A. La Rosa Lecture Notes

INTRODUCTION TO QUANTUM MECHANICS

PART-III THE HAMILTONIAN OPERATOR and the SCHRODINGER EQUATION

CHAPTER-9
WAVEFUNCTIONS, OBSERVABLES and OPERATORS

References:

Feynman Lectures Vol. III; Chapter 16, 20

"Introduction to Quantum Mechanics" by David Griffiths; Chapter 3.

B. H. Bransden & C. J. oachin, Quantum mechanics, Prentice Hall, 2nd Ed. 2000

CHAPTER-9
WAVEFUNCTIONS, OBSERVABLES and OPERATORS

Quantum theory is based on two mathematical items: **wavefunctions and operators**.

- The state of a system is represented by a wavefunction. An exact knowledge of the wavefunction is the maximum one can have of the system: all possible information about the system can be calculated from this wavefunction.
- Quantities such as position, momentum, or energy, which one measures experimentally, are called **observables**. In classical physics, observables are represented by ordinary variables. In quantum mechanics observables are represented by **operators**; i.e. by quantities that operate on the wavefunction giving a new wavefunction.

Before undertaking the detailed description of observables and operators, let's make a summary of the different notations we have been using so far, as well as refreshing some results from the Fourier analysis made in Chapter 4.

9.1 Summary of previous notations

- Section 8.2.A "*From a discrete basis to a continuum basis*," in Chapter-8, introduced the different notations used to describe amplitude probabilities when working with a continuum basis.

  For example, when writing

$$|\,\phi\,\rangle = \int |\,x\,\rangle\,[\,A_{\phi}(x)\,]\,dx \tag{1}$$

  the amplitude probability $A_{\phi}(x)$ is typically expressed under different but equally valid notations,

$$\langle\, x\,|\phi\rangle = A_{\phi}(x) = \phi(x) \tag{2}$$

- In Chapter 4, Section 4.1.D "*Spectral decomposition in complex variable. The Fourier Transform*," we obtained,

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \underbrace{F(k)}_{\text{Fourier coefficients}} \underbrace{e^{ikx}}_{\text{Base-functions}} dk$$

where the weight coefficients F(k) of the complex harmonic functions components are given by,

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx'} \psi(x')dx'$$

and referred to as the Fourier transform of the function Ψ.

For the purpose of this chapter, it would be more convenient to express the last two expressions in terms of the variable p,

$$p = \hbar k$$

which leads to,

$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} A(p)\, e^{i(p/\hbar)x} dp \qquad (3)$$

where

$$A(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-i(p/\hbar)x'} \psi(x')dx' \qquad (4)$$

- Expressions (3) and (4) have a clearer physics interpretation. Indeed, according to the de Broglie postulate a plane wave of wavelength λ, $e^{i(2\pi/\lambda)x}$, can be associated to a particle of linear momentum $p = h/\lambda$. Thus,

$$\frac{1}{\sqrt{2\pi\hbar}} e^{i(p/\hbar)x} \qquad (5)$$

Represents a plane wave of definite linear momentum p.

(where the factor $1/\sqrt{2\pi\hbar}$ has been chosen for later convenience).

Based on (5) we define the state $|\,\phi_p\rangle$,

$$|\,\phi_p\rangle \equiv \int_{-\infty}^{\infty} |\,x\rangle \underbrace{\phi_p(x)}\,\mathrm{d}x = \int_{-\infty}^{\infty} |\,x\rangle \underbrace{\frac{1}{\sqrt{2\pi\hbar}}\,e^{i(p/\hbar)x}}\,\mathrm{d}x \qquad (6)$$

Representation of the momentum state $|\,\phi_p\rangle$ *in the space-coordinate basis* $\{\,|\,x\rangle\,\}$

Expression (5) can then be identified with $\langle x|\phi_p\rangle$,

$$\frac{1}{\sqrt{2\pi\hbar}}\,e^{i(p/\hbar)x} = \langle\, x|\,\phi_p\rangle \equiv \phi_p(x) \qquad (7)$$

Amplitude probability that a particle, in a state of momentum p, be found at the coordinate x.

- Notice then that the wavefunction given in (3) can be interpreted as a linear combination of states $|\,\phi_p\rangle$

$$|\,\Psi\rangle = \int_{-\infty}^{\infty} \mathrm{A}(p)\,|\,\phi_p\rangle\, dp \qquad (8)$$

where

$$\mathrm{A}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \mathrm{e}^{-ikx'}\,\psi(x')dx' = \langle\phi_p|\Psi\rangle \qquad (9)$$

Or, using (9) in (8),

$$|\,\Psi\rangle = \int_{-\infty}^{\infty} \langle\phi_p|\Psi\rangle\,|\,\phi_p\rangle\, dp \qquad (10)$$

9.2 The underlying math typically used for describing the wavefunction

Chapter 8 helped to provide some clues on the proper interpretation of the wavefunction (the solutions of the Schrodinger equation.) This came through the analysis of the particular case of an electron moving in a discrete lattice: the wavefunction is pictured as an *amplitude probability* (a complex number) for an electron to jump to a neighbor atom site. Notice, however, that when taking the limiting case of the lattice spacing tending to zero, one ends up with a situation in which the electron is propagating through a continuum line space. Thus, this limiting case takes us to the study of a particle moving in a continuum space.

In analogy to the discrete lattice, where the location of the atoms guided the selection of the state basis $\{\,|n\rangle\,\}$, in the continuum space we consider the following continuum set,

$$\{\ |\,x\,\rangle\,;\quad 0 < x < \infty\,\} \quad \textit{a continuum base of space coordinates} \tag{11}$$

in order to describe the most general state $|\Psi\rangle$ of a particle.

$$|\Psi\rangle = \int_{-\infty}^{\infty} |\,x\,\rangle \underbrace{\langle\, x|\ \Psi\,\rangle}_{\text{number}}\, dx \;=\; \int_{-\infty}^{\infty} |\,x\,\rangle\ \underbrace{\Psi(x)}_{\text{number}}\, dx \tag{12}$$

It turns out, however, that the continuum base of space coordinates may not be, sometimes, the most convenient way to express the state $|\Psi\rangle$. Alternatively,

$$\{\,|\ \phi_p\,\rangle\ ,\ -\infty < p < \infty\quad\} \quad \text{the continuum base of momentum-coordinates} \tag{13}$$

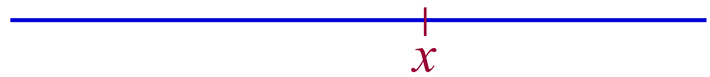
can also be used,

$$|\Psi\rangle = \int_{-\infty}^{\infty} |\,\phi_p\,\rangle\ \langle\phi_p|\,\Psi\,\rangle\ dp \tag{14}$$

The two representations of a given state, namely in the *space coordinates* and *momentum coordinates,* are explained with a bit more detail below.

9.2.A Representation of the wavefunction in the spatial coordinates basis $\{\,|\,x\,\rangle\ ,\quad -\infty < x < \infty\,\}$

$|x\rangle$ stands for a state in which a particle is located around at a spatial coordinate x. (15)



For every value x along the line one conceives a corresponding state. If one includes all the points on the line, a complete set results $\{ |\, x \rangle$, $-\infty < x < \infty \}$, which will be used to describe a general quantum state and, hence, to describe the one-dimension motion of a particle.

A given state $|\Psi\rangle$ gives a particular way in which an electron is distributed along a line. One way of specifying this state is by giving all the amplitude-probabilities that the electron will be found in each of the base states $|\, x\rangle$. We write these amplitudes as $\langle\, x|\, \Psi\, \rangle$. We must give an infinite set of amplitudes, one for each value of x.

With this information in mind, we express the state as

About the notation

- We could use alternative notations, like, for example,

  $|\Psi\rangle = \int_{-\infty}^{\infty} |\, x\, \rangle\, [A\ (x)\,]\ dx$ as to make this expansion to resemble the expansion of a "vector $|\Psi\rangle$" in terms of a base-vectors $|\, x\, \rangle$ with the corresponding coefficients $A(x)$ playing the role of weighting coefficients.

  We could even use $A_{\Psi}(x)$ instead of simply $A(\,x)$, as to emphasize that those coefficients correspond to the state $|\Psi\rangle$. The meaning of this latter notation becomes clearer but, at the same time, it may result too cumbersome. Hence, the notation $\langle x|\, \Psi\rangle$ is frequently preferred, as it also goes along with our definition of amplitude probability in Chapter 6.

- Another common notation for the amplitude probability $\langle x|\Psi\,\rangle$ is $\Psi(x)$.

$$\Psi(x) \equiv \langle\, x\,|\,\Psi\,\rangle \qquad (17)$$

Amplitude probability that the particle initially in the state $|\Psi\rangle$ be found at the state $|\, x\rangle$.

Thus,

$$|\Psi\rangle = \int_{-\infty}^{\infty} |x\rangle \underbrace{\langle x|\Psi\rangle}_{\text{number}} dx = \int_{-\infty}^{\infty} |x\rangle \underbrace{\Psi(x)}\, dx \qquad (18)$$

Warning: $\langle x | \Psi \rangle$ does not mean $\int_{-\infty}^{\infty} [x]^* \Psi(x)\, dx$. Working with the spatial coordinates base $\{ |x\rangle \}$ may constitute the only occasion in which the notation $\langle x| \Psi \rangle$ gets confused with the definition of the scalar product.

9.2.A1 The Delta Dirac[1]

A subproduct of the mathematical manipulation expressing a state in a given basis is the closure relationship that the components of the basis set must comply: the Delta Dirac relationship. This is illustrated for the case of the space-coordinates basis.

$$|\Psi\rangle = \int_{-\infty}^{\infty} |x'\rangle [\langle x'|\Psi\rangle]\, dx'$$

$$\langle x|\Psi\rangle = \langle x| \int_{-\infty}^{\infty} |x'\rangle [\langle x'|\Psi\rangle]\, dx'$$

$$\langle x|\Psi\rangle = \int_{-\infty}^{\infty} \langle x|x'\rangle [\langle x'|\Psi\rangle]\, dx'$$

$$\underbrace{\langle x|\Psi\rangle}_{\Psi(x)} = \int_{-\infty}^{\infty} \langle x|x'\rangle [\underbrace{\langle x'|\Psi\rangle}_{\Psi(x')}]\, dx'$$

Or, equivalently

$$\Psi(x) = \int_{-\infty}^{\infty} \langle x|x'\rangle [\Psi(x')]\, dx'$$

Since for an arbitrary function f, the delta 'function' is defined as[2]

$$f(x) \equiv \int_{-\infty}^{\infty} \delta(x'-x) f(x')\, dx'$$

The last two expressions are consistent if,

$$\langle x|x'\rangle = \delta(x'-x)$$

Thus, we have the following result:

CASE Discrete states		CASE Continuum states
Delta Kroenecker	$\longrightarrow$	Delat Dirac $\delta(x\text{-}x')$
$\langle\, n \,|\, m \,\rangle = \delta_{nm}$		$\langle\, x \,|\, x' \rangle = \delta(\, x - x'\,)$

(19`

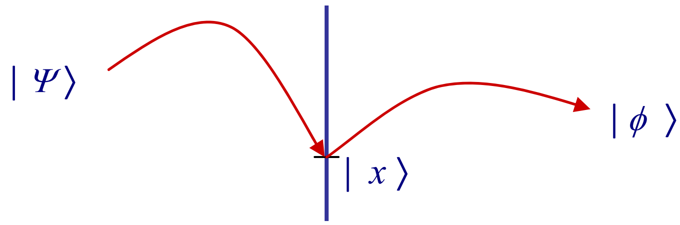
9.2.A2 Compatibility between the physical concept of amplitude probability $\langle\, \phi \,|\, \Psi \rangle$ and the notation used for the inner product $\int_{-\infty}^{\infty} \phi^*(\,x)\; \Psi(x)\, dx$

We know that given a state $|\Psi\rangle$**,** the amplitude probabilities $\langle x \,|\, \Psi \rangle$ that appear in the expansion $|\Psi\rangle = \int_{-\infty}^{\infty} |x\rangle\langle x|\Psi\rangle dx$ are determined by the Hamiltonian equations.

[Recall, in Chapter 8 we used the notation $|\phi(\,t\,)\,\rangle = \sum_n |\, n\rangle\, A_n(\,t\,)$, where the Hamiltonian Eqs. allowed to determine the amplitudes $A_n(\,t\,)$. In this chapter, instead of $A_n(\,t\,)$, we will use $\langle\, n \,|\Psi\,\rangle$, but simply extrapolated to the continuum base.]

Suppose we have an electron in the state $|\Psi\rangle$ and we want to know the amplitude probability (after a given measurement process) for finding the electron in a different state $|\phi\rangle$. That is, we want to evaluate $\langle\, \phi \,|\, \Psi \rangle$.

From what we learned in Chapter 6 (Section 6.2 and 6.3), there are many path way for the state $|\Psi\rangle$ to transit to state $|\phi\rangle$. It could do it by passing first through any of the base-states $|\, x\,\rangle$, in particular for example $|\, x_0\,\rangle$; that is $\langle \phi \,|\, x_0\,\rangle\langle\, x_0 \,|\, \Psi\,\rangle$. Since each state $|\, x\,\rangle$ generates a path, and all the paths (each corresponding to a given state $|\, x\,\rangle$) are equivalent, then, according to the rules established in Chapter 6, the total amplitude probability is given by,



$$\langle \phi | \Psi \rangle = \sum_{all\ x} \langle \phi | x \rangle \langle x | \Psi \rangle$$

The sum over a small region of width dx would be $\langle \phi | x \rangle \langle x | \Psi \rangle$ multiplied by dx. Accordingly, since x varies from $-\infty$ to ∞ the expression above can be written as,

$$\langle \phi | \Psi \rangle = \int_{-\infty}^{\infty} \langle \phi | x \rangle \langle x | \Psi \rangle \, dx \qquad (20)$$

We can here introduce the notation used above, namely $\langle x|\Psi\rangle = \Psi(x)$. Also, since $\langle \phi | x \rangle = \langle x | \phi \rangle^*$ one obtains

$$\langle \phi | \Psi \rangle = \int_{-\infty}^{\infty} \phi^*(x)\, \Psi(x)\, dx \qquad (21)$$

The amplitude probability $\langle \phi | \Psi \rangle$ is equal to the inner product between the functions ϕ and Ψ

9.2.B Representation of the wavefunction in the momentum coordinates basis $\{ | \phi_p \rangle \}$

Representation in the momentum basis $\{ | \phi_p \rangle \}$

$|\phi_p\rangle$ stands for a state of linear momentum p (22)

See also expressions (5), (6) and (7), given above.

In terms of these states, the wavefunction $|\Psi\rangle$ is formally expressed as,

$$|\Psi\rangle = \int_{-\infty}^{\infty} |\phi_p\rangle \underbrace{\langle \phi_p|\Psi\rangle}\, dp \;=\; \int_{-\infty}^{\infty} |\phi_p\rangle \underbrace{A(p)}\, dp \tag{23}$$

where

$$A(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \mathrm{e}^{-ikx'}\, \psi(x')dx' \;=\; \langle\phi_p|\Psi\rangle$$

$\langle\phi_p \,|\, \Psi\rangle \equiv A(p)$ *amplitude probability that a particle initially in the state* $|\Psi\rangle$ *can be found in a state of linear momentum* p.

$|\langle\phi_p \,|\, \Psi\rangle|^2\, \mathrm{d}p =$ *probability to find the particle with a momentum within the interval* $(p, p+\mathrm{d}p)$.

In short, we can use either

$$|\Psi\rangle = \int_{-\infty}^{\infty} |\phi_p\rangle \langle \phi_p|\Psi\rangle\, dp = \int_{-\infty}^{\infty} |\phi_p\rangle A(p)\, dp \quad \textit{(bra-kets notation)}$$

or

$$\Psi(x) = \int_{-\infty}^{\infty} \Big[\frac{1}{\sqrt{2\pi\hbar}} e^{i(p/\hbar)x}\Big] A(p)\, \mathrm{d}p \qquad \textit{(our Chapter 6 notation)} \tag{24}$$

where $A(p) = \dfrac{1}{\sqrt{2\pi\hbar}} \displaystyle\int_{-\infty}^{\infty} e^{-i(p/\hbar)x'}\, \Psi(x')\, \mathrm{d}x'$

9.3 The Schrödinger Equation as a postulate

9.3.A The Hamiltonian equations expressed in the continuum spatial coordinates. The Schrödinger Equation.[3]

In chapter 7 we obtained the general Hamiltonian equations that describe the time evolution of the wavefunction $|\phi(t)\rangle = \sum_n |n\rangle A_n(t)$,

$$i\hbar \frac{dA_n}{dt} = \sum_j H_{nj}(t)\; A_j \;, \tag{25}$$

Particular case: Chapter 8 described the particular case of an electron moving in a lattice (the latter constituted by atoms separated a distance "b"). When we took the limit $b \rightarrow 0$) the Hamiltonian equations took the form

$$i\hbar \frac{\partial A(x,t)}{\partial t} = -\frac{\hbar^2}{2\, m_{eff}} \frac{\partial^2 A(x,t)}{\partial x^2} + V(x,t) A(x,t) \qquad (26)$$

General case: Let's consider now an arbitrary general case. How does the Hamiltonian equations (25) look like when expressed in the in the continuum space coordinates $\{ \mid x \rangle \; , \; -\infty < x < \infty \}$? Let's work out such general formal expression.

First notice that the amplitudes A_j in (25) account for the state describing the quantum system,

$$\mid \Psi \rangle = \sum_j \mid j \rangle \, A_j$$

Since A_j can also be written as $A_j = \langle \, j \mid \Psi \rangle$, Eq. (25) can also be expressed as,

$$i\hbar \frac{d}{dt} \langle n \mid \Psi \rangle = \sum_j H_{nj} \, \langle \, j \mid \Psi \rangle$$

Let's also recall, from Chapter 7, that the coefficients H_{nj} are obtained from the Hamiltonian operator $\widetilde{\mathrm{H}}$ (specific to the problem being solved.) That is, $H_{nj} \equiv \langle \, n \mid \widetilde{\mathrm{H}} \mid j \, \rangle$. In general, $\widetilde{\mathrm{H}}$ and Ψ depend on t.

$$i\hbar \frac{d}{dt} \langle n \mid \Psi \rangle = \sum_j \langle n \mid \widetilde{\mathrm{H}} \mid j \, \rangle \; \langle \, j \mid \Psi \rangle$$

In the continuum space coordinates we should expect,

$$i\hbar \frac{d}{dt} \underbrace{\langle x \mid \Psi \rangle}_{\Psi(x)} = \int \langle x \mid \widetilde{\mathrm{H}} \mid x' \, \rangle \; \underbrace{\langle \, x' \mid \Psi \rangle}_{\Psi(x')} \, \mathrm{d}x'$$

$$\boxed{i\hbar \frac{d}{dt} \Psi(x) = \int H(x, x') \Psi(x') \, \mathrm{d}x'} \qquad (27)$$

where we have defined $H(x, x') \equiv \langle x \mid \widetilde{\mathrm{H}} \mid x' \rangle$

Quoting Feynman,[4]

“*According to (22), the rate of change of Ψ at x would depend on the value of Ψ at all other points x'* .

> $\langle x | \widetilde{\mathrm{H}} | x' \rangle$ is the amplitude per unit time that the electron will jump from x *to* x'.
>
> *It turns out in nature, however, that this amplitude is zero except for points x' very close to x. …*
>
> *… This means (as we saw in the example of the chain of atoms) that the right-hand side of Eq. (27) can be expressed completely in terms of Ψ and the spatial derivatives of Ψ, all evaluated at x.*

The correct law of physics is

$$\int H(x, x')\ \Psi(x')\,\mathrm{d}x' = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\ \Psi(x) + V(x)\ \Psi(x) \qquad (28)$$

Where did we get that from? Nowhere.
It came out of the mind of Schrodinger, invented in his struggle to find an understanding of the experimental observation of the experimental world. ”

Using (27) in (28) one obtains,

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x,t)\psi = i\hbar\frac{\partial\psi}{\partial t} \qquad \textit{Schrodinger Equation} \qquad (29)$$

“*This equation marked a historic moment constituting the birth of the quantum mechanical description of matter. The great historical moment marking the birth of the **quantum mechanical description of matter** occurred when Schrodinger first wrote down his equation in 1926.*

> *For many years the internal atomic structure of the matter had been a great mystery. No one had been able to understand what held matter together, why there was chemical binding, and especially how it could be that atoms could be stable. (Although Bohr had been able to give a description of the internal motion of an electron in a hydrogen atom which seemed to explain the observed spectrum of light emitted by this atom, the reason that electrons moved this way remained a mystery.)*

Schrodinger's discovery of the proper equations of motion for electrons on an atomic scale provided a theory from which atomic phenomena could be calculated quantitatively, accurately and in detail." Feynman's Lectures, Vol III, page 16-13.

Although the result (29) is kind of a postulate, we do have some clues about how to interpret it, based on the particular case of the dynamics of an electron in a crystal lattice, studied in Chapter 8.

9.3.B Interpretation of the Wavefunction

Einstein's view on the granularity nature of the electromagnetic radiation

In Chapter 4, the proposed harmonic function to describe the motion of a free particle were introduced in analogy to the existent formalism to describe electromagnetic waves,

$$\mathcal{E}(x,t) = \mathcal{E}_o Cos\ [\frac{2\pi}{\lambda} x - \nu t] \qquad \textit{electromagnetic wave}$$

where, the electromagnetic intensity I (energy per unit time crossing a unit cross-section area perpendicular to the direction of radiation propagation) is proportional to $|\mathcal{E}(x,t)|^2$.

Einstein (in the context of trying to explain the results from the photoelectric effect) introduced the *granularity* interpretation of the electromagnetic waves (later called photons), abandoning the more classical *continuum* interpretation.

In Einstein's view, the intensity of radiation $I = \langle \varepsilon_o c \mathcal{E}^2 \rangle$ is interpreted as $I = \langle \varepsilon_o c \mathcal{E}^2 \rangle = \langle N \rangle\ h\ \gamma$ and as a statistical variable. Here $\langle N \rangle$ constitutes the **average** number $\langle N \rangle$ of photons per second crossing a unit area perpendicular to the direction of radiation propagation.

Notice,

$$\langle \mathcal{E}^2 \rangle \sim \langle N \rangle$$

Average values are used in this interpretation because the emission process of photons by a given source is **statistical in nature**. The exact number of photons crossing a unit area per unit time **fluctuates** around an average value $\langle N \rangle$.

Max Born's Probabilistic Interpretation of the wavefunction

In analogy to Einstein's view of radiation, Max Born proposed a similar view to interpret the particle's wave-functions. In Max Born's view, $\left|\psi(x,t)\right|^2$ plays a role similar to $\left|\mathcal{E}(x,t)\right|^2$,

$\left|\psi(x,t)\right|^2$ *is a measure of the probability of finding the particle around a given place* x *and at a given time* t.

This interpretation was introduced years after Schrodinger (1926) had developed a formal quantum mechanics description.

That is, $\left|\psi(x,y,z,t)\right|^2$ plays the role of ***probability density***.

Pictorially, the particle must be at some location where the wavefuntion has an appreciable value.

Deterministic evolution of the wavefunction

The predictions of quantum mechanics are statistical

In order to know the state of motion of a particle, we must make a measurement

But a measurement necessarily disturbs the system in a way that can not be completely determined

However, notice that ψ , being the solution of a differential equation (the Schrodinger equation), **varies with time in a way that is completely *deterministic***. That is, if ψ were known at $t=0$, the Schrodinger equation determines precisely its form at any future time.

But, what happens is that the wavefunction ψ at $t=0$ can not be completely be uniquely determined. This is because, a set of measurements at $t=0$ at most may lead to the determination of $\psi\ \psi^*$ but not uniquely defines ψ .

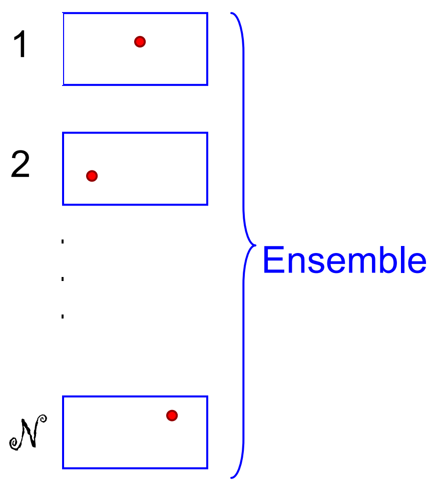
Let’s explain the statistical interpretation a bit further in the context of an ensemble of identical systems.

Ensemble[5]

Imagine a very large number of identical, independent systems, each of them consisting of a single particle moving under the influence of a given external force.

All these systems are identically prepared.

The whole ensemble is assumed to be described by a complex-variable single wavefunction $\psi = \psi(x, y, z, t))$, which contains all the information that can be obtained about them.



Ψ describes the whole ensemble

Ψ is used to make a probabilistic prediction on what may happen in a particular member of the ensemble.

It is postulated that:

> If measurement of the particle’s position are made on each of the $\mathcal{N}$ member of the ensemble, the fraction of times the particle will be found within the volume element $d^3\mathbf{r} = dx\ dy\ dz$ around the position $\mathbf{r} = (x, y, z, t)$ at the time t is given by
>
> $$\psi(x, y, z, t)\psi^*(x, y, z, t)\ d^3\mathbf{r}$$
>
> where * stands for the complex conjugate number. (30)

Notice that this is nothing but the language of probability; in this case, position probability density P.

$$P(x,y,z,t) = \left|\psi(x,y,z,t)\right|^2$$

Caution: For convenience, we shall often speak of
"*the wavefunction of a particular system*",
BUT it must always be understood that this is shorthand for
"*the wavefunction associated with an ensemble of identical and identically prepared systems*", as required by the statistical nature of the theory.[6]

9.3.C Normalization condition for the wavefunction

The probabilistic interpretation of the wavefunction implies, therefore, the following requirement:

$$\int_{\text{All space}} \psi(\mathrm{x,y,z,t})\ \psi^*(\mathrm{x,y,z,t})\mathrm{d}^3\mathbf{r} \ = 1 \tag{31}$$

because given a particle, the likelihood to find it anywhere should be one. Inherent to this requirement is that,

$$\left|\psi\right|^2(\mathbf{r},\mathrm{t}) \xrightarrow[|\mathbf{r}| \to \infty]{} = 0 \tag{32}$$

Notice that if φ is a solution of the Schrodinger equation, the function $c\varphi$ (c being a constant) is also a solution. The multiplicative factor c therefore has to be chosen such that the function $\mathrm{c}\varphi$ satisfies the condition (31). This process is called **normalizing** the wavefunction.

In general, there will be solutions to the Schrodinger equation (29) whose solution tend to an infinite value. This means they are **non-normalizable** and therefore can not represent a particle probability density. Such functions must be rejected on the grounds of Born's probability interpretation.

Quantum mechanics states are represented by **square- integrable** functions that satisfy the Schrodinger equation.

The particular subset of **square integrable functions** form a vector space call the **Hilbert space**.

QUESTION: Suppose that ψ is normalized at $t=0$. As the time evolves, ψ will change. How do we know if it will remain normalized?

Here we show that the Schrodinger equation has the remarkable property that it automatically preserves the normalization of the wavefunction:

If ψ satisfies the Schrodinger equation

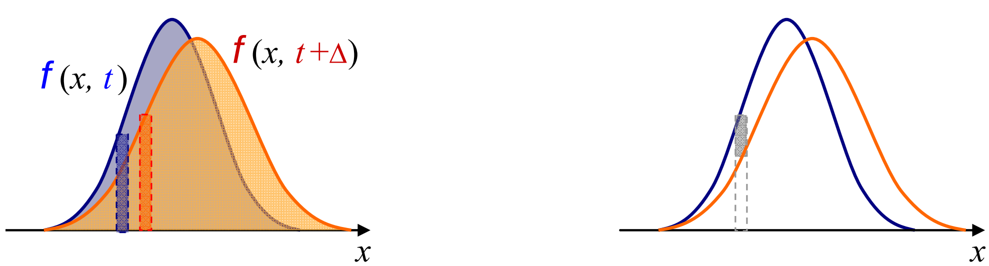
(for the case where the potential is real)

then $\frac{d}{dt}\left[\int_{-\infty}^{\infty}|\psi(x,t)|^2 dx\right] = 0$ (32)

Proof:
Let's start with

$$\frac{d}{dt}\int_{-\infty}^{\infty}|\psi(x,t)|^2 dx = \int_{-\infty}^{\infty}\frac{\partial}{\partial t}|\psi(x,t)|^2 dx \tag{33}$$

We provide below a graphic justification of (33).



$$\frac{1}{\Delta t}\left[\int_{-\infty}^{\infty} f(x, t+\Delta)dx - \int_{-\infty}^{\infty} f(x, t)\, dx\right] = \frac{1}{\Delta t}\int_{-\infty}^{\infty}[f(x, t+\Delta) - f(x, t)]\, dx$$

On the other hand,

$$\frac{\partial}{\partial t}|\psi|^2 = \frac{\partial}{\partial t}(\psi\psi^*) = \psi\frac{\partial\psi^*}{\partial t} + \frac{\partial\psi}{\partial t}\psi^* \tag{34}$$

We use the Schrodinger equation (29) to calculate the time derivatives,

$$\frac{\partial \psi}{\partial t} = \frac{-\mathrm{i}}{\hbar}\left[\frac{\hbar^2}{2\mathrm{m}}\frac{\partial^2 \psi}{\partial x^2} + \mathrm{V}(x,t)\psi\right] = \frac{\mathrm{i}\hbar}{2\mathrm{m}}\frac{\partial^2 \psi}{\partial x^2} + \frac{-\mathrm{i}}{\hbar}\mathrm{V}(x,t)\psi$$

$$\frac{\partial \psi}{\partial t}\psi^* = \frac{\mathrm{i}\hbar}{2\mathrm{m}}\frac{\partial^2 \psi}{\partial x^2}\psi^* + \frac{-\mathrm{i}}{\hbar}\mathrm{V}(x,t)\psi\psi^*$$

Taking the complex conjugate, and assuming that the potential is real,

$$\frac{\partial \psi^*}{\partial t}\psi = \frac{-\mathrm{i}\hbar}{2\mathrm{m}}\frac{\partial^2 \psi^*}{\partial x^2}\psi + \frac{\mathrm{i}}{\hbar}\mathrm{V}(x,t)\psi^*\psi$$

Adding the last two expressions,

$$\psi\frac{\partial \psi^*}{\partial t} + \frac{\partial \psi}{\partial t}\psi^* = \frac{\mathrm{i}\hbar}{2\mathrm{m}}\left[\frac{\partial^2 \psi}{\partial x^2}\psi^* - \frac{\partial^2 \psi^*}{\partial x^2}\psi\right]$$

$$= \frac{\mathrm{i}\hbar}{2\mathrm{m}}\frac{\partial}{\partial x}\left[\frac{\partial \psi}{\partial x}\psi^* - \frac{\partial \psi^*}{\partial x}\psi\right] \qquad (35)$$

Replacing (35) in (34) we obtain,

$$\frac{\partial}{\partial t}|\psi|^2 = \frac{\mathrm{i}\hbar}{2\mathrm{m}}\frac{\partial}{\partial x}\left[\frac{\partial \psi}{\partial x}\psi^* - \frac{\partial \psi^*}{\partial x}\psi\right]$$

Accordingly,

$$\frac{d}{dt}\int_{-\infty}^{\infty}|\psi(x,t)|^2 dx = \int_{-\infty}^{\infty}\frac{\partial}{\partial t}|\psi(x,t)|^2 dx$$

$$= \frac{\mathrm{i}\hbar}{2\mathrm{m}}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left[\frac{\partial \psi}{\partial x}\psi^* - \frac{\partial \psi^*}{\partial x}\psi\right]dx$$

$$= \frac{\mathrm{i}\hbar}{2\mathrm{m}}\left(\frac{\partial \psi}{\partial x}\psi^* - \frac{\partial \psi^*}{\partial x}\psi\right)\Bigg|_{-\infty}^{\infty}$$

The expression on the right is zero because $\psi(x) \xrightarrow[x \to \pm\infty]{} 0$

9.3.D The Philosophy of Quantum Theory

There has been a controversy over the Quantum Theory's philosophic foundations.

- **Neils Bohr** has been the principal architect of what is known as the Copenhagen interpretation (statistical interpretation)
- **Einstein** was the principal critic of Bohr 's interpretation.

  His statement "God does not play dice with the universe", refers to the abandonment of strict causality and individual events by quantum theory.

- **Heisenberg** counteracts arguing:
  "**We have not assumed that the quantum theory** (as oppose to the classical theory) **is a statistical theory**, in the sense that only statistical conclusions can be drawn from exact data.

  In the formulation of the causal law, namely, *'if we know the present exactly, we can predict the future'* it is not the conclusion, but rather the premise which is false. **We cannot know, as a matter of principle, the present in all its details**.

- Louis de Broglie, on the other hand, argues that that limited knowledge of the present may be rather a limitation of the current measurement methods being used.

  He recognizes that
  a) it is certain that the methods of measurement do not allow us to determine simultaneously all the magnitude which would be necessary to obtain a picture of the classical type, and that
  b) perturbations introduced by the measurement, which are impossible to eliminate, prevent us in general from predicting precisely the results which it will produce and allow only statistical predictions.

  The construction of purely probabilistic formulae was thus completely justified.

  But, the assertion that
  i) The uncertain and incomplete character of the knowledge that experiment at its present stage gives us about what really happens in microphysics,

  is the result of

ii) a real indeterminacy of the physical states and of their evolution,

constitutes an extrapolation that does not appear in any way to be justified.

De Broglie considers possible that looking into the future we will be able to interpret the laws of probability and quantum physics as being the statistical results of the development of completely determined values of variables which are at present hidden from us.

- Louis de Broglie's view given above highlights the objection to quantum mechanics' philosophic indeterminism.

  According to Einstein:

  "The belief of an external world independent of the perceiving subject is the basis of all natural science."

  Quantum mechanics, however,

  - regards the interaction between object and observer as the ultimate reality;
  - rejects as meaningless and useless the notion that behind the universe of our perception there lies a hidden objective world ruled by causality;
  - confines itself to the description of the relations among perceptions[7]

Physics has given up on the problem of trying predicting exactly what will happen in a definite circumstance.

9.4 Expectation values

9.4.A Expectation (or mean) value of a particle's position

For a particle in an state $|\Psi\rangle$, the expectation value of its position is defined by:

$$< x > = \int_{-\infty}^{\infty} x \, |\psi(x)|^2 dx \qquad (36)$$

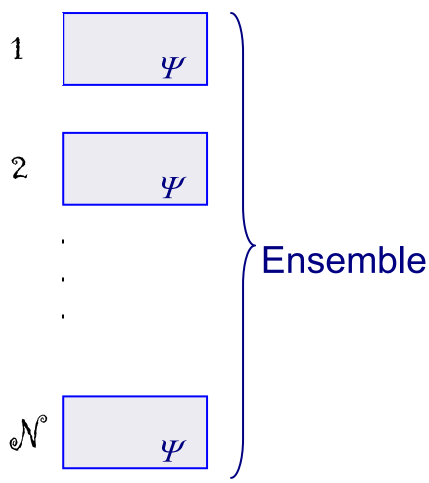
But what does this integral exactly mean?

It is worth to emphasize first what type of interpretation should be avoided.[8]

- Expression (36) <u>does not</u> imply that if you measure the position of the particle over and over again then $\int_{-\infty}^{\infty} x\,|\,\psi(x)|^2 dx$ would be the average of the results.
- In fact, if repeated measurements were to be made on the same particle, the first measurement (whose outcome is unpredictable) will make the wavefunction to collapse to a state of corresponding particle's position x (let's say x_0); subsequent measurements (if they are performed quickly) will simply repeat that same result x_0.

On the contrary, $< x > \equiv \int_{-\infty}^{\infty} x\,|\,\psi(x)|^2 dx$ means the average of measurements performed on *many* particles, all in the state $|\Psi\rangle$. That is,

- An ensemble of particles is prepared, each in the same state, and measurement of the position is performed in all of them. $< x >$ is the average of these results.



$|\Psi\rangle$ describes the whole ensemble

$|\Psi\rangle$ is used to make a probabilistic prediction on what may happen in a particular member of the ensemble.

Fig. 9.1 *Ensemble of identically prepared systems. When we say that a system is in the state $|\Psi\rangle$, we are actually referring to an ensemble of systems all of them in the same state. Thus, $|\Psi\rangle$ represent the ensemble.*

9.4.B Expectation (or mean) value of the particle's momentum

As time goes on, the expectation value $<x>$ may change with time, since the wavefunction evolves with time. Let's calculate its rate of change.

$$\frac{d<x>}{dt} = \frac{d}{dt}\int x\left|\psi(x,t)\right|^2 dx = \int x\frac{\partial}{\partial t}\left|\psi(x,t)\right|^2 dx = \int x\frac{\partial}{\partial t}[\psi\,\psi^*]dx$$

$$= \int x\,\underbrace{[\psi\,\frac{\partial\psi^*}{\partial t} + \frac{\partial\psi}{\partial t}\psi^*]}\,dx$$

For the case where the potential is real, we obtained in expression (35) that,

$$\psi\frac{\partial\psi^*}{\partial t} + \frac{\partial\psi}{\partial t}\psi^* = \frac{i\hbar}{2m}\left[\frac{\partial^2\psi}{\partial x^2}\psi^* - \frac{\partial^2\psi^*}{\partial x^2}\psi\right]$$

$$\frac{d<x>}{dt} = \int x\frac{i\hbar}{2m}\left[\frac{\partial^2\psi}{\partial x^2}\psi^* - \frac{\partial^2\psi^*}{\partial x^2}\psi\right]$$

$$= \int x\frac{i\hbar}{2m}\frac{\partial}{\partial x}\left[\frac{\partial\,\psi}{\partial x}\psi^* - \frac{\partial\psi^*}{\partial x}\psi\right]$$

After integrating by parts, it gives

$$\frac{d<x>}{dt} = -\int\frac{i\hbar}{2m}\left[\frac{\partial\psi}{\partial x}\psi^* - \frac{\partial\psi^*}{\partial x}\psi\right]$$

Integrating one more time by parts (one of the terms,)

$$\frac{d<x>}{dt} = -\frac{i\hbar}{m}\int\frac{\partial\psi}{\partial x}\psi^* dx \qquad (37)$$

We will postulate that the expectation (or mean) value of the linear momentum is equal to $<p> \equiv m\frac{d<x>}{dt}$. Thus,

$$<p> = \int\psi^*\frac{\hbar}{i}\frac{\partial\psi}{\partial x}dx \qquad (38)$$

Look at the functions inside the integral. How does a term like $\frac{\partial\psi}{\partial x}$ lead to the average value of the linear momentum? This appears a bit strange, to say the least. In the following sections we will get a better understanding or interpretation of this result.

9.4.C Expectation (average) values are calculated in an ensemble of identically prepared systems

In general, the mean-value of a given physical property f (namely, energy, linear momentum, position, etc.) more generically called **observable** is obtained by making measurement in each of the equally prepared systems in the ensemble (and not by averaging repeated measurements on a single system.)

When making measurements on each of the $\mathcal{N}$ identically prepared systems of the ensemble (see left-side of the figure below) let's assume we get a series of results (see right-side of the figure below) like this:

$\mathcal{N}_1$ systems are found to have a value of f equal to f_1,
from which we deduce that the particular system collapsed to the state $|f_1\rangle$ right after the measurement

$\mathcal{N}_2$ systems are found to have a value of f equal to f_2,
from which we deduce that the particular system collapsed to the state $|f_2\rangle$ right after the measurement

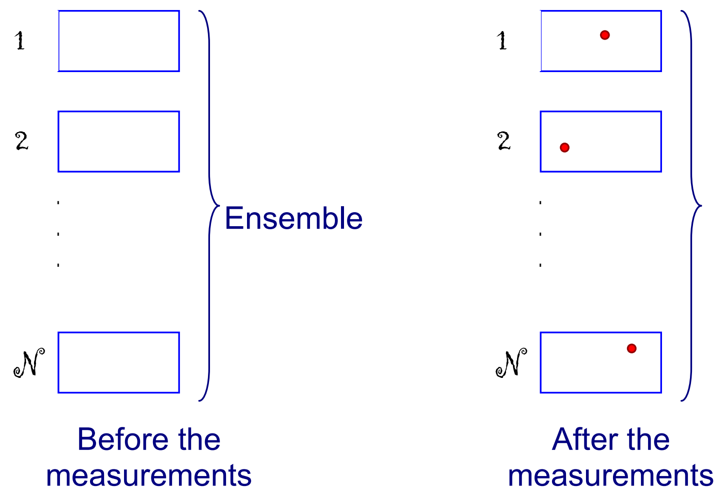
etc.

Accordingly, the average value of f would be calculated as follows,

$$\langle f \rangle_{\text{av}} = \frac{1}{\mathcal{N}} \sum_n f_n \mathcal{N}_n = \sum_n f_n \frac{\mathcal{N}_n}{\mathcal{N}} \qquad (39)$$

Notice that when $\mathcal{N}$ is a very large number, $\frac{\mathcal{N}_{\text{n}}}{\mathcal{N}}$ is nothing but the probability of finding the system in the particular state $|f_n\rangle$. Thus,

$$\langle f \rangle_{\text{av}} = \sum_n f_n \left| \langle f_n | \psi \rangle \right|^2 \qquad (40)$$



9.5 Operators associated to Observables

Quantities such as position, momentum, or energy (which are measured experimentally) are called **observables**.

- In classical physics, observables are represented by ordinary variables;
- In quantum mechanics observables are represented by **operators** (quantities that operate on a function to give a new function.)

  When a system in a state $|\,\Psi\rangle$ enters some apparatus, like, for example, a magnetic field in the Stern Gerlach experiment, or a maser resonant cavity, it may leave in a different state $|\,\phi\rangle$. That is, as a result of its interaction with the apparatus, the state of the system is modified. Symbolically, the apparatus can be represented by a corresponding operator $\tilde{\mathcal{F}}$ such that

$$|\,\phi\rangle = \tilde{\mathcal{F}}\,|\Psi\rangle \tag{41}$$

  Note: We will distinguish the operators (from other quantities) by putting a small hat $\sim$ on top of its corresponding symbol.

We show below how to introduce a quantum mechanics operator associated to a given physical quantity (this is done along the calculation of expectation values).

9.5.A Observables and Operator's Eigenvalues

Let's consider a physical quantity or observable f (for example, f = *angular momentum*) that characterizes the state of a quantum system (f actually characterizes an ensemble of similarly prepared systems.)

In quantum mechanics the values that a given physical quantity (observable) can take are called its ***eigenvalues****;* (42)

The set of these quantum eigenvalues is referred to as the spectrum of eigenvalues of the corresponding quantity f. For simplicity, let' assume for the moment that the spectrum of eigenvalues is discrete:

$|\,\phi_n\rangle$ will denote the state where the quantity f has the value f_n ;

These states will be called **eigenstates**

We will assume they satisfy

$$\langle\, \phi_n \,|\, \phi_m \,\rangle \;=\; \int_{-\infty}^{\infty} \phi_n{}^*(x)\, \phi_m(x)\, dx \;=\delta_{nm} \tag{43}$$

Using the basis constituted by the eigenstates associated to the observable f, $\{\, |\, \phi_n\rangle\ ;\ n = 1, 2, 3, \ldots\}$, an arbitrary state $|\Psi\rangle$ can be represented by the expansion,

$$|\Psi\rangle \;=\; \sum_n |\,\phi_n\rangle \underbrace{A_n} = \sum_n |\,\phi_n\rangle \underbrace{\langle\, \phi_n \,|\, \Psi\,\rangle} \tag{44}$$

where $A_n = \langle\, \phi_n \,|\, \Psi\,\rangle = \int_{-\infty}^{\infty} \phi_n{}^*(x)\ \Psi(x)\, dx$

Since the state $|\Psi\rangle$ must be a normalized state, then

$$\sum_n |\, A_n\,|^2 = \sum_n |\,\langle\, \phi_n \,|\, \Psi\,\rangle|^2 = 1$$

According to expression (40), the mean value of f, when the system is in the state $|\Psi\rangle$, is given by,

$$\langle\, f\,\rangle_{\rm av} = \sum_n f_n\, |\, A_n\,|^2 \;=\; \sum_n f_n\, |\,\langle\, \phi_n \,|\, \Psi\,\rangle|^2 \tag{45}$$

9.5.B Defining an operator $\tilde{\mathcal{F}}$ associated to an observable f. [9,10]

The operator $\tilde{\mathcal{F}}$ to be associated with the observable f is such that, when acting on an arbitrary state $|\Psi\rangle$, satisfies the following:

$$\langle \Psi \,|\, \tilde{\mathcal{F}}\, \Psi\rangle \equiv \langle f \rangle_{\text{av}} \tag{46}$$

Definition of the Operator $\tilde{\mathcal{F}}$ *associated to the observable* f

(the average value is calculated over the ensemble represented by the state $|\Psi\rangle$ *)*

But, how to build the operator $\tilde{\mathcal{F}}$? That is, if the observable quantity were, for example, the linear momentum or the angular momentum, how to build their corresponding quantum mechanics operator?

In this section 9.5.B we derive a very general self consistent expression that shows how an operator, associated to a given observable, should look like (see expression (48) below). In the subsequent sections (9.5.C and 9.5.D) we provide a specific construction of the position and momentum operators

General procedure

If the system is in the state

$$|\Psi\rangle = \sum_n |\phi_n\rangle A_n = \sum_n |\phi_n\rangle \langle \phi_n \,|\, \Psi\rangle,$$

the requirement to build the operator $\tilde{\mathcal{F}}$ is,

$$\begin{aligned}\langle \Psi \,|\, \tilde{\mathcal{F}}\, \Psi\rangle \equiv \langle f \rangle_{\text{av}} &= \sum_n f_n \,|A_n|^2 \\ &= \sum_n f_n \,|\langle \phi_n \,|\Psi\rangle|^2 \\ &= \sum_n f_n A_n^{\,*} A_n = \sum_n f_n \underbrace{\langle \Psi|\, \phi_n\rangle} \langle \phi_n \,|\Psi\rangle\end{aligned}$$

$$\textit{Since} \quad A_n = \langle \phi_n \,|\, \Psi\rangle = \int_{-\infty}^{\infty} \phi_n^{\,*}(x)\; \Psi(x)\, dx$$

$$A_n^{\,*} = \underbrace{\langle \Psi|\, \phi_n\rangle} = \int_{-\infty}^{\infty} \phi_n(x)\; \Psi^{*}(x)\, dx$$

$$\langle \Psi \mid \tilde{\mathcal{F}}\, \Psi \rangle = \sum_n f_n \underbrace{\int_{-\infty}^{\infty} \phi_n(x)\ \Psi^*(x)\, dx}\, \langle \phi_n \mid \Psi \rangle$$

Interchanging the order of the summation and integral,

$$\langle \Psi \mid \tilde{\mathcal{F}}\, \Psi \rangle = \int_{-\infty}^{\infty} \Psi^*(x) \underbrace{\sum_n f_n \langle \phi_n \mid \Psi \rangle\, \phi_n(x)}_{[\tilde{\mathcal{F}}\, \Psi](x)}\ dx \qquad (47)$$

The last expression implies: $[\tilde{\mathcal{F}}\, \Psi](x) = \sum_n f_n \langle \phi_n \mid \Psi \rangle\ \phi_n(x) = \sum_n f_n A_n \phi_n(x).$

or simply

$$\tilde{\mathcal{F}}\, \Psi = \sum_n \underbrace{f_n}_{\text{numbers}} \underbrace{\langle \phi_n \mid \Psi \rangle}_{\text{numbers}}\ \underbrace{\phi_n}_{\text{function}} = \sum_n f_n A_n\ \phi_n \qquad (48)$$

If $\tilde{\mathcal{F}}$ exists, it will have this form

Alternatively, using the brackets notation,

$$\tilde{\mathcal{F}} \mid \Psi \rangle = \sum_n f_n \langle \phi_n \mid \Psi \rangle\ \mid \phi_n \rangle = \sum_n f_n A_n \mid \phi_n \rangle \qquad (48)'$$

In the case that Ψ were one of the eigenfunctions, (48) gives,

$$\tilde{\mathcal{F}}\, \phi_n = f_n\, \phi_n \qquad (49)$$

That is, the eigenfunctions of a give physical quantity f are the solutions of the equation

$$\tilde{\mathcal{F}}\, \Psi = f\, \Psi$$

where f is a constant.

But, notice, (48) gives just a self-consistent expression for the operator $\tilde{\mathcal{F}}$; that is, an expression that is compatible with the requirement that $\langle \Psi \mid \tilde{\mathcal{F}}\, \Psi \rangle \equiv \langle f \rangle_{\text{av}}$. But there are many unknowns in (48): for example, what are eigenfunctions $\mid \phi_n \rangle$. (Accordingly, $\tilde{\mathcal{F}}$ is not known yet.)

"Of course, while the operator $\tilde{\mathcal{F}}$ is still defined by (48), which itself contain the eigenfunctions ϕ_n, no further conclusions can be drawn from the results we have obtained.
However, as we shall see below, the form of the operators for various physical quantities can be determined from direct physical considerations, which subsequently, using the above properties of the operators, will enable us to find the eigenfunctions and eigenvalues by solving the equation $\tilde{\mathcal{F}}\,\Psi = f\,\Psi$." [11]

9.5.C Definition of the Position Operator $\tilde{X}$

We are looking for operator $\tilde{X}$ such that $\langle \Psi | \tilde{X}\,\Psi \rangle$ equals the mean value of the position when the system is in the state $|\Psi\rangle$,

$$\langle \Psi \mid \tilde{X}\,\Psi \rangle \equiv \, < x > = \int_{-\infty}^{\infty} x\,|\,\psi(x)|^2\,dx, \qquad \tilde{X} = ? \tag{50}$$

Using $|\Psi\rangle = \int_{-\infty}^{\infty} |\,x\,\rangle\langle\, x\,|\Psi\rangle\,dx \;=\; \int_{-\infty}^{\infty} |\,x\,\rangle\; \Psi(x)\mathrm{d}x$, expression (50) requires,

$$\int_{-\infty}^{\infty} \Psi^{*}(x)\,[\,\tilde{X}\,\Psi](x)\,dx \;=\; \int_{-\infty}^{\infty} [\Psi^{*}(x)]\,x\,[\Psi(x)]\,dx$$

which implies,

$$[\,\tilde{X}\,\Psi](x) \;=\; x\,[\Psi(x)] \tag{51}$$

Notice, we can not say $[\,\tilde{X}\,\Psi] \;=\; x\,[\Psi]$; it would be incorrect. More appropriate is first to define the identity function I, for which $I(x) = x$, in terms of which (51) can be written as,

$$[\,\tilde{X}\,\Psi](x) \;=\; I\,\Psi(x)$$

That is,

$$\tilde{X}\,\Psi = I\,\Psi \tag{51'}$$

(Note: Frequently we will find (51) written in the following form,

$\tilde{X}\ \Psi\ =\ x\ \Psi$, but it is incorrect.)

$$\tilde{X}\ \Psi = I\Psi \qquad (I \text{ is the identity function})$$

$$[\ \tilde{X}\ \Psi](x)\ =\ x\ \Psi(x) \tag{52}$$

$$\langle \Psi \mid \tilde{X}\ \Psi \rangle = \int_{-\infty}^{\infty} [\ \Psi^{*}(x)\ ]\ [\ \tilde{X}\ \Psi\ (x)\ ]\ dx$$

$$= \int_{-\infty}^{\infty} [\ \Psi^{*}(x)\ ]\ x\ [\ \Psi(x)]\ \equiv < x >$$

9.5.D Definition of the Linear Momentum Operator

Here we construct the quantum Linear Momentum Operator, and give its representation in both the momentum-coordinates and spatial-coordinates basis. It will help illustrate that operators are general mathematical concepts whose representation depends on the base states being used.

The tasks of defining this operator is facilitated by the fact that the eigenfunctions and eigenvalues of the linear momentum operator are already known. Thus Sections 9.5.D1 and 9.5.D1 may appear to be trivial; still it helps to illustrate the connection between an operator and the mean value of the corresponding observable.

9.5.D1 The Linear Momentum Operator $\tilde{\mathcal{P}}$ expressed in the momentum base states $\{ \mid \phi_p \rangle \}$

The observable is the linear momentum p. That is,

The quantity f referred above (Section 9.5.B) is the linear momentum p.

For a given p the corresponding state is denoted as $\mid \phi_p \rangle$. (53)

The eigenstate $|\phi_p\rangle$ has the eigenvalue p .

Based on this information, find out the Linear Momentum Operator.

Since in this case we already know the eigen-states and the eigen-values (as given in (53) above), then we can apply the general formula given in (48), $|\tilde{\mathcal{F}}\,\Psi\rangle = \sum_n f_n \langle\phi_n|\Psi\rangle\,|\phi_n\rangle = \sum_n f_n A_n\,|\phi_n\rangle$,

where $|\Psi\rangle = \sum_n |\phi_n\rangle A_n$

In our particular case, we identify (using (8) and (9) given above):

$$|\Psi\rangle = \sum_n |\phi_n\rangle A_n \rightarrow \int_{-\infty}^{\infty} \mathrm{A}(p)|\phi_p\rangle\, dp \tag{54}$$

$$\text{where } \mathrm{A}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \mathrm{e}^{-ikx'}\,\psi(x')dx' = \langle\phi_p|\Psi\rangle$$

$$f_n \rightarrow p, \quad |\phi_n\rangle \rightarrow |\phi_p\rangle, \quad A_n \rightarrow \mathrm{A}(p), \quad \tilde{\mathcal{F}} \rightarrow \tilde{\mathcal{P}}.$$

Accordingly,

$$\tilde{\mathcal{P}}|\Psi\rangle = \sum_n f_n A_n |\phi_n\rangle \rightarrow \int_{-\infty}^{\infty} p\ \mathrm{A}(p)\,|\phi_p\rangle\, dp\ , \tag{55}$$

In particular

$$\tilde{\mathcal{P}}|\phi_p\rangle = p\,|\phi_p\rangle$$

In short,

$\tilde{\mathcal{P}}\|\phi_p\rangle = p\,\|\phi_p\rangle$ Or equivalently $\underbrace{\tilde{\mathcal{P}}\,\phi_p}_{\text{Eigen-function}} = \underbrace{p}_{\text{Eigenvalue}}\,\underbrace{\phi_p}_{\text{Eigenfunction}}$.	*The Linear Momentum Operator* $\tilde{\mathcal{P}}$ *acting on the momentum states*	(56)

Since $\langle \phi_{p'} | \phi_p \rangle = \delta(p - p')$, we obtain

$(\phi_{p'}, \widetilde{\mathcal{P}}\, \phi_p) = p\, \delta(p-p')$ or in the kets notation $\langle \phi_{p'} | \widetilde{\mathcal{P}}\, \phi_p \rangle = p\, \delta(p-p')$	*Components of the matrix representation of the Linear Momentum Operator* $\widetilde{\mathcal{P}}$ *in the momentum basis*	(57)

Summary

In short, if the expansion of a state $|\Psi\rangle$ in the momentum basis is known; that is,

$$|\Psi\rangle = \int_{-\infty}^{\infty} \langle \phi_p | \Psi \rangle\, |\phi_p\rangle\, dp = \int_{-\infty}^{\infty} \mathrm{A}(p) |\phi_p\rangle\, dp$$; or equivalently,

$$\Psi = \int_{-\infty}^{\infty} \langle \phi_p | \Psi \rangle\, \phi_p\, dp = \int_{-\infty}^{\infty} \mathrm{A}(p)\, \phi_p\, dp \qquad (58)$$

then the operator $\widetilde{\mathcal{P}}$, defined through the requirement $\langle \Psi \,|\, \widetilde{\mathcal{P}}\, \Psi \rangle = \langle p \rangle_{\mathrm{av}}$, satisfies

$$\widetilde{\mathcal{P}}\, \Psi = \widetilde{\mathcal{P}} \left(\int_{-\infty}^{\infty} \mathrm{A}(p)\, \phi_p\, dp \right) = \int_{-\infty}^{\infty} dp\; \mathrm{A}(p)\, \widetilde{\mathcal{P}}\, \phi_p = \int_{-\infty}^{\infty} dp\; \mathrm{A}(p)\, p\, \phi_p$$

9.5.D2 The linear momentum operator in the spatial coordinates basis

What about if the expansion of $|\Psi\rangle$ in the momentum basis is not known, and, instead, its expansion in the spatial coordinate is available? What to do to find $\widetilde{\mathcal{P}}\, \Psi$ (without having to go through the trouble of expressing $|\Psi\rangle$ in terms of the momentum basis as expression (58) requires)? It is shown below that an alternative way to express the linear momentum does exist.

For $|\Psi\rangle = \int_{-\infty}^{\infty} A(p)|\phi_p\rangle \, dp$, or equivalently $\Psi(x) = \int_{-\infty}^{\infty} A(p)\, \phi_p(x)\, dp$

From (55)

$$\widetilde{\mathcal{P}}|\Psi\rangle = \int_{-\infty}^{\infty} p \;\; A(p)\,|\,\phi_p\rangle \, dp \;\; ,$$

$$\langle\, x\,|\,\widetilde{\mathcal{P}}|\Psi\rangle = \int_{-\infty}^{\infty} p \;\; A(p) \; \langle\, x\,|\,|\,\phi_p\rangle \, dp \;\; ,$$

$$[\widetilde{\mathcal{P}}\;\Psi](x) = \int_{-\infty}^{\infty} p \;\; A(p) \;\; \phi_p(x) = \;\; dp \;\; ,$$

Using (7) $\frac{1}{\sqrt{2\pi\hbar}} \; e^{i(p/\hbar)x} = \langle\, x|\;\phi_p\,\rangle = \phi_p(x)$

$$[\widetilde{\mathcal{P}}\;\Psi](x) = \int_{-\infty}^{\infty} p \;\; A(p) \;\; \frac{1}{\sqrt{2\pi\hbar}} \; e^{i(p/\hbar)x} \; dp \;\; ,$$

$$= \int_{-\infty}^{\infty} \;\; A(p) \;\; \frac{\hbar}{i}\frac{d}{dx} \;\; \frac{1}{\sqrt{2\pi\hbar}} \; e^{i(p/\hbar)x} \; dp \;\; ,$$

$$= \frac{\hbar}{i}\frac{d}{dx} \int_{-\infty}^{\infty} \;\; A(p) \;\; \frac{1}{\sqrt{2\pi\hbar}} \; e^{i(p/\hbar)x} \; dp \;\; ,$$

$$= \frac{\hbar}{i}\frac{d}{dx} \int_{-\infty}^{\infty} \;\; A(p) \;\; \phi_p(x) \, dp \;\; ,$$

$$= \frac{\hbar}{i}\frac{d}{dx} \; \Psi(x)$$

Hence,

$$\widetilde{\mathcal{P}}\;\Psi = \frac{\hbar}{i}\frac{d}{dx} \; \Psi$$

$\widetilde{\mathcal{P}}\,\Psi = \dfrac{\hbar}{i}\dfrac{d}{dx}\Psi$ $\widetilde{\mathcal{P}} \rightarrow \dfrac{\hbar}{i}\dfrac{d}{dx}$	*Representation of the Linear Momentum Operator $\widetilde{\mathcal{P}}$ in the spatial coordinates*

(59)

According to (58),

$$\langle p \rangle_{\text{av}} = \langle \Psi \mid \widetilde{\mathcal{P}}\,\Psi \rangle = \langle \Psi \mid \frac{\hbar}{i}\frac{d}{dx}\Psi \rangle = \int \psi^* \frac{\hbar}{i}\frac{d}{d\,x}\psi\, dx \tag{60}$$

Notice, we have obtained the result (38) in a more formal way.

9.5.D3 Construction of the operators $\widetilde{\mathcal{P}}$, $\widetilde{\mathcal{P}}^2$, $\widetilde{\mathcal{P}}^3$

- Construction of the Linear Momentum $\widetilde{\mathcal{P}}$

  Starting from the definition

$$\langle p \rangle_{\text{av}} = \int_{-\infty}^{\infty} \langle \Psi | \phi_p \rangle\, p \langle \phi_p | \Psi \rangle\, dp$$

Since $\langle \phi_p | \Psi \rangle$ is the p-component of the Fourier transform of Ψ

$$p \langle \phi_p | \Psi \rangle = p \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \mathrm{e}^{-i(p/\hbar)x'}\, \psi(x')dx'$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} p\, \mathrm{e}^{-i(p/\hbar)x'}\, \psi(x')dx'$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \frac{-\hbar}{i}\left[\frac{d}{d}\, \mathrm{e}^{-i(p/\hbar)x'}\right] \psi(x')dx'$$

Integrating by parts□

$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \left[\mathrm{e}^{-i(p/\hbar)x'}\right] \frac{\hbar}{i}\frac{d\Psi}{dx}(x')dx'$$

$$p \langle \phi_p | \Psi \rangle = \langle \phi_p | \frac{\hbar}{i}\frac{d\Psi}{dx} \rangle \tag{61}$$

$$\langle p \rangle_{\text{av}} = \int_{-\infty}^{\infty} \langle \Psi | \phi_p \rangle \langle \phi_p | \frac{\hbar}{i} \frac{d\Psi}{dx} \rangle \, dp \tag{62}$$

One way to procced from here is to express explicitly the Fourier component $\langle \Psi | \phi_p \rangle$ as well as the Fourier component $\langle \phi_p | \frac{\hbar}{i} \frac{d\Psi}{dx} \rangle$, and then when implementing the three integrals to use the properties of the Delta Dirac.

Alternatively we follow below a procedure a bit unconventional (i.e. less rigorous)

$$\langle p \rangle_{\text{av}} = \langle \Psi | \int_{-\infty}^{\infty} | \phi_p \rangle \langle \phi_p | \frac{\hbar}{i} \frac{d\Psi}{dx} \rangle \, dp$$

$$= \langle \Psi | \left[\int_{-\infty}^{\infty} | \phi_p \rangle \langle \phi_p | \, dp \right] | \frac{\hbar}{i} \frac{d\Psi}{dx} \rangle$$

But since $1 = \int_{-\infty}^{\infty} \langle \Psi | \phi_p \rangle \langle \phi_p | \Psi \rangle \, dp$

$$1 = \langle \Psi | \left[\int_{-\infty}^{\infty} | \phi_p \rangle \langle \phi_p | \, dp \right] | \Psi \rangle$$

It implies

$$\left[\int_{-\infty}^{\infty} | \phi_p \rangle \langle \phi_p | \, dp \right] = 1$$

$$\langle p \rangle_{\text{av}} = \langle \Psi | \frac{\hbar}{i} \frac{d\Psi}{dx} \rangle$$

Hence, we find that the linear momentum operator is $\frac{\hbar}{i} \frac{d}{dx} \equiv \widetilde{\mathcal{P}}$

- Construction of the operator associated to $\left\langle p^2 \right\rangle_{\text{av}}$

By definition:

$$\left\langle p^2 \right\rangle_{\text{av}} = \int_{-\infty}^{\infty} \langle \Psi | \phi_p \rangle p^2 \langle \phi_p | \Psi \rangle \, dp$$

We concentrate first in evaluating the factor $p^2 \langle \phi_p \mid \Psi \rangle$. Following a similar procedure as above, we obtain,

$$p^2 \langle \phi_p \mid \Psi \rangle = \langle \phi_p \mid (\frac{\hbar}{i})^2 \frac{d^2 \Psi}{dx^2} \rangle$$

which will lead to

$$\langle p \rangle_{\text{av}} = \langle \Psi | \left(\frac{\hbar}{i} \frac{d}{dx} \right)^2 \Psi \rangle$$

Thus, the operator associated to $< p^2 >_{\text{av}}$ is $\left(\frac{\hbar}{i} \frac{d}{dx} \right)^2 = \tilde{\mathcal{P}}^2$

9.5.E Mean energy in terms of the Hamiltonian operator

In Chapter 7, the Hamiltonian Operator $\tilde{\mathcal{H}}$ was recognized through its matrix representation H , the latter being interpreted as an energy matrix due to the fact that, when working with stationary states, the components of the matrix were the energy of the corresponding stationary states. In the language of eigenvalues used in this chapter we can write,

$$\tilde{\mathcal{H}} \mid E_n \rangle = E_n \mid E_n \rangle \qquad (63)$$

where

$\{ \mid E_n \rangle \text{ , } n=1, 2, 3, \ldots \}$ is the basis constituted by stationary states

Let's calculate the expectation (or mean) value of energy for a system in a state $|\Psi\rangle$ where,

$$|\Psi\rangle = \sum_n | E_n \rangle \underbrace{\langle E_n | \Psi \rangle} = \sum_n | E_n \rangle \underbrace{B_n} \qquad (64)$$

Its mean energy is given by,

$$\langle E \rangle_{\text{av}} \equiv \sum_n E_n |\langle E_n | \psi \rangle|^2 = \sum_n \langle E_n | \Psi \rangle^* E_n \langle E_n \mid \Psi \rangle$$

$$= \sum_n \underbrace{\langle \Psi | E_n \rangle E_n} \langle E_n \mid \Psi \rangle$$

This factor can be expressed in terms of the Hamiltonian operator

From (61): $\langle \Psi | \tilde{\mathcal{H}} | E_n \rangle = E_n \langle \Psi | E_n \rangle$

$$= \sum_n \underbrace{\langle \Psi | \tilde{\mathcal{H}} | E_n \rangle} \langle E_n | \Psi \rangle$$

$$= \langle \Psi | \tilde{\mathcal{H}} \underbrace{\sum_n |E_n\rangle \langle E_n | \Psi \rangle}_{= |\Psi\rangle}$$

$$\langle E \rangle_{\text{av}} = \langle \Psi | \tilde{\mathcal{H}} | \Psi \rangle \tag{65}$$

We have found again (as we did for the linear momentum and the position operators) an elegant way to express a mean value (in this case for the energy) that does not make reference to the particular base states. Although the stationary state basis $\{ | E_n \rangle \ \textit{for}\ n = 1, 2, 3, \ldots \}$ may be convenient to use in some cases, a different base may be convenient in other cases. In effect, for a general basis $\{ | j \rangle \ \textit{for}\ j = 1, 2, 3, \ldots \}$ we will have,

$$\langle E \rangle_{\text{av}} = [\sum_i \langle i | \Psi \rangle^* \langle i |] \ \tilde{\mathcal{H}} \ [\sum_j | j \rangle \langle j | \Psi \rangle]$$

$$= \sum_{i,j} \langle \Psi | i \rangle \langle i | \tilde{\mathcal{H}} | j \rangle \langle j | \Psi \rangle \tag{66}$$

Representation of the Hamiltonian Operator in the spatial coordinate basis

In (63), let's take the case of spatial coordinate basis

$$\langle E \rangle_{\text{av}} = \langle \Psi | \tilde{\mathcal{H}} | \Psi \rangle$$

$$= [\int_{-\infty}^{\infty} \langle x | \Psi \rangle^* \langle x | \, dx] \ \tilde{\mathcal{H}} \ [\int_{-\infty}^{\infty} | x' \rangle \langle x' | \Psi \rangle \, dx']$$

$$= [\int_{-\infty}^{\infty} \langle x | \Psi \rangle^* \langle x | \, dx] \ [\int_{-\infty}^{\infty} \tilde{\mathcal{H}} | x' \rangle \langle x' | \Psi \rangle \, dx']$$

$$= \int_{-\infty}^{\infty} \langle x | \Psi \rangle^* \int_{-\infty}^{\infty} \langle x | \tilde{\mathcal{H}} | x' \rangle \langle x' | \Psi \rangle \, dx' \, dx \,]$$

Defining $H(x, x') \equiv \langle x | \tilde{\mathcal{H}} | x' \rangle$

$$\langle E\rangle_{av} = \int_{-\infty}^{\infty} \langle x|\Psi\rangle^{*} \int_{-\infty}^{\infty} H(x,x') \langle x'|\Psi\rangle dx'\, dx$$

$$= \int_{-\infty}^{\infty} \Psi(x)^{*} \int_{-\infty}^{\infty} H(x,x')\, \Psi(x')\, dx'\, dx$$

But Schrodinger established that (see expression (28) above)

$$\int_{-\infty}^{\infty} H(x,x')\, \Psi(x')\, dx' = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x) + V(x)\Psi(x)$$

Accordingly

$$\langle E\rangle_{av} = \int_{-\infty}^{\infty} \Psi(x)^{*} \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x) + V(x)\Psi(x)\right] dx$$

$$\langle E\rangle_{av} = \langle\Psi|\,\tilde{\mathcal{H}}\,|\Psi\rangle$$

$$= \int_{-\infty}^{\infty} \Psi(x)^{*} \underbrace{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]}\, \Psi(x)\, dx$$

$$\tilde{\mathcal{H}} \rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \qquad (67)$$

Representation of the Hamiltonian Operator in the spatial coordinates basis

Summary

Observable	mean value	Operator	Operator in the spatial coordinates representation
position	$< x >$	$\tilde{X}$	$\tilde{X}$
		$< x > = \langle\Psi \mid \tilde{X}\,\Psi\rangle$	$\tilde{X}\,\Psi = x\,\Psi$
momentum	$< p >$	$\tilde{\mathcal{P}}$	$\frac{\hbar}{i}\frac{d}{dx}$

		$< p > = \langle \Psi \mid \tilde{\mathcal{P}}\ \Psi \rangle$	$\tilde{\mathcal{P}}\ \Psi = \frac{\hbar}{i}\frac{d}{dx}\Psi$
Energy	$< E >$	$\tilde{\mathcal{H}}$	$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$
		$< E > = \langle \Psi \mid \tilde{\mathcal{H}}\ \Psi \rangle$	

9.6 Properties of Operators

9.6.A Hermitian conjugate (or adjoint) operators

$\tilde{\Omega}^+$ is called the *Hermitian conjugate* operator of the operator $\tilde{\Omega}$ if for any state $|\Psi\rangle$ and $|\phi\rangle$ the following relationship holds,

$$\langle\ \tilde{\Omega}^+ \phi \mid \Psi \rangle \ \equiv\ \langle \phi \mid \tilde{\Omega}\ \Psi \rangle \qquad (68)$$

Since $\langle a \mid b \rangle = \langle b \mid a \rangle^*$, we have $\langle \tilde{\Omega}^+ \phi | \Psi \rangle^* = \langle\ \Psi \mid \tilde{\Omega}^+ \phi\ \rangle$, which can be re-written as,

$$\langle\ \Psi \mid \tilde{\Omega}^+ \phi\ \rangle\ =\ \langle \phi \mid \tilde{\Omega}\, \Psi \rangle^*$$

The amplitude probability that the state $\tilde{\Omega}^+|\phi\rangle$ *be found in the state* $|\Psi\rangle$
is equal to
the complex conjugate that the state $\tilde{\Omega}\ |\Psi\ \rangle$ *be found in the state* $|\phi\ \rangle$.

$$\begin{tikzcd} |\ \Psi\rangle \arrow[r, bend left, "\tilde{\Omega}"] & |\ \phi\rangle \arrow[l, bend left, "\tilde{\Omega}^+"] \end{tikzcd}$$

Matrix Representation

In the expression above, if we take $|\Psi\rangle$ as the base state $|\ n\ \rangle$, and $|\phi\rangle$ as the base state $|\ m\ \rangle$, we obtain a relationship between the matrix representation of $\tilde{\Omega}$ and $\tilde{\Omega}^+$.

$$[\tilde{\Omega}^{+}]_{nm} = [\tilde{\Omega}]_{mn}{}^{*} \qquad (69)$$

(Notice the order of the indexes are reversed)

$\tilde{\Omega}^{+}$ is also called the **Hermitian adjoint** operator of $\tilde{\Omega}$.

Properties:

- $$(\tilde{A}\,\tilde{B})^{+} = \tilde{B}^{+}\,\tilde{A}^{+} \qquad (70)$$

Example: What is the *Hermitian conjugate* operator of the operator $\tilde{X}$?

$$\langle\, \tilde{X}^{+}\phi \mid \Psi \rangle \;\equiv\; \langle \phi \mid \tilde{X}\;\Psi \rangle = \int_{-\infty}^{\infty} \phi^{*}(x)\;[\tilde{X}\,\Psi](x)\,dx$$

$$= \int_{-\infty}^{\infty} \phi^{*}(x)\;x\;\Psi(x)\,dx \;=\; \int_{-\infty}^{\infty} x\,\phi^{*}(x)\;\;\Psi(x)\,dx$$

$$= \int_{-\infty}^{\infty} [x\,\phi(x)]^{*}\;\;\Psi(x)\,dx = \int_{-\infty}^{\infty} [\,\tilde{X}\,\phi(x)]^{*}\;\;\Psi(x)\,dx$$

$$= \langle\, \tilde{X}\,\phi \mid \Psi \rangle$$

That is,

$$\tilde{X}^{+} = \tilde{X} \qquad (71)$$

Example: What is the *Hermitian conjugate* operator of the operator $\tilde{D} = \dfrac{d}{d\,x}$?

$$\langle\, \tilde{D}^{+}\phi|\Psi\rangle \;\equiv\; \langle\phi\,|\tilde{D}\;\Psi\rangle = \int_{-\infty}^{\infty} \phi^{*}(x)\,[\,\frac{\mathrm{d}}{\mathrm{d}\,x}\,\Psi](x)\,dx \;=\; \int_{-\infty}^{\infty} \phi^{*}(x)\;\;\frac{\mathrm{d}\psi}{\mathrm{d}\,x}(x)\,dx$$

Integrating by parts

$$= -\int_{-\infty}^{\infty} \frac{\mathrm{d}\phi^{*}}{\mathrm{d}\,x}(x)\;\;\Psi(x)\,dx \;=\; \int_{-\infty}^{\infty} [\,-\tilde{\mathrm{D}}\phi(x)]^{*}\;\;\Psi(x)\,dx$$

$$= \;\langle\, -\tilde{D}\,\phi|\Psi\rangle$$

That is, $\tilde{D}^{+} = -\tilde{D}$

9.6.B Hermitian or self-adjoint operators

Many important operators of quantum mechanics have the special property that when you take the Hermitian adjoint you get back the same operator.

$$\tilde{\Omega}^{+} = \tilde{\Omega} \qquad (72)$$

Such operators are called the "**self-adjoint**" or "**Hermitian"** operators.

Example: The position operator $\tilde{\mathcal{X}}$ is a self adjoint operator because $\tilde{\mathcal{X}}^{+} = \tilde{\mathcal{X}}$, as shown in the example in the previous section.

Example: Let's see if the linear momentum operator $\tilde{\mathcal{P}}$ is self adjoint

$$\langle\, \tilde{\mathcal{P}}^{+} \phi | \Psi \rangle \equiv \langle \phi \mid \tilde{\mathcal{P}}\, \Psi \rangle = \int_{-\infty}^{\infty} \phi^{*}(\,x)\,[\,\frac{\hbar}{i}\,\frac{\mathrm{d}}{\mathrm{d}\,x}\,\Psi\,](x)\,dx \;=\; \frac{\hbar}{i}\int_{-\infty}^{\infty} \phi^{*}(\,x)\,\frac{\mathrm{d}\psi}{\mathrm{d}\,x}(x)\,dx$$

Integrating by parts

$$= -\frac{\hbar}{i}\int_{-\infty}^{\infty} \frac{\mathrm{d}\phi^{*}}{\mathrm{d}\,x}(\,x)\;\;\Psi(x)\,dx \;\;=\;\; \int_{-\infty}^{\infty} [\frac{\hbar}{i}\,\frac{\mathrm{d}\phi}{\mathrm{d}\,x}(\,x)\,]^{*}\;\;\Psi(x)\,dx$$

$$= \langle\;\; \tilde{\mathcal{P}}\,\phi \mid \Psi \rangle$$

That is,

$$\tilde{\mathcal{P}}^{+} = \tilde{\mathcal{P}} \qquad (73)$$

9.6.C Observables and Hermitian (or self-adjoint) operators

In section 9.5 above we defined quantum mechanics operators associated to observables. The definition involved the calculation of mean values of observables. From the fact that mean values are real, we can draw some conclusions concerning the properties of these operators.

$$\langle f \rangle_{\mathrm{av}} = \langle\; \Psi \mid \tilde{\mathcal{F}}\;\; \Psi \rangle = \langle\; \Psi \mid \tilde{\mathcal{F}}\;\; \Psi \rangle^{*} = \langle\; \tilde{\mathcal{F}}\;\; \Psi \mid \Psi \rangle$$

But, by definition

$$\langle\; \Psi \mid \tilde{\mathcal{F}}\;\; \Psi \rangle \equiv \langle\; \tilde{\mathcal{F}}^{+}\; \Psi \mid \Psi \rangle$$

The last two results imply,

$$\tilde{\mathcal{F}}^{+} = \tilde{\mathcal{F}} \qquad (68)$$

Operators corresponding to observables must be hermitians

The eigenvalues of a Hermitian operator are real.

Let $\tilde{\mathcal{F}}\,\phi_j = \lambda_j\,\phi_j$ (69)

Since $\langle \tilde{\mathcal{F}}\,\Psi \,|\Psi\rangle = \langle\Psi|\,\tilde{\mathcal{F}}\,\Psi\rangle$, then in particular $\langle \tilde{\mathcal{F}}\,\phi_j \,|\,\phi_j\,\rangle = \langle\phi_j|\,\tilde{\mathcal{F}}\,\phi_j\,\rangle$

Using (69)

$$\langle\, \lambda_j\,\phi_j \,\mid\, \phi_j\,\rangle = \langle\, \phi_j \mid \lambda_j\,\phi_j \,\rangle$$

$$\lambda_j^*\langle\, \phi_j \,\mid\, \phi_j\,\rangle = \lambda_j\langle\, \phi_j \,\mid\, \phi_j\,\rangle$$

which implies

$$\lambda_j^* = \lambda_j \tag{70}$$

Eigenfunctions of a Hermitian operator corresponding to different eigenvalues are orthogonal

For a given operator $\hat{\Omega}$, a states that satisfy $\hat{\Omega}|\Psi\rangle = \lambda\,|\Psi\rangle$ is called "eigen-state" of that operator, λ being the corresponding eigen-value. If a set of a few of them exist, we can denote them by

$$\hat{\Omega}\mid\Omega_j\,\rangle = \Omega_j\,\mid\Omega_j\,\rangle\quad j = 1, 2, 3, \ldots$$

Hermitian operators have the following properties:

- ➢ The eigenvalues of a Hermitian operator are real.
- ➢ The eigen-sates of a Hermitian operator corresponding to two different eigen-values are orthogonal.
- \- The sum of two Hermitian operators is also Hermitian

9.6.D Observables

When working in a space of finite dimension, it can be demonstrated that it is always possible to form a basis with the eigen-vectors of a Hermitian operator. But, when the space is infinite dimensional, this is not necessarily the case. This is the reason why it is useful to introduce the concept of an observable.

An Hermitian operator $\hat{\Omega}$ is an *observable* if its orthonormal eigen-vectors form a basis

9.7 Generalization: Expectation value of a physical quantity Q

If we review the demonstration that led to (65) we will realize that we can generalize the result to any other physical quantity. That is, the average value of a physical quantity Q can be expressed in terms of its corresponding operator $\hat{\mathbf{Q}}$.

$$\langle Q \rangle_{\text{av}} = \langle\, \Psi | \hat{\mathbf{Q}} |\, \Psi \rangle \tag{71}$$

The standard procedure is to express a general state $|\Psi\rangle$ in terms of the eigen-states of the operator $\hat{\mathbf{Q}}$, that is $\hat{\mathbf{Q}} |Q_n\rangle = Q_n \,|\, Q_n\rangle$, and then to calculate the expectation value $\langle \mathrm{Q} \rangle_{\text{av}} = \sum_n \mathrm{Q_n} \,|\langle\, \mathrm{Q_n} \,|\Psi\rangle|^2$. The latter will lead to (65).

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Alternative derivations

Definition of the Position Operator $\widetilde{X}$

Similar to the case of the linear momentum operator (as described above), the proper definition of the position operator is facilitated by the fact that the eigenfunctions and eigenvalues are known (or postulated), as shown below.

We will define an operator $\widetilde{X}$ such that $\langle \Psi | \widetilde{X}\, \Psi \rangle$ equals the mean value of the position,

$$\langle \Psi | \widetilde{X}\, \Psi \rangle \equiv < x > = \int_{-\infty}^{\infty} x \left| \psi(x) \right|^2 dx \qquad \text{(A)}$$

Let $|\Psi\rangle = \int_{-\infty}^{\infty} |x\rangle \langle x | \Psi \rangle\, dx = \int_{-\infty}^{\infty} |x\rangle\, \Psi(x) dx$

Let's assume: The eigenstate $|x\rangle$ has the eigenvalue x

Expression (48) $|\widetilde{\mathcal{F}}\, \Psi\rangle = \sum_n f_n \langle \phi_n | \Psi \rangle\, |\phi_n\rangle = \sum_n f_n A_n\, |\phi_n\rangle$ becomes

$$|\widetilde{X}\, \Psi\rangle = \int_{-\infty}^{\infty} x \langle x | \Psi \rangle\, |x\rangle\, dx = \int_{-\infty}^{\infty} x\, \Psi(x)\, |x\rangle\, dx$$

$$\langle x' | \widetilde{X}\, \Psi\rangle = \langle x' | \int_{-\infty}^{\infty} x\, \Psi(x)\, |x\rangle\, dx = \int_{-\infty}^{\infty} x\, \Psi(x)\, \langle x' | x \rangle\, dx$$

Using (8) $\langle x' | x \rangle = \delta(x - x')$

$$\langle x' | \widetilde{X}\, \Psi\rangle = \int_{-\infty}^{\infty} x\, \Psi(x)\, \delta(x - x')\, dx = x'\, \Psi(x')$$

$$\widetilde{X}\, \Psi(x) = x\, \Psi(x)$$

$$[\, \widetilde{X}\, \Psi](x) = x\, \Psi(x) \qquad \text{(B)}$$

$$\langle \Psi | \widetilde{X}\, \Psi \rangle \equiv < x > = \int_{-\infty}^{\infty} [\, \Psi^*(x)\,]\, [\, \widetilde{X}\, \Psi(x)\,]\, dx$$

$$= \int_{-\infty}^{\infty} [\, \Psi^*(x)\,]\; x\, [\, \Psi(x)]$$

[1] See Section 16-4 in Feynman Lectures: Vol III (See Fig 16-2 in this reference for an illustration of the Delta Dirac).

[2] See Feynman Lectures, Vol III, page 16-9 and 16-10.

[3] See Feynman Lectures, Vol III, Section 16-5.

[4] See Feynman Lectures, Vol III, page 16-12

[5] It is interesting to observe new strategies beyond the ensemble approach: B. L. Altshuler, JETP Lett. 41, 648 (1985). P. A. Lee and A. D. Stone, Phys. Rev. Lett. 55, 1622 (1985). See also the introduction article by Igor V. Lerner, “So Small Yey Still Giant,” Science 316, 63 (2007).

[6] B. H. Brasden and C. J. Joachain, “Quantum Mechanics,” 2nd Edition, page 56.

[7] Eisberg, Resnick, “Quantum Physics,” page 80, 2nd Edition Wiley (1985).

[8] D. Griffiths, Introduction to Quantum Mechanics,” Second Eddition,; Pearson Prentice Hall (2005), page 15.

[9] L. D. Landau and E.M. Lifshitz, “Quantum Mechanics, Non-Relativistic Theory,” Prgamon Press, 1965; Chapter 1, Section 3. He introduces the concept of Quantum operators in the context of finding mean values of observables.

[10] Feynman Lectures, Vol III, Section 20-4 and Section 20-5. Feynman also introduces the concept of Quantum operators in the context of finding mean values of observables.

[11] L. D. Landau and E.M. Lifshitz, “Quantum Mechanics, Non-Relativistic Theory,” Prgamon Press, 1965; Chapter 1, Section 3.