QUANTUM MECHANICS

with

Basic Field Theory

BIPIN R. DESAI

CAMBRIDGE

CAMBRIDGE www.cambridge.org/9780521877602

This page intentionally left blank

Quantum Mechanics with Basic Field Theory

Students and instructors alike will find this organized and detailed approach to quantum mechanics ideal for a two-semester graduate course on the subject.

This textbook covers, step-by-step, important topics in quantum mechanics, from traditional subjects like bound states, perturbation theory and scattering, to more current topics such as coherent states, quantum Hall effect, spontaneous symmetry breaking, superconductivity, and basic quantum electrodynamics with radiative corrections. The large number of diverse topics are covered in concise, highly focused chapters, and are explained in simple but mathematically rigorous ways. Derivations of results and formulas are carried out from beginning to end, without leaving students to complete them.

With over 200 exercises to aid understanding of the subject, this textbook provides a thorough grounding for students planning to enter research in physics. Several exercises are solved in the text, and password-protected solutions for remaining exercises are available to instructors at www.cambridge.org/9780521877602.

Bipin R. Desai is a Professor of Physics at the University of California, Riverside, where he does research in elementary particle theory. He obtained his Ph.D. in Physics from the University of California, Berkeley. He was a visiting Fellow at Clare Hall, Cambridge University, UK, and has held research positions at CERN, Geneva, Switzerland, and CEN Saclay, France. He is a Fellow of the American Physical Society.

Quantum Mechanics with Basic Field Theory

Bipin R. Desai

University of California at Riverside

CAMBRIDGE
UNIVERSITY PRESS

CAMBRIDGE UNIVERSITY PRESS
Cambridge, New York, Melbourne, Madrid, Cape Town, Singapore,
São Paulo, Delhi, Dubai, Tokyo

Cambridge University Press
The Edinburgh Building, Cambridge CB2 8RU, UK

Published in the United States of America by Cambridge University Press, New York

www.cambridge.org
Information on this title: www.cambridge.org/9780521877602

First published in print format 2009

ISBN-13 978-0-511-68761-7 eBook (Adobe Reader)

ISBN-13 978-0-521-87760-2 Hardback

To Ba, Bapuji, and Blaire

Contents

Preface

While writing this book I was reminded at times of what Professor Francis Low used to say when I took his class on undergraduate electromagnetism at the University of Illinois, Urbana-Champaign. "Be sure to understand the subject thoroughly," he said, "otherwise, your only other chance will be when you have to teach it." Knowing now what I know by having written this book, I would add that, if at that point one still does not understand the subject, there will be yet another opportunity when writing a book on it. That was certainly the case with me and this book.

For the last twenty years or so I have taught a one-year graduate course in quantum mechanics at the University of California, Riverside. I have used several books, including the text by Schiff which also happens to be the text I used when I was taking my graduate courses at the University of California, Berkeley (along with my class notes from Professor Eyvind Wichmann who taught the quantum electrodynamics course). However, it became clear to me that I would need to expand the subject matter considerably if I wanted the book not only to be as thorough and up-to-date as possible but also organized so that one subject followed the other in a logical sequence. I hope I have succeeded.

Traditionally, books on graduate quantum mechanics go up to relativity and in some cases even cover the Dirac equation. But relativistic equations lead to the troublesome negative-energy solutions. It would be unsatisfactory then to just stop there and not go to second quantization, to show how the negative-energy states are reinterpreted as positive-energy states of antiparticles. It was, therefore, logical to cover elementary second quantization, which in a sense is many-body quantum mechanics with quantization conditions. And once this topic was addressed it would be unfair not to cover the great successes of many-body systems in condensed matter, in particular, superconductivity and Bose–Einstein condensation. A logical concurrent step was to include also full relativistic quantum field theory, at least basic quantum electrodynamics (QED) and then finish on a triumphant note describing the stunning success of QED in explaining the anomalous magnetic moment and the Lamb shift. With the vast acreage that I wanted to cover, it seemed only appropriate to include as well the modern subject of spontaneous symmetry breaking, which has its applications both in condensed matter physics and in particle physics. This then was the rationale behind this book's content and organization.

I have organized the book with small chapters in what I believe to be a logical order. One can think of the layout of the chapters in terms of the following blocks, each with a common thread, with chapters arranged in an increasing degree of complexity within each block

Chs. 1, 2, 3	Basic Formalism
Chs. 4, 5, 6, 7	Free Particles
Chs. 8, 9, 10, 11, 12	Exactly Solvable Bound State Problems
Chs. 13, 14, 15	Two-Level Problems
Chs. 16, 17, 18	Perturbation Theory
Ch. 24	New approximation methods
Ch. 25	Lagrangian and Feynman integral formalisms
Chs. 19, 20, 21, 22, 23	Scattering Theory
Chs. 26, 27, 28, 29, 30	Symmetry, Rotations, and Angular Momentum
Chs. 31, 32, 33, 34, 35, 36	Relativistic theory with Klein–Gordon, Dirac, and Maxwell's equations
Chs. 37, 38, 39, 40	Second Quantization, Condensed Matter Problems
Chs. 41, 42	Classical Fields and Spontaneous Symmetry Breaking
Chs. 43, 44, 45	Quantum Electrodynamics and Radiative Corrections

In the chapters on scattering theory, one may find an extra coverage in this book on the properties of the S-matrix especially with reference to its analytical properties. This is thanks to my thesis advisor at Berkeley, Professor Geoffrey Chew who emphasized the importance of these properties to his students.

I believe it is feasible to complete the first 32 chapters in one year (two semesters or three quarters). The remaining chapters beginning with the Dirac equation could well be taught in the first semester or first quarter of an advanced quantum mechanics course. Since these topics cover quantum field theory applied to both particle physics and condensed matter physics, it could be taken by students specializing in either subject.

Except at the beginning of each chapter, this book does not have as much narrative or as many long descriptive paragraphs as one normally finds in other textbooks. I have instead spent extra space on deriving and solving the relevant equations. I feel that the extra narrative can always be supplemented by the person teaching the course.

There are an adequate number of problems in this book. They are fairly straightforward. I suppose I still have scars left from the days when I took graduate quantum mechanics from Professor Edward Teller at Berkeley, who gave very inspiring lectures full of interesting and topical episodes while on the blackboard he usually wrote down just the basic formulas. But then he turned around and gave, as homework, a huge number of some of the toughest problems this side of the Atlantic! Those assignments routinely took care of our entire weekends.

I have many people to thank, beginning with Dustin Urbaniec and Omar Moreno who did a good bit of the typing for me, and Barbara Simandl who did all the figures. I am also grateful to a number of graduate students from my Quantum Mechanics course for pointing out errors in my write-up; in particular, I am thankful to Eric Barbagiovanni, for suggesting a number of improvements. I must also thank Dr. Steve Foulkes, a former graduate student at UC Riverside, who read a number of chapters and, following my instructions not to show any mercy in criticizing what he read, did exactly that! I also wish to thank my colleagues who critically read parts of the manuscript: Professors Robert Clare (who also directed me to Cambridge University Press), Leonid Pryadkov, G. Rajasekaran and Utpal Sarkar.

At Cambridge University Press, my special thanks to Simon Mitton, with whom I corresponded in the early years, for his kind support and encouragement; to John Fowler and Lindsay Barnes for their constant help and, more importantly, for their patience with this long project.

There is one individual, Alex Vaucher, whom I must single out, without whose help this book would neither have been started nor completed. After finishing my graduate course on Quantum Mechanics at UC Riverside some years ago, he strongly encouraged me to write this book. He supplied the necessary software and, knowing how computer-ignorant I was, continued to provide me with technical instructions during all phases of this project. Initially the two of us were planning to collaborate on this book but, because of his full time position with the Physics and Astronomy department at the University of California, Los Angeles, he was not able to participate. My deepest gratitude to him.

Physical constants

Planck's constant	$\hbar$	6.581×10^{-16} eV s
Velocity of light in vacuum	c	2.9979×10^{10} cm/s
Fine structure constant	$\alpha = e^2/\hbar c$	$1/137.04$
Rest mass of the electron	mc^2	0.511 MeV
Mass of the proton	Mc^2	938.28 MeV
Bohr radius	$\hbar^2/me^2$	5.2918×10^{-9} cm
Bohr magneton	$e\hbar/2mc$	0.58×10^{-8} eV/gauss
Boltzmann constant	k	8.62×10^{-5} eV/K
1 eV		1.6×10^{-12} erg

1 Basic formalism

We summarize below some of the postulates and definitions basic to our formalism, and present some important results based on these postulates. The formalism is purely mathematical in nature with very little physics input, but it provides the structure within which the physical concepts that will be discussed in the later chapters will be framed.

1.1 State vectors

It is important to realize that the Quantum Theory is a linear theory in which the physical state of a system is described by a vector in a complex, linear vector space. This vector may represent a free particle or a particle bound in an atom or a particle interacting with other particles or with external fields. It is much like a vector in ordinary three-dimensional space, following many of the same rules, except that it describes a very complicated physical system. We will be elaborating further on this in the following.

The mathematical structure of a quantum mechanical system will be presented in terms of the notations developed by Dirac.

A physical state in this notation is described by a "ket" vector, $|\rangle$, designated variously as $|\alpha\rangle$ or $|\psi\rangle$ or a ket with other appropriate symbols depending on the specific problem at hand. The kets can be complex. Their complex conjugates, $|\rangle^*$, are designated by $\langle|$ which are called "bra" vectors. Thus, corresponding to every ket vector there is a bra vector. These vectors are abstract quantities whose physical interpretation is derived through their so-called "representatives" in the coordinate or momentum space or in a space appropriate to the problem under consideration.

The dimensionality of the vector space is left open for the moment. It can be finite, as will be the case when we encounter spin, which has a finite number of components along a preferred direction, or it can be infinite, as is the case of the discrete bound states of the hydrogen atom. Or, the dimensionality could be continuous (indenumerable) infinity, as for a free particle with momentum that takes continuous values. A complex vector space with these properties is called a Hilbert space.

The kets have the same properties as a vector in a linear vector space. Some of the most important of these properties are given below:

(i) $|\alpha\rangle$ and $c\,|\alpha\rangle$, where c is a complex number, describe the same state.
(ii) The bra vector corresponding to $c\,|\alpha\rangle$ will be $c^*\,\langle\alpha|$.

(iii) The kets follow a linear superposition principle

$$a\,|\alpha\rangle + b\,|\beta\rangle = c\,|\gamma\rangle \tag{1.1}$$

where a, b, and c are complex numbers. That is, a linear combination of states in a vector space is also a state in the same space.

(iv) The "scalar product" or "inner product" of two states $|\alpha\rangle$ and $|\beta\rangle$ is defined as

$$\langle\beta|\,\alpha\rangle. \tag{1.2}$$

It is a complex number and not a vector. Its complex conjugate is given by

$$\langle\beta|\,\alpha\rangle^* = \langle\alpha|\,\beta\rangle. \tag{1.3}$$

Hence $\langle\alpha|\,\alpha\rangle$ is a real number.

(v) Two states $|\alpha\rangle$ and $|\beta\rangle$ are orthogonal if

$$\langle\beta|\,\alpha\rangle = 0. \tag{1.4}$$

(vi) It is postulated that $\langle\alpha|\,\alpha\rangle \geq 0$. One calls $\sqrt{\langle\alpha|\,\alpha\rangle}$ the "norm" of the state $|\alpha\rangle$. If a state vector is normalized to unity then

$$\langle\alpha|\,\alpha\rangle = 1. \tag{1.5}$$

If the norm vanishes, then $|\alpha\rangle = 0$, in which case $|\alpha\rangle$ is called a null vector.

(vii) The states $|\alpha_n\rangle$ with $n = 1, 2, \ldots,$ depending on the dimensionality, are called a set of basis kets or basis states if they span the linear vector space. That is, any arbitrary state in this space can be expressed as a linear combination (superposition) of them. The basis states are often taken to be of unit norm and orthogonal, in which case they are called orthonormal states. Hence an arbitrary state $|\phi\rangle$ can be expressed in terms of the basis states $|\alpha_n\rangle$ as

$$|\phi\rangle = \sum_n a_n\,|\alpha_n\rangle \tag{1.6}$$

where, as stated earlier, the values taken by the index n depends on whether the space is finite- or infinite-dimensional or continuous. In the latter case the summation is replaced by an integral. If the $|\alpha_n\rangle$'s are orthonormal then $a_n = \langle\alpha_n\,|\phi\rangle$. It is then postulated that $|a_n|^2$ is the probability that the state $|\phi\rangle$ will be in state $|\alpha_n\rangle$.

(viii) A state vector may depend on time, in which case one writes it as $|\alpha(t)\rangle$, $|\psi(t)\rangle$, etc. In the following, except when necessary, we will suppress the possible dependence on time.

(ix) The product $|\alpha\rangle\,|\beta\rangle$, has no meaning unless it refers to two different vector spaces, e.g., one corresponding to spin, the other to momentum; or, if a state consists of two particles described by $|\alpha\rangle$ and $|\beta\rangle$ respectively.

(x) Since bra vectors are obtained through complex conjugation of the ket vectors, the above properties can be easily carried over to the bra vectors.

1.2 Operators and physical observables

A physical observable, like energy or momentum, is described by a linear operator that has the following properties:

(i) If A is an operator and $|\alpha\rangle$ is a ket vector then

$$A\,|\alpha\rangle = \text{another ket vector.} \tag{1.7}$$

Similarly, for an operator B,

$$\langle\alpha|\,B = \text{another bra vector} \tag{1.8}$$

where B operates to the left

(ii) An operator A is linear if, for example,

$$A\,[\lambda\,|\alpha\rangle + \mu\,|\beta\rangle] = \lambda A\,|\alpha\rangle + \mu A\,|\beta\rangle \tag{1.9}$$

where λ and μ are complex numbers. Typical examples of linear operators are derivatives, matrices, etc. There is one exception to this rule, which we will come across in Chapter 27 which involves the so called time reversal operator where the coefficients on the right-hand side are replaced by their complex conjugates. In this case it is called an antilinear operator.

If an operator acting on a function gives rise to the square of that function, for example, then it is called a nonlinear operator. In this book we will be not be dealing with such operators.

(iii) A is a called a unit operator if, for any $|\alpha\rangle$,

$$A\,|\alpha\rangle = |\alpha\rangle, \tag{1.10}$$

in which case one writes

$$A = \mathbf{1}. \tag{1.11}$$

(iv) A product of two operators is also an operator. In other words, if A and B are operators then AB as well as BA are operators. However, they do not necessarily commute under multiplication, that is,

$$AB \neq BA \tag{1.12}$$

in general. The operators commute under addition, i.e., if A and B are two operators then

$$A + B = B + A. \tag{1.13}$$

They also exhibit associativity, i.e., if A, B, and C are three operators then

$$A + (B + C) = (A + B) + C. \tag{1.14}$$

Similarly $A(BC) = (AB)C$.

(v) B is called an inverse of the operator A if

$$AB = BA = \mathbf{1}, \tag{1.15}$$

in which case one writes

$$B = A^{-1}. \tag{1.16}$$

(vi) The quantity $|\alpha\rangle\langle\beta|$ is called the "outer product" between states $|\alpha\rangle$ and $|\beta\rangle$. By multiplying it with a state $|\gamma\rangle$ one obtains

$$[|\alpha\rangle\langle\beta|]\,\gamma\rangle = [\langle\beta|\,\gamma\rangle]\,|\alpha\rangle \tag{1.17}$$

where on the right-hand side the order of the terms is reversed since $\langle\beta|\,\gamma\rangle$ is a number. The above relation implies that when $|\alpha\rangle\langle\beta|$ multiplies with a state vector it gives another state vector. A similar result holds for the bra vectors:

$$\langle\gamma\,[|\alpha\rangle\langle\beta|] = [\langle\gamma\,|\alpha\rangle]\,\langle\beta|\,. \tag{1.18}$$

Thus $|\alpha\rangle\langle\beta|$ acts as an operator.

(vii) The "expectation" value, $\langle A\rangle$, of an operator A in the state $|\alpha\rangle$ is defined as

$$\langle A\rangle = \langle\alpha|\,A\,|\alpha\rangle\,. \tag{1.19}$$

1.3 Eigenstates

(i) If the operation $A|\alpha\rangle$ gives rise to the same state vector, i.e., if

$$A|\alpha\rangle = (\text{constant}) \times |\alpha\rangle \tag{1.20}$$

then we call $|\alpha\rangle$ an "eigenstate" of the operator A, and the constant is called the "eigenvalue" of A. If $|\alpha\rangle$'s are eigenstates of A with eigenvalues a_n, assumed for convenience to be discrete, then these states are generally designated as $|a_n\rangle$. They satisfy the equation

$$A|a_n\rangle = a_n|a_n\rangle \tag{1.21}$$

with $n = 1, 2, \ldots$ depending on the dimensionality of the system. In this case one may also call A an eigenoperator.

(ii) If $|\alpha_n\rangle$ is an eigenstate of both operators A and B, such that

$$A|\alpha_n\rangle = a_n|\alpha_n\rangle\,, \quad \text{and} \quad B|\alpha_n\rangle = b_n|\alpha_n\rangle \tag{1.22}$$

then we have the results

$$AB\,|\alpha_n\rangle = b_n A\,|\alpha_n\rangle = b_n a_n\,|\alpha_n\rangle\,, \tag{1.23}$$

$$BA\,|\alpha_n\rangle = a_n B\,|\alpha_n\rangle = a_n b_n\,|\alpha_n\rangle\,. \tag{1.24}$$

If the above two relations hold for all values of n then

$$AB = BA. \tag{1.25}$$

Thus under the special conditions just outlined the two operators will commute.

1.4 Hermitian conjugation and Hermitian operators

We now define the "Hermitian conjugate" $A^\dagger$, of an operator A and discuss a particular class of operators called "Hermitian" operators which play a central role in quantum mechanics.

(i) In the same manner as we defined the complex conjugate operation for the state vectors, we define $A^\dagger$ through the following complex conjugation

$$[A\,|\alpha\rangle]^* = \langle\alpha|\,A^\dagger \tag{1.26}$$

and

$$\langle\beta|\,A\,|\alpha\rangle^* = \langle\alpha|\,A^\dagger\,|\beta\rangle\,. \tag{1.27}$$

If on the left-hand side of (1.26), $|\alpha\rangle$ is replaced by $c\,|\alpha\rangle$ where c is a complex constant, then on the right-hand side one must include a factor c^*.

(ii) From (1.26) and (1.27) it follows that if

$$A = |\alpha\rangle\,\langle\beta| \tag{1.28}$$

then

$$A^\dagger = |\beta\rangle\,\langle\alpha|\,. \tag{1.29}$$

At this stage it is important to emphasize that $|\alpha\rangle$, $\langle\beta|\,\alpha\rangle$, $|\alpha\rangle\,\langle\beta|$, and $|\alpha\rangle\,|\beta\rangle$ are four totally different mathematical quantities which should not be mixed up: the first is a state vector, the second is an ordinary number, the third is an operator, and the fourth describes a product of two states.

(iii) The Hermitian conjugate of the product operator AB is found to be

$$(AB)^\dagger = B^\dagger A^\dagger. \tag{1.30}$$

This can be proved by first noting from (1.27) that for an arbitrary state $|\alpha\rangle$

$$[(AB)\,|\alpha\rangle]^* = \langle\alpha|\,(AB)^\dagger\,. \tag{1.31}$$

If we take

$$B\,|\alpha\rangle = |\beta\rangle \tag{1.32}$$

where $|\beta\rangle$ is another state vector, then the left-hand side of (1.31) can be written as

$$[(AB)\,|\alpha\rangle]^* = [A\,|\beta\rangle]^* . \tag{1.33}$$

From the definition given in (1.26) we obtain

$$[A\,|\beta\rangle]^* = \langle\beta|\,A^\dagger = \Big[\langle\alpha|\,B^\dagger\Big]A^\dagger = \langle\alpha|\,B^\dagger A^\dagger \tag{1.34}$$

where we have used the fact that $\langle\beta| = [B\,|\alpha\rangle]^* = \langle\alpha|\,B^\dagger$. Since $|\alpha\rangle$ is an arbitrary vector, comparing (1.31) and (1.34), we obtain (1.30).

(iv) Finally, if

$$A = A^\dagger \tag{1.35}$$

then the operator A is called "Hermitian."

1.5 Hermitian operators: their eigenstates and eigenvalues

Hermitian operators play a central role in quantum mechanics. We show below that the eigenstates of Hermitian operators are orthogonal and have real eigenvalues.

Consider the eigenstates $|a_n\rangle$ of an operator A,

$$A\,|a_n\rangle = a_n\,|a_n\rangle \tag{1.36}$$

where $|a_n\rangle$'s have a unit norm. By multiplying both sides of (1.36) by $\langle a_n|$ we obtain

$$a_n = \langle a_n|\,A\,|a_n\rangle . \tag{1.37}$$

Taking the complex conjugate of both sides we find

$$a_n^* = \langle a_n|\,A\,|a_n\rangle^* = \langle a_n|\,A^\dagger\,|a_n\rangle = \langle a_n|\,A\,|a_n\rangle . \tag{1.38}$$

The last equality follows from the fact that A is Hermitian ($A^\dagger = A$). Equating (1.37) and (1.38) we conclude that $a_n^* = a_n$. Therefore, the eigenvalues of a Hermitian operator must be real.

An important postulate based on this result says that since physically observable quantities are expected to be real, the operators representing these observables must be Hermitian.

We now show that the eigenstates are orthogonal. We consider two eigenstates $|a_n\rangle$ and $|a_m\rangle$ of A,

$$A\,|a_n\rangle = a_n\,|a_n\rangle\,, \tag{1.39}$$

$$A\,|a_m\rangle = a_m\,|a_m\rangle\,. \tag{1.40}$$

Taking the complex conjugate of the second equation we have

$$\langle a_m|\,A = a_m\,\langle a_m| \tag{1.41}$$

where we have used the Hermitian property of A, and the fact that the eigenvalue a_m is real. Multiplying (1.39) on the left by $\langle a_m|$ and (1.41) on the right by $|a_n\rangle$ and subtracting, we obtain

$$(a_m - a_n)\,\langle a_m|\,a_n\rangle = 0. \tag{1.42}$$

Thus, if the eigenvalues α_m and α_n are different we have

$$\langle a_m|\,a_n\rangle = 0, \tag{1.43}$$

which shows that the two eigenstates are orthogonal. Using the fact that the ket vectors are normalized, we can write the general orthonormality relation between them as

$$\langle a_m|\,a_n\rangle = \delta_{mn} \tag{1.44}$$

where δ_{mn} is called the Kronecker delta, which has the property

$$\begin{aligned} \delta_{mn} &= 1 \ \text{ for } \ m = n \\ &= 0 \ \text{ for } \ m \neq n. \end{aligned} \tag{1.45}$$

For those cases where there is a degeneracy in the eigenvalues, i.e., if two different states have the same eigenvalue, the treatment is slightly different and will be deferred until later chapters.

We note that the operators need not be Hermitian in order to have eigenvalues. However, in these cases none of the above results will hold. For example, the eigenvalues will not necessarily be real. Unless otherwise stated, we will assume the eigenvalues to be real.

1.6 Superposition principle

A basic theorem in quantum mechanics based on linear vector algebra is that an arbitrary vector in a given vector space can be expressed as a linear combination – a superposition – of a complete set of eigenstates of any operator in that space. A complete set is defined to

be the set of all possible eigenstates of an operator. Expressing this result for an arbitrary state vector $|\phi\rangle$ in terms of the eigenstates $|a_n\rangle$ of the operator A, we have

$$|\phi\rangle = \sum_n c_n |a_n\rangle \tag{1.46}$$

where the summation index n goes over all the eigenstates with $n = 1, 2, \ldots$. If we multiply (1.46) by $\langle a_m|$ then the orthonormality relation (1.44) between the $|a_n\rangle$'s yields

$$c_m = \langle a_m | \phi\rangle. \tag{1.47}$$

It is then postulated that $|c_m|^2$ is the probability that $|\phi\rangle$ contains $|a_m\rangle$. That is, $|c_m|^2$ is the probability that $|\phi\rangle$ has the eigenvalue a_m. If $|\phi\rangle$ is normalized to unity, $\langle\phi|\,\phi\rangle = 1$, then

$$\sum_n |c_n|^2 = 1. \tag{1.48}$$

That is, the probability of finding $|\phi\rangle$ in state $|a_n\rangle$, summed over all possible values of n, is one.

Since (1.46) is true for any arbitrary state we can express another state $|\psi\rangle$ as

$$|\psi\rangle = \sum_n c'_n |a_n\rangle\,. \tag{1.49}$$

The scalar product $\langle\psi\,|\phi\rangle$ can then be written, using the orthonormality property of the eigenstates, as

$$\langle\psi\,|\phi\rangle = \sum_m c'^{*}_m c_m \tag{1.50}$$

with $c'_m = \langle a_m|\,\psi\rangle$ and $c_m = \langle a_m|\,\phi\rangle$.

The above relations express the fact that the state vectors can be expanded in terms of the eigenstates of an operator A. The eigenstates $|a_n\rangle$ are then natural candidates to form a set of basis states.

1.7 Completeness relation

We consider now the operators $|a_n\rangle\,\langle a_n|$, where the $|a_n\rangle$'s are the eigenstates of an operator A, with eigenvalues a_n. A very important result in quantum mechanics involving the sum of the operators $|a_n\rangle\,\langle a_n|$ over the possibly infinite number of eigenvalues states that

$$\sum_n |a_n\rangle\,\langle a_n| = \mathbf{1} \tag{1.51}$$

where the $\mathbf{1}$ on the right-hand side is a unit operator. This is the so called "completeness relation".

To prove this relation we first multiply the sum on the left hand of the above equality by an arbitrary eigenvector $|a_m\rangle$ to obtain

$$\left[\sum_n |a_n\rangle \langle a_n|\right] |a_m\rangle = \sum_n |a_n\rangle \langle a_n| a_m\rangle = \sum_n |a_n\rangle \delta_{nm} = |a_m\rangle \tag{1.52}$$

where we have used the orthonormality of the eigenvectors. Since this relation holds for any arbitrary state $|a_m\rangle$, the operator in the square bracket on the left-hand side acts as a unit operator, thus reproducing the completeness relation.

If we designate

$$P_n = |a_n\rangle \langle a_n| \tag{1.53}$$

then

$$P_n |a_m\rangle = \delta_{nm} |a_m\rangle . \tag{1.54}$$

Thus P_n projects out the state $|a_n\rangle$ whenever it operates on an arbitrary state. For this reason P_n is called the projection operator, in terms of which one can write the completeness relation as

$$\sum_n P_n = \mathbf{1}. \tag{1.55}$$

One can utilize the completeness relation to simplify the scalar product $\langle \psi | \phi \rangle$, where $|\phi\rangle$ and $|\psi\rangle$ are given above, if we write, using (1.51)

$$\langle \psi | \phi \rangle = \langle \psi | \mathbf{1} | \phi \rangle = \langle \psi | \left[\sum_n |a_n\rangle \langle a_n|\right] |\phi\rangle = \sum_n \langle \psi | a_n\rangle \langle a_n | \phi\rangle = \sum_n c_n'^* c_n. \tag{1.56}$$

This is the same result as the one we derived previously as (1.50).

1.8 Unitary operators

If two state vectors $|\alpha\rangle$ and $|\alpha'\rangle$ have the same norm then

$$\langle \alpha | \alpha \rangle = \langle \alpha' | \alpha' \rangle. \tag{1.57}$$

Expressing each of these states in terms of a complete set of eigenstates $|a_n\rangle$ we obtain

$$|\alpha\rangle = \sum_n c_n |a_n\rangle \quad \text{and} \quad |\alpha'\rangle = \sum_n c_n' |a_n\rangle . \tag{1.58}$$

The equality in (1.57) leads to the relation

$$\sum_n |c_n|^2 = \sum_n |c_n'|^2 , \tag{1.59}$$

which signifies that, even though c_n may be different from c'_n, the total sum of the probabilities remains the same.

Consider now an operator A such that

$$A\,|\alpha\rangle = \left|\alpha'\right\rangle. \tag{1.60}$$

If $|\alpha\rangle$ and $\left|\alpha'\right\rangle$ have the same norm, then

$$\langle\alpha\,|\,\alpha\rangle = \left\langle\alpha'\right|\,\alpha'\rangle = \langle\alpha|\,A^{\dagger}A\,|\alpha\rangle\,. \tag{1.61}$$

This implies that

$$A^{\dagger}A = \mathbf{1}. \tag{1.62}$$

The operator A is then said to be "unitary." From relation (1.60) it is clear that A can change the basis from one set to another. Unitary operators play a fundamental role in quantum mechanics.

1.9 Unitary operators as transformation operators

Let us define the following operator in term of the eigenstates $|a_n\rangle$ of operator A and eigenstates $|b_n\rangle$ of operator B,

$$U = \sum_n |b_n\rangle\,\langle a_n|\,. \tag{1.63}$$

This is a classic example of a unitary operator as we show below. We first obtain the Hermitian conjugate of U,

$$U^{\dagger} = \sum_n |a_n\rangle\,\langle b_n|\,. \tag{1.64}$$

Therefore,

$$UU^{\dagger} = \left[\sum_n |b_n\rangle\,\langle a_n|\right]\sum_m |a_m\rangle\,\langle b_m| = \sum\sum |b_n\rangle\,\langle a_n|\,a_m\rangle\,\langle b_m| = \sum |b_n\rangle\,\langle b_n| = \mathbf{1} \tag{1.65}$$

where we have used the orthonormality relation $\langle a_n|\,a_m\rangle = \delta_{nm}$ and the completeness relation for the state vectors $|b_n\rangle$ discussed in the previous section. Hence U is unitary.

We note in passing that

$$\sum_n |a_n\rangle\,\langle a_n| \tag{1.66}$$

is a unit operator which is a special case of a unitary operator when $\langle b_n| = \langle a_n|$.

We also note that

$$U\,|a_m\rangle = \sum_n |b_n\rangle\,\langle a_n|\,a_m\rangle = \sum_n |b_n\rangle\,\delta_{nm} = |b_m\rangle\,. \tag{1.67}$$

Hence U transforms the eigenstate $|a_m\rangle$ into $|b_m\rangle$. In other words, if we use $|a_n\rangle$'s as the basis for the expansion of a state vector then U will convert this basis set to a new basis formed by the $|b_n\rangle$'s. Thus U allows one to transform from the "old basis" given by $|a_n\rangle$'s to the "new basis" given by the $|b_n\rangle$'s. One can do the conversion in the reverse order by multiplying both sides of (1.67) by $U^\dagger$ on the left:

$$U^\dagger U\,|a_m\rangle = U^\dagger\,|b_m\rangle\,. \tag{1.68}$$

Hence, from the unitary property of U, we find

$$U^\dagger\,|b_m\rangle = |a_m\rangle\,. \tag{1.69}$$

Furthermore, the matrix element of an operator, A, in the old basis set can be related to its matrix elements in the new basis as follows

$$\langle b_n|\,A\,|b_m\rangle = \langle b_n|\,UU^\dagger AUU^\dagger\,|b_m\rangle = \langle a_n|\,U^\dagger AU\,|a_m\rangle \tag{1.70}$$

where we have used the property $U^\dagger U = \mathbf{1}$ and the relations (1.69). This relation will be true for all possible values of $|a_n\rangle$'s and $|b_n\rangle$'s. Therefore, it can be expressed as an operator relation in terms of the "transformed" operator A^T. We then write

$$A^T = U^\dagger AU. \tag{1.71}$$

Finally, if $|a_n\rangle$'s are the eigenstates of the operator A,

$$A\,|a_n\rangle = a_n\,|a_n\rangle \tag{1.72}$$

and relation (1.67) connecting $|a_n\rangle$ and $|b_n\rangle$ holds, where $|b_n\rangle$'s are the eigenstates of an operator B, then we can multiply (1.72) by U on both sides to obtain

$$UA\,|a_n\rangle = a_n U\,|a_n\rangle \tag{1.73}$$

and write

$$UAU^\dagger\,[U\,|a_n\rangle] = a_n\,[U\,|a_n\rangle]\,. \tag{1.74}$$

Hence

$$UAU^\dagger\,|b_n\rangle = a_n\,|b_n\rangle\,. \tag{1.75}$$

Thus $|b_n\rangle$ is the eigenstate of $UAU^\dagger$ with the same eigenvalues as the eigenvalues of A. However, since $|b_n\rangle$'s are eigenstates of the operator B we find that $UAU^\dagger$ and B are in some sense equivalent.

1.10 Matrix formalism

We define the "matrix element" of an operator A between states $|\alpha\rangle$ and $|\beta\rangle$ as

$$\langle\beta\,|A|\,\alpha\rangle\,, \tag{1.76}$$

which is a complex number. To understand the meaning of this matrix element we note that when A operates on $|\alpha\rangle$ it gives another ket vector. This state when multiplied on the left by $\langle\beta|$ gives a number. When there are many such $|\alpha\rangle$'s and $\langle\beta|$'s then we have a whole array of numbers that can be put into the form of a matrix. Specifically, the matrix formed by the matrix elements of A between the basis states $|b_n\rangle$, with $n = 1, 2, \ldots, N$ depending on the dimensionality of the space, is then a square matrix $\langle b_m\,|A|\,b_n\rangle$ written as follows:

$$\{A\} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & . & A_{1N} \\ A_{21} & A_{22} & A_{23} & . & . \\ A_{31} & A_{32} & A_{33} & . & . \\ . & . & . & . & . \\ A_{N1} & . & . & . & A_{NN} \end{bmatrix} \tag{1.77}$$

where

$$A_{mn} = \langle b_m\,|A|\,b_n\rangle\,. \tag{1.78}$$

The matrix (1.77) is then called the matrix representation of A in terms of the states $|b_n\rangle$. It gives, in a sense, a profile of the operator A and describes what is an abstract object in terms of a matrix of complex numbers. The matrix representation will look different if basis sets formed by eigenstates of some other operator are used.

The matrices follow the normal rules of matrix algebra. Some of the important properties are given below, particularly as they relate to the Hermitian and unitary operators.

(i) The relation between the matrix elements of $A^\dagger$ and A is given by

$$\langle\alpha|\,A^\dagger\,|\beta\rangle = \langle\beta|\,A\,|\alpha\rangle^*\,. \tag{1.79}$$

Thus the matrix representation of $A^\dagger$ can be written as

$$\{A^\dagger\} = \begin{bmatrix} A_{11}^* & A_{21}^* & A_{31}^* & . & A_{N1}^* \\ A_{12}^* & A_{22}^* & A_{23}^* & . & . \\ A_{13}^* & A_{23}^* & A_{33}^* & . & . \\ . & . & . & . & . \\ A_{1N}^* & . & . & . & A_{NN}^* \end{bmatrix} \tag{1.80}$$

where A is represented by the matrix (1.77).

(ii) If the operator A is Hermitian then

$$\langle\beta|\,A\,|\alpha\rangle = \langle\beta|\,A^\dagger\,|\alpha\rangle\,. \tag{1.81}$$

Using the property (1.79) we find

$$\langle\beta|\,A\,|\alpha\rangle = \langle\alpha|\,A\,|\beta\rangle^* . \tag{1.82}$$

In particular, the matrix elements with respect to the eigenstates $|b_n\rangle$ satisfy

$$\langle b_m\,|A|\,b_n\rangle = \langle b_n\,|A|\,b_m\rangle^* . \tag{1.83}$$

A Hermitian operator will, therefore, have the following matrix representation:

$$\{A\} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & . & A_{1N} \\ A_{12}^* & A_{22} & A_{23} & . & . \\ A_{13}^* & A_{23}^* & A_{33} & . & . \\ . & . & . & . & . \\ A_{1N}^* & . & . & . & A_{NN} \end{bmatrix} . \tag{1.84}$$

We note that the same result is obtained by equating the matrices A and $A^\dagger$ given by (1.77) and (1.80) respectively. We also note that the diagonal elements $A_{11}, A_{22}, \ldots$ of a Hermitian operator are real since the matrix elements satisfy the relation $A_{mn}^* = A_{nm}$.

(iii) The matrix representation of an operator A in terms of its eigenstates is a diagonal matrix because of the orthonormality property (1.44). It can, therefore, be written as

$$\{A\} = \begin{bmatrix} A_{11} & 0 & 0 & . & 0 \\ 0 & A_{22} & 0 & . & . \\ 0 & 0 & A_{33} & . & . \\ . & . & . & . & . \\ 0 & . & . & . & A_{NN} \end{bmatrix} \tag{1.85}$$

where $A_{mm} = a_m$ where a_m's are the eigenvalues of A. The matrix representation of A in terms of eigenstates $|b_n\rangle$ of an operator B that is different from A and that does not share the same eigenstates is then written as

$$\{A\} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & . & A_{1N} \\ A_{21} & A_{22} & A_{23} & . & . \\ A_{31} & A_{32} & A_{33} & . & . \\ . & . & . & . & . \\ A_{N1} & . & . & . & A_{NN} \end{bmatrix} \tag{1.86}$$

where $A_{mn} = \langle b_m\,|A|\,b_n\rangle$. If the operator B has the same eigenstates as A then the above matrix will, once again, be diagonal.

(iv) We now illustrate the usefulness of the completeness relation by considering several operator relations. First let us consider the matrix representation of the product of two operators $\{AB\}$ by writing

$$\langle b_m\,|AB|\,b_n\rangle = \langle b_m\,|A\mathbf{1}B|\,b_n\rangle = \sum_p \langle b_m\,\big|A\left[|b_p\rangle\langle b_p|\right]B\big|\,b_n\rangle . \tag{1.87}$$

In the second equality we have inserted a unit operator between the operators A and B and then replaced it by the sum of the complete set of states. Hence the matrix representation of AB is simply the product of two matrices:

$$\{AB\} = \begin{bmatrix} A_{11} & A_{12} & . & . & A_{1N} \\ A_{21} & A_{22} & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ A_{N1} & . & . & . & A_{NN} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} & . & . & B_{1N} \\ B_{21} & B_{22} & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ B_{N1} & . & . & . & B_{NN} \end{bmatrix}. \tag{1.88}$$

Next we consider the operator relation

$$A\,|\alpha\rangle = |\beta\rangle\,. \tag{1.89}$$

It can be written as a matrix relation if we multiply both sides of the equation by the eigenstates $\langle b_m|$ of an operator B and then insert a complete set of states $\left|b_p\right\rangle$ with $p = 1, 2, \ldots$:

$$\langle b_m|\,A\left[\sum_p \left|b_p\right\rangle\langle b_p\right]|\alpha\rangle = \sum_p \langle b_m|\,A\left|b_p\right\rangle\langle b_p\,|\alpha\rangle = \langle b_m\,|\beta\rangle\,. \tag{1.90}$$

This is a matrix equation in which A is represented by the matrix in (1.86), and $|\alpha\rangle$ and $|\beta\rangle$ are represented by the column matrices

$$\begin{bmatrix} \langle b_1\,|\alpha\rangle \\ \langle b_2\,|\alpha\rangle \\ . \\ \langle b_N\,|\alpha\rangle \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} \langle b_1\,|\beta\rangle \\ \langle b_2\,|\beta\rangle \\ . \\ \langle b_N\,|\beta\rangle \end{bmatrix} \tag{1.91}$$

respectively, and hence the above relation can be written in terms of matrices as

$$\begin{bmatrix} A_{11} & A_{12} & . & . & A_{1N} \\ A_{21} & A_{22} & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ A_{N1} & . & . & . & A_{NN} \end{bmatrix} \begin{pmatrix} \langle b_1\,|\alpha\rangle \\ \langle b_2\,|\alpha\rangle \\ . \\ . \\ \langle b_N\,|\alpha\rangle \end{pmatrix} = \begin{pmatrix} \langle b_1\,|\beta\rangle \\ \langle b_2\,|\beta\rangle \\ . \\ . \\ \langle b_N\,|\beta\rangle \end{pmatrix}. \tag{1.92}$$

We can now follow the rules of matrix multiplications and write down N simultaneous equations.

(v) A matrix element such as $\langle\psi\,|\,A\,|\phi\rangle$ can itself be expressed in terms of a matrix relation by using the completeness relation

$$\begin{aligned} \langle\psi\,|\,A\,|\phi\rangle &= \langle\psi|\left[\sum_m |b_m\rangle\langle b_m|\right] A \left[\sum_n |b_n\rangle\langle b_n|\right]|\phi\rangle \\ &= \sum_m\sum_n \langle\psi\,|b_m\rangle\langle b_m|\,A\,|b_n\rangle\langle b_n|\,\phi\rangle. \end{aligned} \tag{1.93}$$

The right-hand side in the matrix form is then

$$\begin{pmatrix} \langle\psi|b_1\rangle & \langle\psi|b_2\rangle & \dots & \langle\psi|b_N\rangle \end{pmatrix} \begin{bmatrix} A_{11} & A_{12} & . & . & A_{1N} \\ A_{21} & A_{22} & . & . & . \\ . & . & A_{33} & . & . \\ . & . & . & . & . \\ A_{N1} & . & . & . & A_{NN} \end{bmatrix} \begin{pmatrix} \langle b_1|\phi\rangle \\ \langle b_2|\phi\rangle \\ . \\ . \\ \langle b_N|\phi\rangle \end{pmatrix}, \tag{1.94}$$

which after a long multiplication reduces to a single number which is, of course, the single matrix element $\langle\psi|A|\phi\rangle$.

Often it is more convenient to write the above product by utilizing the relation $\langle\psi|b_m\rangle = \langle b_m|\psi\rangle^*$,

$$\begin{pmatrix} \langle b_1|\psi\rangle^* & \langle b_2|\psi\rangle^* & \dots & \langle b_N|\psi\rangle^* \end{pmatrix} \begin{bmatrix} A_{11} & A_{12} & A_{13} & . & A_{1N} \\ A_{21} & A_{22} & A_{23} & . & . \\ A_{31} & A_{32} & A_{33} & . & . \\ . & . & . & . & . \\ A_{N1} & . & . & . & A_{NN} \end{bmatrix} \begin{pmatrix} \langle b_1|\phi\rangle \\ \langle b_2|\phi\rangle \\ . \\ . \\ \langle b_N|\phi\rangle \end{pmatrix}. \tag{1.95}$$

(vi) The trace of a matrix A is defined as a sum of its diagonal elements,

$$\mathrm{Tr}(A) = \sum_n \langle a_n|A|a_n\rangle = \sum_n A_{nn}, \tag{1.96}$$

where $|a_n\rangle$'s form an orthonormal basis set. An important property of a trace is

$$\mathrm{Tr}(AB) = \mathrm{Tr}(BA) \tag{1.97}$$

This can be proved by noting that

$$\mathrm{Tr}(AB) = \sum_n \langle a_n|AB|a_n\rangle = \sum_n\sum_m \langle a_n|A|a_m\rangle\langle a_m|B|a_n\rangle \tag{1.98}$$

where we have used the completeness relation for the basis sets $|a_m\rangle$. Since the matrix elements are numbers and no longer operators, they can be switched. Hence using completeness for the $|a_m\rangle$'s we have

$$\mathrm{Tr}(AB) = \sum_m\sum_n \langle a_m|B|a_n\rangle\langle a_n|A|a_m\rangle = \sum_m \langle a_m|BA|a_m\rangle = \mathrm{Tr}(BA), \tag{1.99}$$

which is the desired result. This leads to the generalization involving a product of an arbitrary number of operators that

$$\mathrm{Tr}(ABC\dots) = \text{ invariant} \tag{1.100}$$

under a cyclic permutation of the product $ABC\dots$.

1.11 Eigenstates and diagonalization of matrices

Consider the case where we know the matrix elements of A with respect to the basis given by $|a_n\rangle$. That is, we know $\langle a_m| A |a_n\rangle$ where $|a_n\rangle$'s are not necessarily the eigenstates of A. We call $|a_n\rangle$'s the old basis. We now wish to obtain the eigenstates and eigenvalues of A. Let $|b_n\rangle$'s be the eigenstates of A, we will call them the new basis, which satisfy

$$A |b_n\rangle = b_n |b_n\rangle . \tag{1.101}$$

We proceed in a manner very similar to the previous problem. We multiply both sides of (1.101) by $\langle a_m|$ and insert a complete set of states $\left|a_p\right\rangle$,

$$\sum_p \langle a_m| A \left|a_p\right\rangle \left\langle a_p\right| b_n\rangle = b_n \langle a_m| b_n\rangle. \tag{1.102}$$

The above relation can be written as a matrix relation by taking $m = 1, 2, \ldots, N$ for a fixed value of n

$$\begin{bmatrix} A_{11} & A_{12} & . & . & A_{1N} \\ A_{21} & A_{22} & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ A_{N1} & . & . & . & A_{NN} \end{bmatrix} \begin{pmatrix} \langle a_1 |b_n\rangle \\ \langle a_2 |b_n\rangle \\ . \\ . \\ \langle a_N |b_n\rangle \end{pmatrix} = b_n \begin{pmatrix} \langle a_1 |b_n\rangle \\ \langle a_2 |b_n\rangle \\ . \\ . \\ \langle a_N |b_n\rangle \end{pmatrix} \tag{1.103}$$

where, as stated earlier, the matrix elements $A_{mp} = \langle a_m| A \left|a_p\right\rangle$ are known. The relation (1.103) can be written as

$$\begin{bmatrix} A_{11} - b_n & A_{12} & . & . & A_{1N} \\ A_{21} & A_{22} - b_n & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ A_{N1} & . & . & . & A_{NN} - b_n \end{bmatrix} \begin{pmatrix} \langle a_1 |b_n\rangle \\ \langle a_2 |b_n\rangle \\ . \\ . \\ \langle a_N |b_n\rangle \end{pmatrix} = 0, \tag{1.104}$$

which is valid for each value of n. Thus, effectively, the above relation corresponds to "diagonalization" of the matrix formed by the A_{mn}.

A solution of equation (1.104) is possible only if the determinant of the $N \times N$ matrix vanishes for each value of n. Hence the eigenvalues b_n are the roots of the determinant equation

$$\det [A - \lambda I] = 0 \tag{1.105}$$

where I is a unit matrix. The different values of λ correspond to the different eigenvalues b_n. The corresponding elements $\langle a_m | b_n \rangle$ can then be determined by solving N simultaneous equations in (1.104).

1.11.1 Diagonalization through unitary operators

Let us bring in the unitary operators, which will shed further light on determining eigenstates and eigenvalues of A. Let U be the unitary operator that transforms the old basis to the new basis,

$$|b_n\rangle = U\,|a_n\rangle\,. \tag{1.106}$$

This transformation preserves the norms of the two basis sets since U is unitary. Equation (1.101) can be expressed as

$$AU\,|a_n\rangle = b_n U\,|a_n\rangle\,. \tag{1.107}$$

We now multiply both sides on the left by $U^\dagger$; then

$$U^\dagger AU\,|a_n\rangle = b_n U^\dagger\,U\,|a_n\rangle = b_n\,|a_n\rangle \tag{1.108}$$

where we have used the unitary property $U^\dagger\,U = \mathbf{1}$. Once again we multiply on the left, this time by $\langle a_m|$. We find

$$\langle a_m|\,U^\dagger AU\,|a_n\rangle = b_n \langle a_m\,|a_n\rangle = b_n \delta_{mn}. \tag{1.109}$$

The right-hand side corresponds to a diagonal matrix. Thus the operator U must be such that $U^\dagger AU$ is a diagonal matrix and we write

$$A_D = U^\dagger AU. \tag{1.110}$$

Once we find U then we can immediately obtain the eigenstates $|b_n\rangle$ from (1.106) and eigenvalues b_n from (1.109).

Taking the trace of both sides of (1.10) we obtain

$$\mathrm{Tr}(A_D) = \mathrm{Tr}(U^\dagger AU). \tag{1.111}$$

Since A_D is a diagonal operator with matrix elements given by the eigenvalues of A, the trace on the left of the above equation is simply the sum of the eigenvalues. For the right-hand side we note, using the invariance of a trace under cyclic permutation, that

$$\mathrm{Tr}(U^\dagger AU) = \mathrm{Tr}(AUU^\dagger) = \mathrm{Tr}(A). \tag{1.112}$$

Thus

$$\mathrm{Tr}(A) = \text{sum of the eigenvalues of the operator } A. \tag{1.113}$$

This result holds even though A itself is not diagonal in the basis set $|a_n\rangle$.

In a two-channel system, i.e., in a system that consists of only two eigenstates, U is relatively easy to express. One writes

$$U = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}, \tag{1.114}$$

which is manifestly unitary. One then imposes the condition

$$U^\dagger A U = \text{diagonal matrix}. \tag{1.115}$$

This is accomplished by taking the off-diagonal elements to be zero. From this relation one can determine the angle θ and, therefore, the matrix U. The diagonal elements of the matrix (1.116) give the eigenvalues, while the eigenstates $|b_n\rangle$ are obtained in terms of U and $|a_n\rangle$ through (1.107). We will return to this formalism in Chapter 13 when we focus on two-channel phenomena.

1.12 Density operator

The expectation value $\langle \alpha | A | \alpha \rangle$, taken with respect to a state $|\alpha\rangle$, of an operator A was defined earlier. It was defined with respect to a single state, often referred to as a pure quantum state. Instead of a pure quantum state one may, however, have a collection of states, called an ensemble of states. If each state in this ensemble is described by the same ket $|\alpha\rangle$ then one refers to it as a pure ensemble.

When all the states in an ensemble are not the same then it is called a mixed ensemble. If one is considering a mixed ensemble where w_α describes the probability that a state $|\alpha\rangle$ is present in the ensemble, w_β describes the probability that a state $|\beta\rangle$ is present, and so on, then, instead of the expectation value, $\langle \alpha | A | \alpha \rangle$, the relevant quantity is the ensemble average, which is defined as

$$\langle A \rangle_{av} = \sum_\alpha w_\alpha \langle \alpha | A | \alpha \rangle \tag{1.116}$$

where the sum runs over all the states in the ensemble. Naturally, if $w_\alpha = 1$, with all other w_i's zero, then only the state $|\alpha\rangle$ contributes in the sum, in which case we have a pure ensemble and the ensemble average is then the same as the expectation value. We note that a mixed ensemble is also referred to as a statistical mixture.

Below we outline some important properties of $\langle \alpha | A | \alpha \rangle$ and $\langle A \rangle_{av}$.

Inserting a complete set of states $|b_n\rangle$ with $n = 1, 2, \ldots$ in the expression for the expectation value $\langle \alpha\, |A|\, \alpha \rangle$ we can write

$$\langle \alpha\, |A|\, \alpha \rangle = \sum_n \sum_m \langle \alpha | b_n \rangle \, \langle b_n\, |A|\, b_m \rangle \, \langle b_m | \alpha \rangle \tag{1.117}$$

$$= \sum_n \sum_m \langle b_n\, |A|\, b_m \rangle \, \langle b_m | \alpha \rangle \, \langle \alpha | b_n \rangle \tag{1.118}$$

where we have made an interchange of some of the matrix elements, which is allowed because they are numbers and no longer operators. We now introduce a "projection operator" defined by

$$P_\alpha = |\alpha\rangle\langle\alpha|. \tag{1.119}$$

It has the property

$$P_\alpha |\beta\rangle = |\alpha\rangle\langle\alpha|\beta\rangle = \delta_{\alpha\beta}|\alpha\rangle \tag{1.120}$$

where we have taken the states $|\alpha\rangle$, $|\beta\rangle \ldots$ as orthonormal. Thus P_α projects out the state $|\alpha\rangle$ when operating on any state. Furthermore,

$$P_\alpha^2 = |\alpha\rangle \, \langle\alpha|\alpha\rangle \, \langle\alpha| = |\alpha\rangle\langle\alpha| = P_\alpha, \tag{1.121}$$

$$P_\alpha^\dagger = (\langle\alpha|) \, (|\alpha\rangle) = |\alpha\rangle\langle\alpha| = P_\alpha. \tag{1.122}$$

The completeness theorem gives

$$\sum_\alpha P_\alpha = \sum_\alpha |\alpha\rangle\langle\alpha| = \mathbf{1}. \tag{1.123}$$

From (1.119) and (1.120) we can write $\langle \alpha\, |A|\, \alpha \rangle$ in terms of P_α by noting that

$$\langle b_m | \alpha \rangle \, \langle \alpha | b_n \rangle = \langle b_m\, |P_\alpha|\, b_n \rangle \tag{1.124}$$

where $|b_n\rangle$'s are eigenstates of an operator. Therefore,

$$\langle \alpha\, |A|\, \alpha \rangle = \sum_n \sum_m \langle b_n\, |A|\, b_m \rangle \, \langle b_m\, |P_\alpha|\, b_n \rangle \tag{1.125}$$

$$= \sum_n \langle b_n |\, AP_\alpha \, | b_n \rangle \tag{1.126}$$

where we have used the completeness relation $\sum_m |b_m\rangle\langle b_m| = \mathbf{1}$ for the eigenstates $|b_m\rangle$. Thus,

$$\langle \alpha\, |A|\, \alpha \rangle = \mathrm{Tr}\, (AP_\alpha) \tag{1.127}$$

where "Tr" indicates trace. If we take

$$A = \mathbf{1} \tag{1.128}$$

then

$$\mathrm{Tr}\,(P_\alpha) = 1. \tag{1.129}$$

We consider now a mixed ensemble that contains the states $|\alpha\rangle, |\beta\rangle, \ldots$ etc. with probabilities $w_\alpha, w_\beta \ldots$, respectively. We define a density operator ρ as

$$\rho = \sum_\alpha w_\alpha P_\alpha = \sum_\alpha w_\alpha |\alpha\rangle\langle\alpha|. \tag{1.130}$$

Since w_α, being the probability, is real and P_α is Hermitian, ρ is, therefore, Hermitian,

$$\rho^\dagger = \rho. \tag{1.131}$$

From (1.117) and (1.128) the ensemble average is

$$\langle A\rangle_{av} = \sum_\alpha w_\alpha \mathrm{Tr}\,(AP_\alpha)\,. \tag{1.132}$$

We note that since w_α is a number and not a matrix, and, at the same time, since the operator A is independent of α, and thus does not participate in the summation over α, we can reshuffle the terms in (1.133) to obtain

$$\langle A\rangle_{av} = \mathrm{Tr}\left(A\sum_\alpha w_\alpha P_\alpha\right) = \mathrm{Tr}\,(A\rho) = \mathrm{Tr}\,(\rho A)\,. \tag{1.133}$$

The last equality follows from the property that the trace of a product of two matrices is invariant under interchange of the matrices.

From (1.117) we find, by taking $A = \mathbf{1}$, that

$$\langle \mathbf{1}\rangle_{av} = \sum_\alpha \omega_\alpha \langle\alpha\,|\mathbf{1}|\,\alpha\rangle = \sum_\alpha \omega_\alpha = \mathbf{1}. \tag{1.134}$$

Therefore, from (1.134), we get

$$\langle \mathbf{1}\rangle_{av} = \mathrm{Tr}\,(\rho)\,. \tag{1.135}$$

Finally, (1.135) and (1.136) imply

$$\mathrm{Tr}\,(\rho) = 1. \tag{1.136}$$

We will discuss the properties of ρ in Chapter 14 for the specific case of the spin ½ particles, and again in the chapter on two-level problems.

1.13 Measurement

When a measurement of a dynamical variable is made on a system and a specific, real, value for a physical observable is found, then that value is an eigenvalue of the operator

representing the observable. In other words, irrespective of the state, the act of measurement itself kicks the state into an eigenstate of the operator in question.

From the superposition principle, the state of a system, say $|\phi\rangle$, can always be expressed as a superposition of basis states, which we take to be normalized kets. One can choose these states to be the eigenstates of the operator, e.g., $|a_n\rangle$. Thus one can write the superposition as

$$|\phi\rangle = \sum_n c_n |a_n\rangle . \tag{1.137}$$

When a single measurement is made, one of the eigenstates of this operator in this superposition will be observed and the corresponding eigenvalue will be measured. In other words, the state $|\phi\rangle$ will "collapse" to a state $|a_n\rangle$. The probability that a particular eigenvalue, e.g., a_n will be measured in a single measurement is given by $|c_n|^2$. But a second measurement of an identical system may yield another eigenstate with a different eigenvalue and a different probability. Repeated measurements on identically prepared systems, will then give the probability distribution of the eigenvalues and yield information on the nature of the system. In practice, one prefers to make measurements on a large number of identical systems, which gives the same probability distribution.

Similar arguments follow if a measurement is made to determine whether the system is in state $|\psi\rangle$. In this case the original state $|\phi\rangle$ will "jump" into the state $|\psi\rangle$ with the probability $|\langle\psi\ |\phi\rangle|^2$.

The concept of measurement and the probability interpretation in quantum mechanics is a complex issue that we will come back to when we discuss Stern–Gerlach experiments in Chapter 7 and entangled states in Chapter 30.

1.14 Problems

1. Define the following two state vectors as column matrices:

$$|\alpha_1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad |\alpha_2\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

with their Hermitian conjugates given by

$$\langle\alpha_1| = \begin{bmatrix} 1 & 0 \end{bmatrix} \quad \text{and} \quad \langle\alpha_2| = \begin{bmatrix} 0 & 1 \end{bmatrix}$$

respectively. Show the following for $i, j = 1, 2$:

(i) The $|\alpha_i\rangle$'s are orthonormal.

(ii) Any column matrix

$$\begin{bmatrix} a \\ b \end{bmatrix}$$

can be written as a linear combination of the $|\alpha_i\rangle$'s.

(iii) The outer products $|\alpha_i\rangle\langle\alpha_j|$ form 2×2 matrices which can serve as operators.
(iv) The $|\alpha_i\rangle$'s satisfy completeness relation

$$\sum_i |\alpha_i\rangle\langle\alpha_i| = \mathbf{1}$$

where $\mathbf{1}$ represents a unit 2×2 matrix.
(v) Write

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

as a linear combination of the four matrices formed by $|\alpha_i\rangle\langle\alpha_j|$.
(vi) Determine the matrix elements of A such that $|\alpha_1\rangle$ and $|\alpha_2\rangle$ are simultaneously the eigenstates of A satisfying the relations

$$A|\alpha_1\rangle = +|\alpha_1\rangle \quad \text{and} \quad A|\alpha_2\rangle = -|\alpha_2\rangle\,.$$

(The above properties signify that the $|\alpha_i\rangle$'s span a Hilbert space. These abstract representations of the state vectors actually have a profound significance. They represent the states of particles with spin ½. We will discuss this in detail in Chapter 5.)

2. Show that if an operator A is a function of λ then

$$\frac{dA^{-1}}{d\lambda} = -A^{-1}\frac{dA}{d\lambda}A^{-1}.$$

3. Show that a unitary operator U can be written as

$$U = \frac{\mathbf{1}+iK}{\mathbf{1}-iK}$$

where K is a Hermitian operator. Show that one can also write

$$U = e^{iC}$$

where C is a Hermitian operator. If

$$U = A + iB.$$

Show that A and B commute. Express these matrices in terms of C. You can assume that

$$e^M = 1 + M + \frac{M^2}{2!} + \cdots$$

where M is an arbitrary matrix.

4. Show that

$$\det\left(e^A\right) = e^{\mathrm{Tr}(A)}.$$

5. For two arbitrary state vectors $|\alpha\rangle$ and $|\beta\rangle$ show that

$$\mathrm{Tr}\left[|\alpha\rangle\langle\beta|\right] = \langle\beta|\alpha\rangle.$$

6. Consider a two-dimensional space spanned by two orthonormal state vectors $|\alpha\rangle$ and $|\beta\rangle$. An operator is expressed in terms of these vectors as

$$A = |\alpha\rangle\langle\alpha| + \lambda\,|\beta\rangle\langle\alpha| + \lambda^*\,|\alpha\rangle\langle\beta| + \mu\,|\beta\rangle\langle\beta|\,.$$

Determine the eigenstates of A for the case where (i) $\lambda = 1, \mu = \pm 1$, (ii) $\lambda = i, \mu = \pm 1$. Do this problem also by expressing A as a 2×2 matrix with eigenstates as the column matrices.

2 Fundamental commutator and time evolution of state vectors and operators

In the previous chapter we outlined the basic mathematical structure essential for our studies. We are now ready to make contact with physics. This means introducing the fundamental constant $\hbar$, the Planck constant, which controls the quantum phenomena. Our first step will be to discuss the so-called fundamental commutator, also known as the canonical commutator, which is proportional to $\hbar$ and which essentially dictates how the quantum processes are described. We then examine how time enters the formalism and thus set the stage for writing equations of motion for a physical system.

2.1 Continuous variables: *X* and *P* operators

Eigenvalues need not always be discrete as we stated earlier. For example, consider a one-dimensional, continuous (indenumerable) infinite-dimensional position space, the x-space. One could have an eigenstate $|x'\rangle$ of a continuous operator X,

$$X|x'\rangle = x'|x'\rangle \tag{2.1}$$

where x'corresponds to the value of the x-variable.

The ket $|x'\rangle$ has all the properties of the kets $|\alpha\rangle$ and of the eigenstates $|a_n\rangle$ that were outlined in the previous chapter. The exceptions are those cases where the fact that x is a continuous variable makes an essential difference.

δ-function $\delta(x - x')$, which has the following properties:

$$\delta(x - x') = 0 \text{ for } x \neq x', \tag{2.2}$$

$$\int_{-\infty}^{\infty} dx\, \delta(x - x') = 1. \tag{2.3}$$

From these two definitions it follows that

$$\int_{-\infty}^{\infty} dx f(x)\, \delta(x - x') = f(x'). \tag{2.4}$$

The properties of the delta function are discussed in considerable detail in Appendix 2.9.

The orthogonality condition involving the Kronecker δ-function that we used for the discrete variables is now replaced by

$$\langle x|\, x'\rangle = \delta(x - x') \tag{2.5}$$

The completeness relation is then expressed as

$$\int_{-\infty}^{\infty} dx\ |x\rangle\, \langle x| = \mathbf{1} \tag{2.6}$$

where the summation in the discrete case is replaced by an integral. Just as in the discrete case one can prove this relation quite simply by multiplying the two sides of (2.6) by the ket $|x'\rangle$. We obtain

$$\left[\int_{-\infty}^{\infty} dx\ |x\rangle\, \langle x|\right] |x'\rangle = \int_{-\infty}^{\infty} dx\ |x\rangle\, \langle x|\, x'\rangle = |x'\rangle\,. \tag{2.7}$$

Thus the left-hand side of (2.6), indeed, acts as a unit operator.

We also note that

$$\langle x\,|X|\,x'\rangle = x\,\delta(x - x'). \tag{2.8}$$

It does not matter if we have the factor x or x' on the right-hand side multiplying the δ-function since the δ-function vanishes unless $x = x'$. The matrix element $\langle x\,|X|\,x'\rangle$, in this continuous space, is called the "representative" of the operator X in the x-space.

A "wavefunction" in the x-space, $\phi(x)$, corresponding to a state vector $|\phi\rangle$ is defined as

$$\phi(x) = \langle x|\, \phi\rangle \tag{2.9}$$

and from the properties of the bra and ket vectors outlined earlier,

$$\phi^*(x) = \langle \phi|\, x\rangle. \tag{2.10}$$

The function $\phi(x)$ is then a manifestation of an abstract vector $|\phi\rangle$ in the x-space which we also call the "representative" of $|\phi\rangle$ in the x-space. The linear superposition principle stated in (1.1) can be written in the following form by taking the representatives in the x-space,

$$a\alpha(x) + b\beta(x) = c\gamma(x) \tag{2.11}$$

where $\alpha(x) = \langle x|\, \alpha\rangle$ etc.

The product $\langle \psi|\, \phi\rangle$ can be expressed in the x-space by inserting a complete set of intermediate states:

$$\langle \psi|\, \phi\rangle = \langle \psi|\, \mathbf{1}\, |\phi\rangle = \int_{-\infty}^{\infty} dx\, \langle \psi|\, x\rangle\, \langle x|\, \phi\rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x)\phi(x) \tag{2.12}$$

In particular, if the states $|\phi\rangle$ are normalized, $\langle\phi|\,\phi\rangle = 1$, then replacing $\langle\psi|$ by $\langle\phi|$ in the above relation we obtain the normalization condition in the x-space for the wavefunction $\phi(x)$,

$$\int_{-\infty}^{\infty} dx\, \phi^*(x)\phi(x) = 1. \tag{2.13}$$

For the integrals to be finite, it is important to note that $\phi(x)$ and $\psi(x)$ must vanish as $x \to \pm\infty$.

As with the x-variables, one can also consider the momentum variable, p, in one dimension (p-space) which can be continuous. If P is the momentum operator with eigenstates $|p'\rangle$ then

$$P|p'\rangle = p'|p'\rangle \tag{2.14}$$

with

$$\langle p|p'\rangle = \delta(p - p') \tag{2.15}$$

and

$$\langle p|P|p'\rangle = p\delta(p - p'). \tag{2.16}$$

A wavefunction in the p-space, $f(p)$, for an abstract vector $|f\rangle$ is defined as

$$f(p) = \langle p|f\rangle \tag{2.17}$$

with the normalization condition

$$\int_{-\infty}^{\infty} dp f^*(p) f(p) = 1. \tag{2.18}$$

If the state vectors depend on time then the above conditions can be expressed in terms of $\phi(x,t)$ and $f(p,t)$.

2.2 Canonical commutator [*X, P*]

The commutator between two operators B and C is defined as

$$[B, C] = BC - CB \tag{2.19}$$

It is itself an operator. As we saw earlier, it will vanish if B and C have a common eigenstate.

The commutator between the canonical variables X and P plays a fundamental role in quantum mechanics, which in the one-dimensional case is given by

$$[X, P] = i\hbar \mathbf{1} \tag{2.20}$$

where the right-hand side has the Planck constant, $\hbar$, multiplied by a unit operator. The appearance of $\hbar$ signals that we are now in the regime of quantum mechanics.

The relation (2.20) shows that $[X, P]$ does not vanish, and, therefore, X and P cannot have a common eigenstate, i.e., they cannot be measured simultaneously. The commutator, however, allows us to connect two basic measurements: one involving the x-variable and the other involving the p-variable. If the right-hand side were zero then it would correspond to classical physics, where the two measurements can be carried out simultaneously

To obtain the representatives of the momentum operator in the x-space, we proceed by taking the matrix elements of both sides of (2.20),

$$\langle x|(XP - PX)|x'\rangle = i\hbar\delta(x - x'). \tag{2.21}$$

The left-hand side is simplified by inserting a complete set of intermediate states,

$$\langle x|(XP - PX)|x'\rangle = \int_{-\infty}^{\infty} dx'' \, \langle x|X|x''\rangle\langle x''|P|x'\rangle - \int_{-\infty}^{\infty} dx'' \, \langle x|P|x''\rangle\langle x''|X|x'\rangle. \tag{2.22}$$

For the right-hand side of the above equation we use the relation (2.8) and replace the matrix elements of X by Dirac δ-functions. The integrals are further simplified by using (2.4) and (2.8). We thus obtain

$$x\langle x|P|x'\rangle - \langle x|P|x'\rangle x' = i\hbar\delta(x - x'). \tag{2.23}$$

We notice that when $x \neq x'$ the right-hand side of the above equation vanishes. The left-hand side, however, does not vanish when $x \neq x'$ unless $\langle x| P \left|x'\right\rangle$ itself has a δ-function in it. Writing it as

$$\langle x|P|x'\rangle = \delta(x - x')P(x) \tag{2.24}$$

where $P(x)$ is an operator expressed in terms of the x-variable, we obtain the following from (2.23), and (2.24) after cancelling the δ-function from both sides,

$$xP(x) - P(x)x = i\hbar. \tag{2.25}$$

This is an operator relation in which the operators are expressed as functions of x. This relation becomes meaningful only upon operating it on a wavefunction. Multiplying both sides by a wavefunction $\phi(x)$ on the right, we obtain

$$[xP(x) - P(x)x]\,\phi(x) = i\hbar\phi(x), \tag{2.26}$$

which we can write as

$$xP(x)\left[\phi(x)\right] - P(x)\left[x\phi(x)\right] = i\hbar\phi(x). \tag{2.27}$$

Considering the left-hand side in (2.26), we note that since $P(x)$ is assumed to be a linear operator that operates on the quantities to the right of it, we will have two types of terms $P(x)\left[\phi(x)\right]$ and $P(x)\left[x\phi(x)\right]$. Furthermore, relation (2.27) suggests that $P(x)$ will be a derivative operator, in which case one can simplify the second term involving the product $\left[x\phi(x)\right]$ by using the product rule for first order derivatives and writing

$$P(x)\left[x\phi(x)\right] = \left[P(x)x\right]\phi(x) + x\left[P(x)\phi(x)\right] \tag{2.28}$$

where the square bracket in $\left[P(x)x\right]\phi(x)$ implies that $P(x)$ operates only on x and not on $\phi(x)$. Thus the left-hand side of (2.27) can be written as

$$x\left[P(x)\phi(x)\right] - \left[P(x)x\right]\phi(x) - x\left[P(x)\phi(x)\right] = -\left[P(x)x\right]\phi(x). \tag{2.29}$$

The equation (2.27) now reads

$$-\left[P(x)x\right]\phi(x) = i\hbar\phi(x). \tag{2.30}$$

Since on the left-hand side of (2.30), $P(x)$ operates only on x and does not operate on $\phi(x)$, we can remove $\phi(x)$ from both sides and obtain the relation

$$-\left[P(x)x\right] = i\hbar. \tag{2.31}$$

It is easy to confirm that the following linear differential operator for $P(x)$ satisfies the above relation:

$$P(x) = -i\hbar\frac{d}{dx}. \tag{2.32}$$

This is then the representation of the operator P in the x-space. In terms of matrix elements in the x-space we can write this relation as

$$\langle x'|P|x\rangle = \delta(x - x')\left(-i\hbar\frac{d}{dx}\right). \tag{2.33}$$

A matrix element that one often comes across is $\langle x'|P|\phi\rangle$ which can be expressed, by inserting a complete set of states, as

$$\langle x'|P|\phi\rangle = \int_{-\infty}^{\infty} dx''\,\langle x'|P|x''\rangle\langle x''|\phi\rangle. \tag{2.34}$$

Using (2.33) we obtain

$$\langle x'|P|\phi\rangle = -i\hbar\frac{d}{dx'}\phi(x'). \tag{2.35}$$

2.3 P as a derivative operator: another way

We describe another way in which the relation (2.35) can be established. Let us start with the fundamental commutator written as

$$[P, X] = -i\hbar. \tag{2.36}$$

Consider

$$[P, X^2] = PX^2 - X^2P. \tag{2.37}$$

This relation can be rewritten as

$$[P, X^2] = [P, X]X + X[P, X] = -2i\hbar X \tag{2.38}$$

where we have used the relation (2.36). Expressing the right-hand side as a derivative we obtain

$$[P, X^2] = -i\hbar \frac{d}{dX}(X^2). \tag{2.39}$$

Proceeding in a similar manner one can show that

$$[P, X^n] = -ni\hbar X^{n-1} = -i\hbar \frac{d}{dX}(X^n). \tag{2.40}$$

Consider now the commutator $[P, f(X)]$ where $f(X)$ is a regular function which can be expanded in a Taylor series around $X = 0$,

$$f(X) = a_0 + a_1 X + \cdots + a_n X^n + \cdots. \tag{2.41}$$

Using the result (2.40) we conclude that

$$[P, f(X)] = -i\hbar \frac{df(X)}{dX}. \tag{2.42}$$

We operate the two sides on a state vector $|\phi\rangle$,

$$[P, f(X)]|\phi\rangle = -i\hbar \frac{df(X)}{dX}|\phi\rangle. \tag{2.43}$$

The left-hand side is

$$(Pf - fP)|\phi\rangle = [(Pf)|\phi\rangle + fP|\phi\rangle] - f(P|\phi\rangle) = (Pf)|\phi\rangle. \tag{2.44}$$

In the above relation (Pf) means P operates on f alone. Since $|\phi\rangle$ is any arbitrary state vector one can remove the factor $|\phi\rangle$. Hence

$$(Pf) = -i\hbar \frac{df(X)}{dX}. \tag{2.45}$$

Thus

$$P = -i\hbar \frac{d}{dX}. \tag{2.46}$$

Taking the matrix element of the above, we find

$$\langle x'|P|\phi\rangle = -i\hbar \frac{d}{dx'}\phi(x'), \tag{2.47}$$

confirming our result (2.35).

2.4 *X* and *P* as Hermitian operators

Let us now show that X and P are Hermitian, as they should be since they correspond to physically measurable quantities.

For X it is quite trivial as we demonstrate below. From the definition of Hermitian conjugate we notice that the matrix element of $X^\dagger$ is given by

$$\langle x'|X^\dagger|x\rangle = \langle x|X|x'\rangle^* = x\delta(x - x'). \tag{2.48}$$

where we have taken account of the fact that x' and $\delta(x - x')$ are real. The matrix element of X is given by

$$\langle x'|X|x\rangle = x\delta(x - x'). \tag{2.49}$$

Therefore,

$$X = X^\dagger. \tag{2.50}$$

The Hermitian conjugate of P can be obtained by first taking the matrix element of P between two arbitrary states $|\psi\rangle$ and $|\phi\rangle$ and then evaluating it by inserting a complete set of states. We obtain

$$\langle \psi|P|\phi\rangle = \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dx'' \, \langle \psi|x'\rangle\langle x'|P|x''\rangle\langle x''|\phi\rangle \tag{2.51}$$

$$= \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dx'' \, \psi^*(x')\delta(x' - x'') \left(-i\hbar \frac{\partial}{\partial x''}\right) \phi(x''), \tag{2.52}$$

remembering that P operates on the functions to the right. Therefore,

$$\langle \psi|P|\phi\rangle = (-i\hbar) \int_{-\infty}^{\infty} dx' \, \psi^*(x') \frac{\partial \phi(x')}{\partial x'}. \tag{2.53}$$

Interchanging ψ and ϕ, we obtain

$$\langle\phi|P|\psi\rangle = (-i\hbar)\int_{-\infty}^{\infty} dx'\,\phi^*(x')\frac{\partial\psi(x')}{\partial x'}. \tag{2.54}$$

Integrating the right-hand side above by parts, and also, to ensure the convergence of the integrals, assuming $\psi(x') \to 0, \phi(x') \to 0$ as $x' \to \pm\infty$, we obtain

$$\langle\phi|P|\psi\rangle = (i\hbar)\int_{-\infty}^{\infty} dx'\,\frac{\partial\phi^*(x')}{\partial x'}\psi(x'). \tag{2.55}$$

Next we consider the matrix element of $P^\dagger$, and use its Hermitian conjugation properties,

$$\langle\phi|P^\dagger|\psi\rangle = \langle\psi|P|\phi\rangle^* = (i\hbar)\int_{-\infty}^{\infty} dx'\,\psi(x')\frac{\partial\phi^*(x')}{\partial x'} \tag{2.56}$$

where we have used (2.53). Comparing this result with that of $\langle\phi|P|\psi\rangle$ in (2.55) we conclude that, since $\psi(x')$ and $\phi(x')$ are arbitrary functions, we must have

$$P^\dagger = P \tag{2.57}$$

and thus P is Hermitian.

We can extend the above relations to three dimensions with the commutation relations given by

$$\left[X_i, P_j\right] = i\hbar\delta_{ij}\mathbf{1}, \tag{2.58}$$

$$\left[X_i, X_j\right] = 0, \tag{2.59}$$

$$\left[P_i, P_j\right] = 0 \tag{2.60}$$

where $i,j = 1,2,3$ correspond to the three dimensions. Thus X_1, X_2, X_3 correspond to the operators X, Y, Z respectively, while P_1, P_2, P_3 correspond to operators P_x, P_y, P_z respectively.

Beginning with the relation

$$[X, P_x] = i\hbar\mathbf{1} \tag{2.61}$$

we conclude, following the same steps as before, that the representation of P_x in the x-space will be given by

$$P_x = -i\hbar\frac{\partial}{\partial x}. \tag{2.62}$$

Note that we now have a partial derivative rather than the total derivative that we had earlier for the one-dimensional case. The above operator satisfies the relation

$$[Y, P_x] = 0 = [Z, P_x]. \tag{2.63}$$

Since P_x commutes with Y and Z, it cannot involve any derivative operators involving the y- and z-coordinates. Therefore, the relation (2.61) remains a correct representation of P_x. Similarly, we have

$$P_y = -i\hbar\frac{\partial}{\partial y}, \;\; P_z = -i\hbar\frac{\partial}{\partial z}. \tag{2.64}$$

Finally, we note that the operators P_x, P_y, and P_z as written above also satisfy the relations (2.60). All the remaining results we derived for the one-dimensional case stay the same for the three-dimensional operators.

2.5 Uncertainty principle

As we discussed earlier, when two operators commute, i.e., when the commutator between two operators vanishes, then these operators can share the same eigenstates. This implies that the observables associated with these operators can be measured simultaneously. A commutator, therefore, quantifies in some sense the degree to which two observables can be measured at the same time.

In quantum mechanics, Planck's constant, $\hbar$, provides a measure of the commutator between the canonical operators X and P through the fundamental commutator (2.20). The uncertainty relation, one of the most famous results in quantum mechanics, relates the accuracies of two measurements when they are made simultaneously.

The uncertainty of an operator A is defined as the positive square root $\sqrt{\langle(\Delta A)^2\rangle}$ where

$$\Delta A = A - \langle A\rangle\,\mathbf{1} \tag{2.65}$$

and $\langle A\rangle$ is given by

$$\langle A\rangle = \langle\phi|A|\phi\rangle, \tag{2.66}$$

which is the expectation value of A with respect to an arbitrary state $|\phi\rangle$. We note that

$$\langle\Delta A\rangle = \langle A - \langle A\rangle\,\mathbf{1}\rangle = \langle A\rangle - \langle A\rangle = \; 0 \tag{2.67}$$

and

$$\left\langle(\Delta A)^2\right\rangle = \left\langle A^2 - 2A\,\langle A\rangle + \langle A\rangle^2\,\mathbf{1}\right\rangle = \left\langle A^2\right\rangle - \langle A\rangle^2\,. \tag{2.68}$$

To derive the uncertainty relation let us consider three Hermitian operators C, D, F that satisfy the commutation relation

$$[C, D] = iF. \tag{2.69}$$

We consider the following relation involving the state vector $|\phi\rangle$,

$$(C + i\lambda D)\,|\phi\rangle = C|\phi\rangle + i\lambda D|\phi\rangle \tag{2.70}$$

where λ is real. We note that

$$|C|\phi\rangle + i\lambda D|\phi\rangle|^2 \geq 0 \tag{2.71}$$

for all values of λ. The left-hand side can be written as

$$\left(\langle\phi|C^\dagger - i\lambda\langle\phi|D^\dagger\right)(C|\phi\rangle + i\lambda D|\phi\rangle) \tag{2.72}$$

$$= \langle\phi|C^\dagger C|\phi\rangle + i\lambda\langle\phi|C^\dagger D|\phi\rangle - i\lambda\langle\phi|D^\dagger C|\phi\rangle + \lambda^2\langle\phi|D^\dagger D|\phi\rangle \tag{2.73}$$

$$= \langle\phi|C^\dagger C|\phi\rangle + i\lambda\langle\phi|\,[C, D]\,|\phi\rangle + \lambda^2\langle\phi|D^\dagger D|\phi\rangle \tag{2.74}$$

$$= |C|\phi\rangle|^2 - \lambda\langle\phi|F|\phi\rangle + \lambda^2|D|\phi\rangle|^2 \tag{2.75}$$

where we have used the Hermitian property of the operators and the commutation relation (2.69).

The relation (2.71) can then be written as

$$|C|\phi\rangle|^2 - \lambda\langle\phi|F|\phi\rangle + \lambda^2|D|\phi\rangle|^2 \geq 0 \tag{2.76}$$

for all values of λ. Let us write

$$x^2 = |D|\phi\rangle|^2, \quad y = \langle\phi|F|\phi\rangle \quad \text{and} \quad z^2 = |C|\phi\rangle|^2. \tag{2.77}$$

The relation (2.76) can be written as a quadratic in λ,

$$\lambda^2 x^2 - \lambda y + z^2 \geq 0 \quad \text{for all values of } \lambda. \tag{2.78}$$

First we confirm that this relation is correct for $\lambda \to \infty$. To determine the sign of the left-hand side of (2.78) for finite values of λ, let us express the relation in terms of its roots in λ:

$$\lambda^2 x^2 - \lambda y + z^2 = x^2\,(\lambda - \lambda_1)\,(\lambda - \lambda_2) \tag{2.79}$$

where λ_1 and λ_2 are the roots, which we write as

$$\lambda_1 = a_0 - \Delta \;\text{ and }\; \lambda_2 = a_0 + \Delta \tag{2.80}$$

where

$$a_0 = \frac{y}{2x^2} \;\text{ and }\; \Delta = \frac{\sqrt{y^2 - 4x^2z^2}}{2x^2}. \tag{2.81}$$

Since x^2 defined by (2.77) is positive definite, the relation (2.78) implies that

$$(\lambda - \lambda_1)(\lambda - \lambda_2) \geq 0. \tag{2.82}$$

However, the left-hand side is negative for

$$\lambda_1 < \lambda < \lambda_2. \tag{2.83}$$

To solve this apparent contradiction we substitute (2.80) for λ_1 and λ_2 in the product

$$(\lambda - \lambda_1)(\lambda - \lambda_2) = (\lambda - a_0 - \Delta)(\lambda - a_0 + \Delta) = (\lambda - a_0)^2 - \Delta^2. \tag{2.84}$$

In order to satisfy (2.82), the right-hand side above must be positive, which implies that $\Delta^2 < 0$, i.e., Δ is pure imaginary,

$$\Delta = i|\Delta|. \tag{2.85}$$

Hence,

$$(\lambda - \lambda_1)(\lambda - \lambda_2) = (\lambda - a_0)^2 + |\Delta|^2 \tag{2.86}$$

This is a positive definite quantity. We note that since F is Hermitian, a_0 defined by (2.81) is real. For Δ to be pure imaginary we must have, from (2.81) and (2.85),

$$4x^2z^2 \geq y^2. \tag{2.87}$$

In terms of the operators C, D, and F this implies

$$\left[|C|\phi\rangle|^2\right]\left[|D|\phi\rangle|^2\right] \geq \frac{1}{4}|\langle\phi|F|\phi\rangle|^2. \tag{2.88}$$

To derive the uncertainty relation we consider two Hermitian operators A and B, and relate them to the operators C and D as follows:

$$C = \Delta A, \quad D = \Delta B. \tag{2.89}$$

Then from the relations (2.65), (2.69), we have

$$[C, D] = [\Delta A, \Delta B] = [A, B] \tag{2.90}$$

and

$$iF = [A, B]\,. \tag{2.91}$$

We, therefore, conclude from (2.88) that

$$\left\langle(\Delta A)^2\right\rangle\left\langle(\Delta B)^2\right\rangle \geq \frac{1}{4}\,|\langle[A, B]\rangle|^2\,. \tag{2.92}$$

This is true for any set of Hermitian operators. We choose $A = X$, and $B = P$. Since $[X, P] = i\hbar\mathbf{1}$ we obtain from (2.92)

$$\left\langle (\Delta X)^2 \right\rangle \left\langle (\Delta P)^2 \right\rangle \geq \frac{\hbar^2}{4} \implies \Delta x \Delta p \geq \frac{\hbar}{2} \tag{2.93}$$

where we have taken Δx and Δp as the uncertainties defined by $\sqrt{\langle (\Delta X)^2 \rangle}$ and $\sqrt{\langle (\Delta P)^2 \rangle}$ respectively. These are the uncertainties in the measurements of the x and p variables. One often writes the relation (2.93) more simply as

$$\Delta x \Delta p \gtrsim \hbar. \tag{2.94}$$

This is the statement of the uncertainty relation in a quantum-mechanical system where the commutation relations between the canonical variables are governed by the Planck constant, $\hbar$.

2.6 Some interesting applications of uncertainty relations

2.6.1 Size of a particle

By "size" we mean Δx in the sense of the uncertainty relations according to which

$$\Delta x \sim \frac{\hbar}{\Delta p}. \tag{2.95}$$

A typical value of Δp is given by the momentum mv of the particle. The maximum possible value of the velocity according to the theory of relativity is the velocity of light, c. The minimum value of Δx is then

$$(\Delta x)_{\min} = \frac{\hbar}{mc}. \tag{2.96}$$

Quantum-mechanically therefore, one does not think of a particle of mass m as a point particle but rather as an object with a finite size, $\hbar/mc$. This is also called the Compton wavelength characteristic of that particle and it enters into calculations whenever a length scale for the particle appears.

2.6.2 Bohr radius and ground-state energy of the hydrogen atom

Classically, an electron of charge $-e$ orbiting around a proton of charge e would lose energy due to radiation and eventually fall into the proton. This is, of course, in contradiction to the observed fact that the electron executes stable orbits. This is explained quantum-mechanically in the simplest terms through the uncertainty principle.

The total energy E of the electron is a sum of the kinetic energy $\left(\frac{1}{2}\right) mv^2$ and the potential energy, which in the case of hydrogen is just the Coulomb potential. Thus, writing the kinetic energy in terms of $p = mv$, the momentum, we have

$$E = \frac{p^2}{2m} - \frac{e^2}{r} \tag{2.97}$$

where r is the distance between the proton and electron. Taking $\Delta p \sim p$ and $\Delta r \sim r$, the uncertainty relation says that

$$pr \sim \hbar. \tag{2.98}$$

Thus, as r for the electron gets small due to the Coulomb attraction, p becomes large due to the uncertainty principle. In other words, as the attractive Coulomb potential moves the electron toward the proton, the increasing kinetic energy pushes the electron away from the system. The electron will then settle down at a minimum of the total energy. We can obtain this minimum by writing

$$E = \frac{\hbar^2}{2mr^2} - \frac{e^2}{r} \tag{2.99}$$

and then taking

$$\frac{\partial E}{\partial r} = 0. \tag{2.100}$$

This gives

$$-\frac{\hbar^2}{mr^3} + \frac{e^2}{r^2} = 0. \tag{2.101}$$

We find

$$r_{\min} = \frac{\hbar^2}{me^2}. \tag{2.102}$$

This is, indeed, the Bohr radius of the hydrogen atom, which is designated as a_0. Substituting this in the expression (2.99) we obtain the minimum value of E given by

$$E_{\min} = -\frac{e^2}{2a_0} \tag{2.103}$$

which is precisely the ground-state energy of the hydrogen atom.

Thus we find that even a simple application of the uncertainty relations can often give meaningful results.

2.7 Space displacement operator

We consider two unitary operators that are of fundamental importance: space displacement, also called translation, and time evolution. The displacement operator, $D(x)$, involves

translation of the space coordinates and, in one dimension, it has the property

$$D(\Delta x')|x'\rangle = |x' + \Delta x'\rangle. \tag{2.104}$$

Hence

$$\langle x'|D^{\dagger}(\Delta x') = \langle x' + \Delta x'| \tag{2.105}$$

where $\Delta x'$ is the displacement. The displacement operator for $\Delta x' = 0$ corresponds to an operator that causes no displacement, hence,

$$D(0) = \mathbf{1}. \tag{2.106}$$

Furthermore, by repeated translations one finds

$$D(\Delta x'')D(\Delta x') = D\left(\Delta x'' + \Delta x'\right) = D(\Delta x')D(\Delta x''). \tag{2.107}$$

This follows from the fact that when all three of the operators that appear in the above equality operate on $\left|x'\right\rangle$, they give the same state, $\left|x' + \Delta x' + \Delta x''\right\rangle$. In particular, taking $\Delta x'' = -\Delta x'$, we find, since $D(0) = \mathbf{1}$,

$$D(\Delta x')D(-\Delta x') = \mathbf{1}. \tag{2.108}$$

Hence

$$D(-\Delta x') = D^{-1}(\Delta x') \tag{2.109}$$

which implies that the inverse of a displacement operator is the same as displacement in the opposite direction.

The set of operators $D(\Delta x')$ for different Δx's form what is called a "group." The precise definition of a group and its detailed properties will be discussed in some of the later chapters, but for now it is important to note that the operator $D(\Delta x')$ varies continuously

Since $D(\Delta x')$ merely translates the coordinates of a state vector, we assume the norm of $\left|x'\right\rangle$ to remain unchanged. Therefore,

$$\langle x'|x'\rangle = \langle x' + \Delta x'|x' + \Delta x'\rangle \Longrightarrow \langle x'|x'\rangle = \langle x'|D^{\dagger}(\Delta x')D(\Delta x')|x'\rangle, \tag{2.110}$$

i.e.,

$$D^{\dagger}(\Delta x')D(\Delta x') = \mathbf{1}. \tag{2.111}$$

Hence D is a unitary operator.

If $\Delta x'$ is infinitesimally small then, since $D(\Delta x')$ is a continuous function of $\Delta x'$, one can expand it in a power series as follows, keeping only the leading term in $\Delta x'$,

$$D(\Delta x') = \mathbf{1} - iK\Delta x'. \tag{2.112}$$

The operator K is called the "generator" of an infinitesimal space displacement transformation. Inserting the above expression in (2.111), we have

$$\mathbf{1} + i\left(K^{\dagger} - K\right)\Delta x' + O(\Delta x')^2 = \mathbf{1} \tag{2.113}$$

where $O\left(\Delta x'\right)^2$ means of the order of $\left(\Delta x'\right)^2$. This term can be neglected since $\Delta x'$ is infinitesimal and because we want to keep only the leading terms in $\Delta x'$. The above result then implies that

$$K^{\dagger} = K. \tag{2.114}$$

The operator K must, therefore, be Hermitian.

We will not prove it here but the fact that the generators of infinitesimal unitary transformations are Hermitian is actually a very general property.

To obtain further insight into K, consider the commutator $\left[X, D(\Delta x')\right]$. When the commutator operates on a state vector $\left|x'\right\rangle$ we obtain

$$\left[X, D(\Delta x')\right]|x'\rangle = XD(\Delta x')|x'\rangle - D(\Delta x')X|x'\rangle \tag{2.115}$$

$$= \left(x' + \Delta x'\right)|x' + \Delta x'\rangle - x'|x' + \Delta x'\rangle \tag{2.116}$$

$$= \Delta x'|x' + \Delta x'\rangle. \tag{2.117}$$

Since $\Delta x'$ is infinitesimal, we can make the expansion

$$|x' + \Delta x'\rangle = |x'\rangle + O\left(\Delta x'\right). \tag{2.118}$$

Substituting (2.118) in (2.117) and neglecting terms of order $\left(\Delta x'\right)^2$, we have from (2.114)

$$\left[X, D(\Delta x')\right] = \Delta x'\mathbf{1} \tag{2.119}$$

where we retain the unit operator on the right to preserve the fact that both sides of (2.119) are operators. Substituting the expression for D in terms of its generator K in (2.119) we obtain

$$\left[X, \left(\mathbf{1} - iK\Delta x'\right)\right] = \Delta x'\mathbf{1}. \tag{2.120}$$

The commutator $[X, \mathbf{1}]$ vanishes, so we have, after canceling $\Delta x'$ from both sides,

$$[X, K] = i. \tag{2.121}$$

Comparing this commutator with the canonical commutator relation $[X, P] = i\hbar\mathbf{1}$, we obtain the important relation

$$K = \frac{P}{\hbar}, \tag{2.122}$$

which leads to the observation that the generator for infinitesimal space displacement transformations of a state vector is proportional to the momentum operator. Thus the space displacement operator can be written as

$$D(\Delta x') = \mathbf{1} - i\frac{P}{\hbar}\Delta x'. \tag{2.123}$$

To confirm that K has the same form as P we proceed by considering the quantity $D(\Delta x)|\phi\rangle$. Inserting a complete set of states we have

$$D(\Delta x)|\phi\rangle = \int_{-\infty}^{\infty} dx\, D(\Delta x)|x\rangle\langle x|\phi\rangle = \int_{-\infty}^{\infty} dx\, |x + \Delta x\rangle\langle x|\phi\rangle. \tag{2.124}$$

We change variables by taking $(x + \Delta x) = x''$, and notice that the limits $\pm\infty$ will remain unchanged. Thus, on the right-hand side above, $\langle x|\phi\rangle$ will be replaced by $\langle (x'' - \Delta x)|\phi\rangle$, which can be expanded in a Taylor series in terms of Δx to give

$$D(\Delta x)|\phi\rangle = \int_{-\infty}^{\infty} dx''\, |x''\rangle\langle x'' - \Delta x|\phi\rangle = \int_{-\infty}^{\infty} dx''|x''\rangle \left[\phi(x'') - \Delta x\frac{d}{dx''}\phi(x'')\right] \tag{2.125}$$

where we have taken $\langle x''|\phi\rangle = \phi(x'')$. Multiplying the two sides above by $\langle x'|$, we have

$$\langle x'|D(\Delta x)|\phi\rangle = \int_{-\infty}^{\infty} dx''\, \langle x'|x''\rangle \left[\phi(x'') - \Delta x\frac{d}{dx''}\phi(x'')\right]. \tag{2.126}$$

Since $\langle x'|x''\rangle = \delta(x' - x'')$, we obtain

$$\langle x'|D(\Delta x)|\phi\rangle = \phi(x') - \Delta x\frac{d}{dx'}\phi(x'). \tag{2.127}$$

Inserting $D(\Delta x) = \mathbf{1} - iK\Delta x$, we find

$$\langle x'|K|\phi\rangle = -i\frac{d}{dx'}\phi(x'). \tag{2.128}$$

Hence K has the same form as P, given by

$$\langle x'|P|\phi\rangle = -i\hbar\frac{d}{dx'}\phi(x'), \tag{2.129}$$

confirming (2.122).

Finally, we can convert D defined in terms of an infinitesimal transformation, to finite transformations. For example, space displacement by a finite amount, x, can be obtained if

we divide x, into N equal parts $\Delta x = x/N$ and then take the products of $D(\Delta x)$ N times in the limit $N \to \infty$,

$$D(x) = \lim_{N\to\infty} D\left(\frac{x}{N}\right) D\left(\frac{x}{N}\right) D\left(\frac{x}{N}\right) \cdots = \lim_{N\to\infty} \left[D\left(\frac{x}{N}\right)\right]^N \tag{2.130}$$

$$= \lim_{N\to\infty} \left[\mathbf{1} - i\frac{1}{N}\frac{Px}{\hbar}\right]^N . \tag{2.131}$$

To determine the right-hand side we note that one can write

$$\lim_{N\to\infty} \left[\mathbf{1} + a\frac{x}{N}\right]^N = \lim_{N\to\infty} \exp\left[N \ln\left(\mathbf{1} + a\frac{x}{N}\right)\right]. \tag{2.132}$$

If we expand the exponent containing the logarithmic function, we obtain

$$N \ln\left(\mathbf{1} + a\frac{x}{N}\right) = N\left[a\left(\frac{x}{N}\right) - \frac{1}{2}a^2\left(\frac{x}{N}\right)^2 + \cdots\right] = ax - \frac{1}{2}(ax)^2\frac{1}{N} + \cdots . \tag{2.133}$$

In the limit $N \to \infty$, the right-hand side is simply ax. Hence

$$\lim_{N\to\infty} \left[\mathbf{1} + a\frac{x}{N}\right]^N = e^{ax}. \tag{2.134}$$

Thus $D(x)$ in (2.131) can be written as

$$D(x) = \exp\left(-i\frac{P}{\hbar}x\right) \tag{2.135}$$

where the exponential of the operators are understood in terms of the power series expansion as

$$e^A = 1 + A + \frac{A^2}{2!} + \cdots . \tag{2.136}$$

We can derive the relation (2.133) analytically also by using the definition of the derivative

$$\frac{dD(x)}{dx} = \lim_{\Delta x\to 0} \frac{D(x + \Delta x) - D(x)}{\Delta x}. \tag{2.137}$$

Let us then write

$$D(x + \Delta x) = D(x)\, D(\Delta x) = D(x)\left(\mathbf{1} - i\frac{P}{\hbar}\Delta x\right). \tag{2.138}$$

Inserting this in (2.137) we obtain

$$\frac{dD(x)}{dx} = \lim_{\Delta x\to 0} \frac{D(x)\left(\mathbf{1} - i\frac{P}{\hbar}\Delta x\right) - D(x)}{\Delta x} = -i\frac{P}{\hbar}D(x). \tag{2.139}$$

The solution of this is an exponential given by

$$D(x) = \exp\left(-i\frac{P}{\hbar}x\right), \tag{2.140}$$

confirming our earlier result.

We can extend the above results to three dimensions quite simply through the following steps for the infinitesimal translation of the state $|x,y,z\rangle$ in three mutually independent directions:

$$\begin{aligned}
&\left|x'+\Delta x', y'+\Delta y', z'+\Delta z'\right\rangle && (2.141)\\
&= D(\Delta x')\left|x', y'+\Delta y', z'+\Delta z'\right\rangle && (2.142)\\
&= \left[D(\Delta x')\right]\left[D(\Delta y')\right]|x', y', z'+\Delta z'\rangle && (2.143)\\
&= \left[D(\Delta x')\right]\left[D(\Delta y')\right]\left[D(\Delta z')\right]|x', y', z'\rangle. && (2.144)
\end{aligned}$$

We then obtain the relation

$$D(\Delta x_i') = \left(\mathbf{1} - i\frac{P_i}{\hbar}\Delta x_i'\right) \tag{2.145}$$

where $i = 1, 2, 3$ correspond to the x, y, z components. For finite transformation one follows the procedure of N infinitesimal transformations in each direction in the limit $N \to \infty$. We can then write

$$D(x,y,z) = D(x)D(y)D(z) = \exp\left(-i\frac{P_x x + P_y y + P_z z}{\hbar}\right). \tag{2.146}$$

In vector notation the transformation can be written compactly as

$$D(\mathbf{r}) = \exp\left(-i\frac{\mathbf{P}\cdot\mathbf{r}}{\hbar}\right) \tag{2.147}$$

where $\mathbf{r} = (x,y,z)$ and $\mathbf{P} = \left(P_x, P_y, P_z\right)$.

2.8 Time evolution operator

Following the same procedure that we followed for the space displacement operator, we define another unitary operator, the time evolution operator, $U(t,t_0)$, which shifts the time parameter of a state from t_0 to t,

$$|\alpha(t)\rangle = U(t,t_0)\,|\alpha(t_0)\rangle. \tag{2.148}$$

We note that

$$U(t_0,t_0) = \mathbf{1}. \tag{2.149}$$

Furthermore, we can write (2.148) in two steps, e.g., we first write it as

$$|\alpha(t)\rangle = U\,(t, t_1)\,|\alpha(t_1)\rangle \tag{2.150}$$

and then write

$$|\alpha(t_1)\rangle = U\,(t_1, t_0)\,|\alpha(t_0)\rangle. \tag{2.151}$$

From (2.148), (2.150), and (2.151) we find, just as with the D-operator,

$$U\,(t, t_0) = U\,(t, t_1)\,U\,(t_1, t_0)\,. \tag{2.152}$$

If the norms of $|\alpha(t_0)\rangle$ and $|\alpha(t)\rangle$ are the same then we have

$$\langle\alpha(t_0)|\alpha(t_0)\rangle = \langle\alpha(t)|\alpha(t)\rangle = \langle\alpha(t_0)|U^{\dagger}\,(t, t_0)\,U\,(t, t_0)\,|\alpha(t_0)\rangle, \tag{2.153}$$

which implies that U is unitary,

$$U^{\dagger}\,(t, t_0)\,U\,(t, t_0) = \mathbf{1}. \tag{2.154}$$

Consider an infinitesimal transformation from t_0 to $t_0 + \Delta t$. As we did for the space displacement operator, D, the operator $U(t_0 + \Delta t, t_0)$ can be expanded in terms of its generator Ω, as follows:

$$U\,(t_0 + \Delta t, t_0) = \mathbf{1} - i\Omega\Delta t. \tag{2.155}$$

From the unitary property of $U\,(t_0 + \Delta t, t_0)$ we have

$$U^{\dagger}\,(t_0 + \Delta t, t_0)\,U\,(t_0 + \Delta t, t_0) = \mathbf{1}. \tag{2.156}$$

Substituting (2.155) we find, following the same arguments as for the generator K of D, that Ω is Hermitian,

$$\Omega^{\dagger} = \Omega. \tag{2.157}$$

As in classical mechanics we identify time evolution with the Hamiltonian, H, of the system and write the following relation that includes the Planck constant $\hbar$:

$$\Omega = \frac{H}{\hbar}. \tag{2.158}$$

An equivalent quantum-mechanical description for the time evolution of a state vector is then given by

$$U(t_0 + \Delta t, t_0) = \mathbf{1} - i\frac{H}{\hbar}\Delta t. \tag{2.159}$$

Thus we can write

$$|\alpha(t + \Delta t)\rangle = U(t + \Delta t, t)\,|\alpha(t)\rangle = \left(\mathbf{1} - i\frac{H}{\hbar}\Delta t\right)|\alpha(t)\rangle. \tag{2.160}$$

We expand $|\alpha(t+\Delta t)\rangle$ for an infinitesimal Δt in a Taylor series in terms Δt, keeping only the first two terms,

$$|\alpha(t+\Delta t)\rangle = |\alpha(t)\rangle + \Delta t \frac{\partial}{\partial t}|\alpha(t)\rangle. \tag{2.161}$$

Comparing this equation with the one above, we obtain the result

$$i\hbar \frac{\partial}{\partial t}|\alpha(t)\rangle = H|\alpha(t)\rangle, \tag{2.162}$$

which is the equation for the time evolution of a state vector in terms of the Hamiltonian H.

As we will discuss further in the next section, this is the time-dependent Schrödinger equation. In comparing space and time transformations, we note that, unlike X which is an operator, t is simply a parameter and not an operator and, therefore, has no commutation properties with H. This is not unexpected since x and t are not on an equal footing in nonrelativistic problems. In the relativistic case, where they are on an equal footing, one finds that instead of elevating t to an operator, x is in fact demoted to being a parameter in the quantum-mechanical treatments, keeping the status of x and t the same.

Let us now obtain an explicit expression for $U(t,t_0)$. We can do this by following the same procedure as we followed for $D(x)$ which is to take the product of N infinitesimal transformations in the limit $N \to \infty$, or to do it analytically. We will follow the analytical path. We first obtain the differential equation for U, by using the definition for the partial derivative

$$\frac{\partial U(t,t_0)}{\partial t} = \lim_{\Delta t \to 0} \frac{U(t+\Delta t,t_0) - U(t,t_0)}{\Delta t}. \tag{2.163}$$

From (2.152) we write $U(t+\Delta t,t_0) = U(t+\Delta t,t)\,U(t,t_0)$ and from (2.159), replacing t_0 by t we write $U(t+\Delta t,t) = \mathbf{1} - iH/\hbar\Delta t$. The above relation then reads

$$\frac{\partial U(t,t_0)}{\partial t} = \lim_{\Delta t \to 0} \frac{\left(\mathbf{1} - i\Delta t \frac{H}{\hbar}\right) U(t,t_0) - U(t,t_0)}{\Delta t}, \tag{2.164}$$

which leads to

$$i\hbar \frac{\partial U(t,t_0)}{\partial t} = HU(t,t_0). \tag{2.165}$$

In other words, as we will elaborate in the next section, U itself satisfies the same time-dependent equation that the ket vector $|\alpha(t)\rangle$ satisfies. We can now integrate the above equation with the condition $U(t_0,t_0) = \mathbf{1}$ and obtain

$$U(t,t_0) = \exp\left[-i\frac{H}{\hbar}(t-t_0)\right] \tag{2.166}$$

where we have assumed that H, is independent of time.

We can also obtain the equation for $U^\dagger$ by taking the Hermitian conjugate of the equation (2.165)

$$-i\hbar\frac{\partial U^\dagger}{\partial t} = U^\dagger H \tag{2.167}$$

where we have made use of the fact that H is Hermitian. The solution of this equation, as expected, directly from (2.167) is

$$U^\dagger(t, t_0) = \exp\left[i\frac{H}{\hbar}(t - t_0)\right]. \tag{2.168}$$

2.9 Appendix to Chapter 2

2.9.1 Dirac delta function

The Dirac delta function, $\delta(x)$, in one dimension, is defined by the following two relations:

$$\delta(x) = 0 \text{ for } x \neq 0, \tag{2.169}$$

$$\int_{-\infty}^{\infty} dx\, \delta(x) = 1. \tag{2.170}$$

The above two relations then also imply that the limits of integration can be different from $\pm\infty$, as long as they include the point $x = 0$. Indeed, one can write

$$\int_b^c dx\, \delta(x) = 1 \text{ for } b < 0 < c. \tag{2.171}$$

One can extend the definition to include a point that is not the origin:

$$\delta(x - a) = 0 \quad \text{for} \quad x \neq a, \tag{2.172}$$

$$\int_{-\infty}^{\infty} dx\, \delta(x - a) = \int_b^c dx\, \delta(x - a) = 1 \text{ for } b < a < c \tag{2.173}$$

where a is a real number.

Properties of the δ-function

Following are some of the interesting properties satisfied by the δ-function.

Property (a)

$$\delta(-x) = \delta(x). \tag{2.174}$$

This can be proved by noting that $\delta(-x)$ satisfies the same properties as $\delta(x)$ given in (2.169) and (2.170), namely, it vanishes for $x \neq 0$, and, through change of variables, $x \to -x$, its integral over $(-\infty, \infty)$ is found to be the same as that of $\delta(x)$. This establishes the fact that $\delta(x)$ is an even function of x.

Property (b)

$$\int_{-\infty}^{\infty} dx f(x)\delta(x-a) = f(a) \tag{2.175}$$

where $f(x)$ is assumed to be regular, without any singularity, along the interval of integration. The proof is quite simple if we write

$$\int_{-\infty}^{\infty} dx f(x)\delta(x-a) = \int_{a-\epsilon}^{a+\epsilon} dx f(x)\delta(x-a) = f(a)\int_{a-\epsilon}^{a+\epsilon} dx\,\delta(x-a) = f(a) \tag{2.176}$$

where ϵ is a small positive quantity.

Property (c)

$$\delta(ax) = \frac{1}{|a|}\delta(x). \tag{2.177}$$

This relation can be derived by changing variables, $ax = y$, and taking account of the even nature of the δ-function.

Property (d)

$$\delta\left(x^2 - a^2\right) = \frac{\delta(x-a) + \delta(x+a)}{2|a|}. \tag{2.178}$$

To prove this we first note that both sides vanish for $x \neq a$. Furthermore, we can write the integral on the left-hand side in the following manner:

$$\int_{-\infty}^{+\infty} \delta\left(x^2 - a^2\right) = \int_{-\infty}^{+\infty} \delta[(x-a)(x+a)] = \int_{-a-\epsilon}^{-a+\epsilon} \delta[(-2a(x+a))] + \int_{a-\eta}^{a+\eta} \delta[(2a(x-a))] \tag{2.179}$$

where ϵ and η are small positive quantities. From (2.177) we recover the right-hand side of (2.178).

Property (e)

$$\delta(f(x)) = \sum_n \frac{\delta(x-x_n)}{\left|\frac{df}{dx}\right|_{x=x_n}} \tag{2.180}$$

where $f(x)$ is a regular function, and x_n are the (real) zeros of $f(x)$. This is a generalization of the case (d) where there were only two zeros, $x = \pm a$. To prove this one expands $f(x)$ around each of its zeros, e.g., around $x = x_n$:

$$f(x) = f(x_n) + (x - x_n)\left(\frac{df}{dx}\right)_{x=x_n} + \cdots = (x - x_n)\left(\frac{df}{dx}\right)_{x=x_n} \tag{2.181}$$

where in the last equality we have used the fact that $f(x_n) = 0$, and have kept only the leading term in $(x - x_n)$. Therefore,

$$\delta(f(x)) = \delta\left[(x - x_n)\,(df/dx)_{x=x_n}\right]. \tag{2.182}$$

Using (2.177) we obtain (2.180).

As a strict mathematical function, the relation (2.169) for $\delta(x)$ will imply that the right-hand side of (2.170) must also be zero, because a function that is everywhere zero except at one point (or at a finite number of points) gives an integral that will also be zero. However, it can be represented in terms of limiting functions.

Representations of the δ-function

We consider the following four well-known limiting functions and discuss their role in mathematical problems, particularly in quantum mechanics

(i) The most common example of a δ-function behavior in quantum-mechanical problems, or in Fourier transforms, is the following limiting function:

$$\lim_{L\to\infty} \frac{1}{\pi}\frac{\sin Lx}{x}. \tag{2.183}$$

This function oscillates along the $\pm$ x-axis with zeros at $x = \pm\pi/L,\ \pm 2\pi/L, \ldots,$ $\pm n\pi/L, \ldots$ where n is an integer. The spacing between two consecutive zeros is given by π/L. Therefore, as $L \to \infty$, this spacing becomes increasingly narrower with the zeros almost overlapping with each other, while at the same time the function $\sin(Lx/x)$ itself goes to zero as $x \to \pm\infty$. Thus, for all practical purposes this function vanishes along the $\pm$ x-axis. That is,

$$\lim_{L\to\infty} \frac{1}{\pi}\frac{\sin Lx}{x} \to 0 \text{ for } x \neq 0. \tag{2.184}$$

The only exceptional point is the origin itself, $x = 0$. At this point $\sin Lx = Lx$ and $\sin(Lx/\pi x) = L/\pi$ which grows as $L \to \infty$. Thus the function goes to infinity at one point, while vanishing everywhere else, which is a classic situation for a δ-function. As far as its integral is considered, one can show, using standard techniques – through the complex variables method – that

$$\frac{1}{\pi}\int_{-\infty}^{\infty} dx \frac{\sin Lx}{x} = 1, \tag{2.185}$$

independent of L.

Thus as a limiting function one can express the δ-function as

$$\delta(x) = \lim_{L\to\infty} \frac{1}{\pi} \frac{\sin Lx}{x}. \tag{2.186}$$

The following equivalent integral form,

$$\frac{1}{2}\int_{-L}^{L} dk\, e^{ikx} = \frac{\sin Lx}{x} \tag{2.187}$$

enables us, through the relation (2.186), to write

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ikx} \tag{2.188}$$

where it is understood that

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ikx} = \lim_{L\to\infty} \frac{1}{2\pi}\int_{-L}^{L} dk\, e^{ikx}. \tag{2.189}$$

More generally, one can write

$$\delta(x-a) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ik(x-a)}. \tag{2.190}$$

(ii) The following Gaussian also mimics a δ-function behavior:

$$\lim_{\beta\to\infty} \sqrt{\frac{\beta}{\pi}} \exp(-\beta x^2). \tag{2.191}$$

We note that for $x \neq 0$ the right-hand side vanishes in the limit $\beta \to \infty$, but at $x = 0$, in the same limit, it goes to infinity like $\sqrt{\beta/\pi}$. This is once again a typical δ-function behavior. From the well-known Gaussian integral

$$\int_{-\infty}^{\infty} dy \exp(-y^2) = \sqrt{\pi} \tag{2.192}$$

we deduce, by a change of variables $\sqrt{\beta}x = y$, that

$$\sqrt{\frac{\beta}{\pi}}\int_{-\infty}^{\infty} dx \exp(-\beta x^2) = 1. \tag{2.193}$$

Thus, one can write

$$\delta(x) = \lim_{\beta\to\infty}\sqrt{\frac{\beta}{\pi}}\exp(-\beta x^2). \tag{2.194}$$

Another way of writing the above result is by taking $\beta = 1/\left[\alpha\left(t-t'\right)\right]$, and writing a very general condition, replacing x by $\left(x-x'\right)$,

$$\delta(x-x') = \lim_{t\to t'}\sqrt{\frac{1}{\alpha\left(t-t'\right)\pi}}\exp\left[-\frac{\left(x-x'\right)^2}{\alpha\left(t-t'\right)}\right]. \tag{2.195}$$

(iii) Here is another δ-function type behavior:

$$\lim_{\epsilon\to 0}\frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2}. \tag{2.196}$$

We find that for $x \neq 0$, this function vanishes in the limit $\epsilon \to 0$. However, if $x = 0$, the function behaves like $1/\pi\epsilon$ and goes to infinity in the same limit (the limit has to be taken after the value of x is chosen). Furthermore, one can easily show through standard integration techniques that

$$\frac{1}{\pi}\int_{-\infty}^{\infty} dx\frac{\epsilon}{x^2+\epsilon^2} = 1. \tag{2.197}$$

Once again we can identify

$$\delta(x) = \lim_{\epsilon\to 0}\frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2}. \tag{2.198}$$

This form often occurs in the so-called dispersion relations and in Green's function problems, e.g.,

$$\lim_{\epsilon\to 0}\frac{1}{\pi}\int_0^{\infty} dx'\frac{f(x')}{x'-x-i\epsilon} \tag{2.199}$$

where one writes

$$\begin{aligned}\lim_{\epsilon\to 0}\left[\frac{1}{x'-x-i\epsilon}\right] &= \lim_{\epsilon\to 0}\left[\frac{\left(x'-x\right)}{(x'-x)^2+\epsilon^2}\right] + \lim_{\epsilon\to 0}\left[\frac{i\epsilon}{(x'-x)^2+\epsilon^2}\right] \\ &= \lim_{\epsilon\to 0}\left[\frac{\left(x'-x\right)}{(x'-x)^2+\epsilon^2}\right] + i\pi\,\delta(x'-x).\end{aligned} \tag{2.200}$$

This relation is often written as

$$\frac{1}{x'-x-i\epsilon} = P\left(\frac{1}{x'-x}\right) + i\pi\delta(x'-x) \tag{2.201}$$

where P in the first term on the right stands for what is called the "principal part." It vanishes at the point $x' = x$ and hence excludes that point when integrated over it. The contribution of the singularity at $x' = x$ is now contained in the second term. Thus,

$$\lim_{\epsilon\to 0}\frac{1}{\pi}\int_0^\infty dx'\frac{f(x')}{x'-x-i\epsilon} = \frac{1}{\pi}P\int_0^\infty dx'\frac{f(x')}{x'-x} + if(x). \tag{2.202}$$

(iv) Finally, an interesting representation is given by the function,

$$\frac{d}{dx}\theta(x) \tag{2.203}$$

where $\theta(x)$ is called the step-function,

$$\theta(x) = 0 \quad \text{for} \quad x \le 0, \tag{2.204}$$

$$\text{and } \theta(x) = 1 \quad \text{for} \quad x > 0. \tag{2.205}$$

Notice that the derivative on either side of $x = 0$ vanishes, but at the point $x = 0$ it becomes infinite. The integral can be carried out and is given by

$$\int_{-\infty}^{\infty} dx\frac{d}{dx}\theta(x) = \theta(\infty) - \theta(-\infty) = 1. \tag{2.206}$$

We also note that the above result holds if we take the integration limits to be $(-L, +L)$. Thus, one can write

$$\delta(x) = \frac{d}{dx}\theta(x). \tag{2.207}$$

This θ-function representation appears in Green's function calculations, often for finite-dimensional problems.

In summary, we note that for the above representations of $\delta(x)$, as long as $x \neq 0$, each of the functions on the right-hand side vanishes. But when they are integrated over an interval that includes the point $x = 0$, the result is 1, keeping in mind that the limits are to be taken after the integration is carried out. Thus the limiting process is nonuniform.

Three dimensions

We define the δ-function in the Cartesian system as a product of three one-dimensional δ-functions as follows:

$$\delta^{(3)}(\mathbf{r}-\mathbf{r}') = \delta(x-x')\delta(y-y')\delta(z-z'). \tag{2.208}$$

Therefore, it satisfies

$$\delta^{(3)}(\mathbf{r}-\mathbf{r}') = 0 \quad \text{if} \quad x \neq x' \ \text{ or } \ y \neq y' \ \text{ or } z \neq z' \tag{2.209}$$

and

$$\int_{(\infty)} d^3r\, \delta^{(3)}(\mathbf{r}-\mathbf{r}') = 1, \tag{2.210}$$

which implies, as in the one-dimensional case, that

$$\int_{(\infty)} d^3\mathrm{r} f(\mathbf{r})\delta^{(3)}(\mathbf{r}-\mathbf{r}') = f(\mathbf{r}'). \tag{2.211}$$

Since

$$\delta(x-x') = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ik(x-x')}, \tag{2.212}$$

we can express the three-dimensional δ-function as the product

$$\delta^{(3)}(\mathbf{r}-\mathbf{r}') = \left[\frac{1}{2\pi}\int_{-\infty}^{\infty} dk_x\, e^{ik_x(x-x')}\right]\left[\frac{1}{2\pi}\int_{-\infty}^{\infty} dk_y\, e^{ik_y(y-y')}\right]\left[\frac{1}{2\pi}\int_{-\infty}^{\infty} dk_z\, e^{ik_z(z-z')}\right], \tag{2.213}$$

which can be written in a compact form as

$$\delta^{(3)}(\mathbf{r}-\mathbf{r}') = \frac{1}{(2\pi)^3}\int d^3k e^{i\mathbf{k}.(\mathbf{r}-\mathbf{r})} \tag{2.214}$$

where d^3k is the three-dimensional volume element in the k-space given by

$$d^3k = dk_x\, dk_y\, dk_z. \tag{2.215}$$

We have defined the vector $\mathbf{k}$ as a three-dimensional vector with components (k_x, k_y, k_z) so that

$$\mathbf{k}.(\mathbf{r}-\mathbf{r}') = k_x(x-x') + k_y(y-y') + k_z(z-z'). \tag{2.216}$$

In spherical coordinates, (r, θ, ϕ), the δ-function is easily defined, once again, in terms of products of three one-dimensional δ-functions:

$$\delta^{(3)}(\mathbf{r}-\mathbf{r}') = A(r,\theta,\phi)\delta(r-r')\delta(\theta-\theta')\delta(\phi-\phi') \tag{2.217}$$

where the relation between the Cartesian and spherical coordinates is given by

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta. \tag{2.218}$$

The parameter A in (2.217) can be determined from the definition (2.214):

$$1 = \int_{(\infty)} d^3r\,\delta^{(3)}(\mathbf{r}-\mathbf{r}') = \int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\phi\, J\, A(r,\theta,\phi)\delta(r-r')\delta(\theta-\theta')\delta(\phi-\phi') \tag{2.219}$$

where on the right-hand side we have converted d^3r from Cartesian to spherical coordinates through the relation

$$d^3r = dx\,dy\,dz = J\,dr\,d\theta\,d\phi \tag{2.220}$$

with J as the Jacobian, $\dfrac{\partial(x,y,z)}{\partial(r,\theta,\phi)}$, defined as

$$J = \det\begin{bmatrix} \dfrac{\partial x}{\partial r} & \dfrac{\partial x}{\partial\theta} & \dfrac{\partial x}{\partial\phi} \\ \dfrac{\partial y}{\partial r} & \dfrac{\partial y}{\partial\theta} & \dfrac{\partial y}{\partial\phi} \\ \dfrac{\partial z}{\partial r} & \dfrac{\partial z}{\partial\theta} & \dfrac{\partial z}{\partial\phi} \end{bmatrix}. \tag{2.221}$$

We find

$$J = r^2\sin\theta. \tag{2.222}$$

Substituting this in the above relation, we obtain

$$d^3r = r^2\sin\theta\,dr\,d\theta\,d\phi. \tag{2.223}$$

Relation (2.219) gives

$$\int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\phi\, \left(r^2\sin\theta\right) A(r,\theta,\phi)\delta(r-r')\delta(\theta-\theta')\delta(\phi-\phi') = 1. \tag{2.224}$$

Hence,

$$A(r,\theta,\phi) = \frac{1}{r^2\sin\theta} \tag{2.225}$$

and

$$\delta^{(3)}(\mathbf{r}-\mathbf{r}') = \frac{1}{r^2\sin\theta}\delta(r-r')\delta(\theta-\theta')\delta(\phi-\phi'). \tag{2.226}$$

It is often more convenient to use $\cos\theta$ as a variable rather than θ so that we can write the integrals more simply

$$\int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\phi\, r^2 \sin\theta \to \int_0^\infty dr\, r^2 \int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\phi, \tag{2.227}$$

in which case we obtain the relation

$$\delta^{(3)}(\mathbf{r}-\mathbf{r}') = \frac{1}{r^2}\delta(r-r')\delta(\cos\theta-\cos\theta')\delta(\phi-\phi'). \tag{2.228}$$

This expression is consistent with the relation (2.180) for converting $\delta(\theta-\theta')$ to $\delta(\cos\theta-\cos\theta')$.

2.10 Problems

1. The state vectors $|\gamma\rangle$, $|\alpha\rangle$ and $|\beta\rangle$ are related as

   $$|\gamma\rangle = |\alpha\rangle + \lambda|\beta\rangle$$

   where λ is an arbitrary complex constant. By choosing an appropriate λ and the fact that $\langle\gamma|\gamma\rangle \geq 0$, derive the Schwarz inequality relation

   $$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2.$$

2. For the above problem consider a state $|\phi\rangle$ such that

   $$\Delta A|\phi\rangle = |\alpha\rangle, \Delta B|\phi\rangle = |\beta\rangle$$

   where A and B are Hermitian operators and ΔA and ΔB are the corresponding uncertainties. Expressing the product $\Delta A\Delta B$ as a sum of a commutator and an anticommutator,

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

   and using the Schwarz inequality relation derived above, show that

   $$|\Delta A\Delta B|^2 \geq \frac{1}{4}|[A,B]|^2.$$

   From this result show that the uncertainty relation follows

   $$\Delta x\Delta p \geq \frac{\hbar}{2}.$$

3. Put $B = H$ in the above relation and show that

$$\Delta A \Delta H \geq \frac{1}{2}\hbar \left| \frac{d}{dt} \langle A \rangle (t) \right|.$$

Defining the time uncertainty Δt as

$$\frac{1}{\Delta t} = \frac{1}{\Delta A} \left| \frac{d}{dt} \langle A \rangle (t) \right|,$$

show that one obtains

$$\Delta E \Delta t \geq \frac{1}{2}\hbar,$$

which is often called the energy–time uncertainty relation.

4. Use uncertainty relations to estimate the bound-state energies corresponding to
   (i) the linear potential

$$V(r) = Kr;$$

   (ii) the Coulomb potential (hydrogen atom)

$$V(r) = -\frac{Ze^2}{r}.$$

5. Show that the operator in spherical coordinates given by $-i\hbar\partial/\partial r$ is not Hermitian. Consider then the operator

$$-i\hbar \left(\frac{\partial}{\partial r} + \frac{a}{r} \right).$$

Determine a so that it is Hermitian.

6. Show that the operator

$$D = \mathbf{p}.\left(\frac{\mathbf{r}}{r}\right) + \left(\frac{\mathbf{r}}{r}\right).\mathbf{p}$$

is Hermitian. Obtain its explicit form in spherical coordinates. Compare your result with that of problem 5.

7. For the operator D defined above, obtain

$$\text{(i) } [D, x_i], \quad \text{(ii) } [D, p_i], \quad \text{and} \quad \text{(iii) } [D, L_i]$$

where $\mathbf{L}\,(= \mathbf{r} \times \mathbf{p})$ is the angular momentum operator. Also show that

$$e^{i\alpha D/\hbar} x_i e^{-i\alpha D/\hbar} = e^{\alpha} x_i.$$

8. Using the fundamental commutator relation, determine $\left[x, p^2\right]$, $\left[x^2, p\right]$ and $\left[x^2, p^2\right]$.

9. Consider the operator which corresponds to finite displacement

$$F(d) = e^{-ipd/\hbar}.$$

Show that

$$[x, F(d)] = dF(d).$$

If for a state $|\alpha\rangle$ we define $|\alpha_d\rangle = F(d)\,|\alpha\rangle$, then show that the expectation values with respect to the two states satisfy

$$\langle x\rangle_d = \langle x\rangle + d.$$

10. For a Hamiltonian given by

$$H = \frac{p^2}{2m} + V(x),$$

evaluate the commutator $[H, x]$ and the double commutator $[[H, x], x]$. From these derive the following identity involving the energy eigenstates and eigenvalues:

$$\sum_k (E_k - E_n)|\langle k|x|n\rangle|^2 = \frac{\hbar^2}{2m}.$$

11. For a Hamiltonian given by

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}),$$

use the properties of the double commutator $\left[\left[H, e^{i\mathbf{k}\cdot\mathbf{r}}\right], e^{-i\mathbf{k}\cdot\mathbf{r}}\right]$ to obtain

$$\sum_n (E_n - E_s)\,|\langle n|e^{i\mathbf{k}.\mathbf{r}}|s\rangle|^2.$$

3 Dynamical equations

We are now ready to derive the equation of motion of the state vectors and operators that determine the dynamics of a physical system. These equations are considered within the framework of three commonly used pictures: the Schrödinger, the Heisenberg and the interaction pictures.

3.1 Schrödinger picture

Here the motion of the system is expressed in terms of time- and space-variation of the wavefunctions. Consequently the operators in the coordinate representation are expressed in terms of time and space derivatives. The Hamiltonian operator, as we discussed in the preceding section, is expressed as

$$H \rightarrow i\hbar \frac{\partial}{\partial t}. \tag{3.1}$$

The Hamiltonian operator corresponds to the energy of the particle. In other words, if a state $|a_n(t)\rangle$ is an eigenstate of energy, E_n, then it satisfies the eigenvalue equation

$$H\,|a_n(t)\rangle = E_n\,|a_n(t)\rangle \tag{3.2}$$

where the time dependence of the state vector has been made explicit. Therefore,

$$H\,|a_n(t)\rangle = i\hbar \frac{\partial}{\partial t}\,|a_n(t)\rangle = E_n\,|a_n(t)\rangle\,. \tag{3.3}$$

The solution of this equation is quite simple, given by,

$$|a_n(t)\rangle = |a_n(0)\rangle \exp\left(-\frac{iE_n}{\hbar}t\right) \tag{3.4}$$

where we have normalized the eigenvector to its $t = 0$ value.

Confining to one dimension, the eigenfunction in the x-space is given by

$$\phi_n(x,t) = \langle x|\, a_n(t)\rangle. \tag{3.5}$$

Equation (3.4) then reads

$$\phi_n(x,t) = \phi_n(x,0) \exp\left(-\frac{iE_n}{\hbar}t\right). \tag{3.6}$$

We now discuss the properties of the Hamiltonian. In a dynamical system, the motion of a particle is described in terms of the Hamiltonian, H, which is written as

$$H = T + V \tag{3.7}$$

where T is the kinetic energy and V the potential energy. Thus, for a state vector $|\phi\rangle$ one can write

$$H\,|\phi\rangle = T\,|\phi\rangle + V\,|\phi\rangle\,. \tag{3.8}$$

In terms of operators X and P, H is given by

$$H = \frac{P^2}{2m} + V(X) \tag{3.9}$$

where V is assumed to be a function of x only, thus $V(X)\,|x\rangle = V(x)\,|x\rangle$. Implicit in this statement is the assumption that the interaction is local, i.e., $\langle x'|\,V(X)\,|x\rangle = V(x)\delta(x'-x)$. Furthermore, we assume V to be real.

In the coordinate-space the momentum operator, P, is given by

$$P \to -i\hbar\frac{\partial}{\partial x}. \tag{3.10}$$

Writing

$$\langle x\,|\phi(t)\rangle = \phi(x,t) \tag{3.11}$$

and

$$\langle x\,|V(X)|\,\phi(t)\rangle = V(x)\phi(x,t), \tag{3.12}$$

the equation of motion in the Schrödinger picture is then described by the following differential equation for the wavefunction $\phi(x,t)$:

$$i\hbar\frac{\partial\phi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\phi(x,t)}{\partial x^2} + V(x)\phi(x,t). \tag{3.13}$$

This is the classic Schrödinger equation.

If $\phi(x,t)$ is an eigenstate of energy E_n, which we previously designated as $\phi_n(x,t)$, then it satisfies the equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi_n(x,t)}{\partial x^2} + V(x)\phi_n(x,t) = E_n\phi_n(x,t). \tag{3.14}$$

The t-dependence of the energy eigenfunctions is already known from our previous results as

$$\phi_n(x,t) = u_n(x)\exp\left(-\frac{iE_n}{\hbar}t\right) \tag{3.15}$$

where

$$u_n(x) = \phi_n(x, 0). \tag{3.16}$$

The equation for $u_n(x)$ will now be in terms of the total derivative, given by

$$-\frac{\hbar^2}{2m}\frac{d^2u_n(x)}{dx^2} + V(x)u_n(x) = E_n u_n(x). \tag{3.17}$$

This equation can easily be extended to three dimensions by writing

$$-\frac{\hbar^2}{2m}\nabla^2 u_n(\mathbf{r}) + V(\mathbf{r})u_n(\mathbf{r}) = E_n u_n(\mathbf{r}) \tag{3.18}$$

where

$$\nabla^2 = \frac{\partial}{\partial x^2} + \frac{\partial}{\partial y^2} + \frac{\partial}{\partial z^2} \tag{3.19}$$

and

$$u_n(\mathbf{r}) = u_n(x, y, z), \qquad V(\mathbf{r}) = V(x, y, z). \tag{3.20}$$

Solving the above equations for different potentials and boundary conditions will be our task in the coming chapters.

3.2 Heisenberg picture

In the Schrödinger picture the state vectors evolve with time, while the operators are independent of time. In the Heisenberg picture, which we will describe below, the state vectors are fixed in time while the operators evolve as a function of time. The quantities in the two pictures are related to each other, however, due to the fact that the results of any experiment should be the same when described in either of the two pictures.

The Schrödinger picture deals with the equations for the wavefunctions. It is more often used because its framework allows for easier calculations, while the Heisenberg picture effectively involves equations between operators.

We designate the states and the operators in the Schrödinger picture with subscript S, i.e., as $|\alpha_S(t)\rangle$ and A_S respectively. As we have already stated, in this picture the states depend on time, while the operators do not (except for special cases which we ignore). Consider now the matrix element

$$\langle \alpha_S(t) | A_S | \beta_S(t) \rangle. \tag{3.21}$$

From our earlier discussions we can connect $|\alpha_S(t)\rangle$ to $|\alpha_S(0)\rangle$ through the unitary operator $U(t,0) = U(t)$,

$$|\alpha_S(t)\rangle = U(t)\,|\alpha_S(0)\rangle \tag{3.22}$$

where, as we found in the previous section,

$$U(t) = e^{-iHt/\hbar} \tag{3.23}$$

where H is the Hamiltonian, assumed to be independent of time. The matrix element (3.21) can be written as

$$\langle \alpha_S(t)\,|A_S|\,\beta_S(t)\rangle = \left\langle \alpha_S(0)\,\middle|\,U^\dagger(t)A_S U(t)\,\middle|\,\beta_S(0)\right\rangle. \tag{3.24}$$

Let $|\alpha_H\rangle$ be the state vector in the Heisenberg picture. It is independent of time and we define it to be the same as the state vector in the Schrödinger picture at $t = 0$. That is,

$$|\alpha_H\rangle = |\alpha_S(0)\rangle\,. \tag{3.25}$$

As we stated earlier, the measurement of an observable is reflected in the value of the matrix element of the corresponding operator. The matrix elements of an operator in the Schrödinger and Heisenberg pictures must, therefore, be the same, as the result of any measurement must be independent of the type of picture which one uses to describe it. If A_H is the operator in the Heisenberg picture then we must have

$$\langle \alpha_S(t)\,|A_S|\,\beta_S(t)\rangle = \langle \alpha_H\,|A_H|\,\beta_H\rangle\,. \tag{3.26}$$

From (3.22) and (3.23) we conclude that

$$A_H = U^\dagger(t)A_S U(t) = e^{iHt/\hbar}A_S e^{-iHt/\hbar}. \tag{3.27}$$

In the Heisenberg picture, therefore, it is the operators that change as a function of time.

Taking the time-derivatives on both sides of the equation (3.27) above, we obtain

$$\frac{dA_H}{dt} = (iH/\hbar)\left(e^{iHt/\hbar}A_S e^{-iHt/\hbar}\right) + \left(e^{iHt/\hbar}A_S e^{-iHt/\hbar}\right)(-iH/\hbar) \tag{3.28}$$

where we have assumed that A_H does not have any explicit dependence on time. From (3.27) and (3.28) we obtain

$$i\hbar\frac{dA_H}{dt} = [A_H, H]\,. \tag{3.29}$$

Thus, in the Heisenberg representation the time dependence is governed by the commutator of the operator with the Hamiltonian.

In the following we will confine our attention entirely to the Heisenberg picture and suppress the index H. The space and momentum operators, X and P respectively, will then satisfy

$$i\hbar\frac{dX}{dt} = [X, H], \tag{3.30}$$

$$i\hbar\frac{dP}{dt} = [P, H]. \tag{3.31}$$

We see, at once, that if an operator commutes with H, i.e.,

$$[A, H] = 0 \tag{3.32}$$

then A is an "invariant." It stays constant as a function of time and is called the constant of the motion. Since H is given by

$$H = \frac{P^2}{2m} + V(X), \tag{3.33}$$

the evaluation of the right-hand side above proceeds by the application of the fundamental commutator $[X, P]$ (2.20).

The Heisenberg picture plays an important role in many problems, including the harmonic oscillator problem (Chapter 9) among other topics, and in quantum field theory (Chapter 43).

3.3 Interaction picture

The interaction picture accommodates certain aspects of both the Schrödinger and Heisenberg representations and is used most often when the interaction Hamiltonian, representing the potential, depends on time. Consider the following Hamiltonian:

$$H = H_0 + H_I(t) \tag{3.34}$$

where $H_0 (= p^2/2m)$ represents the kinetic energy and is independent of time, while H_I corresponds to the interaction potential, which now depends on time. We have thus replaced $V(X)$ which we used in the previous two pictures by $H_I(t)$.

The time evolution operator $U(t, t_0)$ satisfies the equation

$$\frac{\partial U(t, t_0)}{\partial t} = -i\frac{H}{\hbar}U(t, t_0) = -i\frac{H_0}{\hbar}U(t, t_0) - i\frac{H_I}{\hbar}U(t, t_0). \tag{3.35}$$

We introduce an operator $U_I(t, t_0)$, which is defined as

$$U_I(t, t_0) = e^{iH_0/\hbar(t-t_0)}U(t, t_0). \tag{3.36}$$

Since it is a product of two unitary operators, $U_I(t, t_0)$ is also a unitary operator. Taking the time derivative of both sides we obtain

$$\frac{\partial U_I(t,t_0)}{\partial t} = e^{iH_0/\hbar(t-t_0)}\left(i\frac{H_0}{\hbar}\right)U(t,t_0) + e^{i\frac{H_0}{\hbar}(t-t_0)}\frac{\partial U(t,t_0)}{\partial t}. \tag{3.37}$$

Using (3.35) and (3.36) we obtain

$$\frac{\partial U_I(t,t_0)}{\partial t} = -\frac{i}{\hbar}e^{i\frac{H_0(t-t_0)}{\hbar}}H_I(t)\,e^{-i\frac{H_0(t-t_0)}{\hbar}}U_I(t,t_0). \tag{3.38}$$

We now define

$$H_I'(t) = e^{i\frac{H_0(t-t_0)}{\hbar}}H_I(t)\,e^{-i\frac{H_0(t-t_0)}{\hbar}}. \tag{3.39}$$

The equation for U_I now reads

$$\frac{\partial U_I(t,t_0)}{\partial t} = -\frac{iH_I'(t)}{\hbar}U_I(t,t_0). \tag{3.40}$$

We note from (3.36) that, since $U(t_0,t_0) = \mathbf{1}$, we must have $U_I(t_0,t_0) = \mathbf{1}$. Integrating both sides of (3.40) we obtain

$$U_I(t,t_0) = \mathbf{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,H_I'(t')\,U_I(t',t_0). \tag{3.41}$$

Through recursion of (3.41) we obtain the following series expansion.

$$U_I(t,t_0) = \mathbf{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,H_I'(t') + \left(-\frac{i}{\hbar}\right)^2\int_{t_0}^{t} dt'\,H_I(t')\int_{t_0}^{t'} dt''\,H_I(t'') + \cdots. \tag{3.42}$$

Since the order of integration is unimportant, we can write

$$\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''H_I'(t')\,H_I'(t'') = \int_{t_0}^{t} dt''\int_{t_0}^{t''} dt'\,H_I'(t')\,H_I'(t'). \tag{3.43}$$

Hence

$$\begin{aligned}&\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\,H_I'(t')\,H_I'(t'')\\ &= \frac{1}{2}\left[\int_{t_0}^{t} dt'\int_{t_0}^{t'} dt''\,H_I'(t')\,H_I'(t'') + \int_{t_0}^{t} dt''\int_{t_0}^{t''} dt'\,H_I'(t')\,H_I'(t')\right].\end{aligned} \tag{3.44}$$

To obtain a simple expression for U_I, let us define the "time-ordered product" of two operators $A(t')$ and $B(t'')$ as

$$T\left[A(t')B(t'')\right] = \theta(t'-t'')A(t')B(t'') + \theta(t''-t')B(t'')A(t') \tag{3.45}$$

where the θ-function is defined by

$$\theta\left(t_1 - t_2\right) = 0, \quad t_1 < t_2 \tag{3.46}$$

$$= 1, \quad t_1 > t_2. \tag{3.47}$$

This function is also called a "step-function." The relation (3.43) can then be written as

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \, H_I'\left(t'\right) H_I'\left(t''\right) = \frac{1}{2} \int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' \, T\left(H_I'\left(t'\right) H_I'\left(t''\right)\right) \tag{3.48}$$

where, following the definition (3.45),

$$T\left(H_I'\left(t'\right) H_I'\left(t''\right)\right) = \theta\left(t' - t''\right) H_I'\left(t'\right) H_I'\left(t''\right) + \theta\left(t'' - t'\right) H_I'\left(t''\right) H_I'\left(t'\right). \tag{3.49}$$

We note that the upper limits in the double integral are now the same, which will make it very convenient to write the series.

Even though it is somewhat complicated, one can define the time-ordered product when a product of more than two H_I's is involved. We will not pursue this matter further. For now we note that (3.42) leads to

$$U_I\left(t, t_0\right) = \mathbf{1} + \sum_{n=1}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \, T\left(H_I'\left(t_1\right) H_I'\left(t_2\right) ... H_I'\left(t_n\right)\right). \tag{3.50}$$

One can write this more compactly as

$$U_I\left(t, t_0\right) = T\left(\exp\left[-i \int_{t_0}^{t} dt \, H_I'\left(t'\right)\right]\right) \tag{3.51}$$

since the series in (3.50) is the same as the exponential series. In contrast, in the Schrödinger picture where the Hamiltonian H is independent of time, the time evolution operator is

$$U\left(t, t_0\right) = e^{-i\frac{H}{\hbar}\left(t - t_0\right)}. \tag{3.52}$$

We write $|\alpha_I\left(t\right)\rangle$ as a state vector in the interaction picture, which we normalize by assuming the following relation at $t = 0$ involving the state vectors in the Schrödinger and Heisenberg pictures,

$$|\alpha_I\left(0\right)\rangle = |\alpha_H\rangle = |\alpha_S\left(0\right)\rangle. \tag{3.53}$$

To obtain the time dependence of $|\alpha_I\left(t\right)\rangle$ we employ the unitary operator $U_I\left(t, t_0\right)$. We take $t_0 = 0$ to conform to the initial conditions, and define $U\left(t, 0\right) = U(t)$ and $U_I\left(t, 0\right) = U_I(t)$. From (3.36), and (3.53) we obtain

$$|\alpha_S\left(t\right)\rangle = U(t)\,|\alpha_S\left(0\right)\rangle = e^{-i\frac{H_0 t}{\hbar}} U_I(t)\,|\alpha_S\left(0\right)\rangle = e^{-i\frac{H_0 t}{\hbar}} U_I(t)\,|\alpha_I\left(0\right)\rangle. \tag{3.54}$$

Since the matrix elements of an operator in different pictures must be the same, we have

$$\left\langle \alpha_S(t) \left| A_S \right| \beta_S(t) \right\rangle = \left\langle \alpha_I(t) \left| A_I(t) \right| \beta_I(t) \right\rangle. \tag{3.55}$$

Using (3.54) we obtain

$$\left\langle \alpha_S(t) \left| A_S \right| \beta_S(t) \right\rangle = \langle \alpha_I(0) | U_I^\dagger e^{i\frac{H_0 t}{\hbar}} A_S e^{-i\frac{H_0 t}{\hbar}} U_I \left| \beta_I(0) \right\rangle. \tag{3.56}$$

The definitions of $|\alpha_I(t)\rangle$ and $A_I(t)$ follow quite simply as

$$|\alpha_I(t)\rangle = U_I(t) |\alpha_I(0)\rangle \tag{3.57}$$

and

$$A_I(t) = U_I^\dagger e^{i\frac{H_0 t}{\hbar}} A_S e^{-i\frac{H_0 t}{\hbar}} U_I. \tag{3.58}$$

The relations (3.58) when substituted in (3.56) reproduce (3.55).

To obtain the time dependence of $|\alpha_I(t)\rangle$ we note from the relation of $|\alpha_S(t)\rangle$ given by (3.54) that

$$|\alpha_S(0)\rangle = U_I^\dagger e^{i\frac{H_0 t}{\hbar}} |\alpha_S(t)\rangle. \tag{3.59}$$

Substituting this in (3.53) we obtain

$$|\alpha_I(t)\rangle = e^{i\frac{H_0 t}{\hbar}} |\alpha_S(t)\rangle. \tag{3.60}$$

Taking the derivatives of both sides of (3.60) we obtain

$$\begin{aligned} i\hbar \frac{\partial |\alpha_I(t)\rangle}{\partial t} &= -e^{i\frac{H_0 t}{\hbar}} H_0 |\alpha_S(t)\rangle + e^{i\frac{H_0 t}{\hbar}} i\hbar \frac{\partial}{\partial t} |\alpha_S(t)\rangle \\ &= -e^{i\frac{H_0 t}{\hbar}} H_0 |\alpha_S(t)\rangle + e^{i\frac{H_0 t}{\hbar}} (H_0 + H_I(t)) |\alpha_S(t)\rangle \\ &= e^{iH_0 t/\hbar} H_I(t) |\alpha_S(t)\rangle \\ &= e^{iH_0 t/\hbar} H_I(t) e^{-iH_0 t/\hbar} e^{iH_0 t/\hbar} |\alpha_S(t)\rangle. \end{aligned} \tag{3.61}$$

Hence

$$i\hbar \frac{\partial |\alpha_I(t)\rangle}{\partial t} = H_I'(t) |\alpha_I(t)\rangle. \tag{3.62}$$

We note that $H_I(t)$ and $H_I'(t)$ are operators in the Schrödinger representation:

$$H_I(t) = (H_I(t))_S \qquad \text{and} \qquad H_I'(t) = (H_I(t))_S. \tag{3.63}$$

The time derivative of A_I can be calculated from (3.58). After certain mathematical steps similar to the case of A_H it is found to be

$$i\hbar \frac{dA_I(t)}{dt} = [A_I, H_0]. \tag{3.64}$$

Thus relations (3.62) and (3.64) show that, in the interaction picture, the time dependence of the state vectors is governed by the interaction Hamiltonian, while the time evolution of the operators is determined by the free Hamiltonian.

3.4 Superposition of time-dependent states and energy–time uncertainty relation

Let us assume that an arbitrary state $|\psi(t)\rangle$ can be expanded as a sum of an infinite number of energy eigenstates $|a_n(t)\rangle$. At $t = 0$ we write

$$|\psi(0)\rangle = \sum_n c_n |a_n(0)\rangle \tag{3.65}$$

where

$$\sum_n |c_n|^2 = 1. \tag{3.66}$$

The eigenstates $|a_n(t)\rangle$ are expressed in terms of their eigenvalues E_n as

$$|a_n(t)\rangle = |a_n(0)\rangle \exp(-iE_n t/\hbar). \tag{3.67}$$

Hence

$$|\psi(t)\rangle = \sum_n c_n |a_n(0)\rangle \exp(-iE_n t/\hbar). \tag{3.68}$$

Let us now consider the product $\langle\psi(0)|\psi(t)\rangle$ to determine the evolution of $|\psi(t)\rangle$ with respect to $|\psi(0)\rangle$. We find

$$\langle\psi(0)|\psi(t)\rangle = \sum_n |c_n|^2 \exp(-iE_n t/\hbar). \tag{3.69}$$

We consider this sum for the case of continuous or near continuous values of the energy eigenstates. We note that since $\Delta n = 1$ we can convert the above sum as follows:

$$\sum_n \to \sum_n \Delta n = \sum_n \frac{\Delta n}{\Delta E}\Delta E \to \int dE\, \rho(E) \tag{3.70}$$

where $\rho(E)$ $(= dn/dE)$ is the density of states. We obtain

$$\langle\psi(0)|\psi(t)\rangle = \int dE\, \rho(E)\, |c(E)|^2 \exp(-iEt/\hbar) = \int dE\, g(E) \exp(-iEt/\hbar) \tag{3.71}$$

where $c(E)$ replaces c_n in the continuum limit and

$$g(E) = \rho(E)\, |c(E)|^2, \tag{3.72}$$

which is normalized as

$$\int dE\, g(E) = 1. \tag{3.73}$$

For the purposes of illustration and to simplify our discussion, we assume $g(E)$ to be peaked at $E = E_0$ and write

$$g(E) = g_0 \exp\left[-(E - E_0)^2 / 4(\Delta E)^2\right] \tag{3.74}$$

where ΔE corresponds to the width of the peak. We then write

$$\langle \psi(0) | \psi(t) \rangle = \exp(-iE_0 t/\hbar) g_0 \int dE \exp\left[-(E - E_0)^2 / 4(\Delta E)^2\right] \exp(-i(E - E_0)\, t/\hbar). \tag{3.75}$$

To carry out the integration we make the change of variables

$$(E - E_0) = y \tag{3.76}$$

and take

$$A = \frac{1}{4(\Delta E)^2} \quad \text{and} \quad B = -i\frac{t}{2\hbar}. \tag{3.77}$$

Therefore, the term in the exponent is given by

$$-\frac{(E - E_0)^2}{4(\Delta E)^2} - i\frac{(E - E_0)\, t}{\hbar} = -Ay^2 + 2By \tag{3.78}$$

and the integral can be written as

$$\int dy\, \exp\left[-Ay^2 + 2By\right] = \exp\left[B^2/A\right] \int du\, \exp[-Au^2] \tag{3.79}$$

where

$$u = y - \frac{B}{A}. \tag{3.80}$$

The integral can be obtained quite simply. It is given by

$$\int_{-\infty}^{\infty} du\, \exp[-Au^2] = \sqrt{\frac{\pi}{A}}. \tag{3.81}$$

Hence, using the normalization condition (3.75) we find

$$\langle \psi(0) | \psi(t) \rangle = \exp(-iE_0 t/\hbar) e^{-(\Delta E)^2 t^2/\hbar^2}. \tag{3.82}$$