PUSAT PENGAJIAN SAINS FIZIK
SCHOOL OF FIZIK
Universiti Sains Malaysia,
11800 USM, Pulau Pinang
Tel. no.: 04-6533888 ext : 5311
Fax no.: 04-6535143

INDUSTRIAL TRAINING REPORT

INDUSTRIAL TRAINING
(ZCE 299)

SEMESTER 2
ACADEMIC SESSION (2010/201)

NAME	: Ng Wei Chun
MATRIC NUMBER	: 105525
COURSE	: PURE PHYSICS
DATE START / DATE END	: 16th May 2011 / 9th September 2011
NAME OF COMPANY	: School of Physics, USM
ADDRESS OF COMPANY	: USM
NAME OF PROJECT	: Representations in Quantum Mechanics
NAME OF ACADEMIC ADVISOR	: Dr. Azhar Bin Abdul Rahman
NAME OF TRAINING ADVISOR	: Dr. Myo Thaik
TRAINING ADVISOR E-MAIL	: mmmt474@gmail.com

Acknowledgment

Thank God for giving me this great opportunity to go through this student training scheme program. The completion of this project has required a lot of helps.

Firstly, I would like to express my gratitude to Dr. Myo Thaik, who has supervised me throughout the training. He has never hold back for his guidance, knowledge, and pointing out an easy and systematic pathway for me. His passions in theoretical physics and the willingness to share more have inspired me a lot and allow me to know more, even outside the scope of the title.

To my family, I would like to give special thanks for their moral support and encouragement, even it is holiday term and they miss out the chance to have any family gather.

As well, to my friends, who have given me information and advice directly and indirectly. Especially thanks to Wong Ze Hao, who have given me brilliant tips in solving some mathematics and provide me a place to work on during holiday period where library is not available in long hours.

Abstract

We can have three common interpretations regarding the representation in quantum mechanics: representation in term of bases system, representation in the type of vector spaces, and representation of time dependency for state vectors and operators. The formulation of quantum mechanics itself is already based on two different bases systems, discrete bases and continuous bases. In other way, we are more familiar in the ordinary spatial coordinates of x_i, but it is sometimes even useful where we need to have the wave function be written in position space, p_i. Finally, we have three pictures of quantum mechanics to readily relate the time evolution factors.

Contents

Acknowledgment……………………………………………………………………….i

Abstract………………………………………………………………………………..ii

Contents……………………………………………………………………………iii

Background of School of Physics……………………………………………………..iv

Chapter 1: Introduction……………………………………………………………1

Chapter 2: Mathematical Formalism and Dirac Bra-Kets Notation………………2

2.1 Phase Space………………………………………………………………..2

2.2 The Hilbert Space………………………………………………………….2

2.3 Dirac Notation……………………………………………………………..3

2.4 Operators…………………………………………………………………..5

2.5 Representation in Discrete Bases…………………………………………8

2.6 Representation in Continuous Bases……………………………………..10

2.7 One-Dimensional Delta Function………………………………………...11

Chapter 3: Schrödinger Equation……………………………………………………..12

3.1 Wave Function…………………………………………………….......12

3.2 Schrödinger Equation in Position space…………………………………14

3.3 Schrödinger Equation in Momentum space……………………………...18

Chapter 4: Applications of Schrödinger Equation………………………………...21

4.1 The Free Particle…………………………………………………………21

4.2 Simple Harmonic Oscillator……………………………………………...23

4.3 Hydrogen Atom…………………………………………………………..26

Chapter 5: The Pictures of Quantum Mechanics…………………………………36

5.1 Time Evolution of State…………………………………………………36

5.2 The Schrödinger Picture…………………………………………………39

5.3 The Heisenberg Picture…………………………………………………..39

5.4 The Interaction Picture (or) the Dirac Picture……………………………40

Reference……………………………………………………………………………...vi

Summary……………………………………………………………………………...vii

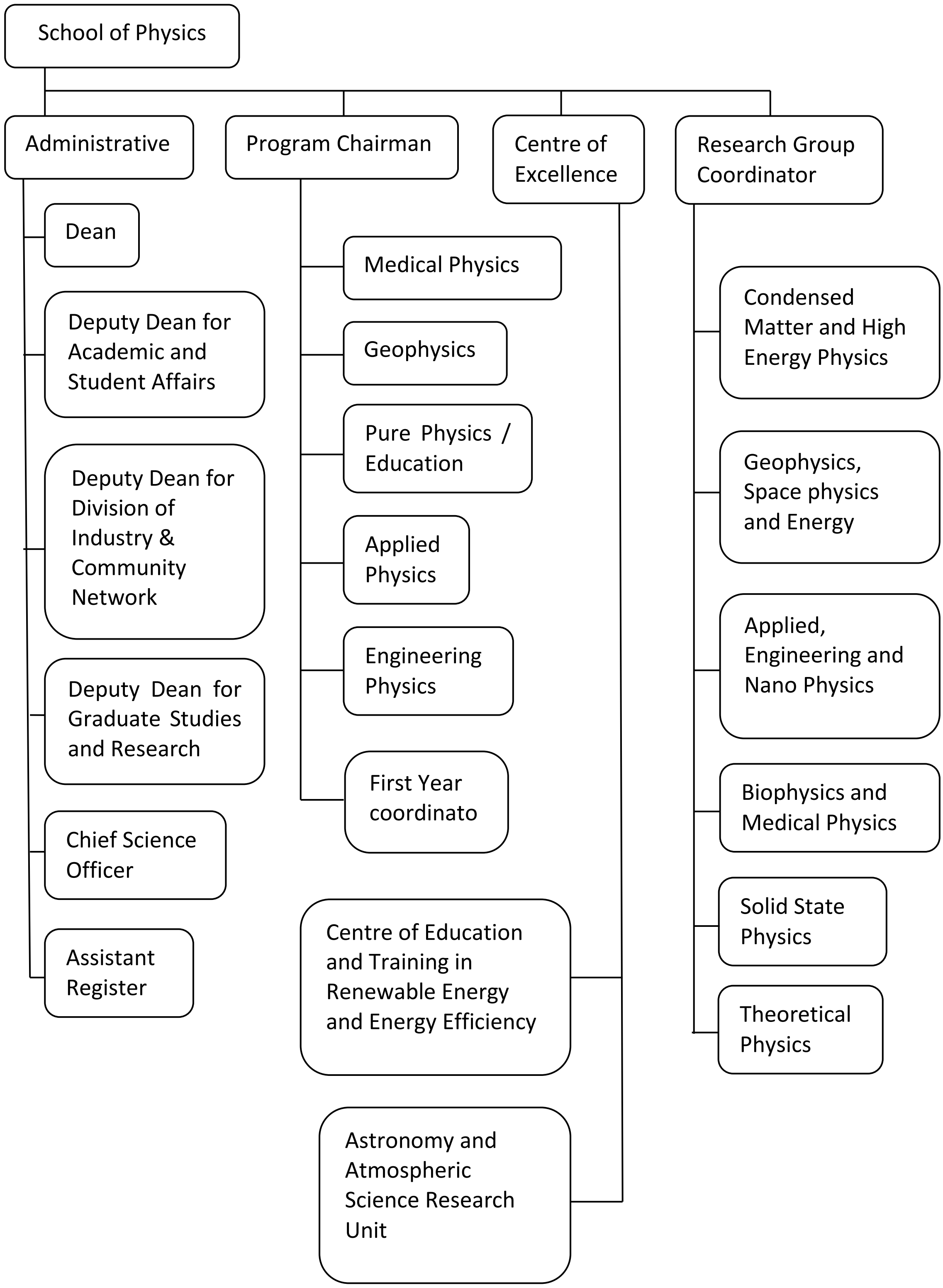
Background of School of Physics

History

When Science University of Malaysia (USM) established at the year of 1969, the School of Physics was among the very first school which was set up along with two other schools. The School of Physics is located behind the first Hamzah Sendut Library, and side to side with school of Industrial Technologies. According to the main website of School of Physics, the main objective is to produce competent, knowledgeable, creative, and innovative Physics and Applied Physics graduates for the nation’s rapid growth and progress. They strive to make generation of Malaysian scientifically and culturally stimulation, resplendent, and fertile, because paramount among these, we believe that to be scientifically illiterate is tantamount to being essentially uncultured. Moreover, the industrial significant of this school is intricately connected to the flow of discoveries in physics field which eventually lead to a growth in various industries such as microelectronics, optical, and nuclear technologies. School of Physics is providing many state-of-the-art pertinent facilities and know-how for the study of physics and its related disciplines.

The area which the School of Physics specialized in Theoretical Physics, Geophysics, Medical Physics, Applied Physics and Engineering Physics. Since the recent acknowledgement of Science University of Malaysia (USM) under the criteria of accelerated program for excellence (apex), the School of Physics has focus more on research and development. The school of physics carries out researches in diverse areas of physics. Among the research activities carried out are radiation monitoring, radiation dosimetry, and industrial applications of radioisotopes; X-ray fluorescence, powder and single crystal spectrometry; material testing (mechanical, electrical, and optical) and device fabrication and characterization calibration of electronic equipment; solar energy collector design; bioenergy; geophysical exploration; engineering seismology; groundwater prospecting and hydro geological studies using geophysical methods; and semiconductor materials and devices fabrication processes.

Organization Chart



CHAPTER 1
INTRODUCTION

The theory of quantum mechanics deals in essence with solving the following eigenvalue problem:

$$\boxed{\hat{H}|\psi\rangle = E|\psi\rangle} \tag{1.1}$$

where $\hat{H}$ is the Hamiltonian of the system. This equation is general and does not depend on any coordinate system or representation. But to solve it, we need to represent it in a given basis system. Historically follow, quantum mechanics was formulated in two different ways:

- Schrödinger's wave mechanics in continuous basis system, and
- Heisenberg's matrix mechanics in discrete basis system.

Though, they are proved to be equivalence a few years after the formulation using the theory of unitary transformations.

Representation in quantum mechanics means the form of equation for eigenvalue problem (1.1) we are going to represent in with proper basis systems and phase space: of position space or momentum space.

There are many representations of wave function and operators, and the connection between various representations is provided by unitary transformations as well. Each class of representation, also called a picture, differs from others in the way it treats the time evolution of the system. The most encountered pictures in quantum mechanics are: the Schrödinger picture, the Heisenberg picture, and the interaction picture.

The Schrödinger picture is useful when describing phenomena with time-independent Hamiltonians, whereas Heisenberg pictures and the interaction pictures are useful when describing phenomena with time-dependent Hamiltonians.

CHAPTER 2

MATHEMATICAL FORMALISM AND DIRAC BRA-KETS NOTATION

2.1 Phase Space

It is essentials to understand the concept of phase space, for we need to represent the eigenvalue equation (1.1) in either position space or momentum space. Position space can easily understand as our ordinary spatial coordinate system. While in momentum space we need suitable transformations to represent the wave function.

Definition of Phase space

For a system with n degrees of freedom, the 2n-dimensional space with coordinates (q_1, q_2, … q_n, p_1, p_2, … p_n), where the 'q's describe the degrees of freedom of the system and the 'p's are the corresponding momenta. Each point represents a state of the system. As the system changes with time the represented points trace out a curve in phase space called trajectory.

2.2 The Hilbert Space

A Hilbert space is a function space consists of a set of vectors $\psi, \phi, \chi, \ldots$ and a set of scalars $a, b, c, \ldots$ which satisfy the following four properties:

a) Hilbert space is a linear space.

b) Hilbert space has a defined scalar product that is strictly positive. The scalar product of ψ and φ is: $(\psi, \phi) = \psi^* \phi =$ complex number. So, the quantity $(\psi, \phi) \neq (\phi, \psi)$ since in general $\psi^* \phi \neq \phi^* \psi$.

c) Hilbert space is separable.

d) Hilbert space is complete.

2.2.1 Square-Integrable Function

The scalar product of two functions $\psi(x)$ and $\phi(x)$ is given as:

$$(\psi, \phi) = \int \psi^*(x) \phi(x) dx \tag{2.1}$$

In order for the function space to possess a scalar product, we must have $(\psi, \phi) < \infty$ finite. It is thus necessary that every admissible function be *square integrable*:

$$(\psi, \psi) = \int |\psi(x)|^2 \, dx < \infty \tag{2.2}$$

In short, the space spanned by square-integrable functions is a Hilbert space.

2.3 Dirac Notation

Dirac introduced the concepts of kets, bras, and bra-kets.

A) Kets: element of a vector space

Dirac denoted the state vector ψ by the symbol $|\psi\rangle$, which he called the ket vector or simply ket. Kets belong to Hilbert space or in short, the ket-space.

B) Bras: element of a dual space

From linear algebra, a dual space can be associated with every vector space. Dirac denoted the element $\langle\psi|$ if a dual space as a bra vector, or simply a bra. For every ket $|\psi\rangle$ there exists a unique bra $\langle\psi|$ and vice versa. Here, bras belong to dual (Hilbert) space.

C) Bra-ket: Dirac notation for the scalar product

Also known as inner product, denoted by the symbol $\langle\ |\ \rangle$. Dirac call this bra-ket. For instance,

$$(\phi,\psi) \to \langle\phi|\psi\rangle \tag{2.3}$$

when a ket (or bra) is multiplied by a complex number, we get a ket (or bra). In wave mechanics we deal with wave function $\psi(\vec{r},t)$ which are also elements of Hilbert space, but in general formalism of quantum mechanics, we deal with abstract kets $|\psi\rangle$. Like wave function, a ket represents the system completely, and hence, knowing $|\psi\rangle$ means knowing all its amplitudes in all possible representations. In the position coordinate representation, the scalar product $\langle\phi|\psi\rangle$ is given by:

$$\boxed{\langle\phi|\psi\rangle = \int \phi^*(\vec{r},t)\psi(\vec{r},t)d^3r} \tag{2.4}$$

2.3.1 Properties of kets, bras and bra-kets

a) Every kets has a corresponding bra

As explained in 2.3 B): $$|\psi\rangle \leftrightarrow \langle\psi| \tag{2.5}$$

one-to-one correspondence between bras and kets:

$$a|\psi\rangle + b|\phi\rangle \leftrightarrow a^*\langle\psi| + b^*\langle\phi| \tag{2.6}$$

where a and b are complex number. Also:

$$|a\psi\rangle = a|\psi\rangle \qquad , \qquad \langle a\psi| = a^*\langle\psi| \tag{2.7}$$

b) Scalar product

Since the scalar product is a complex number, the ordering matters, for

$$\langle \phi|\psi\rangle^* = \langle \psi|\phi\rangle \tag{2.8}$$

By using (2.4),

$$\begin{aligned}\langle \phi|\psi\rangle^* &= \left(\int \phi^*(\vec{r},t)\psi(\vec{r},t)d^3r\right)^* \\ &= \int \psi^*(\vec{r},t)\phi(\vec{r},t)d^3r \\ &= \langle \psi|\phi\rangle \end{aligned} \tag{2.9}$$

Also,

$$\langle \psi|a_1\psi_1 + a_2\psi_2\rangle = a_1\langle \psi|\psi_1\rangle + a_2\langle \psi|\psi_2\rangle \tag{2.10}$$

$$\langle a_1\phi_1 + a_2\phi_2|\psi\rangle = a_1^*\langle \phi_1|\psi\rangle + a_2^*\langle \phi_2|\psi\rangle \tag{2.11}$$

$$\langle a_1\phi_1 + a_2\phi_2|b_1\psi_1 + b_2\psi_2\rangle = a_1^*b_1\langle \phi_1|\psi_1\rangle + a_1^*b_2\langle \phi_1|\psi_2\rangle + a_2^*b_1\langle \phi_2|\psi_1\rangle + a_2^*b_2\langle \phi_2|\psi_2\rangle \tag{2.12}$$

c) The norm is real and positive

For any $|\psi\rangle$, the norm $\sqrt{\langle \psi|\psi\rangle}$ is real and positive.

$\langle \psi|\psi\rangle$ is equal to zero only for the case where $|\psi\rangle = 0$ and if the state $|\psi\rangle$ is normalized, $\langle \psi|\psi\rangle = 1$.

d) Schwarz inequality

For any two states $|\psi\rangle$ and $|\phi\rangle$, we have

$$|\langle \psi|\phi\rangle|^2 \le \langle \psi|\psi\rangle\langle \phi|\phi\rangle \tag{2.13}$$

If $|\psi\rangle$ and $|\phi\rangle$ are linearly dependent, where $|\psi\rangle = \alpha|\phi\rangle$, where α is a scalar, this relation becomes an equality. The Schwarz inequality (2.13) is analogous to the following relation of the real *Euclidean space*:

$$\left|\vec{A}\cdot\vec{B}\right|^2 \le \left|\vec{A}\right|^2\left|\vec{B}\right|^2 \tag{2.14}$$

e) Triangle inequality

$$\sqrt{\langle \psi+\phi|\phi+\psi\rangle} \le \sqrt{\langle \psi|\psi\rangle} + \sqrt{\langle \phi|\phi\rangle} \tag{2.15}$$

Again, if $|\psi\rangle$ and $|\phi\rangle$ are linearly dependent, $|\psi\rangle = \alpha|\phi\rangle$ and if the scalar α is real and positive, the inequality becomes an equality. The inequality in Euclidean space is given by

$$\left|\vec{A}+\vec{B}\right| \le \left|\vec{A}\right| + \left|\vec{B}\right| \tag{2.16}$$

f) Orthogonal states

Two kets, $|\psi\rangle$ and $|\phi\rangle$, are said to be orthogonal if they have vanishing scalar product:

$$\langle\psi|\phi\rangle = 0 \tag{2.17}$$

g) Orthonormal states

Two kets, $|\psi\rangle$ and $|\phi\rangle$, are said to be orthonormal if they are orthogonal and each are normalized. That is:

$$\langle\psi|\phi\rangle = 0 \quad , \quad \langle\psi|\psi\rangle = 1 \quad , \quad \langle\phi|\phi\rangle = 1 \tag{2.18}$$

2.4 Operators

2.4.1 Definitions

An operator $\hat{A}$ is a mathematical rule that when apply to a ket $|\psi\rangle$ transform it into another ket $|\psi'\rangle$ of the same space. The same goes to bra $\langle\phi|$.

$$\hat{A}|\psi\rangle = |\psi'\rangle \quad , \quad \langle\phi|\hat{A} = \langle\phi'| \tag{2.19}$$

Similarly to wave functions:

$$\hat{A}\psi(\vec{r}) = \psi'(\vec{r}) \quad , \quad \phi(\vec{r})\hat{A} = \phi'(\vec{r}) \tag{2.20}$$

The product of two operators is not commutative:

$$\hat{A}\hat{B} \neq \hat{B}\hat{A} \tag{2.21}$$

However, the product is associative.

$$\hat{A}\hat{B}\hat{C} = \hat{A}(\hat{B}\hat{C}) = (\hat{A}\hat{B})\hat{C} \tag{2.22}$$

The order when the product $\hat{A}\hat{B}$ operates on a ket $|\psi\rangle$ is important,

$$\hat{A}\hat{B}|\psi\rangle = \hat{A}\big(\hat{B}|\psi\rangle\big) \tag{2.23}$$

An operator $\hat{A}$ is said to be linear if it obey the distributive law.

$$\hat{A}(a_1|\psi_1\rangle + a_2|\psi_2\rangle) = a_1\hat{A}|\psi_1\rangle + a_2\hat{A}|\psi_2\rangle \tag{2.24}$$

and

$$(\langle\psi_1|a_1 + \langle\psi_2|a_2)\hat{A} = a_1\langle\psi_1|\hat{A} + a_2\langle\psi_2|\hat{A} \tag{2.25}$$

2.4.2 Hermitian adjoin

The Hermitian adjoin $\hat{A}^\dagger$ of an operator $\hat{A}$ is defined by the relation

$$\langle\psi|\hat{A}^\dagger|\phi\rangle = \langle\phi|\hat{A}|\psi\rangle^* \tag{2.26}$$

In algebra, adjoin meant *conjugate transpose*. So, for a complex number α, $\alpha^\dagger = \alpha^*$. While for bras and kets, $(|\psi\rangle^\dagger) = \langle\psi|$ and $(\langle\psi|)^\dagger = |\psi\rangle$.

We have properties:

$$\left(\hat{A}^\dagger\right)^\dagger = \hat{A} \tag{2.27}$$

$$\left(\alpha\hat{A}\right)^{\dagger} = \alpha^{*}\hat{A}^{\dagger} \tag{2.28}$$

$$\left(\hat{A}^{n}\right)^{\dagger} = \left(\hat{A}^{\dagger}\right)^{n} \tag{2.29}$$

$$\left(\hat{A} + \hat{B} + \hat{C} + \hat{D}\right)^{\dagger} = \hat{A}^{\dagger} + \hat{B}^{\dagger} + \hat{C}^{\dagger} + \hat{D}^{\dagger} \tag{2.30}$$

$$\left(\hat{A}\hat{B}\hat{C}\hat{D}\right)^{\dagger} = \hat{D}^{\dagger}\hat{C}^{\dagger}\hat{B}^{\dagger}\hat{A}^{\dagger} \tag{2.31}$$

$$\left(\hat{A}\hat{B}\hat{C}\hat{D}|\psi\rangle\right)^{\dagger} = \langle\psi|\hat{D}^{\dagger}\hat{C}^{\dagger}\hat{B}^{\dagger}\hat{A}^{\dagger} \tag{2.32}$$

The Hermitian adjoin of the operator $|\psi\rangle\langle\phi|$ is given by

$$(|\psi\rangle\langle\phi|)^{\dagger} = |\phi\rangle\langle\psi| \tag{2.33}$$

Operators act inside kets and bras as follows:

$$\left|\alpha\hat{A}\psi\right\rangle = \alpha\hat{A}|\psi\rangle \quad , \quad \left\langle\alpha\hat{A}\psi\right| = \alpha^{*}\langle\psi|\hat{A}^{\dagger} \tag{2.34}$$

For that, we have $\left\langle\alpha\hat{A}^{\dagger}\psi\right| = \alpha^{*}\langle\psi|\left(\hat{A}^{\dagger}\right)^{\dagger} = \alpha^{*}\langle\psi|\hat{A}$. Hence we can write:

$$\left\langle\psi\middle|\hat{A}\middle|\phi\right\rangle = \left\langle\hat{A}^{\dagger}\psi\middle|\phi\right\rangle = \left\langle\psi\middle|\hat{A}\phi\right\rangle \tag{2.35}$$

2.4.3 Hermitian and skew-Hermitian operators

An operator $\hat{A}$ is said to be Hermitian if,

$$\boxed{\hat{A} = \hat{A}^{\dagger} \quad \text{or} \quad \left\langle\psi\middle|\hat{A}\middle|\phi\right\rangle = \left\langle\phi\middle|\hat{A}\middle|\psi\right\rangle^{*}} \tag{2.36}$$

On the other hand, an operator $\hat{B}$ is said to be skew-Hermitian if,

$$\boxed{\hat{B} = -\hat{B}^{\dagger} \quad \text{or} \quad \left\langle\psi\middle|\hat{B}\middle|\phi\right\rangle = -\left\langle\phi\middle|\hat{B}\middle|\psi\right\rangle^{*}} \tag{2.37}$$

2.4.4 Commutator algebra

The commutator of two operator $\hat{A}$ and $\hat{B}$, denoted by $\left[\hat{A},\hat{B}\right]$ is defined by:

$$\boxed{\left[\hat{A},\hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}} \tag{2.38}$$

And the anti-commutator $\left\{\hat{A},\hat{B}\right\}$ is defined by:

$$\boxed{\left\{\hat{A},\hat{B}\right\} = \hat{A}\hat{B} + \hat{B}\hat{A}} \tag{2.39}$$

If $\hat{A}\hat{B} = \hat{B}\hat{A}$, the two operators are said to commute. Of course, any operator commutes with itself:

$$\left[\hat{A},\hat{A}\right] = 0 \tag{2.40}$$

If the two operators are Hermitian, and their product is also Hermitian, these operators commute:

$$\left(\hat{A}\hat{B}\right)^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger} = \hat{B}\hat{A} \quad \text{, also} \quad \left(\hat{A}\hat{B}\right)^{\dagger} = \hat{A}\hat{B} \quad \text{thus,} \quad \hat{A}\hat{B} = \hat{B}\hat{A} \tag{2.41}$$

We have the following properties:

Anti-symmetry: $$[\hat{A},\hat{B}] = -[\hat{B},\hat{A}] \tag{2.42}$$

Linearity: $$[\hat{A},\hat{B}+\hat{C}+\cdots] = [\hat{A},\hat{B}] + [\hat{A},\hat{C}] + \cdots \tag{2.43}$$

Adjoin of a commutator: $$[\hat{A},\hat{B}]^{\dagger} = [\hat{B}^{\dagger},\hat{A}^{\dagger}] \tag{2.44}$$

Distributive: $$[\hat{A},\hat{B}\hat{C}] = [\hat{A},\hat{B}]\hat{C} + \hat{B}[\hat{A},\hat{C}] \tag{2.45}$$

$$[\hat{A}\hat{B},\hat{C}] = \hat{A}[\hat{B},\hat{C}] + [\hat{A},\hat{C}]\hat{B} \tag{2.46}$$

Jacobi identity: $$\left[\hat{A},[\hat{B},\hat{C}]\right] + \left[\hat{B},[\hat{C},\hat{A}]\right] + \left[\hat{C},[\hat{A},\hat{B}]\right] = 0 \tag{2.47}$$

Operator commute with scalars: $$[\hat{A},b] = 0 \tag{2.48}$$

2.4.5 Unitary operators, $\hat{U}$

$$\hat{U}^{\dagger} = \hat{U}^{-1} \qquad \text{and} \qquad \hat{U}\hat{U}^{\dagger} = \hat{U}^{\dagger}\hat{U} = \hat{I} \tag{2.49}$$

2.4.6 Eigenvalues and eigenvectors of an operator

If the action of an operator $\hat{A}$ on $|\psi\rangle$ give:

$$\boxed{\hat{A}|\psi\rangle = a|\psi\rangle} \tag{2.50}$$

Where a is a complex number, then the state vector $|\psi\rangle$ is eigenvector (eigenstate) of operator $\hat{A}$, while a is an eigenvalue of $\hat{A}$.

We have some useful theorems pertaining to the eigenvalue problem.

Theorem 2.1

For a Hermitian operator, say $\hat{A} = \hat{A}^{\dagger}$ for $\hat{A}|\phi_n\rangle = a_n|\phi_n\rangle$.We have the eigenvalues a_n are real and the eigenvectors belonging to distinct eigenvalues are orthogonal.

Proof:

$$\hat{A}|\phi_n\rangle = a_n|\phi_n\rangle \;\Rightarrow\; \langle\phi_m|\hat{A}|\phi_n\rangle = a_n\langle\phi_m|\phi_n\rangle \tag{2.51}$$

$$\langle\phi_m|\hat{A}^{\dagger} = a_m^*\langle\phi_m| \;\Rightarrow\; \langle\phi_m|\hat{A}^{\dagger}|\phi_n\rangle = a_m^*\langle\phi_m|\phi_n\rangle \tag{2.52}$$

Take the difference, and such that $\hat{A} = \hat{A}^{\dagger}$,

$$(a_n - a_m^*)\langle\phi_m|\phi_n\rangle = 0 \tag{2.53}$$

With two possible cases:

case $m = n$: since $\langle\phi_n|\phi_n\rangle > 0$, the vanishing term $a_n - a_n^* = 0$, for $a_n = a_n^*$, a_n must be real.

case $m \neq n$: for $a_n \neq a_m$, with $a_m^* = a_m$, the vanishing term $\langle\phi_m|\phi_n\rangle = 0$, that is $|\phi_m\rangle$ and $|\phi_n\rangle$ must be orthogonal. When $|\phi_n\rangle$ is normalized, then $\langle\phi_m|\phi_n\rangle = \delta_{mn}$, where $\delta_{mn} = \begin{cases} 1\,, m = n \\ 0\,, m \neq n \end{cases}$ is the *Kronecker delta*.

Theorem 2.2

For two non-degenerate Hermitian operators, $\hat{A}$ and $\hat{B}$ to commute, they share the same set of eigenvectors.

Proof:

consider $\hat{A}|\phi_n\rangle = a_n|\phi_n\rangle$ (2.54)

for $\hat{A}\left(\hat{B}|\phi_n\rangle\right) = \hat{B}\left(\hat{A}|\phi_n\rangle\right) = a_n\left(\hat{B}|\phi_n\rangle\right)$ (2.55)

Since $|\phi_n\rangle$ is unique, we must allow $\hat{B}|\phi_n\rangle \propto |\phi_n\rangle$ (2.56)

and with a constant, say $\hat{B}|\phi_n\rangle = b_n|\phi_n\rangle$ (2.57)

we see that $|\phi_n\rangle$ is also eigenstate for operator $\hat{B}$.

2.5 Representation in Discrete Bases

Consider the set of $\{|\phi_n\rangle\}$ which make up a discrete, complete and orthonormal basis, of the Hilbert space. We have the orthonormality of the base kets being expressed by:

$$\langle\phi_m|\phi_n\rangle = \delta_{mn} \tag{2.58}$$

The *completeness* of the basis is given by

$$\sum_{n=1}^{\infty}|\phi_n\rangle\langle\phi_n| = \hat{I} \tag{2.59}$$

where $\hat{I}$ is the unit operator.

2.5.1 Matrix representation of kets and bras

The completeness property of this basis enables us to expand any state vector $|\psi\rangle$ in terms of the base kets $|\phi_n\rangle$:

$$|\psi\rangle = \hat{I}|\psi\rangle = \left(\sum_{n=1}^{\infty}|\phi_n\rangle\langle\phi_n|\right)|\psi\rangle = \sum_{n=1}^{\infty}a_n|\phi_n\rangle \tag{2.60}$$

where the coefficient a_n, which is equal to $\langle\phi_n|\psi\rangle$, represents the projection of $|\psi\rangle$ onto $|\phi_n\rangle$; a_n is the component of $|\psi\rangle$ along the vector $|\phi_n\rangle$. So, within the basis $\{|\phi_n\rangle\}$, the ket $|\psi\rangle$ can be represented by a column vector:

$$|\psi\rangle \rightarrow \begin{pmatrix} \langle\phi_1|\psi\rangle \\ \langle\phi_2|\psi\rangle \\ \vdots \\ \langle\phi_n|\psi\rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \\ \vdots \end{pmatrix} \tag{2.61}$$

While the bra $\langle\psi|$ can be represented by a row vector:

$$\langle\psi| \rightarrow \begin{pmatrix}\langle\psi|\phi_1\rangle & \langle\psi|\phi_2\rangle & \cdots & \langle\psi|\phi_n\rangle & \cdots\end{pmatrix}$$
$$= \begin{pmatrix}\langle\phi_1|\psi\rangle^* & \langle\phi_2|\psi\rangle^* & \cdots & \langle\phi_n|\psi\rangle^* & \cdots\end{pmatrix}$$
$$= \begin{pmatrix}a_1^* & a_2^* & \cdots & a_n^* & \cdots\end{pmatrix} \tag{2.62}$$

Using this representation, we see that a bra-ket $\langle\psi|\phi\rangle$ is a complex number equal to the matrix product of the row matrix corresponding to the bra $\langle\psi|$ with the column matrix corresponding to the ket $|\phi\rangle$:

$$\langle\psi|\phi\rangle = \begin{pmatrix}a_1^* & a_2^* & \cdots & a_n^* & \cdots\end{pmatrix}\begin{pmatrix}b_1\\ b_2\\ \vdots\\ b_n\\ \vdots\end{pmatrix} = \sum_n a_n^* b_n \tag{2.63}$$

where $b_n = \langle\phi_n|\phi\rangle$. We see that, within this representation, the matrices representing $|\psi\rangle$ and $\langle\psi|$ are Hermitian adjoins of each other.

2.5.2 Matrix representation of operators

For each linear operator $\hat{A}$, we can write

$$\hat{A} = \hat{I}\hat{A}\hat{I} = \left(\sum_{n=1}^{\infty}|\phi_n\rangle\langle\phi_n|\right)\hat{A}\left(\sum_{m=1}^{\infty}|\phi_m\rangle\langle\phi_m|\right) = \sum_{nm} A_{nm}|\phi_n\rangle\langle\phi_m| \tag{2.64}$$

where A_{nm} is the nm matrix element of the operator $\hat{A}$:

$$A_{nm} = \langle\phi_n|\hat{A}|\phi_m\rangle \tag{2.65}$$

We see that the operator $\hat{A}$ is represented, within the basis $\{|\phi_n\rangle\}$, by a square matrix:

$$A = \begin{pmatrix}A_{11} & A_{12} & A_{13} & \cdots\\ A_{21} & A_{22} & A_{23} & \cdots\\ A_{31} & A_{32} & A_{33} & \cdots\\ \vdots & \vdots & \vdots & \ddots\end{pmatrix} \tag{2.66}$$

For instance, the unit operator $\hat{I}$ is represented by a unit matrix:

$$\hat{I} = \begin{pmatrix}1 & 0 & \cdots\\ 0 & 1 & \cdots\\ \vdots & \vdots & \ddots\end{pmatrix} \tag{2.67}$$

In summary, kets are represented by a column vectors, bras by row vectors and operators by square matrices.

2.5.3 Matrix representation of the eigenvalue problem

As in equation (2.50), we want to find the eigenvalues a and the eigenvectors $|\psi\rangle$ of an operator $\hat{A}$ such that $\hat{A}|\psi\rangle = a|\psi\rangle$, where a is a complex number. Inserting the unit operator between $\hat{A}$ and $|\psi\rangle$ and multiplying by $\langle\phi_m|$, we have:

$$\left\langle \phi_m \middle| \hat{A} \left(\sum_n |\phi_n\rangle\langle\phi_n| \right) \middle| \psi \right\rangle = a \left\langle \phi_m \middle| \left(\sum_n |\phi_n\rangle\langle\phi_n| \right) \middle| \psi \right\rangle \tag{2.68}$$

or

$$\sum_n A_{mn}\langle\phi_n|\psi\rangle = a \sum_n \langle\phi_n|\psi\rangle\, \delta_{nm} \tag{2.69}$$

which can be rewritten as

$$\sum_n [A_{mn} - a\delta_{nm}]\langle\phi_n|\psi\rangle = 0 \tag{2.70}$$

with $A_{nm} = \langle\phi_n|\hat{A}|\phi_m\rangle$.

The system of equations can have nonzero solutions only if its determinant vanishes:

$$\det(A_{mn} - a\delta_{nm}) = 0 \tag{2.71}$$

2.6 Representation in Continuous Bases

2.6.1 General treatment

The orthonormality condition of the base kets of the continuous basis $|\chi_k\rangle$ is express not by the usual discrete Kronecker delta as in (2.58) but by *Dirac's continuous delta function*:

$$\langle\chi_k|\chi_{k'}\rangle = \delta(k' - k) \tag{2.72}$$

where k and k' are continuous parameters and where $\delta(k' - k)$ is the Dirac delta function, which is defined by

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx} dk \tag{2.73}$$

As for the *completeness* condition for this continuous basis, it is given by an integral over the continuous variable

$$\int_{-\infty}^{\infty} dk\, |\chi_k\rangle\langle\chi_k| = \hat{I} \tag{2.74}$$

where $\hat{I}$ is the unit operator.

Every state vector $|\psi\rangle$ can be expanded in terms of the complete set of basis kets $|\chi_k\rangle$:

$$|\psi\rangle = \hat{I}|\psi\rangle = \left(\int_{-\infty}^{\infty} dk\, |\chi_k\rangle\langle\chi_k|\right)|\psi\rangle = \int_{-\infty}^{\infty} dk\, b(k)\langle\chi_k| \tag{2.75}$$

where $b(k) = \langle\chi_k|\psi\rangle$ represents the projection of $|\psi\rangle$ on $|\chi_k\rangle$.

The norm of the continuous base kets is infinite, from (2.72) and (2.73),

$$\langle\chi_k|\chi_k\rangle = \delta(0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk \to \infty \tag{2.76}$$

this implies that the kets $|\chi_k\rangle$ are not square-integrable and hence are not elements of the Hilbert space. Despite the divergence of the norm of $|\chi_k\rangle$, the scalar product $\langle\chi_k|\psi\rangle$ is finite.

2.7 One-Dimensional Delta Function

Dirac delta function, $\delta(x)$ in one-dimension is :

$$\delta(x) = \begin{cases} 0 \text{ , if } x \neq 0 \\ \infty \text{ , if } x = 0 \end{cases} \qquad \text{with} \qquad \int_{-\infty}^{\infty} \delta(x)dx = 1 \tag{2.77}$$

We should mention that the δ-function is not a function in the usual mathematical sense. It can be expressed as the limit of analytical function such as

$$\delta(x) = \lim_{\varepsilon\to 0} \frac{\sin(x/\varepsilon)}{\pi x} \tag{2.78}$$

The Fourier transform of $\delta(x)$, which can be obtained from:

$$\begin{aligned} \delta(x) &= \lim_{\varepsilon\to 0} \frac{\sin(x/\varepsilon)}{\pi x} \\ &= \lim_{\varepsilon\to 0} \left[\frac{1}{2i\pi x}\left(e^{ix/\varepsilon} - e^{-ix/\varepsilon}\right)\right] \qquad \text{, since } \sin z = \frac{1}{2i}(e^z - e^{-z}) \\ &= \frac{1}{2\pi} \lim_{\varepsilon\to 0} \int_{-1/\varepsilon}^{+1/\varepsilon} e^{ikx} dk \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk \end{aligned} \tag{2.79}$$

The same result as mentioned in (2.73).

Now, $\delta(x-a)$ would be a spike of area 1 at point a instead of 0. Thus, if you multiply $\delta(x-a)$ by an ordinary function $f(x)$, it's the same as multiplying by $f(a)$ because the product is zero anyway except at the point a:

$$f(x)\delta(x-a) = f(a)\delta(x-a) \tag{2.80}$$

In particular,

$$\int_{-\infty}^{\infty} f(x)\delta(x-a)dx = f(a)\int_{-\infty}^{\infty} \delta(x-a)dx = f(a) \tag{2.81}$$

So, we come to a general result:

$$\boxed{\int dx\delta(x-x')f(x) = f(x')} \tag{2.82}$$

CHAPTER 3
SCHRÖDINGER EQUATION

3.1 Wave Function

Inspired by de Broglie's hypothesis, Schrödinger's wave mechanics deals with the dynamic of microscopic particles by means of *wave function* $\psi(\vec{r},t)$. Quantum mechanics describe the state of a particle by Born's statistical interpretation of the wave function, where $|\psi(\vec{r},t)|^2$ gives the probability of finding the particle at certain point of space at time t.

3.1.1 Wave function in position space

Let's write down the eigenvalue equation for the position operator $\hat{\vec{r}}$, denoting the position eigenstates as $|\vec{r}\rangle$ and the eigenvalues as $\vec{r}$, the position vector:

$$\hat{\vec{r}}|\vec{r}\rangle = \vec{r}|\vec{r}\rangle \tag{3.1}$$

We have the orthonormality and completeness conditions given as:

$$\langle\vec{r}|\vec{r}'\rangle = \delta^3(\vec{r}-\vec{r}') \tag{3.2}$$

$$\int d^3\vec{r}|\vec{r}\rangle\langle\vec{r}| = \hat{I} \tag{3.3}$$

where $\hat{I}$ is the unit operator.

So every state vector $|\psi\rangle$ can be expanded as:

$$|\psi\rangle = \left(\int d^3\vec{r}|\vec{r}\rangle\langle\vec{r}|\right)|\psi\rangle = \int d^3\vec{r}\,\psi(\vec{r})|\vec{r}\rangle \tag{3.4}$$

where $\psi(\vec{r})$ denotes the components of $|\psi\rangle$ in the $|\vec{r}\rangle$ basis:

$$\boxed{\langle\vec{r}|\psi\rangle = \psi(\vec{r})} \tag{3.5}$$

This is known as the wave function for the state vector $|\psi\rangle$ in position space. According to the *probabilistic interpretation of Born*, the quantity

$$\langle\psi|\psi\rangle = \left\langle\psi\middle|\left(\int d^3\vec{r}|\vec{r}\rangle\langle\vec{r}|\right)\middle|\psi\right\rangle = \int \psi^*(\vec{r})\psi(\vec{r})d^3\vec{r} = \int|\psi(\vec{r})|^2 d^3\vec{r} \tag{3.6}$$

represents the *probability* of finding the system in the volume element $d^3\vec{r}$, while the integrand $|\psi(\vec{r})|^2$ is the *probability density*.

3.1.2 Wave function in momentum space

The basis $|\vec{p}\rangle$ of the momentum space is obtained from the eigenstates of the momentum operator $\hat{\vec{p}}$:

$$\hat{\vec{p}}|\vec{p}\rangle = \vec{p}|\vec{p}\rangle \tag{3.7}$$

where $\vec{p}$ is the momentum vector. Just like in the position representation, the orthonormality and the completeness conditions of momentum space basis $|\vec{p}\rangle$ are:

$$\langle\vec{p}|\vec{p}'\rangle = \delta^3(\vec{p}-\vec{p}') \qquad \text{and} \qquad \int d^3\vec{p}|\vec{p}\rangle\langle\vec{p}| = \hat{I} \tag{3.8}$$

Expanding $|\phi\rangle$ in this basis, we obtain:

$$|\phi\rangle = \left(\int d^3\vec{p}|\vec{p}\rangle\langle\vec{p}|\right)|\phi\rangle = \int d^3\vec{p}\ \phi(\vec{p})|\vec{p}\rangle \tag{3.9}$$

where $\phi(\vec{p})$ denotes the components of $|\phi\rangle$ in the $|\vec{p}\rangle$ basis:

$$\boxed{\langle\vec{p}|\phi\rangle = \phi(\vec{p})} \tag{3.10}$$

This is known as the wave function for the state vector $|\vec{p}\rangle$ in momentum space.

3.1.3 Transformation relation of wave function in position and momentum space

Let's have $\qquad \psi(x) = \langle x|\varphi\rangle \qquad$ and $\qquad \phi(p) = \langle p|\varphi\rangle \qquad$ (3.11)

and retain the meaning of wave function in one-dimension, we can have:

$$\begin{aligned}\psi(x) &= \langle x|\varphi\rangle = \left\langle x\middle|\left(\int dp|p\rangle\langle p|\right)\middle|\varphi\right\rangle \\ &= \int dp\langle x|p\rangle\phi(p)\end{aligned} \tag{3.12}$$

and

$$\begin{aligned}\phi(p) &= \langle p|\varphi\rangle = \left\langle p\middle|\left(\int dx|x\rangle\langle x|\right)\middle|\varphi\right\rangle \\ &= \int dx\langle p|x\rangle\psi(x)\end{aligned} \tag{3.13}$$

Note that, the different in the transformation is at the $\langle x|p\rangle$ and $\langle p|x\rangle$. Let's introduce

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar} \tag{3.14}$$

so as to complete the transformation as *Fourier transformation*:

$$\boxed{\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int \phi(p)e^{ipx/\hbar}dp} \tag{3.15}$$

and

$$\boxed{\phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int \psi(x)e^{-ipx/\hbar}dx} \tag{3.16}$$

Equation (3.15) and (3.16) are the wave function in the position space and the wave function in the momentum space, respectively.

To understand the normalized factor $\frac{1}{\sqrt{2\pi\hbar}}$, multiply both side of (3.15) with $\frac{1}{\sqrt{2\pi\hbar}}\int e^{-ip'x/\hbar}dx$ to give:

$$\begin{aligned}\frac{1}{\sqrt{2\pi\hbar}}\int \psi(x)e^{-ip'x/\hbar}dx &= \int dp\ \phi(p)\left(\frac{1}{\sqrt{2\pi\hbar}}\int e^{i(p-p')x/\hbar}dx\right) \\ &= \int dp\ \phi(p)\delta(p-p') \\ &= \phi(p')\end{aligned} \tag{3.17}$$

Change the variable p' as p to give back $\phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int \psi(x)e^{-ipx/\hbar}dx$.

3.2 Schrödinger Equation in Position space

3.2.1 Understand Schrödinger equation from classical wave

For a classical one-dimensional wave equation:

$$\frac{\partial^2\Psi(x,t)}{\partial t^2} = c^2\frac{\partial^2\Psi(x,t)}{\partial x^2} \tag{3.18}$$

Having general solution in the form:

$$\begin{aligned}\Psi(x,t) &= Ae^{i(kx-\omega t)} \\ &= Ae^{i(p_x x-Et)/\hbar}\end{aligned} \tag{3.19}$$

where $p_x = \hbar k$ and $E = \hbar\omega$; A a constant.

Now, we take the derivatives:

$$\frac{\partial\Psi(x,t)}{\partial t} = -\frac{iE}{\hbar}\Psi(x,t) \quad \text{and} \quad \frac{\partial^2\Psi(x,t)}{\partial x^2} = -\frac{{p_x}^2}{\hbar^2}\Psi(x,t) \tag{3.20}$$

for a classical relation $E = \frac{{p_x}^2}{2m}$; $E\Psi(x,t) = \frac{{p_x}^2}{2m}\Psi(x,t)$, equate relation in (3.20):

$$-\frac{\hbar}{i}\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} \tag{3.21}$$

multiply both side by $-i^2 = 1$ to give:

$$\boxed{i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}} \tag{3.22}$$

This is the *time-dependent Schrödinger equation* of a free particle in one-dimension.

For a particle moving in a potential force field where we have:

$$\vec{F}(\vec{r},t) = -\vec{\nabla}V(\vec{r},t) \tag{3.23}$$

so that the total energy is given as the sum:

$$E = \frac{\vec{p}^2}{2m} + V(\vec{r}, t) \tag{3.24}$$

while in one-dimension,

$$E = \frac{{p_x}^2}{2m} + V(x, t) \tag{3.25}$$

thus,

$$E\Psi(x, t) = \left[\frac{{p_x}^2}{2m} + V(x, t)\right]\Psi(x, t) \tag{3.26}$$

We can write in operator form for (3.26) according to (3.22) as:

$$i\hbar\frac{\partial\Psi(x, t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x, t)\right]\Psi(x, t) \tag{3.27}$$

In three-dimensional case, we change the operator accordingly for which:

$\vec{r} = x\hat{\imath} + y\hat{\jmath} + z\hat{k}$ and $\vec{\nabla} = \frac{\partial}{\partial x}\hat{\imath} + \frac{\partial}{\partial y}\hat{\jmath} + \frac{\partial}{\partial z}\hat{k}$

$$\boxed{i\hbar\frac{\partial\Psi(\vec{r}, t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r}, t)\right]\Psi(\vec{r}, t)} \tag{3.28}$$

The *time-dependent Schrödinger equation***.**

From the understanding of classical regime, the total energy is called the *Hamiltonian* with criteria that the energy force field is conserved. By operator $\hat{H}$:

$$\hat{H} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r}, t) \tag{3.29}$$

we have:

$$i\hbar\frac{\partial\Psi(\vec{r}, t)}{\partial t} = \hat{H}\Psi(\vec{r}, t) \tag{3.30}$$

3.2.2 Stationary state

Stationary state is when the probability density and other observables are constant in time. That is, in a case available, although $\Psi(x, t) = \psi(x)e^{-iEt/\hbar}$ does depends on time, but the probability density based on Born's interpretation:

$|\Psi(x, t)|^2 = \Psi^*\Psi = \psi^* e^{iEt/\hbar}\psi e^{-iEt/\hbar} = |\psi(x)|^2$ does not.

So, the interpretation allows us to have V independent of time and as well, to write $\Psi(x, t) = \psi(x)\varphi(t)$ and solve Schrödinger equation by method of *separation of variables*. First we take the derivatives for $\frac{\partial\Psi}{\partial t} = \psi\frac{d\varphi}{dt}$ and $\frac{\partial^2\Psi}{\partial x^2} = \varphi\frac{d^2\psi}{dx^2}$.

Substitute into equation (3.27) with $V = V(x, t)$ is now $V = V(x)$ to have:

$$i\hbar\psi\frac{d\varphi}{dt} = -\frac{\hbar^2}{2m}\varphi\frac{d^2\psi}{dx^2} + V\psi\varphi \tag{3.31}$$

Divide by $\psi\varphi$:

$$\frac{i\hbar}{\varphi}\frac{d\varphi}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E \tag{3.32}$$

We introduce the separation constant E such that the equation can be re-written in two separated ordinary differential equation:

$$\frac{i\hbar}{\varphi}\frac{d\varphi}{dt} = E \tag{3.33}$$

and

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi} \tag{3.34}$$

Solve (3.33) as $\int i\hbar\frac{d\varphi}{\varphi} = \int Edt$ to give the general solution as $\varphi(t) = e^{-iEt/\hbar}$. This is why we have $\Psi(x,t) = \psi(x)\varphi(t) = \psi(x)e^{-iEt/\hbar}$.

While equation (3.34) is called the *time-independent Schrödinger equation*.

3.2.3 The conservation of probability

The conservation of probability is a crucial feature of the Schrödinger equation; it allows a normalized wave function to stay normalized at the progress of time. To prove it, let's consider a normalized wave function:

$$\langle\Psi(x,t)|\Psi(x,t)\rangle = \int|\Psi(x,t)|^2dx = 1 \tag{3.35}$$

To observe the wave function evolve in time, we take the time derivatives of:

$$\frac{d}{dt}\int|\Psi(x,t)|^2dx = \int\frac{\partial}{\partial t}|\Psi(x,t)|^2dx \tag{3.36}$$

By the product rule,

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{\partial}{\partial t}(\Psi^*\Psi) = \Psi^*\frac{\partial\Psi}{\partial t} + \frac{\partial\Psi^*}{\partial t}\Psi \tag{3.37}$$

Now, the Schrödinger equation says that

$$\frac{\partial\Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi \tag{3.38}$$

and taking the complex conjugate of (3.38) to give $\frac{\partial\Psi^*}{\partial t}$ as:

$$\frac{\partial\Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^* \tag{3.39}$$

So,

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\right) = \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\right] \tag{3.40}$$

We can rewrite the equation as:

$$\boxed{\frac{\partial\rho(x,t)}{\partial t}+\frac{\partial J(x,t)}{\partial x}=0} \tag{3.41}$$

where $\rho(x,t)=\Psi^*(x,t)\Psi(x,t)$ is called the *probability density*;

while $J(x,t)=\frac{i\hbar}{2m}\left(\Psi\frac{\partial\Psi^*}{\partial x}-\Psi^*\frac{\partial\Psi}{\partial x}\right)$ is the *probability current density*.

Equation (3.41) is interpreted as the *conservation of probability*.

Come back to equation (3.36), we'll see that when evaluate throughout the entire x,

$$\int_{-\infty}^{+\infty}\frac{\partial}{\partial t}|\Psi(x,t)|^2dx=\left[\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x}-\frac{\partial\Psi^*}{\partial x}\Psi\right)\right]_{-\infty}^{+\infty} \tag{3.42}$$

but $\Psi(x,t)$ must goes to zero as $x\to\pm\infty$ so that $\Psi(x,t)$ remain normalized. It follows that

$$\frac{d}{dt}\int|\Psi(x,t)|^2dx=0 \tag{3.43}$$

and hence, the integral is a constant in time, which is consistence with (3.35).

3.2.4 Expectation values and the time-rate change of the system

For a particle in state $|\Psi(x,t)\rangle$, the *expectation value* of any observable, $Q(x,t)$ is:

$$\langle Q\rangle=\langle\Psi|\hat{Q}|\Psi\rangle=\int\hat{Q}|\Psi(x,t)|^2dx \tag{3.44}$$

Taking the time derivative of (3.44):

$$\frac{d}{dt}\langle Q\rangle=\frac{d}{dt}\langle\Psi|\hat{Q}|\Psi\rangle=\left\langle\frac{\partial\Psi}{\partial t}\middle|\hat{Q}\middle|\Psi\right\rangle+\left\langle\Psi\middle|\frac{\partial\hat{Q}}{\partial t}\middle|\Psi\right\rangle+\left\langle\Psi\middle|\hat{Q}\middle|\frac{\partial\Psi}{\partial t}\right\rangle \tag{3.45}$$

We can have $\frac{\partial\Psi}{\partial t}$ from the Schrödinger equation (3.30): $i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}=\hat{H}\Psi(\vec{r},t)$. So,

$$\frac{d}{dt}\langle Q\rangle=-\frac{1}{i\hbar}\langle\hat{H}\Psi|\hat{Q}|\Psi\rangle+\frac{1}{i\hbar}\langle\Psi|\hat{Q}|\hat{H}\Psi\rangle+\left\langle\Psi\middle|\frac{\partial\hat{Q}}{\partial t}\middle|\Psi\right\rangle \tag{3.46}$$

But $\hat{H}$ is hermitian, so $\langle\hat{H}\Psi|\hat{Q}|\Psi\rangle=\langle\Psi|\hat{H}\hat{Q}|\Psi\rangle$ and $\langle\Psi|\hat{Q}|\hat{H}\Psi\rangle=\langle\Psi|\hat{Q}\hat{H}|\Psi\rangle$, hence

$$\boxed{\frac{d}{dt}\langle Q\rangle=\frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle+\langle\frac{\partial\hat{Q}}{\partial t}\rangle} \tag{3.47}$$

This relation shows the *time evolution of expectation values*; two important result stem from this relation.

First, if Q does not depend explicitly on time, then the term $\partial\hat{Q}/\partial t$ vanish, and $\frac{d}{dt}\langle Q\rangle=\frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle$.

Second, besides not depending explicitly on time, if the $\hat{Q}$ commutes with $\hat{H}$, then $\langle Q \rangle$ is constant in time.

3.3 Schrödinger Equation in Momentum space

3.3.1 Momentum and position operator in momentum space

The momentum operator:

$$\begin{aligned}
\langle p \rangle = \langle \psi | \hat{p} | \psi \rangle &= \int \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi dx \\
&= \int \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \left[\frac{1}{\sqrt{2\pi\hbar}} \int \phi e^{ipx/\hbar} dp\right] dx \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int \psi^* \left[\int \phi(-i\hbar) \left(\frac{ip}{\hbar}\right) e^{ipx/\hbar} dp\right] dx \\
&= \int \phi p \left(\frac{1}{\sqrt{2\pi\hbar}} \int \psi^* e^{ipx/\hbar} dx\right) dp \\
&= \int \phi p \left(\frac{1}{\sqrt{2\pi\hbar}} \int \psi e^{-ipx/\hbar} dx\right)^* dp \\
&= \int \phi p \phi^* dp
\end{aligned}$$

So, in position space, $$\hat{p} = -i\hbar \frac{\partial}{\partial x} \tag{3.48}$$

while in momentum space, $$\hat{p}_p = p \tag{3.49}$$

For position operator:

$$\begin{aligned}
\langle x \rangle = \langle \psi | \hat{x} | \psi \rangle &= \int \psi^* x \psi dx \\
&= \int \left(\frac{1}{\sqrt{2\pi\hbar}} \int \phi^* e^{-ipx/\hbar} dp\right) x \psi dx \\
&= \int \phi^* \left(\frac{1}{\sqrt{2\pi\hbar}} \int x \psi e^{-ipx/\hbar} dx\right) dp \\
&= \int \phi^* \left(i\hbar \frac{\partial}{\partial p}\right) \left(\frac{1}{\sqrt{2\pi\hbar}} \int \psi e^{-ipx/\hbar} dx\right) dp \\
&= \int \phi^* \left(i\hbar \frac{\partial}{\partial p}\right) \phi dp
\end{aligned}$$

So, in position space, $$\hat{x} = x \tag{3.50}$$

while in momentum space, $$\hat{x}_p = i\hbar \frac{\partial}{\partial p} \tag{3.51}$$

3.3.2 Transforming the Schrödinger equation into momentum space

From the time-dependent Schrödinger equation in position space,

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \quad (3.52)$$

multiply both side by $\frac{1}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar}$ and integrate over the entire x to obtain:

$$\begin{aligned}\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} i\hbar\frac{\partial\psi}{\partial t}e^{-ipx/\hbar}dx &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi\right)\left(e^{-ipx/\hbar}\right)dx \\ &= i\hbar\frac{\partial}{\partial t}\left(\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi e^{-ipx/\hbar}dx\right) \\ &= i\hbar\frac{\partial}{\partial t}\phi(p,t)\end{aligned} \quad (3.53)$$

For the spatial term:

$$\begin{aligned}\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}\right)e^{-ipx/\hbar}dx &= -\frac{\hbar^2}{2m}\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\frac{\partial^2\psi}{\partial x^2}e^{-ipx/\hbar}dx \\ &= -\frac{\hbar^2}{2m}\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi\frac{\partial^2}{\partial x^2}\left(e^{-ipx/\hbar}\right)dx \quad ;\text{ IBP} \\ &= \frac{p^2}{2m}\left(\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi e^{-ipx/\hbar}dx\right) \\ &= \frac{p^2}{2m}\phi(p,t)\end{aligned} \quad (3.54)$$

where we have used two integration by parts to move the derivatives onto the exponential term. This is true as long as $\psi(x,t)$ is linearly dependent with $e^{-ipx/\hbar}$.

Next, the potential energy function can be expanded in Taylor series to yield

$$\begin{aligned}\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}(V\psi)\left(e^{-ipx/\hbar}\right)dx &= \sum_{n=0}^{\infty}\frac{V^{(n)}(0)}{n!}\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}x^n\psi e^{-ipx/\hbar}dx \\ &= \sum_{n=0}^{\infty}\frac{V^{(n)}(0)}{n!}\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi\left(i\hbar\frac{\partial}{\partial p}\right)^n\left(e^{-ipx/\hbar}\right)dx \\ &= \sum_{n=0}^{\infty}\frac{V^{(n)}(0)}{n!}\left(i\hbar\frac{\partial}{\partial p}\right)^n\phi(p,t) \\ &= V\left(i\hbar\frac{\partial}{\partial p}\right)\phi(p,t)\end{aligned} \quad (3.55)$$

Combine results from (3.53), (3.54) and (3.55) to give *time-dependent Schrödinger equation in momentum space* as:

$$\boxed{i\hbar\frac{\partial}{\partial t}\phi(p,t) = \frac{p^2}{2m}\phi(p,t) + V\left(i\hbar\frac{\partial}{\partial p}\right)\phi(p,t)} \tag{3.56}$$

if the potential function does not depend explicitly on time, we can write

$$\phi(p,t) = \phi(p)e^{-iEt/\hbar} \tag{3.57}$$

and obtain in the same way as in position space, the *time-independent Schrödinger equation in momentum space*:

$$\boxed{E\phi(p) = \frac{p^2}{2m}\phi(p) + V\left(i\hbar\frac{\partial}{\partial p}\right)\phi(p)} \tag{3.58}$$

CHAPTER 4
APPLICATIONS OF SCHRÖDINGER EQUATION

4.1 The Free Particle

4.1.1 The free particle in position space

Due to $V(x) = 0$ for all x, we are left with time-independent Schrödinger equation in the form:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \tag{4.1}$$

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x) = -k^2\psi(x) \tag{4.2}$$

for $k = \frac{1}{\hbar}\sqrt{2mE}$. Since we don't have any boundary of wall to restrict the value of k, the general solution shall take the form:

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \tag{4.3}$$

where A and B are two arbitrary constants.

By include the time progression term, $e^{-i\omega t}$, the wave function become:

$$\begin{aligned}\psi(x,t) &= Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)} && ; E = \hbar\omega = \frac{p^2}{2m} = \frac{\hbar^2k^2}{2m} \\ &= Ae^{i\left(kx-\frac{\hbar k^2}{2m}t\right)} + Be^{-i\left(kx+\frac{\hbar k^2}{2m}t\right)} && \text{so that } \omega = \frac{\hbar k^2}{2m} \\ &= Ae^{ik\left(x-\frac{\hbar k}{2m}t\right)} + Be^{-ik\left(x+\frac{\hbar k}{2m}t\right)} \end{aligned} \tag{4.4}$$

here $e^{ik\left(x-\frac{\hbar k}{2m}t\right)}$ represent a wave travelling to $+x$ direction, while $e^{-ik\left(x+\frac{\hbar k}{2m}t\right)}$ represent a wave travel to $-x$ direction. In other form, we rewrite:

$$\psi_k(x,t) = Ae^{ik\left(x-\frac{\hbar k}{2m}t\right)} \qquad \text{with } k = \pm\frac{1}{\hbar}\sqrt{2mE} \tag{4.5}$$

Here we have three subtleties.

First, the wave has well defined momenta and energy:

$$p = \pm\hbar k \qquad \text{implies that } \Delta p = 0$$

$$E = \frac{\hbar^2k^2}{2m} \qquad \text{implies that } \Delta E = 0$$

while x and t can take on any value, $\Delta x \to \infty$ and $\Delta t \to \infty$.

Second subtlety, the speed of the quantum wave, $v_{wave} = \frac{\omega}{k} = \frac{\hbar k}{2m}$ and the speed of the particle, $v_{particle} = \frac{p}{m} = \frac{\hbar k}{m} = 2v_{wave}$. Evidently the particle travels twice as fast as the wave that represents it.

Third, the wave function is not normalizable, $\int_{-\infty}^{\infty} \psi_k{}^* \psi_k dx = |A|^2 \int_{-\infty}^{\infty} dx \to \infty$ is not square integrable, which represent not a physical entity.

For that, the free particle cannot have definite energy, but a continuous range. The general solution now takes the form of wave packets:

$$\boxed{\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int \phi(k) e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} dk} \tag{4.6}$$

where $\phi(k)$ is the amplitude of the wave packet and is given by the Fourier transform of $\psi(x,0)$ as in:

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int \psi(x,0) e^{-ikx} dx \tag{4.7}$$

in order to fit the initial wave function:

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int \phi(k) e^{ikx} dk \tag{4.8}$$

4.1.2 The free particle in momentum space

In momentum space, time-dependent Schrödinger equation reads:

$$i\hbar \frac{\partial}{\partial t} \phi(p,t) = \frac{p^2}{2m} \phi(p,t) + V\left(i\hbar \frac{\partial}{\partial p}\right) \phi(p,t) \tag{4.9}$$

but, since $V\left(i\hbar \frac{\partial}{\partial p}\right) = 0$, we are left with:

$$i\hbar \frac{\partial}{\partial t} \phi(p,t) = \frac{p^2}{2m} \phi(p,t) \tag{4.10}$$

$$i\hbar \frac{\partial \phi(p,t)}{\phi(p,t)} = \frac{p^2}{2m} \partial t \ \to \ \int \frac{d\phi}{\phi} = -\int \frac{ip^2}{2m\hbar} dt \tag{4.11}$$

$$\ln \phi(p,t) = -\frac{ip^2}{2m\hbar} t + c \tag{4.12}$$

$$\phi(p,t) = A e^{-\frac{ip^2 t}{2m\hbar}} \qquad \text{where } A = e^c \tag{4.13}$$

4.2 Simple Harmonic Oscillator

4.2.1 Simple harmonic oscillator in position representation

The potential for stationary state in this case will be $V(x) = \frac{1}{2}m\omega^2x^2$. So, the problem is to solve the time-independent Schrödinger equation of the form:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi \tag{4.14}$$

By change of variable: $\xi = \sqrt{\frac{m\omega}{\hbar}}x$; $d\xi = \sqrt{\frac{m\omega}{\hbar}}dx$;

$$\frac{d\psi}{dx} = \frac{d\psi}{d\xi}\frac{d\xi}{dx} = \sqrt{\frac{m\omega}{\hbar}}\frac{d\psi}{d\xi} \quad ; \quad \frac{d^2\psi}{dx^2} = \frac{d}{d\xi}\left(\sqrt{\frac{m\omega}{\hbar}}\frac{d\psi}{d\xi}\right)\frac{d\xi}{dx} = \frac{m\omega}{\hbar}\frac{d^2\psi}{d\xi^2}$$

We have:
$$-\frac{\hbar^2}{2m}\frac{m\omega}{\hbar}\frac{d^2\psi}{d\xi^2} + \frac{1}{2}m\omega^2\frac{\hbar}{m\omega}\xi^2\psi = E\psi \tag{4.15}$$

Multiply by $-\frac{2}{\hbar\omega}$ and by putting $K = \frac{eE}{\hbar\omega}$, we get:

$$\frac{d^2\psi}{d\xi^2} = \left(\xi^2 - \frac{2E}{\hbar\omega}\right)\psi = (\xi^2 - K)\psi \tag{4.16}$$

Start by taking the region of large ξ (large x) which will dominate over K, then $\frac{d^2\psi}{d\xi^2} \approx \xi^2\psi$. The general solution is approximated as:

$$\psi(\xi) = Ae^{-\xi^2/2} + Be^{\xi^2/2} \tag{4.17}$$

Since $e^{\xi^2/2} \to \infty$ as $\xi \to \infty$, take $B = 0$, then we will have the *asymptotic form* of:

$$\psi(\xi) = (\quad)e^{-\xi^2/2} \tag{4.18}$$

To take out the exponential part, take

$$\psi(\xi) = h(\xi)e^{-\xi^2/2} \tag{4.19}$$

to have:
$$\frac{d\psi}{d\xi} = \frac{dh}{d\xi}e^{-\xi^2/2} - \xi he^{-\xi^2/2}$$

$$\frac{d^2\psi}{d\xi^2} = \frac{d^2h}{d\xi^2}e^{-\xi^2/2} - 2\xi\frac{dh}{d\xi}e^{-\xi^2/2} - he^{-\xi^2/2} + \xi^2he^{-\xi^2/2}$$

Then, the Schrödinger equation becomes:

$$\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + \xi^2h - h = \xi^2h - Kh$$

$$\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K-1)h = 0 \tag{4.20}$$

Use power series method to solve, in which

$$h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j \quad ; \quad \frac{dh}{d\xi} = \sum_{j=1}^{\infty} j a_j \xi^{j-1} \quad ; \quad \frac{d^2h}{d\xi^2} = \sum_{j=2}^{\infty} j(j-1) a_j \xi^{j-2}$$

$$\sum_{j=2}^{\infty} j(j-1) a_j \xi^{j-2} - 2\sum_{j=1}^{\infty} j a_j \xi^j + (K-1)\sum_{j=0}^{\infty} a_j \xi^j = 0$$

$$\sum_{j=0}^{\infty} (j+2)(j+1) a_{j+2} \xi^j - 2\sum_{j=1}^{\infty} j a_j \xi^j + (K-1)\sum_{j=0}^{\infty} a_j \xi^j = 0$$

So, $2a_2 + (K-1)a_0 = 0$ and $(j+2)(J+1)a_{j+2} - 2ja_j + (K-1)a_j = 0$.

We obtain: $a_2 = \frac{1-K}{2} a_0$ and $a_{j+2} = \frac{2j+1-K}{(j+2)(j+1)} a_j$.

Thus, by now we should have:

$$\begin{aligned} h(\xi) &= a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3 + \cdots \\ &= (a_0 + a_2\xi^2 + a_4\xi^4 + \cdots) + (a_1\xi + a_3\xi^3 + +a_5\xi^5 \cdots) \\ &= h_{even}(\xi) + h_{odd}(\xi) \end{aligned} \tag{4.21}$$

However, when j get larger, the *recursion relation* becomes: $a_{j+2} = \frac{2}{j} a_j$, along with the approximate solution: $a_j \approx \frac{C}{(j/2)!}$, and this yield:

$$h(\xi) \approx C \sum \frac{1}{(j/2)!} \xi^j \approx C \sum \frac{1}{k!} \xi^{2k} \approx C e^{\xi^2} \tag{4.22}$$

This is the asymptotic behavior that we don't want. To solve this unwanted, the power series must terminate at some *highest* j, call it n such that the recursion formula give $a_{n+2} = 0$. Thus, we must have $K = 2n + 1$ for $n = 0,1,2, ...$

Then, the energy must have values:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad ; n = 0,1,2, \ldots \tag{4.23}$$

Beyond the value of K, the recursion relation now becomes: $a_{j+2} = \frac{-2(n-j)}{(j+2)(j+1)} a_j$.

if $n = 0$, pick $a_1 = 0$ and $j = 0$ to give $h_0(\xi) = a_0$ and hence:

$$\psi_0(\xi) = a_0 e^{-\xi^2/2}$$

for $n = 1$, pick $a_0 = 0$ and $j = 1$ so $h_1(\xi) = a_1\xi$ and hence:

$$\psi_1(\xi) = a_1 \xi e^{-\xi^2/2}$$

for $n = 1$, $j = 0$ yields $a_2 = -2a_0$ and $j = 2$ gives $a_4 = 0$, so $h_2(\xi) = a_0(1 - 2\xi^2)$ and $\psi_2(\xi) = a_0(1 - 2\xi^2)e^{-\xi^2/2}$ and carry on.

They are so called *Hermite polynomials*, $H_n(\xi)$. With proper normalized stationary states for the harmonic oscillator is:

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2} \tag{4.24}$$

$$\boxed{\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{-\frac{m\omega x^2}{2\hbar}}} \tag{4.25}$$

4.2.2 Simple harmonic oscillator in momentum representation

We know in momentum representation, the momentum and position operators are:

$$\hat{p}_p = p \qquad \text{and} \qquad \hat{x}_p = i\hbar\frac{\partial}{\partial p}$$

so, the Hamiltonian operator in momentum space shall takes the form:

$$\hat{H}_p = \frac{\hat{p}_p{}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}_p{}^2 = \frac{p^2}{2m} - \frac{1}{2}m\omega^2\hbar^2\frac{\partial^2}{\partial p^2} \tag{4.26}$$

At the same time, the time-independent Schrödinger equation can be rewritten as:

$$\left(\frac{p^2}{2m} - \frac{1}{2}m\omega^2\hbar^2\frac{d^2}{dp^2}\right)\phi = E\phi \tag{4.27}$$

divide both sides of the equation by $m^2\omega^2$, and further rearrange to give:

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dp^2} + \frac{p^2}{2m^3\omega^2}\phi = \frac{E}{m^2\omega^2}\phi \tag{4.28}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dp^2} + \frac{1}{2}m\tilde{\omega}^2p^2\phi = \tilde{E}\phi \tag{4.29}$$

where we have introduced:

$$\tilde{\omega} = \frac{1}{m^2\omega} \qquad \text{and} \qquad \tilde{E} = \frac{E}{m^2\omega^2} \tag{4.30}$$

Look into the similarity in the form as compared to the time-independent Schrödinger equation (4.14). Thus, the solution can be stated readily exploiting the earlier results. The energy according to (4.23), are:

$$\tilde{E}_n = \left(n + \frac{1}{2}\right)\hbar\tilde{\omega} \qquad ; n = 0,1,2,\ldots \tag{4.31}$$

or, by the relations (4.30),

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \qquad ; n = 0,1,2,\ldots \tag{4.32}$$

Also, directly from (4.25), the wave function for simple harmonic oscillator in momentum space should be:

$$\phi_n(p) = \left(\frac{m\tilde{\omega}}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\tilde{\omega}}{\hbar}}p\right) e^{-\frac{m\tilde{\omega}p^2}{2\hbar}} \tag{4.33}$$

Again by (4.30),

$$\boxed{\phi_n(p) = \left(\frac{1}{\pi m\hbar\omega}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{1}{m\hbar\omega}}p\right) e^{-\frac{p^2}{2m\hbar\omega}}} \tag{4.34}$$

4.3 Hydrogen Atom

4.3.1 Schrödinger equation in spherical coordinates

For a general statement in term of Hamiltonian operator:

$$i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi \tag{4.35}$$

where
$$\hat{H} = T + V = \frac{\vec{p}^2}{2m} + V = -\frac{\hbar^2}{2m}\nabla^2 + V \tag{4.36}$$

So, we have in term of *laplacian* $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$:

$$\boxed{i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi} \tag{4.37}$$

and in *spherical coordinate*, what matters is the form of laplacian, where

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2}{\partial\varphi^2}\right) \tag{4.38}$$

with $r = radius, \theta = polar\ angle, \varphi = azimuthal\ angle$

Now, we can solve the Schrödinger equation by *separation of variables*:

$$\psi(r,\theta,\varphi) = R(r)Y(\theta,\varphi) \tag{4.39}$$

$$\frac{\partial\psi}{\partial r} = Y\frac{dR}{dr} \quad , \quad \frac{\partial\psi}{\partial\theta} = R\frac{\partial Y}{\partial\theta} \quad \text{and} \quad \frac{\partial^2\psi}{\partial\varphi^2} = R\frac{\partial^2 Y}{\partial\varphi^2}$$

Substitute back into $E\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$ to get

$$ERY = -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 Y\frac{dR}{dr}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\, R\frac{\partial Y}{\partial\theta}\right) + \frac{R}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}\right] + VRY \tag{4.40}$$

divide by $\psi = RY$, multiply by $\frac{2m}{\hbar^2}$, leave Y to right hand side and move all to left:

$$\frac{2m}{\hbar^2}(E-V)+\frac{1}{r^2R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)$$
$$=-\frac{1}{Yr^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)-\frac{1}{Yr^2\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2} \tag{4.41}$$

Multiply both sides with r^2 and further re-arrange to give a clear separation:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}(E-V)=-\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}\right] \tag{4.42}$$

Equate the equation to a *separation constant* $l(l+1)$ so as to separate it into two differential equation of the form:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}(E-V)=l(l+1) \tag{4.43}$$

$$\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}\right]=-l(l+1) \tag{4.44}$$

4.3.2 Spherical harmonics

Solve the *angular equation* (4.44) of $Y(\theta,\varphi)$ first. Multiply $Y\sin^2\theta$ to get:

$$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+Y\sin^2\theta\, l(l+1)=-\frac{\partial^2 Y}{\partial\varphi^2} \tag{4.45}$$

and introduce separation of variable second time as: $Y(\theta,\varphi)=\Theta(\theta)\Phi(\varphi)$;

$$\frac{\partial Y}{\partial\theta}=\Phi\frac{d\Theta}{d\theta} \quad ; \quad \frac{\partial^2 Y}{\partial\varphi^2}=\Theta\frac{d^2\Phi}{d\varphi^2}$$

Substitute back into (4.45) and divide by $Y=\Theta\Phi$:

$$\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+l(l+1)\sin^2\theta=-\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2}=m^2 \tag{4.46}$$

Meanwhile, use yet another separation constant m^2 to give:

$$\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+l(l+1)\sin^2\theta=m^2 \tag{4.47}$$

and

$$\frac{d^2\Phi}{d\varphi^2}=-m^2\Phi \tag{4.48}$$

For $\Phi(\varphi)$, the general solution take the form:

$$\Phi(\varphi)=c_1e^{im\varphi}+c_2e^{-im\varphi}\equiv ce^{im\varphi} \tag{4.49}$$

by letting m take both $\pm Z$. To be precise, consider the *periodic boundary condition* of $\Phi(\varphi)=\Phi(\varphi+2\pi)$; $ce^{im\varphi}=ce^{im(\varphi+2\pi)}$ or in other words, $e^{im2\pi}=1$ and thus $m=0,\pm1,\pm2,\ldots$

While for $\Theta(\theta)$, rearrange equation (4.47) to get:

$$\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) + [l(l+1)\sin^2\theta - m^2]\Theta = 0 \tag{4.50}$$

use the change of variable $x = \cos\theta$, then$\sin^2\theta = 1 - x^2$; $\frac{dx}{d\theta} = -\sin\theta$ and

$$\frac{d\Theta}{d\theta} = \frac{d\Theta}{dx}\frac{dx}{d\theta} = -\sin\theta \frac{d\Theta}{dx}$$

$$\begin{aligned}\frac{d}{d\theta}\left(-\sin^2\theta \frac{d\Theta}{d\theta}\right) &= -2\sin\theta\cos\theta \frac{d\Theta}{dx} - \sin^2\theta \frac{d}{d\theta}\frac{d\Theta}{dx} \\ &= -2x\sin\theta \frac{d\Theta}{dx} - \sin^2\theta \frac{d}{dx}\left(\frac{d\Theta}{dx}\right)\frac{dx}{d\theta} \\ &= -2x\sin\theta \frac{d\Theta}{dx} - \sin^3\theta \frac{d^2\Theta}{dx^2}\end{aligned}$$

Then,

$$-2x\sin^2\theta \frac{d\Theta}{dx} - \sin^4\theta \frac{d^2\Theta}{dx^2} + [l(l+1)\sin^2\theta - m^2]\Theta = 0 \tag{4.51}$$

divide by $\sin^2\theta = 1 - x^2$ to yield:

$$(1-x^2)\frac{d^2\Theta}{dx^2} - 2x\frac{d\Theta}{dx} + \left[l(l+1) - \frac{m^2}{1-x^2}\right]\Theta = 0 \qquad \text{, with } |x| < 1 \tag{4.52}$$

This is *associated Legendre equation* and the general solution shall take the form:

$$\Theta(x) = d_1 P_l^m(x) + d_2 Q_l^m(x) \tag{4.53}$$

Since $Q_l^m(x)$ is not bounded at both end, the term is vanished by taking $d_2 = 0$, so

$$\Theta(x) = d_1 P_l^m(x) \tag{4.54}$$

where $P_l^m(x)$ is the *associated Legendre function*, defined as:

$$P_l^m(x) = (1-x^2)^{|m|/2}\left(\frac{d}{dx}\right)^{|m|} P_l(x) \tag{4.55}$$

with $P_l(x)$ is l th *Legendre polynomial* and is convenient to define by *Rodrigues formula*:

$$P_l(x) = \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l (x^2-1)^l \tag{4.56}$$

from which $l \geq 0$ and $|m| \leq l$ to have $P_l^m \neq 0$. So, the range of l and m are as:

$$l = 0,1,2,\dots \quad ; \quad m = -l, -l+1, \dots, -1,0,1, \dots, l-1, l \tag{4.57}$$

While in term of θ, we substitute back $x = \cos\theta$ into (4.54),

#

$$\Theta(\theta) = d_1 P_l^m(\cos\theta) \tag{4.58}$$

Collectively, we have:

$$Y(\theta, \varphi) = b e^{im\varphi} P_l^m(\cos\theta) \tag{4.59}$$

where $b = cd_1$ are to determine by the *initial normalization condition*:

$$\int |\psi|^2 \, d^3\vec{r} = 1$$

with $\psi(r, \theta, \varphi) = R(r)Y(\theta, \varphi)$

and $d^3\vec{r} = r^2 \sin\theta \, dr d\theta d\varphi$ (4.60)

So that:

$$\int |R|^2 r^2 dr \iint |Y|^2 \sin\theta \, d\theta d\varphi = 1 \tag{4.61}$$

It eases if we normalize $R(r)$ and $Y(\theta, \varphi)$ separately as:

$$\int_0^\infty |R|^2 r^2 dr = 1 \tag{4.62}$$

and

$$\int_{\varphi=0}^{2\pi} \int_{\theta=0}^{\pi} |Y|^2 \sin\theta \, d\theta d\varphi = 1 \tag{4.63}$$

For $Y(\theta, \varphi)$, the normalized function are given as:

#

$$\boxed{Y_l^m(\theta, \varphi) = \varepsilon \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}} e^{im\varphi} P_l^m(\cos\theta)} \tag{4.64}$$

and are known as *spherical harmonics*, where $\varepsilon = \begin{cases} (-1)^m, & m \geq 0 \\ 1, & m \leq 0 \end{cases}$

They are also orthogonal:

$$\int_{\varphi=0}^{2\pi} \int_{\theta=0}^{\pi} [Y_l^m(\theta, \varphi)]^* \left[Y_{l'}^{m'}(\theta, \varphi)\right] \sin\theta \, d\theta d\varphi = 1 \tag{4.65}$$

4.3.3 The radial equation

Now, solve the *radial equation* of $R(r)$ from (4.43), multiply by R:

$$\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) - \frac{2mr^2 R}{\hbar^2}[V(r) - E] = l(l+1)R \tag{4.66}$$

We can simplify further by change of variable: $u(r) = rR(r)$ such that $R = \frac{u}{r}$

$$\frac{dR}{dr} = \frac{r\frac{du}{dr} - u}{r^2} \quad , \quad \frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) = r\frac{d^2u}{dr^2}$$

$$r\frac{d^2u}{dr^2} - \frac{2mru}{\hbar^2}[V(r) - E] = l(l+1)\frac{u}{r} \tag{4.67}$$

$$\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} - Vu + Eu = \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}u \tag{4.68}$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu} \tag{4.69}$$

This is the radial equation with the *effective potential*:

$$V_{eff} = V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} \tag{4.70}$$

contain an extra *centrifugal term*: $\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}$.

Meanwhile, the normalization condition becomes:

$$\int_0^\infty |u|^2 dr = 1 \tag{4.71}$$

4.3.4 The radial equation for hydrogen

For hydrogen atom, the *Coulombic potential energy* is:

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r} \tag{4.72}$$

then the radial equation becomes:

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[-\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu \tag{4.73}$$

let $\kappa = \frac{\sqrt{-2mE}}{\hbar}$ by taking into consideration that $E < 0$ for bound state, $\frac{1}{\kappa^2} = -\frac{\hbar^2}{2mE}$.

Divide (4.73) by E, we have:

$$\frac{1}{\kappa^2}\frac{d^2u}{dr^2} = \left[1 + \frac{l(l+1)}{\kappa^2 r^2} - \frac{me^2}{2\pi\varepsilon_0\hbar^2\kappa^2 r}\right]u \tag{4.74}$$

By pointing out that $\kappa r = \rho$ and $\frac{me^2}{2\pi\varepsilon_0\hbar^2\kappa} = \rho_0$, then we have:

$$\frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right]u \tag{4.75}$$

We come to have *asymptotic form* of the solutions,

as $\rho \to \infty$,

$$\frac{d^2u}{d\rho^2} = u \tag{4.76}$$

and as $\rho \to 0$,

$$\frac{d^2u}{d\rho^2} = \frac{l(l+1)}{\rho^2}u \tag{4.77}$$

which gives different solutions.

To peel off the asymptotic behavior, introduce a new function $\nu(\rho)$, such that:

$$u(\rho) = \rho^{l+1}e^{-\rho}\nu(\rho) \tag{4.78}$$

first,

$$\frac{du}{d\rho} = \rho^l e^{-\rho}\left[(l+1-\rho)\nu + \rho\frac{d\nu}{d\rho}\right] \tag{4.79}$$

and
$$\frac{d^2u}{d\rho^2} = \rho^l e^{-\rho}\left\{\left[-2l - 2 + \rho + \frac{l(l+1)}{\rho}\right]\nu + 2(l+1-\rho)\frac{d\nu}{d\rho} + \rho\frac{d^2\nu}{d\rho^2}\right\} \tag{4.80}$$

In term of $\nu(\rho)$, the radial equation becomes:

$$\rho\frac{d^2\nu}{d\rho^2} + 2(l+1-\rho)\frac{d\nu}{d\rho} + [\rho_0 - 2(l+1)]\nu = 0 \tag{4.81}$$

To solve this, we use power series method by letting:

$$\nu(\rho) = \sum_{j=0}^{\infty} a_j\rho^j \tag{4.82}$$

$$\frac{d\nu}{d\rho} = \sum_{j=1}^{\infty} ja_j\rho^{j-1} \equiv \sum_{j=0}^{\infty}(j+1)a_{j+1}\rho^j \quad ; \quad \frac{d^2\nu}{d\rho^2} = \sum_{j=0}^{\infty} j(j+1)a_{j+1}\rho^{j-1}$$

Get back to the equation to yield:

$$\sum_{j=0}^{\infty} j(j+1)a_{j+1}\rho^j + 2(l+1)\sum_{j=0}^{\infty}(j+1)a_{j+1}\rho^j - 2\sum_{j=0}^{\infty} ja_j\rho^{j-1} + [\rho_0 - 2(l+1)]\sum_{j=0}^{\infty} a_j\rho^j = 0 \tag{4.83}$$

Equating the terms of like powers yields:

$$j(j+1)a_{j+1} + 2(l+1)(j+1)a_{j+1} - 2ja_j + [\rho_0 - 2(l+1)]a_j = 0$$

$$a_{j+1} = \left\{\frac{2(j+l+1) - \rho_0}{(j+1)(j+2l+2)}\right\}a_j \tag{4.84}$$

-the *recursion relation*

Let $a_0 = A$, and we have obtain a_j for large j as:

$$a_{j+1} \approx \frac{2j}{j(j+1)}a_j = \frac{2}{(j+1)}a_j \quad \text{; thus} \quad a_j \approx \frac{2^j}{j!}A$$

that give us
$$\nu(\rho) = A\sum_{j=0}^{\infty}\frac{2^j}{j!}\rho^j = Ae^{2\rho} \tag{4.85}$$

and hence
$$u(\rho) = A\rho^{l+1}e^{\rho} \tag{4.86}$$

Which again unbounded at large ρ. There's only one way to solve the dilemma, there must be some *maximum* j_{max} such that: $a_{j_{max}+1} = 0$.

Then from the recursion relation, $2(j_{max} + l + 1) - \rho_0 = 0$, and define

$$n = j_{max} + l + 1 \quad , \quad l = 0,1,2,\dots,n-1 \tag{4.87}$$

to give $\rho_0 = 2n$, where n is the *principle quantum number*.

But, we come to note from the earlier substitutions that

$$E = -\frac{\hbar^2\kappa^2}{2m} = -\frac{1}{2m}\frac{me^2\kappa}{2\pi\varepsilon_0\rho_0}\frac{1}{\rho_0}\frac{me^2}{2\pi\varepsilon_0\hbar^2\kappa} = -\frac{me^4}{8\pi^2\varepsilon_0^2\hbar^2\rho_0^2} \tag{4.88}$$

So that the allowed energy are:

$$E_n = -\frac{me^4}{32\pi^2\varepsilon_0^2\hbar^2n^2} = \left[-\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\right]\frac{1}{n^2} = \frac{E_1}{n^2} \tag{4.89}$$

the *Bohr formula*, where $n = 1,2,3, \ldots$.

Also, by taking $\rho_0 = 2n$ into $\rho_0 = \frac{me^2}{2\pi\varepsilon_0\hbar^2\kappa}$, we find that:

$$\kappa = \frac{me^2}{4\pi\varepsilon_0\hbar^2 n} = \frac{1}{an} \qquad \text{where} \qquad a = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = 0.529\text{Å} \tag{4.90}$$

is the *Bohr radius*. Follow from relation, we have $\rho = \kappa r = \frac{r}{an}$

Finally, we come back to $R(r) = \frac{u(r)}{r}$ and by index n and l,

#

$$\boxed{R_{nl}(r) = \frac{1}{r}\rho^{l+1}e^{-\rho}v(\rho)} \tag{4.91}$$

with $v(\rho) = \sum_{j=0}^{\infty} a_j\rho^j$ (4.82) and $a_{j+1} = \frac{2(j+l+1-n)}{(j+1)(j+2l+2)}a_j$ (4.84).

4.3.5 Hydrogen wave function

Now, the wave function for hydrogen should take the form

$$\boxed{\psi_{nlm}(r,\theta,\varphi) = R_{nl}(r)Y_l^m(\theta,\varphi)} \tag{4.92}$$

where $n = 1,2,3, \ldots$

$l = 0,1,2, \ldots, n-1$

$m = -l, -l+1, \ldots, -1,0,1, \ldots, l-1, l$

4.3.6 Ground state wave function for hydrogen atom

The *ground state* is of the case $n = 1$,

$$E_1 = -\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 = -13.6\ eV \tag{4.93}$$

From $n = j_{max} + l + 1$, $j_{max} = 0$ and $l = 0$, also affect $m = 0$.

So, the ground state wave function will be:

$$\psi_{100}(r,\theta,\varphi) = R_{10}(r)Y_0^0(\theta,\varphi) \tag{4.94}$$

The coefficients a_j vanishes at first term, $a_1 = 0$, so $v(\rho) = a_0$ which makes

$$R_{10}(r) = \frac{1}{r}\left(\frac{r}{a}\right)\left(e^{-r/a}\right)a_0 = \frac{a_0}{a}e^{-r/a} \tag{4.95}$$

Normalize it as: $$\int_0^\infty |R_{10}|^2 r^2 dr = \frac{|a_0|^2}{a^2}\int_0^\infty e^{-2r/a}r^2 dr = 1 \tag{4.96}$$

Solve by integration by parts,

$$\begin{aligned}\int_0^\infty r^2 e^{-2r/a}dr &= -\frac{ar^2}{2}e^{-2r/a}\Big|_0^\infty + \int_0^\infty are^{-2r/a}dr \\ &= 0 - a\left(\frac{ar}{2}\right)e^{-2r/a}\Big|_0^\infty + \int_0^\infty \frac{a^2}{2}e^{-2r/a}dr \\ &= 0 + \frac{a^2}{2}\left(-\frac{a}{2}\right)e^{-2r/a}\Big|_0^\infty \\ &= \frac{a^3}{4}\end{aligned} \tag{4.97}$$

So, $\frac{|a_0|^2}{a^2}\left(\frac{a^3}{4}\right) = 1$; $|a_0|^2 = \frac{4}{a}$ and $a_0 = \frac{2}{\sqrt{a}}$. While $Y_0^0 = \sqrt{\frac{1}{4\pi}}$ to make:

$$\boxed{\psi_{100}(r,\theta,\varphi) = \frac{2}{\sqrt{a^3}}\frac{1}{\sqrt{4\pi}}e^{-r/a} = \frac{e^{-r/a}}{\sqrt{\pi a^3}}} \tag{4.98}$$

4.3.7 Ground state wave function of hydrogen atom in momentum space

In position space, the ground state wave function of hydrogen atom is given as in (4.98): $\psi_{100}(r,\theta,\varphi) = \frac{1}{\sqrt{\pi a^3}}e^{-r/a}$, while in momentum space, it should be the *Fourier transform*:

$$\phi_{100}(p,\theta,\varphi) = \frac{1}{\sqrt{(2\pi\hbar)^3}}\int e^{-i\vec{p}\cdot\vec{r}/\hbar}\psi_{100}(r,\theta,\varphi)d^3\vec{r} \tag{4.99}$$

By considering the spherical coordinate system, $d^3\vec{r} = r^2\sin\theta\, dr d\theta d\varphi$ and taking $\vec{p}\cdot\vec{r} = pr\cos\theta$, we would have simplify:

$$\begin{aligned}\phi_{100}(p,\theta,\varphi) &= \frac{1}{\sqrt{(2\pi\hbar)^3}}\int \frac{1}{\sqrt{\pi a^3}}e^{-r/a}e^{-ipr\cos\theta/\hbar}r^2\sin\theta\, dr d\theta d\varphi \\ &= \frac{1}{\sqrt{\pi(2\pi a\hbar)^3}}\int_0^\infty e^{-r/a}r^2 dr\int_0^\pi e^{-ipr\cos\theta/\hbar}\sin\theta\, d\theta\int_0^{2\pi}d\varphi\end{aligned} \tag{4.100}$$

Now, solving the integral separately:

$$\int_0^{2\pi} d\varphi = 2\pi$$

$$\int_0^{\pi} e^{-ipr\cos\theta/\hbar}\sin\theta\, d\theta = -\int_1^{-1} e^{-\frac{ipr}{\hbar}u}du$$

by letting $u = \cos\theta$; $du = -\sin\theta\, d\theta$

$$= -\frac{\hbar}{ipr}\left[-e^{-\frac{ipr}{\hbar}u}\right]_1^{-1}$$

$$= \frac{\hbar}{ipr}\left(e^{\frac{ipr}{\hbar}} - e^{-\frac{ipr}{\hbar}}\right)$$

use $\sin z = \frac{1}{2i}(e^z - e^{-z})$

$$= \frac{2\hbar}{pr}\sin\left(\frac{pr}{\hbar}\right)$$

we should now have:

$$\phi_{100}(p,\theta,\varphi) = \frac{4}{\pi}\frac{\hbar}{\sqrt{(2a\hbar)^3}}\int_0^{\infty} e^{-r/a}r^2\frac{\sin\left(\frac{pr}{\hbar}\right)}{pr}dr$$

$$= \frac{\sqrt{2}\hbar}{p\pi}\frac{1}{\sqrt{(a\hbar)^3}}\int_0^{\infty} re^{-r/a}\sin\left(\frac{pr}{\hbar}\right)dr \tag{4.101}$$

Expand $\sin\left(\frac{pr}{\hbar}\right) = \frac{1}{2i}\left(e^{\frac{pr}{\hbar}} - e^{-\frac{pr}{\hbar}}\right)$, the integral part is:

$$\frac{1}{2i}\int_0^{\infty} re^{-r\left(\frac{1}{a}-i\frac{p}{\hbar}\right)}dr - \frac{1}{2i}\int_0^{\infty} re^{-r\left(\frac{1}{a}+i\frac{p}{\hbar}\right)}dr$$

$$= \frac{1}{2i}\left[\int_0^{\infty} re^{-\left(\frac{1}{a}-i\frac{p}{\hbar}\right)r}dr - \int_0^{\infty} re^{-\left(\frac{1}{a}+i\frac{p}{\hbar}\right)r}dr\right]$$

From general mathematics, by solving *integration by part*,

$$\int xe^{bx}dx = \frac{x}{b}e^{bx} - \int\frac{1}{b}e^{bx} = \frac{xe^{bx}}{b} - \frac{e^{bx}}{b^2} = e^{bx}\left(\frac{x}{b} - \frac{1}{b^2}\right)$$

and by taking $b_{\pm} = -\left(\frac{1}{a} \pm i\frac{p}{\hbar}\right)$, a mere constant here, the integral continue as:

$$\frac{1}{2i}\left[e^{b_- r}\left(\frac{r}{b_-} - \frac{1}{{b_-}^2}\right) - e^{b_+ r}\left(\frac{r}{b_+} - \frac{1}{{b_+}^2}\right)\right]_0^{\infty} = \frac{1}{2i}\left[\frac{1}{{b_-}^2} - \frac{1}{{b_+}^2}\right]$$

$$= \frac{1}{2i}\left[\frac{1}{\left(\frac{1}{a}-i\frac{p}{\hbar}\right)^2} - \frac{1}{\left(\frac{1}{a}+i\frac{p}{\hbar}\right)^2}\right]$$

$$= \frac{1}{2i}\left[\frac{\frac{1}{a^2}+\frac{p^2}{\hbar^2}-\frac{2ip}{a\hbar}-\frac{1}{a^2}-\frac{p^2}{\hbar^2}-\frac{2ip}{a\hbar}}{\left(\frac{1}{a^2}+\frac{p^2}{\hbar^2}\right)^2}\right]$$

$$= \frac{2p}{a\hbar}\frac{1}{\left(\frac{1}{a^2}+\frac{p^2}{\hbar^2}\right)^2}$$

$$= \left(-\frac{2p}{a\hbar}\right)\frac{1}{\frac{1}{a^4}\left(1+\{\frac{ap}{\hbar}\}^2\right)^2}$$

$$= \left(-\frac{2pa^3}{\hbar}\right)\frac{1}{\left[1+(\frac{ap}{\hbar})^2\right]^2}$$

Collectively, we come to have:

$$\phi_{100}(p,\theta,\varphi) = \frac{\sqrt{2}\hbar}{p\pi}\frac{1}{\sqrt{(a\hbar)^3}}\left(-\frac{2pa^3}{\hbar}\right)\frac{1}{\left[1+(\frac{ap}{\hbar})^2\right]^2}$$

$$\boxed{\phi_{100}(p,\theta,\varphi) = \frac{1}{\pi}\left(\frac{2a}{\hbar}\right)^{\frac{3}{2}}\frac{1}{\left[1+(\frac{ap}{\hbar})^2\right]^2}} \tag{4.102}$$

This is in consistent with the ground state wave function of hydrogen atom in momentum space from: Am. J. Phys. 63, 710 (1995) - Barry R. Holstein

Where

$$\phi_{100}(p) = \sqrt{\frac{1}{\pi}}(m\alpha)^{\frac{3}{2}}\frac{8\pi m\alpha}{[\kappa_1^2 + p^2]^2} \tag{4.103}$$

and

$$\psi_{100}(r) = \frac{1}{(2\pi)^3}\int \phi_{100}(p)\, e^{i\vec{p}\cdot\vec{r}} d^3\vec{p} = \left(\frac{m^3\alpha^3}{\pi}\right)^{\frac{1}{2}} e^{-m\alpha r} \tag{4.104}$$

Here, taking by the transformation, $m\alpha = \frac{1}{a}$ and for $\frac{\kappa_n^2}{2m} = \frac{m\alpha^2}{2n^2}$; $\kappa_n^2 = \frac{m^2\alpha^2}{n^2} \Rightarrow \kappa_1^2 = \frac{1}{a^2}$.

$$\phi_{100}(p) = \left(\frac{1}{a^3\pi}\right)^{\frac{1}{2}}\frac{8\pi}{a\left(\frac{1}{a^2}+p^2\right)^2} = \frac{8\sqrt{\pi}a^{\frac{3}{2}}}{(1+a^2p^2)^2} \tag{4.105}$$

Multiply by $\frac{(2\pi\hbar)^{\frac{3}{2}}}{(2\pi)^3} = \left(\frac{\hbar}{2\pi}\right)^{\frac{3}{2}}$ yield:

$$\phi_{100}(p) = \frac{1}{\pi}(2a)^{\frac{3}{2}}\frac{1}{[1+(ap)^2]^2} \qquad \text{when } \hbar = 1 \tag{4.106}$$

CHAPTER 5
THE PICTURES OF QUANTUM MECHANICS

5.1 Time Evolution of State

5.1.1 Time evolution operator

To obtain the *quantum state* at any time t, namely $|\psi(t)\rangle$ based on the initial state $|\psi(t_0)\rangle$, we use the relation:

$$|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle \qquad \text{with } t > t_0 \tag{5.1}$$

where $\hat{U}(t,t_0)$ is known as the *time evolution operator* or *propagator*. From (5.1), note that

$$\hat{U}(t_0,t_0) = \hat{I} \tag{5.2}$$

recall that $\hat{I}$ is the unit operator as suggested in (2.67) by an identity matrix.

Now, to find $\hat{U}(t,t_0)$, we substitute (5.1) into the time-dependent Schrödinger equation (3.30):

$$i\hbar\frac{\partial}{\partial t}\big(\hat{U}(t,t_0)|\psi(t_0)\rangle\big) = \hat{H}\big(\hat{U}(t,t_0)|\psi(t_0)\rangle\big) \tag{5.3}$$

or,

$$\frac{\partial\hat{U}(t,t_0)}{\partial t} = -\frac{i}{\hbar}\hat{H}\hat{U}(t,t_0) \tag{5.4}$$

Solve by assume that the Hamiltonian is independent of time, and take into account for the initial condition (5.2):

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

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

$$\ln\hat{U}(t_0,t_0) = -\frac{i}{\hbar}\hat{H}t_0 + c = 0 \implies c = \frac{i}{\hbar}\hat{H}t_0$$

$$\boxed{\hat{U}(t,t_0) = e^{-i(t-t_0)\hat{H}/\hbar}} \tag{5.5}$$

and, we can get back to (5.1) as:

$$\boxed{|\psi(t)\rangle = e^{-i(t-t_0)\hat{H}/\hbar}|\psi(t_0)\rangle} \tag{5.6}$$

The operator $\hat{U}(t,t_0) = e^{-i(t-t_0)\hat{H}/\hbar}$ represents a *finite time translation*. Notice that it is also a unitary operator, since $\hat{U}^\dagger(t,t_0) = \hat{U}^{-1}(t,t_0) = e^{i(t-t_0)\hat{H}/\hbar} \equiv \hat{U}(t_0,t)$ which automatically reserve for $\hat{U}(t,t_0)\hat{U}^\dagger(t,t_0) = \hat{U}(t,t_0)\hat{U}^{-1}(t,t_0) = \hat{I}$.

5.1.2 The Ehrenfest's theorem

Ehrenfest's theorem tells us that expectation values obey *classical laws*. To illustrate, we take the *time evolution of expectation values* for position and momentum operators, $\hat{\vec{r}}$ and $\hat{\vec{p}}$ of a particle moving in a potential $V(x)$.

Based on equation (3.47) which says for any operator $\hat{Q}$:

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle + \langle\frac{\partial\hat{Q}}{\partial t}\rangle \tag{5.7}$$

The terms $\langle\frac{\partial\hat{Q}}{\partial t}\rangle = 0$ here, since both $\hat{\vec{r}}$ and $\hat{\vec{p}}$ are explicitly independent of time, t. For $\hat{\vec{r}}$, taking in a single dimension, we have:

$$\frac{d}{dt}\langle x\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{x}]\rangle \tag{5.8}$$

Now, we know that $\hat{H} = \frac{\hat{p}_x{}^2}{2m} + V(x)$, and together with the *canonical commutator* relations:

$$[r_i, p_i] = -[p_i, r_i] = i\hbar\delta_{ij} \tag{5.9}$$

We can show that:

$$\begin{aligned}[\hat{H},\hat{x}] &= \left[\left(\frac{\hat{p}_x{}^2}{2m} + V(x)\right),\hat{x}\right] \\ &= \frac{1}{2m}\left[\hat{p}_x{}^2\hat{x} - \hat{x}\hat{p}_x{}^2\right] + [V(x),\hat{x}] \\ &= \frac{1}{2m}\{\hat{p}_x[\hat{p}_x\hat{x}] + [\hat{p}_x\hat{x}]\hat{p}_x\} \\ &= -\frac{i\hbar}{m}\hat{p}_x\end{aligned} \tag{5.10}$$

So,

$$\frac{d}{dt}\langle x\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{x}]\rangle = \frac{i}{\hbar}\langle -\frac{i\hbar}{m}\hat{p}_x\rangle = \frac{\langle p_x\rangle}{m} \tag{5.11}$$

In three dimensional case, we simply have:

$$\boxed{\frac{d}{dt}\langle\vec{r}\rangle = \frac{\langle\vec{p}\rangle}{m}} \tag{5.12}$$

In other hand, working the same way for $\hat{\vec{p}}$:

$$\frac{d}{dt}\langle p_x\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{p}_x]\rangle \tag{5.13}$$

$$[\hat{H},\hat{p}_x]\psi = \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(i\hbar\frac{d}{dx}\psi\right) - i\hbar V\frac{d}{dx}\psi - i\hbar\frac{d}{dx}\left(\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi\right) + i\hbar\frac{d}{dx}(V\psi)$$

$$= \frac{i\hbar^3}{2m}\frac{d^3}{dx^3}\psi - i\hbar V\frac{d}{dx}\psi - \frac{i\hbar^3}{2m}\frac{d^3}{dx^3}\psi + i\hbar\frac{dV}{dx}\psi + i\hbar V\frac{d}{dx}\psi$$

$$= i\hbar\frac{dV}{dx}\psi$$

which gives

$$[\hat{H},\hat{p}_x] = i\hbar\frac{dV}{dx} \tag{5.14}$$

and thus,

$$\frac{d}{dt}\langle p_x\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{p}_x]\rangle = \frac{i}{\hbar}\langle i\hbar\frac{dV}{dx}\rangle = \langle -\frac{dV}{dx}\rangle \tag{5.15}$$

In three dimension,

$$\boxed{\frac{d}{dt}\langle\vec{p}\rangle = \langle-\vec{\nabla}V\rangle} \tag{5.16}$$

The two results, (5.12) and (5.16) imply that the expectation values obey *Newton's second law*.

5.1.3 The Virial theorem

Virial theorem is a relation between mean kinetic energy and mean potential energy. Now, we solve for

$$\frac{d}{dt}\langle xp_x\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{x}\hat{p}_x]\rangle \tag{5.17}$$

$$[\hat{H},\hat{x}\hat{p}_x]\psi = \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(i\hbar x\frac{d\psi}{dx}\right) - i\hbar Vx\frac{d\psi}{dx} - i\hbar x\frac{d}{dx}\left(\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}\right) + i\hbar x\frac{d}{dx}(V\psi)$$

$$= \frac{i\hbar^3}{2m}\left(2\frac{d^2\psi}{dx^2} + x\frac{d^3\psi}{dx^3}\right) - i\hbar Vx\frac{d\psi}{dx} - \frac{i\hbar^3}{2m}x\frac{d^3\psi}{dx^3} + i\hbar xV\frac{d\psi}{dx} + i\hbar x\frac{dV}{dx}\psi$$

$$= \frac{i\hbar^3}{m}\frac{d^2}{dx^2}\psi + i\hbar x\frac{dV}{dx}\psi$$

$$= i\hbar\left(\frac{\hbar^2}{m}\frac{d^2}{dx^2} + x\frac{dV}{dx}\right)\psi$$

So,

$$\frac{d}{dt}\langle xp_x\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{x}\hat{p}_x]\rangle = \frac{i}{\hbar}\langle i\hbar\left(\frac{\hbar^2}{m}\frac{d^2}{dx^2} + x\frac{dV}{dx}\right)\rangle = \langle -\frac{\hbar^2}{m}\frac{d^2}{dx^2} - x\frac{dV}{dx}\rangle \tag{5.18}$$

or,

$$\frac{d}{dt}\langle xp_x\rangle = 2\langle T\rangle - \langle x\frac{dV}{dx}\rangle \tag{5.19}$$

While in three dimension,

$$\frac{d}{dt}\langle\vec{r}\vec{p}\rangle = 2\left\langle -\frac{\hbar^2}{2m}\nabla^2\right\rangle - \langle\vec{r}\cdot\vec{\nabla}V\rangle = 2\langle T\rangle - \langle\vec{r}\cdot\vec{\nabla}V\rangle \tag{5.20}$$

For stationary state, $\frac{d}{dt}\langle\vec{r}\vec{p}\rangle = 0$, so

$$\boxed{2\langle T\rangle = \langle\vec{r}\cdot\vec{\nabla}V\rangle} \tag{5.21}$$

5.2 The Schrödinger Picture

In *Schrödinger picture*, state vectors depend explicitly on time, but operators do not:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \tag{5.22}$$

where $|\psi(t)\rangle$ denotes the state of the system in the Schrödinger picture. As stated before in 5.1.1, $|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle = e^{-i(t-t_0)\hat{H}/\hbar}|\psi(t_0)\rangle$. Let $t_0 = 0$:

$$\boxed{|\psi(t)\rangle = e^{-it\hat{H}/\hbar}|\psi(0)\rangle} \tag{5.23}$$

And we have specific that $\hat{U}(t,t_0)$ is unitary and satisfy the properties:

$$\hat{U}(t,t_0)\hat{U}^\dagger(t,t_0) = \hat{I} \tag{5.24}$$

$$\hat{U}(t,t) = \hat{I} \tag{5.25}$$

$$\hat{U}^\dagger(t,t_0) = \hat{U}^{-1}(t,t_0) = \hat{U}(t_0,t) \tag{5.26}$$

$$\hat{U}(t_1,t_2)\hat{U}(t_2,t_3) = \hat{U}(t_1,t_3) \tag{5.27}$$

5.3 The Heisenberg Picture

In *Heisenberg picture*, operators depend explicitly on time, but state vectors do not. The Heisenberg picture is obtained from the Schrödinger picture by applying $\hat{U}$ on $|\psi(t)\rangle_H$:

$$|\psi(t)\rangle_H = \hat{U}^\dagger(t)|\psi(t)\rangle = |\psi(0)\rangle \tag{5.28}$$

where $|\psi(t)\rangle$ is given by (5.23) while $\hat{U}^\dagger(t)$ can be obtained (5.5) by setting $t_0 = 0$: $\hat{U}^\dagger(t) = \hat{U}^\dagger(t,t_0 = 0) = e^{it\hat{H}/\hbar}$. So, we can actually write (5.28) as:

$$\boxed{|\psi(t)\rangle_H = e^{it\hat{H}/\hbar}|\psi(t)\rangle} \tag{5.29}$$

As $|\psi\rangle_H$ is frozen in time, we have $\frac{d|\psi\rangle_H}{dt} = 0$. However, the expectation value of any operator $\hat{Q}$ in the state $|\psi(t)\rangle$ evolves in time:

$$\langle Q\rangle = \langle\psi(t)|\hat{Q}|\psi(t)\rangle = \langle\psi(0)|e^{it\hat{H}/\hbar}\hat{Q}e^{-it\hat{H}/\hbar}|\psi(0)\rangle$$

$$= \langle \psi(0) | \hat{Q}_H(t) | \psi(0) \rangle$$

$$= \ {}_H\langle \psi(t) | \hat{Q}_H(t) | \psi(t) \rangle_H \qquad (5.30)$$

where $\hat{Q}_H(t)$ is given by:

$$\boxed{\hat{Q}_H(t) = \hat{U}^\dagger(t)\hat{Q}\hat{U}(t) = e^{it\hat{H}/\hbar}\hat{Q}e^{-it\hat{H}/\hbar}} \qquad (5.31)$$

Notice that the left hand side of equation (5.30) is of Schrödinger picture while the right hand side is of Heisenberg picture; this shows that the expectation value of any operator is the same in both pictures. As well, both the Schrödinger picture and Heisenberg picture coincide at $t = 0$, since $|\psi(0)\rangle_H = |\psi(0)\rangle$ and $\hat{Q}_H(0) = \hat{Q}$.

5.3.1 The Heisenberg equation of motion

Assume that $\hat{Q}$ is independent explicitly on time: $\frac{\partial \hat{Q}}{\partial t} = 0$, we have:

$$\begin{aligned}
\frac{\partial \hat{Q}_H(t)}{\partial t} &= \frac{d\hat{U}^\dagger(t)}{dt}\hat{Q}\hat{U}(t) + \hat{U}^\dagger(t)\hat{Q}\frac{d\hat{U}(t)}{dt} \\
&= \frac{i}{\hbar}\hat{H}\hat{U}^\dagger(t)\hat{Q}\hat{U}(t) - \frac{i}{\hbar}\hat{U}^\dagger(t)\hat{Q}\hat{H}\hat{U}(t) \\
&= \frac{i}{\hbar}\hat{H}\hat{Q}_H(t) - \frac{i}{\hbar}\hat{Q}_H(t)\hat{H} \\
&= \frac{i}{\hbar}\left[\hat{H}, \hat{Q}_H(t)\right]
\end{aligned} \qquad (5.32)$$

where we have $\hat{U}(t) = e^{-it\hat{H}/\hbar}$ from (5.5) and $\hat{Q}_H(t) = \hat{U}^\dagger(t)\hat{Q}\hat{U}(t)$ from (5.31); plus for the reason $\hat{U}(t)$ and $\hat{H}$ commute: $\hat{H}\hat{U}(t) = \hat{U}(t)\hat{H}$ in the second line.

We can re-arrange (5.32) to give the *Heisenberg equation of motion* as:

$$\boxed{i\hbar\frac{d\hat{Q}_H(t)}{dt} = \left[\hat{Q}_H(t), \hat{H}\right]} \qquad (5.33)$$

5.4 The Interaction Picture (or) the Dirac Picture

In this picture, both state vectors and operators evolve in time. Therefore we need to find the equation of motion for both the state vectors and operators.

5.4.1 Equation of motion for the state vectors

In *interaction picture*, we define the state vectors based on Schrödinger picture:

$$\boxed{|\psi(t)\rangle_I = e^{it\hat{H}_0/\hbar}|\psi(t)\rangle} \qquad (5.34)$$

Again, at $t = 0$, $|\psi(0)\rangle_I = |\psi(0)\rangle$. The time evolution of $|\psi(t)\rangle$ is governed by the Schrödinger equation (5.22) with $\hat{H} = \hat{H}_0 + \hat{V}$ where $\hat{H}_0$ is time independent, but $\hat{V}$ may depend on time.

To find the time evolution of $|\psi(t)\rangle_I$, take the time derivative of (5.34):

$$\frac{d|\psi(t)\rangle_I}{dt} = \frac{i\hat{H}_0}{\hbar} e^{it\hat{H}_0/\hbar}|\psi(t)\rangle + e^{it\hat{H}_0/\hbar}\left(\frac{d}{dt}|\psi(t)\rangle\right)$$

$$i\hbar\frac{d|\psi(t)\rangle_I}{dt} = -\hat{H}_0|\psi(t)\rangle_I + e^{it\hat{H}_0/\hbar}\left(i\hbar\frac{d}{dt}|\psi(t)\rangle\right)$$

$$= -\hat{H}_0|\psi(t)\rangle_I + e^{it\hat{H}_0/\hbar}\hat{H}|\psi(t)\rangle \quad (5.35)$$

Since $\hat{H} = \hat{H}_0 + \hat{V}$, the last term of (5.35) is:

$$e^{it\hat{H}_0/\hbar}\hat{H}|\psi(t)\rangle = e^{it\hat{H}_0/\hbar}\hat{H}_0|\psi(t)\rangle + e^{it\hat{H}_0/\hbar}\hat{V}|\psi(t)\rangle$$

$$= \hat{H}_0 e^{it\hat{H}_0/\hbar}|\psi(t)\rangle + \left(e^{it\hat{H}_0/\hbar}\hat{V}e^{-it\hat{H}_0/\hbar}\right)e^{it\hat{H}_0/\hbar}|\psi(t)\rangle$$

$$= \hat{H}_0|\psi(t)\rangle_I + \hat{V}_I(t)|\psi(t)\rangle_I \quad (5.36)$$

where $$\hat{V}_I(t) = e^{it\hat{H}_0/\hbar}\hat{V}e^{-it\hat{H}_0/\hbar} \quad (5.37)$$

and $\hat{H}_0$ commute with $e^{it\hat{H}_0/\hbar}$ since any operator commute with itself.

With this, we can re-write (5.35) as:

$$i\hbar\frac{d|\psi(t)\rangle_I}{dt} = -\hat{H}_0|\psi(t)\rangle_I + \hat{H}_0|\psi(t)\rangle_I + \hat{V}_I|\psi(t)\rangle_I \quad (5.38)$$

or simply $$\boxed{i\hbar\frac{d|\psi(t)\rangle_I}{dt} = +\hat{V}_I(t)|\psi(t)\rangle_I} \quad (5.38)$$

This is the Schrödinger equation in the interaction picture. It shows that the time evolution of the state vector is governed by the *interaction* $\hat{V}_I(t)$.

5.4.2 Equation of motion for the operators

The *interaction representation* of any operator $\hat{Q}$ is given, as shown in (5.37), in term of its Schrödinger representation by:

$$\boxed{\hat{Q}_I(t) = e^{it\hat{H}_0/\hbar}\hat{Q}e^{-it\hat{H}_0/\hbar}} \quad (5.40)$$

To obtain the equation of motion, approach the same as in 5.3.1; Take the time derivative of $\hat{Q}_I(t)$ and as mentioned in 5.2 that, $\frac{\partial\hat{Q}}{\partial t} = 0$.

$$\frac{\partial\hat{Q}_I(t)}{\partial t} = \left(\frac{d}{dt}e^{it\hat{H}_0/\hbar}\right)\hat{Q}e^{-it\hat{H}_0/\hbar} + e^{it\hat{H}_0/\hbar}\hat{Q}\left(\frac{d}{dt}e^{-it\hat{H}_0/\hbar}\right)$$

$$= \frac{i}{\hbar}\hat{H}_0 e^{it\hat{H}_0/\hbar}\hat{Q}e^{-it\hat{H}_0/\hbar} - \frac{i}{\hbar}e^{it\hat{H}_0/\hbar}\hat{Q}\hat{H}_0 e^{-it\hat{H}_0/\hbar}$$

$$= \frac{i}{\hbar}\hat{H}_0\hat{Q}_I(t) - \frac{i}{\hbar}\hat{Q}_I(t)\hat{H}_0$$

$$= \frac{i}{\hbar}\left[\hat{H}_0, \hat{Q}_I(t)\right] \tag{5.41}$$

where we have used (5.40) and the relation: $\hat{H}_0 e^{-it\hat{H}_0/\hbar} = e^{-it\hat{H}_0/\hbar}\hat{H}_0$ as we did previously in (5.36). Re-arrange the equation to give:

$$\boxed{i\hbar\frac{\partial\hat{Q}_I(t)}{\partial t} = \left[\hat{Q}_I(t), \hat{H}_0\right]} \tag{5.42}$$

This equation is similar to the Heisenberg equation of motion (5.33), except that $\hat{H}$ is replaced by $\hat{H}_0$. The basic difference between the Heisenberg and interaction pictures can be inferred from a comparison of (5.29) with (5.34) and (5.31) with (5.40): in the Heisenberg picture it is $\hat{H}$ that appears in the exponents, whereas in the interaction picture it is $\hat{H}_0$ that appears.

REFERENCE

Quantum Mechanics - Concept and Application (2nd edition, 2009) - Nouredine Zettili
pp. 14-15, pp. 39-40, pp. 79-101, pp. 104-119, pp. 113, pp. 121-126, pp. 130-132, pp. 178-179, pp.179-183, pp. 189-190 , pp. 218-220, pp. 571-574, pp. 653

Introduction to Quantum Mechanics (1995) – David J. Griffiths
pp. 20-23, pp. 31-41, pp. 44-48, pp. 52-53, pp. 95-103 and pp.121-139

Oxford: A Dictionary of Physics (5th edition, 2005)
pp.382: phase space

Quantum Mechanics (2004) - Ernest S. Abers
pp. 49-51

Quantum Mechanics (2007) - P.J. Mulders
pp. 46-47

Quantum Mechanics (2nd edition, 2006) - Richard W. Robinett
pp. 67-69, pp. 104-106 and pp. 111-116

Quantum Mechanics (2nd edition, 2000) - B.H. Bransden and C.J. Joachain
pp. 82-85 and pp.124-127

From Classical to Quantum Mechanics (2004) - G. Esposito, G. Marmo and E.C.G. Sudarshan
pp. 120

PHY-480
pp. 88-89

Am. J. Phys. 63, 710 (1995) - Barry R. Holstein
pp. 712-713

SUMMARY

The major focus of this study is about the representations in quantum mechanics. Most of which are well known and easily found in various texts, but not all. However the variations are prove to be equivalent or in some case mutually related.

In comparison, Heisenberg matrix formulation offers a greater generality, yet it gives no visual idea about the structure of atom, and being less intuitive than Schrödinger wave mechanics. Both have their own stand point when come to solve certain situation. Matrix mechanics is difficult to solve in relatively easy problem, but become practical in solving harmonic oscillator and angular momentum. While in solving the Schrödinger equation, we might come to a very complex differential equation; the complexity in solving the differential equation depends entirely on the form of potential.

In the other hand, we see that position representation is widely adopted in most introductory quantum mechanics text, but we barely come across momentum representation. The observables (x, p) in position space are of the form: $\left(x, -i\hbar\frac{d}{dx}\right)$, and in momentum space: $\left(-i\hbar\frac{d}{dp}, p\right)$. We already come across the equivalence of each representation through the Fourier transformation. We choose between each representation based on the ease in solving the situation.

Last and the most important one, the pictures of quantum mechanics based on the time evolution scale of state vectors (and thus wave functions) and operators. Besides the traditional Schrödinger picture, Heisenberg picture and interaction picture are obtain from Schrödinger picture with modification using time evolution operator.

Student's Log Book

Date: 16th May 2011 - 9th September 2011 | **Day:** 117 days

Activities of the Day / Period

The first part of my project is to understand the mathematical formalism and Dirac bra-kets notation. I also covered up some part for the postulates of quantum mechanics to allow me have a full sight on the situation, before I proceed into the study of representation.

The first representation I come across is about the representation of bases systems, where the different formulation of quantum mechanics is majorly differed.

Secondly, I studied the representation in position space and momentum space. The two are related via the Fourier transformation. Besides working on the transformation of wave function, operators and Schrödinger equation, I also studied the representation of free particles, simple harmonic oscillator and ground state wave function of hydrogen, in momentum space.

Finally, I worked on the three most common pictures of quantum mechanics namely, the Schrödinger picture, the Heisenberg picture and the interaction picture (also known as Dirac picture). They are related by the time evolution unitary operator.

Achievement of the day/period

Instruction: This section indicates student's achievement of the day based on your activities above. Students can tick more than one box provided below.

Technical/Functional Skills

- ○ Adaptable problem-solving skills
- ○ Process evaluation/analyses
- ○ Quantitative/analytical abilities
- ○ Holistic problem solving
- ○ Technical Skills
- ○ Decision-making Ability
- ○ Project management

Soft Skills

- ○ Interpersonal skills/presence
- ○ Creative and critical thinking
- ○ Teamwork skills
- ○ Leadership awareness
- ○ Communication skills
- ○ Self management

Training Advisor's Comments

Name:

Position:

Signature:

Date:

Academic Advisor's Comments

Name:

Position:

Signature:

Date: