] = i\hbar\delta_{ij} \tag{123b}$$

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):

$$\langle(\Delta x)^2\rangle\langle(\Delta p_x)^2\rangle \geq \frac{\hbar^2}{4} \tag{124}$$

$$[p_i, p_j] = 0 \tag{125}$$

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

$$[x_i, x_j] = 0 \tag{126a}$$

$$[p_i, p_j] = 0 \tag{126b}$$

$$[x_i, p_j] = i\hbar\delta_{ij} \tag{126c}$$

4.3 Canonical Commutation Relations

$$[A, A] = 0 \tag{127a}$$

$$[A, B] = -[B, A] \tag{127b}$$

$$[A, c] = 0 \tag{127c}$$

$$[A + B, C] = [A, C] + [B, C] \tag{127d}$$

$$[A, BC] = [A, B]C + B[A, C] \tag{127e}$$

$$[A[B, C]] + [B, [C, A]] + [C, [A, B]] = 0 \tag{127f}$$

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

4.4 Position Space Wave Function

$$x|x'\rangle = x'|x'\rangle \tag{128}$$

$$\langle x''|x'\rangle = \delta(x'' - x') \tag{129}$$

$$|\alpha\rangle = \int dx'|x'\rangle\langle x'|\alpha\rangle \tag{130}$$

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

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

$$\langle x'|\alpha\rangle = \psi_\alpha(x') \tag{131}$$

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

$$\langle\beta|\alpha\rangle = \int dx' \langle\beta|x'\rangle\langle x'|\alpha\rangle = \int dx' \psi_\beta^*(x')\psi_\alpha(x') \tag{132}$$

Again,

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \tag{133}$$

$$\Longrightarrow \; \langle x'|\alpha\rangle = \sum_{a'} \langle x'|a'\rangle\langle a'|\alpha\rangle \tag{134}$$

$$\Longrightarrow \; \psi_\alpha(x') = \sum_{a'} c_{a'} u_{a'}(x') \tag{135}$$

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

Also,

$$\langle\beta|A|\alpha\rangle = \int dx' \int dx'' \langle\beta|x'\rangle\langle x'|A|x''\rangle\langle x''|\alpha\rangle = \int dx' \int dx'' \psi_\beta^*(x')\langle x'|A|x''\rangle\psi_\alpha(x') \tag{136}$$

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

$$\Longrightarrow \; \langle x'|x^2|x''\rangle = (\langle x'|) \cdot ({x''}^2|x''\rangle) = {x'}^2\delta(x' - x'') \tag{137}$$

$$\Longrightarrow \; \langle\beta|x^2|\alpha\rangle = \int dx' \langle\beta|x'\rangle {x'}^2 \langle x'|\alpha\rangle = \int dx' \psi_\beta^*(x'){x'}^2\psi_\alpha(x') \tag{138}$$

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

$$\langle\beta|f(x)|\alpha\rangle = \int dx' \psi_\beta^*(x') f(x')\psi_\alpha(x') \tag{139}$$

4.5 Momentum Operator in Position Basis

We are interested in considering how the momentum operator looks in the x-basis. In other words, we are interested in seeing the representation of where the position eigenkets are used as base kets.

Recall the definition of the momentum as the generator of infinitesimal translations

$$T(\Delta x') \longrightarrow \Big(1 - \frac{ip\Delta x'}{\hbar}\Big) \tag{140}$$

First, we have the operator act on the state ket $|\alpha\rangle$

$$T(\Delta x')|\alpha\rangle = \int dx' T(\Delta x')|x'\rangle\langle x'|\alpha\rangle \tag{141}$$

where we have introduced closure on the RHS involving the position eigenkets. The infinitesimal translation operator acts on the position eigenket $|x'\rangle$ such that

$$T(\Delta x')|\alpha\rangle = \int dx'|x' + \Delta x'\rangle\langle x'|\alpha\rangle \tag{142}$$

We then make a change of origin

$$T(\Delta x')|\alpha\rangle = \int dx'|x'\rangle\langle x' - \Delta x'|\alpha\rangle \tag{143}$$

$$= \int dx'|x'\rangle\Big(\langle x'|\alpha\rangle - \Delta x'\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\Big) \tag{144}$$

We make a comparison of the LHS and the RHS such that

$$\implies \Big(1 - \frac{ip\Delta x'}{\hbar}\Big)|\alpha\rangle = \int dx'|x'\rangle\Big(\langle x'|\alpha\rangle - \Delta x'\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\Big) \tag{145}$$

$$\implies |\alpha\rangle - \frac{ip\Delta x'}{\hbar}|\alpha\rangle = \int dx'|x'\rangle\langle x'|\alpha\rangle - \int dx'|x'\rangle\Delta x'\frac{\partial}{\partial x'}\langle x'|\alpha\rangle \tag{146}$$

$$\implies |\alpha\rangle - \frac{ip\Delta x'}{\hbar}|\alpha\rangle = |\alpha\rangle - \int dx'|x'\rangle\Delta x'\frac{\partial}{\partial x'}\langle x'|\alpha\rangle \tag{147}$$

$$\implies -\frac{ip\Delta x'}{\hbar}|\alpha\rangle = -\int dx'|x'\rangle\Delta x'\frac{\partial}{\partial x'}\langle x'|\alpha\rangle \tag{148}$$

$$\Longrightarrow \boxed{p|\alpha\rangle = \int dx'|x'\rangle\Big(- i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\Big)} \tag{149}$$

or

$$\langle x'|p|\alpha\rangle = \int dx'\langle x'|x'\rangle\Big(- i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\Big) \tag{150}$$

$$= \int dx'|x'\rangle\langle x'|\Big(- i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\Big) \tag{151}$$

$$\Longrightarrow \boxed{\langle x'|p|\alpha\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle} \tag{152}$$

For the matrix element p in the x-representation, we have

$$\langle x'|p|x''\rangle = -i\hbar\frac{\partial}{\partial x'}\delta(x' - x'') \tag{153}$$

From (4.49) we get a very important identity:

$$\begin{aligned} \langle\beta|p|\alpha\rangle &= \int dx'\langle\beta|x'\rangle\Big(- i\hbar\frac{\partial}{\partial x'}\Big) \\ &= \int dx'\psi^*_\beta(x')\Big(- i\hbar\frac{\partial}{\partial x'}\Big)\psi_\alpha(x') \end{aligned} \tag{154}$$

The formalism (4.54) is not a postulate. It has been derived using the basic properties of momentum. By repeatedly applying (4.52), we can also obtain

$$\langle x'|p^n|\alpha\rangle = (-i\hbar)^n\frac{\partial}{\partial x'^n}\langle x'|\alpha\rangle \tag{155}$$

and

$$\langle\beta|p^n|\alpha\rangle = \int dx'\psi^*_\beta(x')(-i\hbar)^n\frac{\partial}{\partial x'^n}\psi_\alpha(x') \tag{156}$$

5 Momentum Space Wave Function

Let us now work in the p-basis. The eigenvalue equation reads $p|p'\rangle = p'|p'\rangle$. We also have the property $\langle p'|p''\rangle = \delta(p' - p'')$.

For an arbitrary state ket $|\alpha\rangle = \int dp' |p'\rangle\langle p'|\alpha\rangle$.

$|\langle p'|\alpha\rangle|^2$ is the probability that a measurement of p yields a result p' in the range $p' \pm dp'$.

The momentum space wave function is $\langle p'|\alpha\rangle = \phi_\alpha(p')$.

If $|\alpha\rangle$ is normalized, then $\int dp' \langle\alpha|p'\rangle\langle p'|\alpha\rangle = \int dp' |\phi_\alpha(p')|^2 = 1$.

What is the relation between x-representation and p-representation? They are connected by a transformation function of the type $\langle x'|p'\rangle$. What is the form of $\langle x'|p'\rangle$?

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

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

$\implies \langle x'|p'\rangle = N \exp\left(\frac{ip'x'}{\hbar}\right)$

Now, $\langle x'|x''\rangle = \int dp' \langle x'|p'\rangle\langle p'|x''\rangle$

$\implies \delta(x' - x'') = |N|^2 \int dp' \exp\left(\frac{ip'(x'-x'')}{\hbar}\right)$

$= 2\pi\hbar|N|^2\delta(x' - x'')$

We choose the usual convention and make N real and positive: $\langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{ip'x'}{\hbar}\right)$

So, $\langle x'|\alpha\rangle = \int dp' \langle x'|p'\rangle\langle p'|\alpha\rangle$

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

and $\langle p'|\alpha\rangle = \int dx' \langle p'|x'\rangle\langle x'|\alpha\rangle$

$\implies \phi_\alpha(p') = \frac{1}{\sqrt{2\pi\hbar}} \int dx' \exp\left(-\frac{ip'x'}{\hbar}\right)\psi_\alpha(x')$

Gaussian Wave Packets

The x-space wave function of a Gaussian wave packet is given by $\langle x'|\alpha\rangle = \frac{1}{x^{1/4}\sqrt{d}} \exp\left(ikx' - \frac{x'^2}{2d^2}\right)$. This is the plane wave with wave number k, modulated by a Gaussian profile centered at the origin.

Let us compute the expectation value of x, x^2, p, and p^2.

$\langle x\rangle = \int_{-\infty}^{\infty} dx' \langle\alpha|x'\rangle x' \langle x'|\alpha\rangle = \int_{-\infty}^{\infty} dx' |\langle x'|\alpha\rangle|^2 x' = 0 \quad \text{(by symmetry)}$

$\langle x^2\rangle = \int_{-\infty}^{\infty} dx' x'^2 |\langle x'|\alpha\rangle|^2 = \frac{1}{\sqrt{\pi}d} \int_{-\infty}^{\infty} dx' x'^2 \exp\left(-\frac{x'^2}{d^2}\right) = \frac{d^2}{2}$

$\implies \langle(\Delta x)^2\rangle = \langle x^2\rangle - \langle x\rangle^2 = \frac{d^2}{2}$

$\langle p \rangle = \hbar k$

$\langle p^2 \rangle = \frac{\hbar^2}{2d^2} + \hbar^2 k^2$

$\implies \langle (\Delta p)^2 \rangle = \langle p^2 \rangle - \langle p \rangle^2 = \frac{\hbar^2}{2d^2}$

Heisenberg's uncertainty relation can now be calculated as $\langle (\Delta x)^2 \rangle \langle (\Delta p)^2 \rangle = \frac{\hbar^2}{4}$

Noting the equality (and not $>$), we can see that the Gaussian wave packet is a minimum uncertainty wave packet.

In momentum space, $\langle p'|\alpha \rangle = \left(\frac{1}{\sqrt{2\pi\hbar}}\right)\left(\frac{1}{\pi^{1/4}\sqrt{d}}\right)\int_{-\infty}^{\infty} dx' \exp\left(\frac{-ip'x'}{\hbar} + ikx' - \frac{x^2}{2d^2}\right) = \sqrt{\frac{d}{\sqrt{\pi}\hbar}} \exp\left(\frac{-(p'-\hbar k)^2 d^2}{2\hbar^2}\right)$

6 Time Evolution Operator

How does a state ket change with time? Let $|\alpha\rangle$ refer to a state ket at time $= t_0$. A state ket at a later time t is described by $|\alpha, t_0; t\rangle$ with $t > t_0$. We note that $\lim_{t \to t_0} |\alpha, t_0; t\rangle = |\alpha\rangle$.

Our tasks is to study the evolution $|\alpha\rangle = |\alpha, t_0\rangle \longrightarrow |\alpha, t_0; t\rangle$. Let us define a time evolution operator $|\alpha, t_0; t\rangle = U(t, t_0)|\alpha, t_0\rangle$.

Suppose $|\alpha, t_0\rangle = \sum_{a'} c_{a'}(t_0)|a'\rangle$ and $|\alpha, t_0; t\rangle = \sum_{a'} c'_a(t)|a'\rangle$.

In general, $|c_{a'}(t)| \neq |c_{a'}(t_0)|$. But $\sum_{a'} |c_{a'}(t_0)|^2 = \sum_{a'} |c_{a'}(t)|^2$.

Normalization of the state is also preserved since $\langle\alpha, t_0|\alpha, t_0\rangle = 1 \longrightarrow \langle\alpha, t_0; t|\alpha, t_0; t\rangle = 1$.

The time evolution operator U must be unitary, or $U^\dagger(t, t_0)U(t, t_0) = 1$.

Composition property: $U(t_2, t_0) = U(t_2, t_1)U(t_1, t_0)$ where $(t_2 > t_1 > t_0)$.

We define an infinitesimal time evolution operator $U(t_0+dt, t_0)$ such that $|\alpha, t_0; t_0+dt\rangle = U(t_0+dt, t_0)|\alpha, t_0\rangle$

and $\lim_{dt \to t_0} U(t_0 + dt, t_0) = 1$.

All of these requirements are satisfied if we write $U(t_0 + dt, t_0) = 1 - i\Omega dt$ where $\Omega = \Omega^\dagger \implies$ Hermitian operator

We can write $U^\dagger(t_0 + dt_1 + dt_2,\ t_0) = U(t_0 + dt_1 + dt_2,\ t_0 + dt_1)U(t_0 + dt_1,\ t_0)$

Also, $U^\dagger(t_0 + dt,\ t_0)U(t + dt,\ t_0) = (1 + i\Omega^\dagger dt)(1 - i\Omega dt) \approx 1$, ignoring $(dt)^2$ and higher terms. Hence, $1 - i\Omega dt$ is unitary.

Note that Ω has dimension of $1/T$ or frequency. Planck's relation: $E = \hbar\omega$.

Let the Hamiltonian H be $H = \hbar\Omega$. This is dimensionally-correct.

$\implies U(t_0 + dt, t_0) = 1 - \frac{iHdt}{\hbar}$

$H \implies$ Hamiltonian operator (Hermitian)

The Schödinger Equation

$U(t + dt,\ t_0) = U(t + dt,\ t)U(t,\ t_0)$ where $t - t_0 \implies$ finite.

$U(t + dt,\ t_0) - U(t,\ t_0) = -i\frac{H}{\hbar}dt\ U(t,\ t_0)$

$\implies \boxed{i\hbar\frac{\partial}{\partial t}U(t,\ t_0) = HU(t,\ t_0)}$ which is the Schödinger equation for time evolution operator.

$\implies i\hbar\frac{\partial}{\partial t}U(t,\ t_0)|\alpha,\ t_0\rangle = HU(t,\ t_0)|\alpha,\ t_0\rangle$

$\implies i\hbar\frac{\partial}{\partial t}|\alpha,\ t_0; t\rangle = H|\alpha,\ t_0; t\rangle$

Case 1 H is independent of time. Example: H for spin magnetic moment interacting with time-independent magnetic field.

Solution to the Schödinger equation for the time evolution operator is given by $U(t,\ t_0) = \exp\left[\frac{-iH(t-t_0)}{\hbar}\right]$.

Proof. RHS $1 - \frac{iH(t-t_0)}{\hbar} + \left[\frac{(-i)^2}{2}\right]\left[\frac{H(t-t_0)}{\hbar}\right]^2 + \cdots$

$\implies \frac{\partial}{\partial t}\exp\left[\frac{-iH(t-t_0)}{\hbar}\right] = -\frac{iH}{\hbar} + \left[\frac{(-i)^2}{2}\right]\cdot 2\left(\frac{H}{\hbar}\right)^2(t-t_0) + \cdots$ which satisfies the Schödinger equation for the time evolution operator.

Case 2 H is time-independent, but Hs at different times commute.

Example. Spin magnetic moment subject to a magnetic field whose magnitude is changing but the direction is fixed.

Solution to the Schödinger equation for the time evolution operator is given by $U(t,\ t_0) = \exp\left(-\frac{i}{\hbar}\right)\int_0^t dt' H(t')$

Case 3 Hs at different times do not commute. Following the above example, this time the direction of the field also changes.

$t = t_1 \to x$-direction

$t = t_2 \to y$-direction

$[S_x,\ S_y] \neq 0$

$H \sim \bar{S}\cdot\bar{B} \implies [H(t_1), H(t_2)] \neq 0$

The solution is given by Dyson series.

Energy Eigenkets

If the base kets are eigenkets of A, $[A,\ H] = 0$ eigenkets of A are also eigenkets of H, called *energy eigenkets*: $H|a'\rangle = E_{a'}|a'\rangle$

Let $t_0 = 0\ \therefore\ \exp\left(\frac{-iHt}{\hbar}\right) = \sum_{a'}\sum_{a''}|a''\rangle\langle a''|\exp\left(\frac{-iHt}{\hbar}\right)|a'\rangle\langle a'|$

$$= \sum_{a'}|a'\rangle\exp\left(\frac{-iE_{a'}t}{\hbar}\right)\langle a'|$$

Suppose the initial ket can be written as

$|\alpha,\ t_0 = 0\rangle = \sum_{a'}|a'\rangle\langle a'|\alpha\rangle = \sum_{a'}|a'\rangle\langle a'|\alpha\rangle\exp\left(\frac{-iE_{a'}t}{\hbar}\right)$

The expansion coefficient changes with time as $c_{a'}(t=0) \to c_{a'}(t) = c_{a'}(t=0)\exp\left(\frac{-iE_{a'}t}{\hbar}\right)$

If $|\alpha,\ t_0 = 0\rangle = |a'\rangle = |a'\rangle$ and $|\alpha,\ t_0 = 0; t\rangle = |a'\rangle\exp\left(\frac{-iE_\alpha t}{\hbar}\right)$

$\implies$ If the system is initially simultaneous eigenstate of A, H, it continues to remain so at all times. Observables compatible with $H \to$ *constants of motion.*

Time Dependence of Expectation Value

Let at $t = 0$, the initial state is an eigenstate of A and where $[A,\ H] = 0$.

Let $\exists$ another observable B such that $[B,\ H] \neq 0; [B,\ A] \neq 0$.

Now, $|a',\ t_0 = 0; t\rangle = U(t, 0)|a'\rangle$

$\therefore\ \langle B\rangle = (\langle a'|U^\dagger(t, 0))B(U(t, 0)|a'\rangle)$

$= \langle a'| \exp\left(\frac{iE_{a'}t}{\hbar}\right) \exp\left(\frac{-iE_{a'}t}{\hbar}\right)|a'\rangle$

$= \langle a'|B|a'\rangle$

Note: $\langle B\rangle = \langle a'|B|a'\rangle$ is independent of time.

$\implies$ Expectation value of an observable taken with respect to an energy eigenstate does not change with time $\to$ stationary state.

The situation is more interesting when the expectation is taken with respect to a superposition of states $\to$ *non-stationary state.*

Suppose, we have $|\alpha,\ t_0\rangle = \sum_{a'} c_{a'}|a'\rangle$

$\therefore\ \langle B\rangle = \left[\sum_{a'} c^*_{a'}\langle a'| \exp\left(\frac{iE_{a'}t}{\hbar}\right)\right] \cdot B \cdot \left[\sum_{a''} c_{a''} \exp\left(\frac{-iE_{a''}t}{\hbar}\right)\right]|a''\rangle$

$= \sum_{a'} \sum_{a''} c^*_{a'} c_{a''} \langle a'|B|a''\rangle \exp\left[\frac{-i(E_{a''} - E_{a'})t}{\hbar}\right]$

$\implies$ The expectation value has an oscillating term whose angular frequencies are

$\omega_{a'a''} = \frac{(E_{a''} - E_{a'})}{\hbar}$

(Bohr's condition of radiation from an atom.)

7 Spin Precession Example

8 More on Unitary Operators

9 Simple Harmonic Oscillator

10 Continuation of Simple Harmonic Oscillators

11 Gauge Transformations in Electromagnetism

12 Gauge Transformations Continued

13 Theory of Angular Momentum

14 Paul Two Component Formalism

15 Density Operators and Ensembles

16 Matrix Elements of Angular Momentum Operators

17 Spherical Coordinates and Angular Momentum Operators

18 Angular Momentum Addition

19 Perturbation Theory

References

S. Mukherjee, *Quantum Mechanics*, Department of Physics and Astronomy, University of Texas Rio Grande Valley, Spring 2018.

S. Mukherjee, *Quantum Mechanics*, Department of Physics and Astronomy, University of Texas Rio Grande Valley, Spring 2019.

J. J. Sakurai, *Modern Quantum Mechanics*, Revised Edition, Addison-Wesley Publishing Company, Inc. (1994)