

QUANTUM LEAPS AND BOUNDS

Introductory Topics

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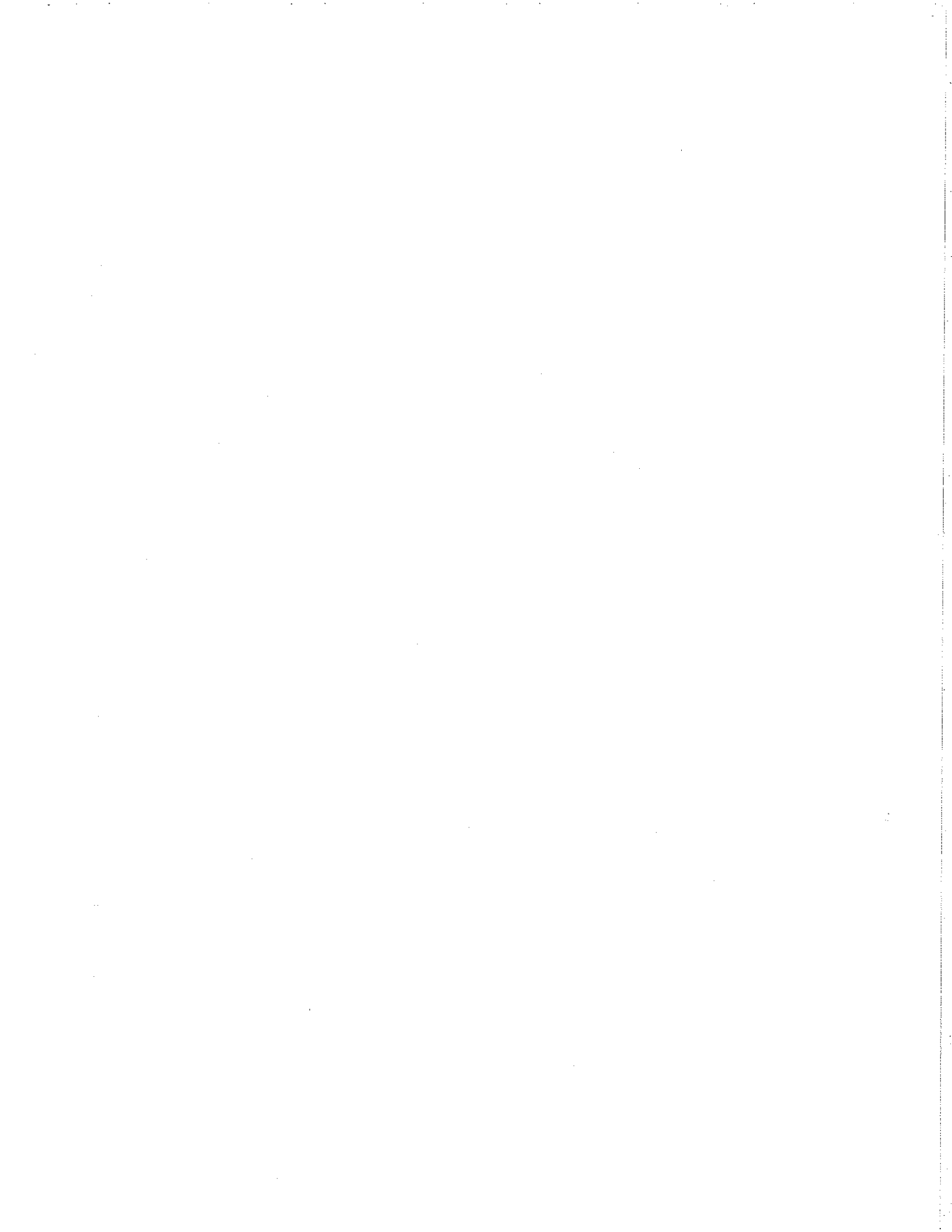
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Preface

The six volumes of notes *Quantum Leaps and Bounds (QLB)* form the basis of the introductory graduate quantum mechanics course I have given in the Department of Physics at the University of British Columbia at various times since 1973.

The six volumes of *QLB* are

- *Introductory Topics*: a collection of miscellaneous topics in introductory quantum mechanics
- *Scattering Theory*: an introduction to the basic ideas of quantum scattering theory by considering the scattering of a relativistic spinless particle from a fixed target
- *Quantum Mechanics in Fock Space*: an introduction to the second-quantization description of nonrelativistic many-body systems
- *Relativistic Quantum Mechanics*: an introduction to incorporating special relativity in quantum mechanics
- *Some Lorentz Invariant Systems*: some examples of systems incorporating special relativity in quantum mechanics
- *Relativistic Quantum Field Theory*: an elementary introduction to the relativistic quantum field theory of spinless bosons, spin $\frac{1}{2}$ fermions and antifermions and to quantum electrodynamics, the relativistic quantum field theory of electrons, positrons and photons

QLB assumes no familiarity with relativistic quantum mechanics. It does assume that students have taken undergraduate courses in nonrelativistic quantum mechanics which include discussion of the nonrelativistic Schrodinger equation and the solutions of some standard problems (e.g., the one-dimensional harmonic oscillator and the hydrogen atom) and perturbation theory and other approximation

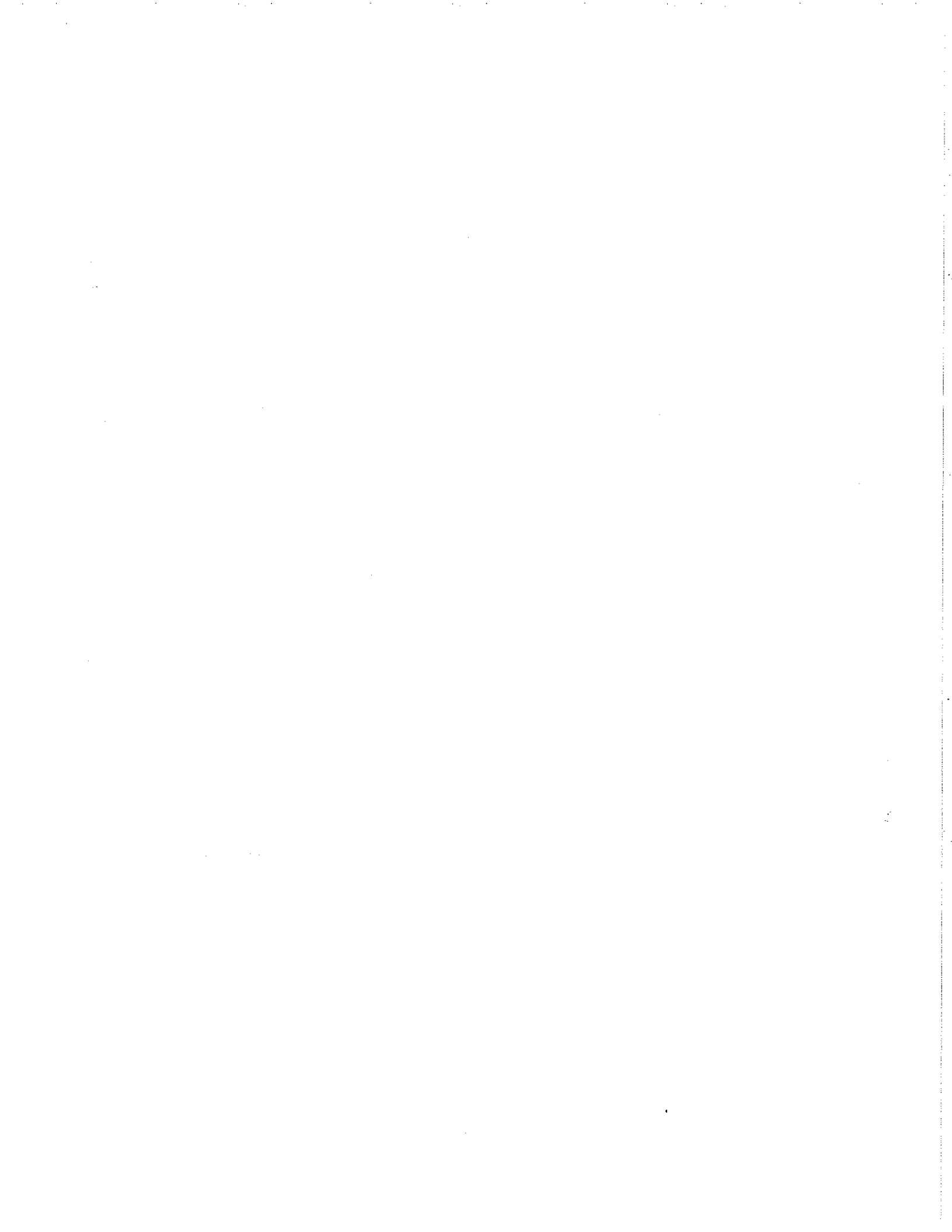
methods.

QLB assumes also that students will take other graduate courses in condensed matter physics, nuclear and particle physics and relativistic quantum field theory. Accordingly, our purpose in *QLB* is to introduce some basic ideas and formalism and thereby give students sufficient background to read the many excellent texts on these subjects.

I am happy to have this opportunity to thank my friends and colleagues I.K. Affleck, R. Barrie, B. Bergersen, M. Bloom, J. Feldman, D.H. Hearn, W.W. Hsieh, R.I.G. Hughes, F.A. Kaempffer, A.H. Monahan, P.A. Kalyniak, R.H. Landau, E.L. Lomon, W. Opechowski, M.H.L. Pryce, A. Raskin, P. Rastall, L. Rosen, G.W. Semenoff, L. Sobrino, F. Tabakin, A.W. Thomas, W.G. Unruh, E.W. Vogt, G.M. Volkoff and N. Weiss for sharing their knowledge of quantum mechanics with me.

I also thank my wife, Henrietta, for suggesting the title for these volumes of notes. Quite correctly, she found my working title *Elements of Intermediate Quantum Mechanics* a bore.

INTRODUCTORY TOPICS



Chapter 1

INTRODUCTORY REMARKS

This volume of *QLB* contains a collection of miscellaneous topics in introductory quantum mechanics. Our purpose here is to define basic concepts and illustrate notation used in all volumes of *QLB* and to give some simple examples of introductory quantum mechanics.

Chapter 2 gives a brief overview of the language, mathematics and machinery of quantum mechanics. Average and uncertainty and pictures of quantum mechanics are discussed more fully in Chapters 3 and 4.

The density operator formalism is discussed in Chapter 5.

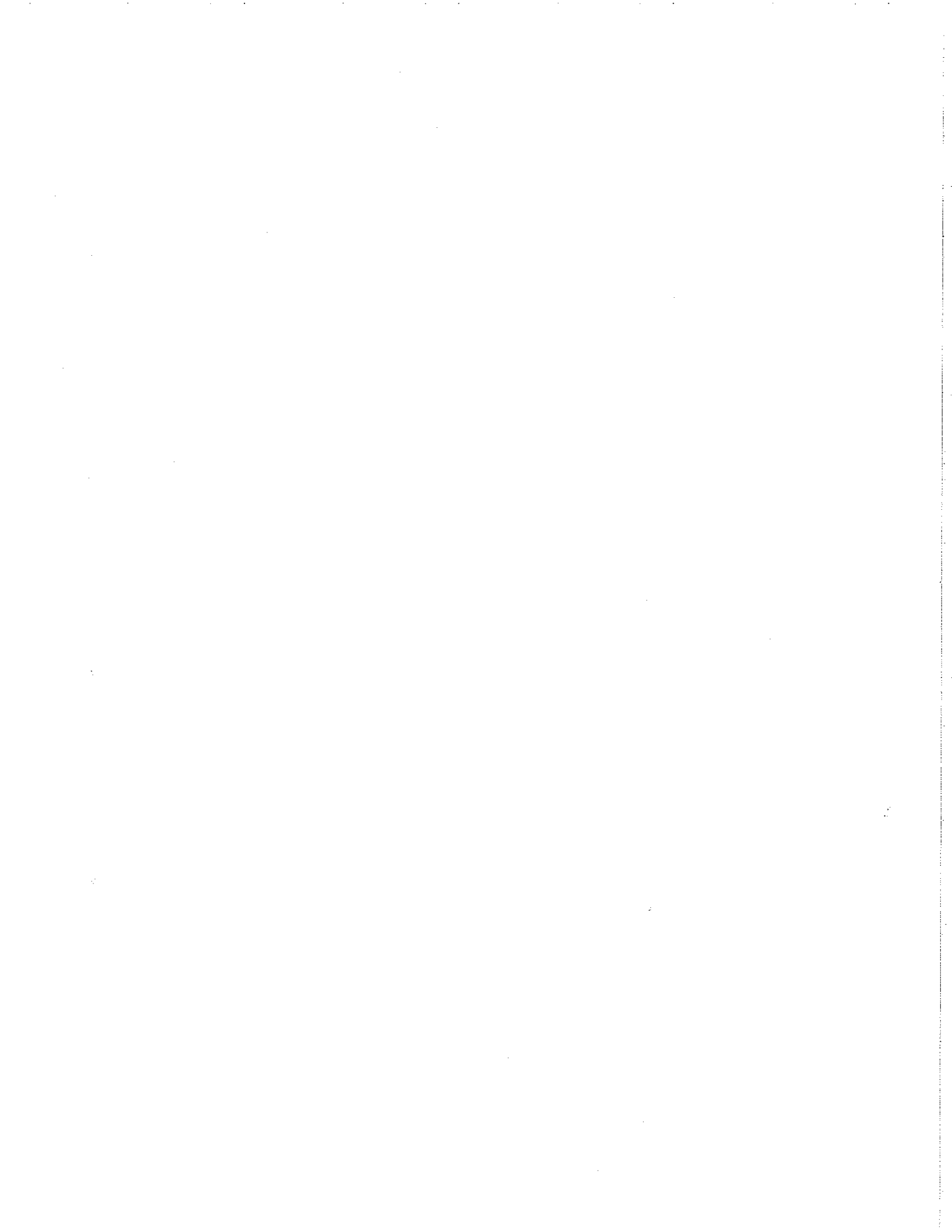
Spin states of a spin $\frac{1}{2}$ and 1 particle are given in Chapters 6 and 7, respectively, and the interaction of a particle with spin with a magnetic field is discussed in Chapter 8.

The mathematical formalism for handling observables with continuous values is discussed in Chapter 9 and the application of this formalism to the special case of a spinless particle confined to move in one dimension is given in Chapter 10.

Ladder operators are defined and discussed in Chapter 11.

The Appendix contains mathematical preliminaries.

The volume concludes with lists of selected reference books, journal articles and theses.



2.1 Introductory remarks

We briefly review the language, mathematics and machinery of quantum mechanics in this chapter.

The language of quantum mechanics is given in Section 2.2; the principles of quantum mechanics are given in Section 2.3; the principles of special relativity are given in Section 2.4; the mathematics of quantum mechanics is given in Section 2.5 and the steps for setting up the machinery of quantum mechanics are given in Section 2.6.

2.2 Language of Quantum Mechanics

1. *Quantum Mechanics* is the description of matter and radiation in all its details and in particular of the happenings on the atomic and subatomic scales. Quantum mechanics deals with states and observables of physical systems. Built into the machinery of quantum mechanics is the notion that a measurement of an observable of a physical system in general disturbs the system and changes its state.
2. A *physical system* is a system of physical objects which can be isolated from the rest of the physical world.
3. A *state* of a physical system is the result of a series of physical manipulations on the system. These manipulations are said to prepare a state of a system or to prepare a system in a state. States are either pure or mixed.
4. A *pure state* of a physical system is characterized by the existence of an experiment which gives a result predictable with certainty when performed

on the system in that state. We generally use lower case Greek letters $|\psi\rangle$, $|\phi\rangle$, $|\chi\rangle$, etc., to denote pure states.

5. A *mixed state* of a physical system is characterized by the absence of any experiment which gives a result predictable with certainty when performed on the system in that state. Mixed states are generally easier to prepare than pure states. We will nevertheless not deal with mixed states in most of *QLB*; unless stated otherwise all states referred to are pure states.¹
6. An *observable* of a physical system is an aspect of the system which is measurable. A measurement consists of the manipulation of apparatuses and the eventual reading or recording of a scale. We generally use upper case Roman letters A , B , C , etc., to denote observables.
7. Observables A and B of a physical system are *compatible* or *simultaneously measurable* if measurement of one subsequent to measurement of the other does not change the state of the system. That is, if a measurement of A yields a and a subsequent measurement of B yields b , then A and B are compatible if a subsequent measurement of A yields a and a subsequent measurement of B yields b .

2.3 Principles of Quantum Mechanics

1. Only *probabilistic statements* about the results of a measurement on a physical system can be made.
2. The *probability* that a system be in the state $|\chi\rangle$ when it is known to be in the state $|\psi\rangle$ is

$$|\langle \chi | \psi \rangle|^2 \quad (2.1)$$

¹ Chapter 5 contains a general description and discussion of mixed states. *QLB: Scattering Theory* Chapter 3 contains a description and discussion of mixed states in scattering theory.

The complex number $\langle \chi | \psi \rangle$ is the **probability amplitude** that the system be in the state $|\chi\rangle$ when it is known to be in the state $|\psi\rangle$.

3. If $|\phi_1\rangle, |\phi_2\rangle, \dots, |\phi_n\rangle$ are all the possible outcomes of a measurement of the state of a system, then for any states $|\chi\rangle$ and $|\psi\rangle$,

$$\langle \chi | \psi \rangle = \sum_{k=1}^n \langle \chi | \phi_k \rangle \langle \phi_k | \psi \rangle \quad (2.2)$$

(2.2) is the **Principle of Superposition**.

2.4 Principles of Special Relativity

1. The laws of physics are the same in all inertial frames.
2. The speed of light in empty space always has the same value.

2.5 Mathematics of Quantum Mechanics

1. A **pure state** of a physical system corresponds to a **unit norm vector** on a separable Hilbert space. Unit vectors which differ only by a phase factor describe the same state. We use the same symbol to denote both the state and the corresponding vector.
2. A **mixed state** of a physical system corresponds to a nonidempotent, unit trace, nonnegative Hermitian operator (**density operator**) on a separable Hilbert space. A mixed state cannot be represented by a unit norm vector.
3. An **observable** of a physical system corresponds to a **Hermitian operator** on a separable Hilbert space. We use the same symbol to denote both the observable and the corresponding Hermitian operator.

4. A *measurement* of the observable A yields one of the *spectral values* a of A . Every spectral value a of A is a possible result of a measurement of A if a system is in a general state $|\psi\rangle$ prior to the measurement of A .
5. If a is an *eigenvalue* of A , the probability of obtaining the value a on measurement of A for a system in the state $|\psi\rangle$ is

$$|\langle \phi_a | \psi \rangle|^2 \quad (2.3)$$

where $|\phi_a\rangle$ is the *eigenvector* of A belonging to eigenvalue a .

The system is in the state $|\phi_a\rangle$ immediately after the measurement of A . $|\phi_a\rangle$ is an *eigenstate* of A .

A measurement in general disturbs a system such that it causes a change in the state of the system. If a system is in an eigenstate $|\phi_a\rangle$ before the measurement of A , however, then measurement of A yields a with certainty and the state of the system is not changed by the measurement.

6. If a is a *continuous spectral value*¹ of A , the probability of obtaining a value in the range $(a, a + da)$ on measurement of A for a system in the state $|\psi\rangle$ is

$$|\psi(a)|^2 da \quad (2.4)$$

where

$$\psi(a) = \langle a | \psi \rangle \quad (2.5)$$

¹ Observables with continuous spectra are discussed more fully in Chapter 9.

and where $|a\rangle$ is the *eigenket* of A corresponding to spectral value a . The system is in the state

$$\int_a^{a+da} da |a\rangle \psi(a) \quad (2.6)$$

immediately after the measurement of A .

7. If a measurement of A for a system in the state $|\psi\rangle$ is made a large number of times (by which one means: first prepare a system in the state $|\psi\rangle$, then measure A , then prepare the system in the state $|\psi\rangle$ again, then measure A again, and so on¹), then

$$\bar{A} = \langle \psi | A | \psi \rangle \quad (2.7)$$

is the *average* of the results obtained.²

8. The *uncertainty* ΔA in the result of measurement of A for a system in the state $|\psi\rangle$ is the root mean square deviation of A . That is,³

$$\Delta A = \sqrt{\langle \psi | (A - \bar{A})^2 | \psi \rangle} = \| (A - \bar{A}) | \psi \rangle \| \quad (2.8)$$

¹ One does not always do it this way in practice. For example, as discussed in *QLB: Scattering Theory*, for experimental efficiency in scattering experiments, one prepares a beam of identical particles and directs this beam at a target of identical particles.

² Average is discussed more fully in Chapter 3.

³ Uncertainty is discussed more fully in Chapter 3.

Alternatively,

$$\Delta A = \sqrt{A^2 - (\overline{A})^2} \quad (2.9)$$

9. For a measurement of two observables A and B for a system in the state $|\psi\rangle$, the uncertainties ΔA and ΔB obey the *uncertainty relation*

$$(\Delta A)(\Delta B) \geq \frac{1}{2} |\overline{[A, B]}| \quad (2.10)$$

where

$$[A, B] = AB - BA \quad (2.11)$$

is the *commutator* of A and B .¹

- i) A and B are *compatible observables* if and only if

$$[A, B] = 0 \quad (2.12)$$

The commutator is therefore a basic mathematical entity in QM since it displays which observables of a physical system are compatible.

¹ (2.10) is derived in Chapter 3. It is shown also how (2.10) leads to the time-energy uncertainty relation.

ii) $|\psi_{opt}\rangle$ is an *optimum state* of A and B if the equality in (2.10) holds.

$|\psi_{opt}\rangle$ satisfies the eigenvalue equation¹

$$\left(\frac{A - \bar{A}}{\Delta A} + i \frac{B - \bar{B}}{\Delta B} \right) |\psi_{opt}\rangle = 0 \quad (2.13)$$

where A and B are chosen such that

$$[\overline{A, B}] = i | [A, B] | \quad (2.14)$$

10. The physical content of quantum mechanics is unchanged if every state $|\psi\rangle$ and every observable A of a physical system are replaced by

$$U |\psi\rangle \quad (2.15)$$

$$UAU^\dagger \quad (2.16)$$

where U is a linear unitary operator or an antilinear antiunitary operator. Each U is thus said to provide a *picture* of quantum mechanics.²

Except where explicitly noted, we always use the *Schrodinger picture* of quantum mechanics, that is, the picture of quantum mechanics where the states of the system change with time and observables which are not explicitly time-dependent remain unchanged in time.

¹ (2.13) is derived in Chapter 3.

² Pictures of quantum mechanics are discussed more fully in Chapter 4.

The *Heisenberg picture* of quantum mechanics, where observables of the system change with time and states remain unchanged in time, will be used occasionally. It will be clear from the context when the Heisenberg picture is being used.

2.6 Machinery of Quantum Mechanics

In order to describe a given physical system using quantum mechanics one does the following:

1. Specify a set of *fundamental dynamical variables* for the system. This is a complete set of independent operators in terms of which all observables of the system can be expressed.
2. Specify the *fundamental algebra* of the set of fundamental dynamical variables. This is a set of algebraic relations satisfied by the set of fundamental dynamical variables.
3. Select a *complete set of compatible observables* for the system.
4. Specify the *Hilbert space* of the system through spectral resolution of the complete set of compatible observables. Thus one constructs an orthonormal basis for the space, each basis ket being a simultaneous eigenvector or simultaneous eigenket of all elements of the set of compatible observables.
5. For a Lorentz invariant¹ or Galilei invariant physical system, determine the *Poincare generators* or *Galilei generators* for the system in terms of the fundamental dynamical variables. In particular, determine the *Hamiltonian* and the *evolution operator* for the system.

There are, unfortunately, no general rules for the accomplishment of these steps.

¹ Lorentz invariant systems are discussed in *QLB: Relativistic Quantum Mechanics*.

Chapter 3 AVERAGE AND UNCERTAINTY

3.1 Introductory remarks

In this chapter we prove various statements about the average and uncertainty of an observable which were stated without proof in Chapter 2. In particular, the eigenvalue equation for the optimum state of two observables is derived and the time-energy uncertainty relation is derived and discussed.

3.2 Average

It is stated in Chapter 2 that if a measurement of an observable A for a physical system in the state $|\psi\rangle$ is made a large number of times then the average \bar{A} of the results obtained is given by (2.7).

Verification of (2.7)

We verify that (2.7) holds for a physical system which can be described in an n -dimensional vector space. The verification for a physical system described in an infinite-dimensional separable Hilbert space is given in Chapter 9.

Central to the description and analysis of a system whose observables have at most n values is:

The Eigenvalue Decomposition Theorem for Hermitian Operators

Every Hermitian operator A defined on an n -dimensional vector space can be written in the form

$$A = \sum_{k=1}^n | a_k \rangle a_k \langle a_k | \quad (3.1)$$

where

$$1 = \sum_{k=1}^n | a_k \rangle \langle a_k | \quad (3.2)$$

$$\langle a_k | a_{k'} \rangle = \delta_{kk'} \quad (3.3)$$

The real numbers a_1, a_2, \dots, a_n are the eigenvalues of A belonging to the eigenvectors $| a_1 \rangle, | a_2 \rangle, \dots, | a_n \rangle$ of A .

(3.2) states that $| a_1 \rangle, | a_2 \rangle, \dots, | a_n \rangle$ span the vector space.

The probability $P(a_k)$ of obtaining the value a_k on measurement of A for the system in the state $| \psi \rangle$ is

$$P(a_k) = \langle \psi | a_k \rangle \langle a_k | \psi \rangle = |\langle a_k | \psi \rangle|^2 \quad (3.4)$$

It follows from (3.2) that

$$\sum_{k=1}^n P(a_k) = \sum_{k=1}^n \langle \psi | a_k \rangle \langle a_k | \psi \rangle = \langle \psi | \psi \rangle = 1 \quad (3.5)$$

as required.

If measurement of A for the system in the state $|\psi\rangle$ is made a large number of times, the average \bar{A} of the results obtained is

$$\bar{A} = \sum_{k=1}^n a_k |\langle a_k | \psi \rangle|^2 \quad (3.6)$$

It follows from (3.1) and (3.6) that

$$\begin{aligned} \bar{A} &= \sum_{k=1}^n a_k |\langle a_k | \psi \rangle|^2 = \sum_{k=1}^n a_k \langle \psi | a_k \rangle \langle a_k | \psi \rangle \\ &= \langle \psi | \sum_{k=1}^n | a_k \rangle a_k \langle a_k | \psi \rangle = \langle \psi | A | \psi \rangle \end{aligned} \quad (3.7)$$

which is (2.7).

3.3 Uncertainty

It is stated in Chapter 2 that for a measurement of two observables A and B for a physical system in the state $|\psi\rangle$, the uncertainties ΔA and ΔB obey (2.10). This statement is proved below.

Proof of (2.10)

Let

$$\tilde{A} = A - \bar{A} \quad (3.8)$$

It follows from (2.8) and from Schwartz's inequality that

$$\begin{aligned} (\Delta A)(\Delta B) &= \| \tilde{A}\psi \| \| \tilde{B}\psi \| \\ &\geq | \langle \tilde{A}\psi | \tilde{B}\psi \rangle | = | \langle \psi | \tilde{A}\tilde{B} | \psi \rangle | \end{aligned} \quad (3.9)$$

Now

$$\tilde{A}\tilde{B} = \frac{1}{2} \{ \tilde{A}, \tilde{B} \} + \frac{1}{2} [\tilde{A}, \tilde{B}] \quad (3.10)$$

and

$$[\tilde{A}, \tilde{B}] = [A, B] \quad (3.11)$$

so

$$\langle \psi | \tilde{A}\tilde{B} | \psi \rangle = \frac{1}{2} \langle \psi | \{ \tilde{A}, \tilde{B} \} | \psi \rangle + \frac{1}{2} \langle \psi | [A, B] | \psi \rangle \quad (3.12)$$

Now

$$\langle \psi | \{ \tilde{A}, \tilde{B} \} | \psi \rangle \quad \text{is a real number} \quad (3.13)$$

and

$$\langle \psi | [A, B] | \psi \rangle \quad \text{is an imaginary number} \quad (3.14)$$

since $\{ \tilde{A}, \tilde{B} \}$ and $i[A, B]$ are Hermitian.

It follows from (3.12) to (3.14) that

$$\begin{aligned} | \langle \psi | \tilde{A}\tilde{B} | \psi \rangle | &= \frac{1}{2} \sqrt{ \left(\langle \psi | \{ \tilde{A}, \tilde{B} \} | \psi \rangle \right)^2 + \left(\langle \psi | [A, B] | \psi \rangle \right)^2 } \\ &\geq \frac{1}{2} | \langle \psi | [A, B] | \psi \rangle | = \frac{1}{2} | \overline{[A, B]} | \end{aligned} \quad (3.15)$$

(2.10) follows from (3.9) and (3.15).

3.4 Optimum state

$|\psi_{opt}\rangle$ is an optimum state of A and B when the equality in (2.10) holds. That is,

$$(\Delta A)(\Delta B) = \frac{1}{2} |\overline{[A, B]}| \quad (3.16)$$

when the system is in the state $|\psi_{opt}\rangle$.

It is stated in Chapter 2 that $|\psi_{opt}\rangle$ satisfies (2.13). This statement is proved below.

Proof of (2.13)

It follows from the proof of (2.10) that (3.16) holds if and only if

$$\|\tilde{A}\psi\| \|\tilde{B}\psi\| = |\langle \tilde{A}\psi | \tilde{B}\psi \rangle| \quad (3.17)$$

and

$$\langle \psi | \{\tilde{A}, \tilde{B}\} | \psi \rangle = 0 \quad (3.18)$$

where \tilde{A} is defined by (3.8).

(3.17) holds if and only if

$$|\tilde{B}\psi\rangle = \lambda |\tilde{A}\psi\rangle \quad (3.19)$$

where λ is a constant, and substitution of (3.19) into (3.18) yields

$$(\lambda + \lambda^*) \langle \tilde{A}\psi | \tilde{A}\psi \rangle = 0 \quad (3.20)$$

(3.20) holds if $\lambda = ir$ where r is real, substitution of which into (3.19) yields

$$\tilde{B} |\psi\rangle = ir \tilde{A} |\psi\rangle \quad (3.21)$$

and

$$\langle \psi | \tilde{B} = -ir \langle \psi | \tilde{A} \quad (3.22)$$

(2.13) follows from (3.21) and (3.22).

Comments

1. Compatible observables

(3.19) and (3.20) hold also if

$$\tilde{A} |\psi\rangle = 0 \quad (3.23)$$

and

$$\tilde{B} |\psi\rangle = 0 \quad (3.24)$$

(3.23) and (3.24) are a special case of (2.13).

In this case, $|\psi\rangle$ is a simultaneous eigenvector of A and B and \bar{A} and \bar{B} are the corresponding eigenvalues.

(3.23) and (3.24) hold when A and B are compatible observables, that is, when

$[A, B] = 0$ (3.25)
--

2. Optimum state of position and momentum

The coordinate-space wave function for the optimum state of position and momentum of a particle with rest mass m and spin s is a gaussian function.

This fact is demonstrated in Chapter 10 for a spinless particle confined to move in one dimension.

3.5 Time-energy uncertainty relation

We show that

$$(\Delta E)(\Delta t_{min}(t)) \geq \frac{1}{2}\hbar \quad (3.26)$$

where ΔE is the uncertainty in the energy of the system and $\Delta t_{min}(t)$ is the smallest time interval required at time t to measure a change in the system.

(3.26) is the time-energy uncertainty relation.

Proof of (3.26)

The proof involves the uncertainty relation (2.10) and equation (4.7) for the average.

Choosing $B = H$ in (2.10) and writing $\Delta H = \Delta E$, it follows from (2.10) and (4.7) that

$$(\Delta E)(\Delta A) \geq \frac{1}{2}\hbar \left| \frac{d\bar{A}(t)}{dt} \right| \quad (3.27)$$

On defining $\Delta t_A(t)$ by

$$\left| \frac{d\bar{A}(t)}{dt} \right| = \frac{\Delta A}{\Delta t_A(t)} \quad (3.28)$$

(3.27) becomes

$$(\Delta E)(\Delta t_A(t)) \geq \frac{1}{2}\hbar \quad (3.29)$$

(3.29) holds for every observable A of the system.

(3.26) follows from (3.29) where $\Delta t_{min}(t)$ be the minimum $\Delta t_A(t)$ for all A .

Comments

1. The meaning of $\Delta t_A(t)$ and $\Delta t_{min}(t)$

It follows from (3.28) that $\Delta t_A(t)$ is the time interval required at time t for the average \bar{A} of A to be changed by the uncertainty ΔA of A .

$\Delta t_A(t)$ is the time interval required at time t to measure a change in \bar{A} .

$\Delta t_{min}(t)$ is the smallest time interval required at time t to measure a change in the average value of some observable of the system.

$\Delta t_{min}(t)$ is the smallest time interval required at time t to measure a change in the system.

2. State whose energy is uncertain

It follows from (3.26) that

- i. if the system is in a state such that the uncertainty in the energy is ΔE , then it takes a time interval of at least

$$\frac{1}{2} \hbar / \Delta E \quad (3.30)$$

to measure a change in the system.

- ii. if it takes a time interval of at least Δt to measure a change in the system, then the system is in a state such that the uncertainty in the energy is

$$\frac{1}{2}\hbar/\Delta t \quad (3.31)$$

3. Comparison with momentum-position uncertainty relations

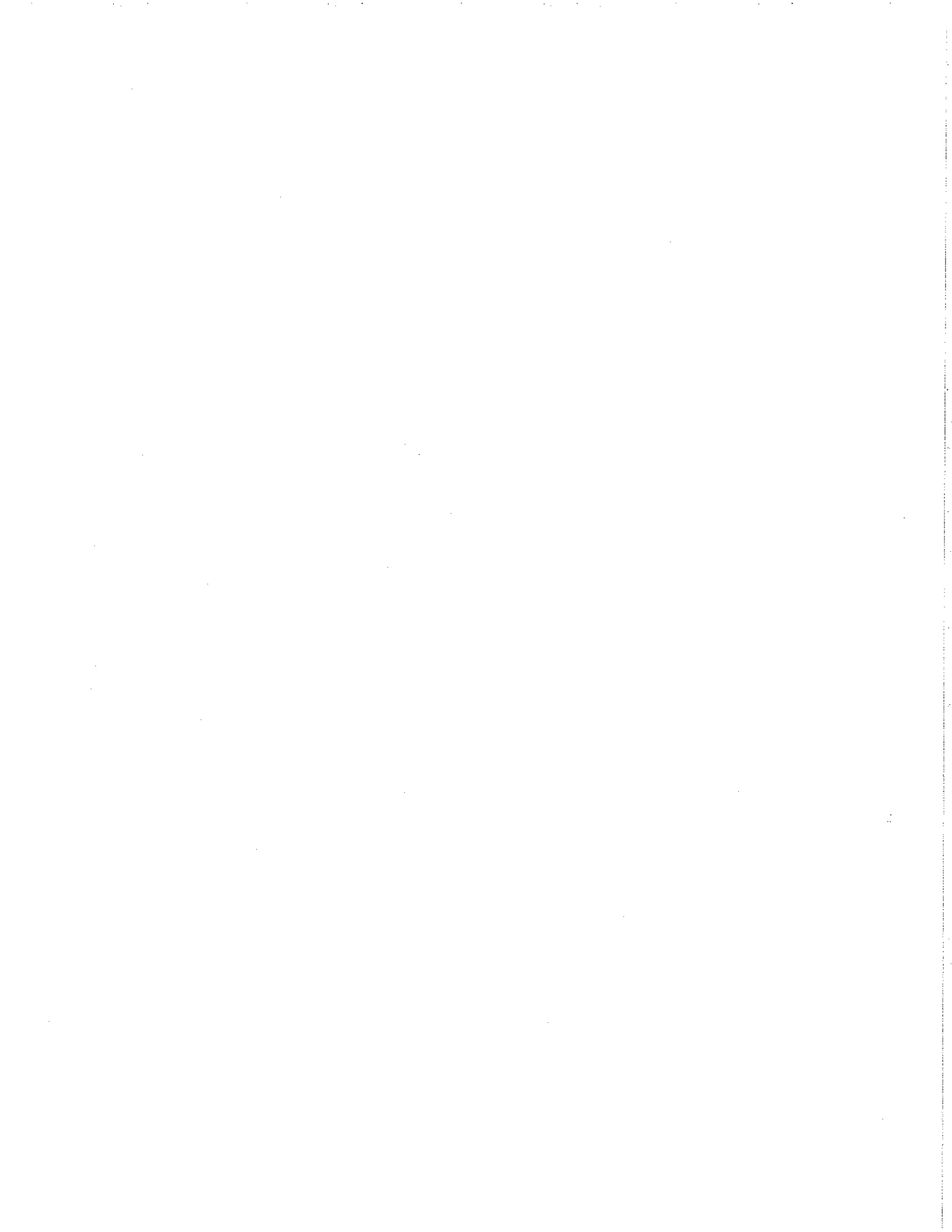
As stated in *QLB: Relativistic Quantum Mechanics* Chapter 6, Heisenberg's Uncertainty Relation for centre of mass motion of a system is

$$(\Delta\hat{X}^j)(\Delta P^k) \geq \frac{1}{2}\hbar\delta_{jk} \quad (3.32)$$

where $\vec{\hat{X}}$ is the centre of mass position of the system and \vec{P} is total momentum of the system.

Given that H/c and \vec{P} are the components of the energy-momentum four-vector, one is tempted to try to package (3.26) and (3.32) into an equation involving a space-time four-vector. As tempting as this is, it does not work because of the asymmetry of position and time in quantum mechanics: $\vec{\hat{X}}$, like \vec{P} and H , is an operator and time is a parameter. This asymmetry is reflected in the derivations of (3.26) and (3.32): the former requiring an interpretation of $\Delta t_{min}(t)$ and the latter following immediately from (2.10) and the fundamental equation

$$[\hat{X}^j, P^k] = i\hbar\delta_{jk} \quad (3.33)$$



4.1 Introductory remarks

The physical content of quantum mechanics is unchanged if every state $|\psi\rangle$ and every observable A of a physical system are replaced by

$$U |\psi\rangle \tag{4.1}$$

$$UAU^\dagger \tag{4.2}$$

where U is a linear unitary operator or an antilinear antiunitary operator. Each U is thus said to provide a picture of quantum mechanics.

In this chapter we consider three pictures of quantum mechanics: the Schrodinger picture, the Heisenberg picture and the interaction (or mixed) picture.

The Schrodinger picture is generally the easiest to conceptualize and work with.

The Heisenberg picture is useful for defining observables (velocity, force, torque) which are time rates of change of other observables.

The interaction picture is useful when there is a natural separation of the Hamiltonian for the system into a simple part and another part (the interaction) which might not be simple.

Except where explicitly noted, the Schrodinger picture is always used in *QLB*.

For simplicity in this chapter, we only consider observables which do not depend explicitly upon time.

4.2 Schrodinger picture

In the Schrodinger picture, an observable of the system is constant in time and a state of the system evolves in time according to

$$|\psi(t)\rangle = U(t) |\psi\rangle \quad (4.3)$$

$|\psi\rangle$ is the state of the system at time zero, $|\psi(t)\rangle$ is the state of the system at time t and

$$U(t) = e^{-iHt/\hbar} \quad (4.4)$$

is the evolution operator for the system. H is the Hamiltonian for the system.

The average $\bar{A}(t)$ of an observable A for the system in the state $|\psi(t)\rangle$ is

$$\bar{A}(t) = \langle \psi(t) | A | \psi(t) \rangle \quad (4.5)$$

It follows on differentiating (4.3) with respect to t that $|\psi(t)\rangle$ satisfies the Schrodinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle \quad (4.6)$$

It follows on differentiating (4.5) with respect to t that $\overline{A}(t)$ satisfies

$$i\hbar \frac{d}{dt} \overline{A}(t) = \overline{[A, H]} \quad (4.7)$$

4.3 Heisenberg picture

In the Heisenberg picture, a state of the system is constant in time and an observable of the system evolves in time according to

$$A(t) = U^\dagger(t) A U(t) \quad (4.8)$$

It follows from (4.3), (4.5) and (4.8) that the average $\overline{A}(t)$ of the observable $A(t)$ for the system in the state $|\psi\rangle$ is

$$\overline{A}(t) = \langle \psi | A(t) | \psi \rangle \quad (4.9)$$

It follows on differentiating (4.8) with respect to t that $A(t)$ satisfies the Heisenberg equation

$$i\hbar \frac{dA(t)}{dt} = [A(t), H] \quad (4.10)$$

4.4 Interaction picture

The interaction picture (or mixed picture) provides an alternative to the Schrodinger and Heisenberg pictures when the Hamiltonian H is written as

$$H = H_0 + H_1 \quad (4.11)$$

The evolution operator (4.4) is written as

$$U(t) = U_0(t)U_1(t) \quad (4.12)$$

$$U_0(t) = e^{-iH_0t/\hbar} \quad (4.13)$$

States and observables evolve in time in the interaction picture. A state evolves in time according to

$$|\psi'(t)\rangle = U_1(t)|\psi\rangle \quad (4.14)$$

An observable evolves in time according to

$$A'(t) = U_0^\dagger(t)AU_0(t) \quad (4.15)$$

The average $\bar{A}(t)$ of the observable $A'(t)$ for the system in the state $|\psi'(t)\rangle$ is

$$\bar{A}(t) = \langle \psi'(t) | A'(t) | \psi'(t) \rangle \quad (4.16)$$

$|\psi'(t)\rangle$ and $A'(t)$ satisfy

$$i\hbar \frac{d}{dt} |\psi'(t)\rangle = H_1'(t) |\psi'(t)\rangle \quad (4.17)$$

$$i\hbar \frac{dA'(t)}{dt} = [A'(t), H_0] = U_0^\dagger(t) [A, H_0] U_0(t) \quad (4.18)$$

Proof of (4.14), (4.15), (4.16) and (4.18)

(4.14), (4.15) and (4.16) follow on substituting (4.3) and (4.12) into (4.5):

$$\begin{aligned} \bar{A}(t) &= \langle \psi(t) | A | \psi(t) \rangle \\ &= \langle U(t)\psi | A | U(t)\psi \rangle = \langle U_0(t)U_1(t)\psi | A | U_0(t)U_1(t)\psi \rangle \quad (4.19) \\ &= \langle U_1(t)\psi | U_0^\dagger(t)AU_0(t) | U_1(t)\psi \rangle = \langle \psi'(t) | A'(t) | \psi'(t) \rangle \end{aligned}$$

(4.18) follows on differentiating (4.15) with respect to t .

Proof of (4.17)

It follows from (4.4) and (4.13) that

$$i\hbar \frac{d}{dt} U(t) = HU(t) \quad (4.20)$$

$$i\hbar \frac{d}{dt} U_0(t) = H_0 U_0(t) \quad (4.21)$$

and from (4.12) and (4.21) that

$$\begin{aligned} i\hbar \frac{d}{dt} U(t) &= i\hbar \frac{d}{dt} U_0(t) U_1(t) \\ &= i\hbar \frac{dU_0(t)}{dt} U_1(t) + i\hbar U_0(t) \frac{dU_1(t)}{dt} \\ &= H_0 U_0(t) U_1(t) + i\hbar U_0(t) \frac{dU_1(t)}{dt} \end{aligned} \quad (4.22)$$

It follows from (4.11), (4.12), (4.20) and (4.22) that

$$i\hbar U_0(t) \frac{dU_1(t)}{dt} = (H - H_0) U_0(t) U_1(t) = H_1 U_0(t) U_1(t) \quad (4.23)$$

from which

$$i\hbar \frac{dU_1(t)}{dt} = U_0^\dagger(t) H_1 U_0(t) U_1(t) = H_1'(t) U_1(t) \quad (4.24)$$

using (4.15). (4.17) follows from (4.14) and (4.24).

5.1 Introductory remarks

The development of quantum mechanics in *QLB* refers for the most part to pure states of a physical system, that is, to states which can be represented mathematically by unit norm vectors in the Hilbert space for the system. This is done merely for convenience in writing. It should be noted that pure states are special states of a physical system: a pure state is characterized by the existence of an experiment which gives a result predictable with certainty when performed on the system in that state. For example, a pure spin state of a particle can be produced by a Stern-Gerlach apparatus since a subsequent experiment with a Stern-Gerlach apparatus can give a result predictable with certainty when performed on a particle in one of the outgoing beams from the first apparatus.

Other states of a system (mixed states) can be prepared and in some cases are easier to prepare. A mixed state results from an incomplete specification of the state of the system by a preparation apparatus; it results from using an inefficient preparation apparatus. A mixed state is characterized by the absence of any experiment which gives a result predictable with certainty when performed on the system in that state. For example, a mixed spin state of a particle will be produced by a “fuzzy” Stern-Gerlach apparatus, that is, by a Stern-Gerlach apparatus which does not have a sufficiently strong magnetic field gradient to produce cleanly separated beams of outgoing particles. No experiment gives a result predictable with certainty when performed on a state prepared by a fuzzy Stern-Gerlach apparatus. Mixed states of spin $\frac{1}{2}$ and spin 1 particles are discussed in Chapters 6 and 7.

A mixed state is represented mathematically by a nonidempotent density operator in the Hilbert space for the physical system. It cannot be represented by a single unit norm vector. Built into the nonidempotent density operator is a set of probabilities which are characterize the preparation apparatus.

We describe the density operator formalism of quantum mechanics in this chapter. The formalism was originally developed by von Neumann in the 1930's; the standard reference is Fano (1957).

The density operator for a pure state is defined in Section 5.2. It is defined in terms of the state vector for the system.

The formalism developed in Section 5.2 for pure states is extended in Section 5.3 to include mixed states. The extended formalism makes no reference to the state vector for the system.

The entropy of a state is defined in Section 5.4. Entropy is a number which characterizes the extent to which a state is mixed; it is a measure of the mixedness of a state.

The density operator for a state with given average energy is given in Section 5.5. The density operator is expressed in terms of the temperature and the partition function. The density operator so defined is appropriate for describing a physical system in thermodynamic equilibrium with its surroundings. The probabilities which are built into the density operator are the Boltzmann factors.

Derivations of some results are given in Section 5.6.

For simplicity throughout this chapter we consider a physical system which can be described in an n -dimensional vector space.

5.2 Density operator for a pure state

A pure state of a physical system may be represented mathematically by a single unit norm vector in the Hilbert space for the physical system.

The density operator $\Psi(t)$ for a pure state at time t is defined as

$$\Psi(t) = |\psi(t)\rangle\langle\psi(t)| \quad (5.1)$$

where $|\psi(t)\rangle$ is the state vector for the system at time t .

Probabilities and averages

We give expressions for probabilities and averages in terms of density operators. Proofs of these expressions are given in Section 5.6.

1. Probability of a state

The probability $P(\chi, \psi, t)$ that a system be found in the state $|\chi(t)\rangle$ when it is known to be in the state $|\psi(t)\rangle$ is

$$P(\chi, \psi, t) = |\langle\chi(t)|\psi(t)\rangle|^2 \quad (5.2)$$

(5.2) may be written equivalently as

$$P(\chi, \Psi, t) = \langle\chi(t)|\Psi(t)|\chi(t)\rangle \quad (5.3)$$

and as

$$P(X, \Psi, t) = \text{Tr}(X(t)\Psi(t)) \quad (5.4)$$

where $X(t) = |\chi(t)\rangle\langle\chi(t)|$ is the density operator corresponding to $|\chi(t)\rangle$.

2. Probability of a value

The probability $P(a_k, \psi, t)$ of observing the value a_k on measurement of A for the system in the state $|\psi(t)\rangle$ is

$$P(a_k, \psi, t) = |\langle a_k | \psi(t) \rangle|^2 \quad (5.5)$$

where $|a_k\rangle$ is the eigenvector of A belonging to eigenvalue a_k .

(5.5) may be written equivalently as

$$P(a_k, \Psi, t) = \langle a_k | \Psi(t) | a_k \rangle \quad (5.6)$$

and as

$$P(a_k, \Psi, t) = \text{Tr}(A_k \Psi(t)) \quad (5.7)$$

where $A_k = |a_k\rangle\langle a_k|$ is the density operator corresponding to $|a_k\rangle$.

3. Average

The average $\bar{A}(t)$ of measurement of A for the system in the state $|\psi(t)\rangle$ is

$$\bar{A}(t) = \langle \psi(t) | A | \psi(t) \rangle \quad (5.8)$$

(5.8) may be written equivalently as

$$\bar{A}(t) = \text{Tr} (A\Psi(t)) \quad (5.9)$$

Comments

1. Mathematical representation of pure states

(5.4), (5.7) and (5.9) express the physical content of quantum mechanics.

(5.4), (5.7) and (5.9) show that the physical content of quantum mechanics for pure states can be expressed entirely in terms of density operators.

Accordingly, a pure state of a physical system corresponds mathematically to a unit norm vector or, equivalently, to an idempotent density operator.

The mathematical properties of the density operator for a pure state are given in Topic 5.2.2.

Properties of the pure state density operator

It follows from definition (5.1) that

I. $\Psi(t)$ evolves in time according to

$$\Psi(t) = U(t)\Psi(0)U^\dagger(t) \quad (5.10)$$

where $U(t) = e^{-iHt/\hbar}$ is the evolution operator for the system.

II. $\Psi(t)$ is Hermitian.

$$\Psi^\dagger(t) = \Psi(t) \quad (5.11)$$

III. $\Psi(t)$ has unit trace.

$$\text{Tr}(\Psi(t)) = 1 \quad (5.12)$$

IV. $\Psi(t)$ is non-negative.

$$\langle \phi | \Psi(t) | \phi \rangle \geq 0 \quad (5.13)$$

for all $|\phi\rangle$.

V. $\Psi(t)$ is idempotent.

$$\Psi^2(t) = \Psi(t) \quad (5.14)$$

5.3 Density operator for a mixed state

In this section we extend the density operator formalism developed in Section 5.2 for pure states to include mixed states of a physical system.

We assume that

The state of the system at time t can be described by a density operator $\Psi(t)$ having Properties I to IV in Topic 5.2.2 and such that

1. the probability $P(X, \Psi, t)$ that the system be found in the state $X(t)$ when it is known to be in the state $\Psi(t)$ is given by (5.4);
2. the probability $P(a_k, \Psi, t)$ of observing the value a_k on measurement of A for the system in the state $\Psi(t)$ is given by (5.7);
3. the average $\bar{A}(t)$ of measurements of A for the system in the state $\Psi(t)$ is given by (5.9).

Comments

1. **A scheme for comparison of theory and experiment**

The above provides a scheme for comparison of theory and experiment.

No reference is made to the state vector for the system.

2. **Comparison with the formalism for pure states**

Comparison with the formalism developed in Section 5.2 for pure states

shows that the original definition (5.1) and Property V in Topic 5.2.2 have been dropped; it is not required that $\Psi(t)$ be idempotent.

3. Mathematical implications

As shown in Section 5.6, it follows from Properties I to IV in Topic 5.2.2 that

$$\Psi(t) = \sum_{k=1}^n |\psi_k(t)\rangle p_k \langle \psi_k(t)| \quad (5.15)$$

$$|\psi_k(t)\rangle = U(t) |\psi_k(0)\rangle \quad (5.16)$$

$$1 = \sum_{k=1}^n |\psi_k(0)\rangle \langle \psi_k(0)| \quad (5.17)$$

$$\langle \psi_k(0) | \psi_{k'}(0) \rangle = \delta_{kk'} \quad (5.18)$$

$$\sum_{k=1}^n p_k = 1 \quad (5.19)$$

$$0 \leq p_k \leq 1 \quad \text{for all } k = 1, 2, \dots, n \quad (5.20)$$

4. Expressions for the probability and the average

Substitution of (5.15) into (5.7) and (5.9) yields

$$P(a_j, \Psi, t) = \sum_{k=1}^n p_k |\langle a_j | \psi_k(t) \rangle|^2 \quad (5.21)$$

$$\bar{A}(t) = \sum_{k=1}^n p_k \langle \psi_k(t) | A | \psi_k(t) \rangle \quad (5.22)$$

5. Special case: idempotent density operator

It follows from (5.15) that (5.14) holds if and only if

$$p_k^2 = p_k \quad \text{for all } k = 1, 2, \dots, n \quad (5.23)$$

That is,

$$p_k = 0 \quad \text{or} \quad 1 \quad \text{for all } k = 1, 2, \dots, n \quad (5.24)$$

The only solutions (5.24) satisfying (5.19) are

$$p_k = 1 \quad \text{for some } k \quad (5.25)$$

$$p_j = 0 \quad \text{for all } j \neq k$$

It follows from (5.15) and (5.25) that

$$\Psi(t) = |\psi(t)\rangle\langle\psi(t)| \quad (5.26)$$

where we have written $|\psi(t)\rangle = |\psi_k(t)\rangle$.

That is, the original definition (5.1) follows on requiring that Property V in Topic 5.2.2 hold.

$|\psi(t)\rangle$ is the state vector for the system.

6. Pure state

If $\Psi(t)$ is idempotent, the system is said to be in a pure state.

If the system is in a pure state, it may be represented mathematically by a single unit norm vector in the Hilbert space for the system.

7. Mixed state

If $\Psi(t)$ is not idempotent, the system is said to be in a mixed state.

If the system is in a mixed state, it cannot be represented mathematically by a single unit norm vector in the Hilbert space for the system.

8. Eigenvalues of the density operator.

The eigenvalues p_1, p_2, \dots, p_n of $\Psi(0)$ are interpreted as the probabilities for preparing the system in the pure states $|\psi_1(0)\rangle, |\psi_2(0)\rangle, \dots, |\psi_n(0)\rangle$ at time zero.

p_1, p_2, \dots, p_n are specified by the characteristics of the preparation apparatus.

9. Average over incoherent states

(5.21) and (5.22) sometimes appear in applications without explicit mention of the density operator or of a mixed state of a physical system.

In such applications, the summations in (5.21) and (5.22), since they involve probabilities and not probability amplitudes, are interpreted as an average over "incoherent" states $|\psi_1(t)\rangle, |\psi_2(t)\rangle, \dots, |\psi_n(t)\rangle$ of the system.

10. Results of measurements for a mixed state

We show in Section 5.6 that

$$P(a_j, \Psi, t) < 1 \quad (5.27)$$

for every observed value a_j of every observable A for a system in any mixed state $\Psi(t)$.

It follows from (5.27) that

No experiment gives a result predictable with certainty when performed on a system in a mixed state.

A mixed state of a system is characterized by the absence of any experiment which gives a result predictable with certainty when performed on the system in that state.

11. Results of measurements for a pure state

We show in Section 5.6 that

$$P(a_j, \Psi, t) = 1 \quad (5.28)$$

for some observed value a_j of an observable A for a system in the pure state $\Psi(t)$.

It follows from (5.28) that

An experiment exists which gives a result predictable with certainty when performed on a system in a pure state.

A pure state of a system is characterized by the existence of an experiment which gives a result predictable with certainty when performed on the system in that state.

5.4 Entropy of a state

The entropy S of a state $\Psi(t)$ is defined by

$$S = -\kappa \overline{\ln \Psi(t)} = -\kappa \text{Tr} (\Psi(t) \ln \Psi(t)) \quad (5.29)$$

where $\kappa = 86.171 \mu\text{eV/K}$ is Boltzmann's constant.

We show below that entropy characterizes the extent to which a state is mixed.

It follows from (5.15) that

$$\ln \Psi(t) = \sum_{k=1}^n | \psi_k(t) \rangle \ln p_k \langle \psi_k(t) | \quad (5.30)$$

and

$$\Psi(t) \ln \Psi(t) = \sum_{k=1}^n | \psi_k(t) \rangle p_k \ln p_k \langle \psi_k(t) | \quad (5.31)$$

and therefore

$$S = -\kappa \sum_{k=1}^n p_k \ln p_k \quad (5.32)$$

Comments

1. Entropy is non-negative

It follows from (5.20) and (5.32) that

$$S \geq 0 \quad (5.33)$$

2. Entropy of a pure state

It follows from (5.25) and (5.32) that

$$S = 0 \quad \text{for a pure state} \quad (5.34)$$

3. Entropy of a mixed state

It follows from (5.69) and (5.32) that

$$S > 0 \quad \text{for a mixed state} \quad (5.35)$$

4. Maximum value of entropy

We show in Section 5.6 that the maximum value of S occurs when

$$p_k = \frac{1}{n} \quad \text{for all } k \quad (5.36)$$

In this case

$$S = S_{max} = \kappa \ln n \quad (5.37)$$

5. Entropy and information

It follows from (5.25) and (5.34) that

$S = 0$ corresponds to maximum information about a system.

It follows from (5.36) and (5.37) that

$S = S_{max}$ corresponds to minimum information about a system.

6. Increase of entropy due to a measurement

Measurement of a system in a pure state of the system and measuring apparatus yields system and apparatus component states which are mixed.

It follows from (5.34) and (5.35) that

The measurement increases the total entropy of the system and measuring apparatus.

5.5 State with given average energy

We consider a state Ψ of a system which has been prepared such that only its average energy \overline{E} is specified.

We show in Section 5.6 that

$$\Psi = \frac{e^{-\beta H}}{Z} \quad (5.38)$$

where

$$Z = \text{Tr } e^{-\beta H} \quad (5.39)$$

$$\beta = \frac{1}{\kappa T} \quad (5.40)$$

where H is the Hamiltonian for the system and κ is Boltzmann's constant.

Comments

1. Stationary state

(5.38) describes a stationary state of the system.

$$\Psi(t) = U^\dagger(t)\Psi U(t) = e^{+iHt/\hbar}\Psi e^{-iHt/\hbar} = \Psi \quad (5.41)$$

2. Temperature

The parameter T in (5.40) is the temperature of the system.

3. Thermodynamic equilibrium

The state Ψ given by (5.38) may be identified with the state of a system in thermodynamic equilibrium with its surroundings.

In this case, T is identified with the temperature of the surroundings.

4. **Partition function**

The function Z defined by (5.39) is the partition function for the system.

5. **Average energy in terms of the partition function**

The average energy \bar{E} of the system in the state Ψ is

$$\bar{E} = \text{Tr}(H\Psi) = -\frac{d}{d\beta} \ln Z \quad (5.42)$$

6. **Free energy**

The free energy F of the system in the state Ψ is defined as

$$F = -\kappa T \ln Z \quad (5.43)$$

7. **Determining the average energy and the entropy**

It follows from (5.29), (5.42) and (5.43) that

$$\bar{E} = \frac{\partial(F/T)}{\partial(1/T)} \quad (5.44)$$

$$S = \frac{\bar{E} - F}{T} \quad (5.45)$$

(5.43) to (5.45) allow determination of the average energy and entropy of the system at temperature T from the partition function for the system.

Comments

1. Boltzmann factors

p_k given by (5.84) is the probability for preparing the system with energy ϵ_k .

p_k is the Boltzmann factor for the state $|\epsilon_k\rangle$.

2. Values of the Boltzmann factors

We label the eigenvalues of the Hamiltonian such that

$$\epsilon_1 \leq \epsilon_2 \leq \dots \leq \epsilon_n \quad (5.46)$$

It follows from (5.84) that

$$\frac{p_{k+1}}{p_k} = e^{-\beta(\epsilon_{k+1} - \epsilon_k)} \quad (5.47)$$

and, therefore,

$$p_1 \geq p_2 \geq \cdots \geq p_n \quad \text{when } T \text{ is positive} \quad (5.48)$$

$$p_1 \leq p_2 \leq \cdots \leq p_n \quad \text{when } T \text{ is negative} \quad (5.49)$$

3. Negative temperature and population inversion

(5.49) implies that a negative temperature corresponds to a population inversion in a sample of particles each prepared in the state Ψ .

That is, the number of particles in the sample whose energy is ϵ_1 is less than the number of particles whose energy is ϵ_2 , and so on.

The above statement does not include effects which arise when the particles in the sample are identical.

Systems of identical particles are discussed in *QLB: Quantum Mechanics in Fock Space*.

4. Infinite temperature limit

It follows from (5.38) to (5.40) that

$$\lim_{T \rightarrow \pm\infty} \Psi = \Psi_{min} = \frac{1}{n} \quad (5.50)$$

Ψ_{min} is the state of the system which has been prepared with the least input information.

For this state,

$$p_k = \frac{1}{n} \quad \text{for all } k = 1, 2, \dots, n \quad (5.51)$$

5. Zero temperature limit through positive temperatures

It follows from (5.38) to (5.40) that

$$\lim_{T \rightarrow 0^+} \Psi = \Psi_1 = | \psi_1 \rangle \langle \psi_1 | \quad (5.52)$$

For the state Ψ_1 ,

$$p_1 = 1 \quad (5.53)$$

$$p_k = 0 \quad \text{for all } k \neq 1 \quad (5.54)$$

6. Zero temperature limit through negative temperatures

It follows from (5.38) to (5.40) that

$$\lim_{T \rightarrow 0^-} \Psi = \Psi_n = | \psi_n \rangle \langle \psi_n | \quad (5.55)$$

For the state Ψ_n ,

$$p_n = 1 \quad (5.56)$$

$$p_k = 0 \quad \text{for all } k \neq n \quad (5.57)$$

7. Planck's Radiation Law

For simplicity throughout this chapter we have considered a physical system which can be described in a finite-dimensional vector space. We now assume that the physical system is a nonrelativistic one-dimensional harmonic oscillator as discussed in Topic 11.2.1. In this case, the Hilbert space is infinite-dimensional and the partition function (5.85) becomes

$$Z = \sum_{k=0}^{\infty} e^{-\beta \epsilon_k} \quad (5.58)$$

where, from (11.22),

$$\epsilon_k = \left(k + \frac{1}{2}\right) \hbar \omega \quad (5.59)$$

where ω is the oscillator angular frequency as given by (11.15).

It follows from (5.58) and (5.59) that

$$Z = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} \quad (5.60)$$

It follows from (5.42) and (5.60) that the average energy of the oscillator is

$$\bar{E} = \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} \quad (5.61)$$

(5.61) is a standard result which leads to Planck's Radiation Law.

5.6 Some derivations

Derivation of (5.4)

Let $|\phi_1\rangle, |\phi_2\rangle, \dots, |\phi_n\rangle$ span the Hilbert space for the physical system. Then

$$1 = \sum_{k=1}^n |\phi_k\rangle\langle\phi_k| \quad (5.62)$$

$$\langle\phi_k|\phi_{k'}\rangle = \delta_{kk'} \quad (5.63)$$

and

$$\begin{aligned}
P(\chi, \psi, t) &= |\langle \chi(t) | \psi(t) \rangle|^2 \\
&= \langle \chi(t) | \psi(t) \rangle \langle \psi(t) | \chi(t) \rangle = P(\chi, \Psi, t) \\
&= \sum_{k=1}^n \langle \chi(t) | \psi(t) \rangle \langle \psi(t) | \phi_k \rangle \langle \phi_k | \chi(t) \rangle \\
&= \sum_{k=1}^n \langle \phi_k | \chi(t) \rangle \langle \chi(t) | \psi(t) \rangle \langle \psi(t) | \phi_k \rangle \\
&= \sum_{k=1}^n \langle \phi_k | X(t)\Psi(t) | \phi_k \rangle = \text{Tr}(X(t)\Psi(t)) = P(X, \Psi, t)
\end{aligned} \tag{5.64}$$

Derivation of (5.7)

The proof of (5.7) is identical to the proof of (5.4) with $|\chi(t)\rangle$ replaced by $|a_k\rangle$.

Derivation of (5.9)

$$\begin{aligned}
\bar{A}(t) &= \langle \psi(t) | A | \psi(t) \rangle \\
&= \sum_{k=1}^n \langle \psi(t) | \phi_k \rangle \langle \phi_k | A | \psi(t) \rangle = \sum_{k=1}^n \langle \phi_k | A | \psi(t) \rangle \langle \psi(t) | \phi_k \rangle \\
&= \sum_{k=1}^n \langle \phi_k | A\Psi(t) | \phi_k \rangle = \text{Tr}(A\Psi(t))
\end{aligned} \tag{5.65}$$



and

$$\begin{aligned}
P(\chi, \psi, t) &= |\langle \chi(t) | \psi(t) \rangle|^2 \\
&= \langle \chi(t) | \psi(t) \rangle \langle \psi(t) | \chi(t) \rangle = P(\chi, \Psi, t) \\
&= \sum_{k=1}^n \langle \chi(t) | \psi(t) \rangle \langle \psi(t) | \phi_k \rangle \langle \phi_k | \chi(t) \rangle \\
&= \sum_{k=1}^n \langle \phi_k | \chi(t) \rangle \langle \chi(t) | \psi(t) \rangle \langle \psi(t) | \phi_k \rangle \\
&= \sum_{k=1}^n \langle \phi_k | X(t)\Psi(t) | \phi_k \rangle = \text{Tr}(X(t)\Psi(t)) = P(X, \Psi, t)
\end{aligned} \tag{5.64}$$

Derivation of (5.7)

The proof of (5.7) is identical to the proof of (5.4) with $|\chi(t)\rangle$ replaced by $|a_k\rangle$.

Derivation of (5.9)

$$\begin{aligned}
\bar{A}(t) &= \langle \psi(t) | A | \psi(t) \rangle \\
&= \sum_{k=1}^n \langle \psi(t) | \phi_k \rangle \langle \phi_k | A | \psi(t) \rangle = \sum_{k=1}^n \langle \phi_k | A | \psi(t) \rangle \langle \psi(t) | \phi_k \rangle \\
&= \sum_{k=1}^n \langle \phi_k | A\Psi(t) | \phi_k \rangle = \text{Tr}(A\Psi(t))
\end{aligned} \tag{5.65}$$

Derivation of (5.15) to (5.20)

It follows from Property II that $\Psi(0)$ has the eigenvalue decomposition

$$\Psi(0) = \sum_{k=1}^n |\psi_k(0)\rangle p_k \langle \psi_k(0)| \quad (5.66)$$

where $|\psi_1(0)\rangle, |\psi_2(0)\rangle, \dots, |\psi_n(0)\rangle$ satisfy (5.17) and (5.18) and where p_1, p_2, \dots, p_n are real numbers.

(5.15) and (5.16) follow from Property I.

(5.19) follows from Property III.

It follows from Property IV that

$$p_k \geq 0 \quad \text{for all } k = 1, 2, \dots, n \quad (5.67)$$

(5.20) follows from (5.19) and (5.67).

Derivation of (5.27)

It follows from (5.15) that $\Psi(t)$ is not idempotent if and only if

$$p_k^2 \neq p_k \quad \text{for all } k = 1, 2, \dots, n \quad (5.68)$$

It follows from (5.19), (5.20) and (5.68) that

$$0 < p_k < 1 \quad \text{for some } k = 1, 2, \dots, n \quad (5.69)$$

when $\Psi(t)$ is not idempotent.

It follows from (5.21) and (5.69) that

$$\begin{aligned} P(a_j, \Psi, t) &= \sum_{k=1}^n p_k |\langle a_j | \psi_k(t) \rangle|^2 < \sum_{k=1}^n |\langle a_j | \psi_k(t) \rangle|^2 \\ &= \sum_{k=1}^n \langle a_j | \psi_k(t) \rangle \langle \psi_k(t) | a_j \rangle = \langle a_j | a_j \rangle = 1 \end{aligned} \quad (5.70)$$

Derivation of (5.28)

It follows from (5.21), (5.25) and (5.26) that

$$P(a_j, \Psi, t) = |\langle a_j | \psi(t) \rangle|^2 = 1 \quad (5.71)$$

if $|\psi(t)\rangle = |a_j\rangle$.

That is, given any observable A , the result of a measurement of A yields the eigenvalue a_j of A with certainty when the system is in the state $|a_j\rangle$.

Derivation of (5.36)

We determine p_1, p_2, \dots, p_n such that S is maximum subject to (5.19).

We use the method of Lagrange multipliers; we write

$$d\left(\sum_{k=1}^n p_k \ln p_k + \alpha \sum_{k=1}^n p_k\right) = 0 \quad (5.72)$$

where α is a Lagrange multiplier. Simplifying the left side of (5.72) yields

$$\sum_{k=1}^n (\ln p_k + \alpha + 1) dp_k = 0 \quad (5.73)$$

from which

$$\ln p_k = -\alpha - 1 \quad (5.74)$$

which shows that p_k is independent of k . (5.36) then follows from (5.19).

Derivation of (5.38)

The eigenvalue decomposition of Ψ is given by (5.15) where the probabilities p_1, p_2, \dots, p_n satisfy (5.19) and (5.20); the entropy S is expressed in terms of p_1, p_2, \dots, p_n by (5.32) and the average energy \bar{E} is expressed in terms of p_1, p_2, \dots, p_n using (5.22):

$$\bar{E} = \sum_{k=1}^n p_k \bar{E}_k \quad (5.75)$$

$$\bar{E}_k = \langle \psi_k | H | \psi_k \rangle \quad (5.76)$$

where $|\psi_k\rangle$ is the eigenvector of Ψ belonging to eigenvalue p_k .

We determine p_1, p_2, \dots, p_n such that S is maximum for given \bar{E} . We use the method of Lagrange multipliers; we write

$$d \left(\sum_{k=1}^n p_k \ln p_k + \alpha \sum_{k=1}^n p_k + \beta \sum_{k=1}^n p_k \bar{E}_k \right) = 0 \quad (5.77)$$

where α and β are Lagrange multipliers.

Solving (5.77) yields

$$p_k = e^{-1-\alpha-\beta\bar{E}_k} \quad (5.78)$$

The constant α is determined using (5.19). It follows that

$$p_k = \frac{e^{-\beta\bar{E}_k}}{Z} \quad (5.79)$$

$$Z = \sum_{k=1}^n e^{-\beta\bar{E}_k} \quad (5.80)$$

We now specify the eigenvectors $|\psi_1\rangle, |\psi_2\rangle, \dots, |\psi_n\rangle$ of Ψ . The Hamiltonian H has the eigenvalue decomposition

$$H = \sum_{k=1}^n |\epsilon_k \rangle \epsilon_k \langle \epsilon_k| \quad (5.81)$$

We assume that

$$|\psi_k \rangle = |\epsilon_k \rangle \quad \text{for all } k = 1, 2, \dots, n \quad (5.82)$$

It follows from (5.81) and (5.82) that

$$\bar{E}_k = \epsilon_k \quad (5.83)$$

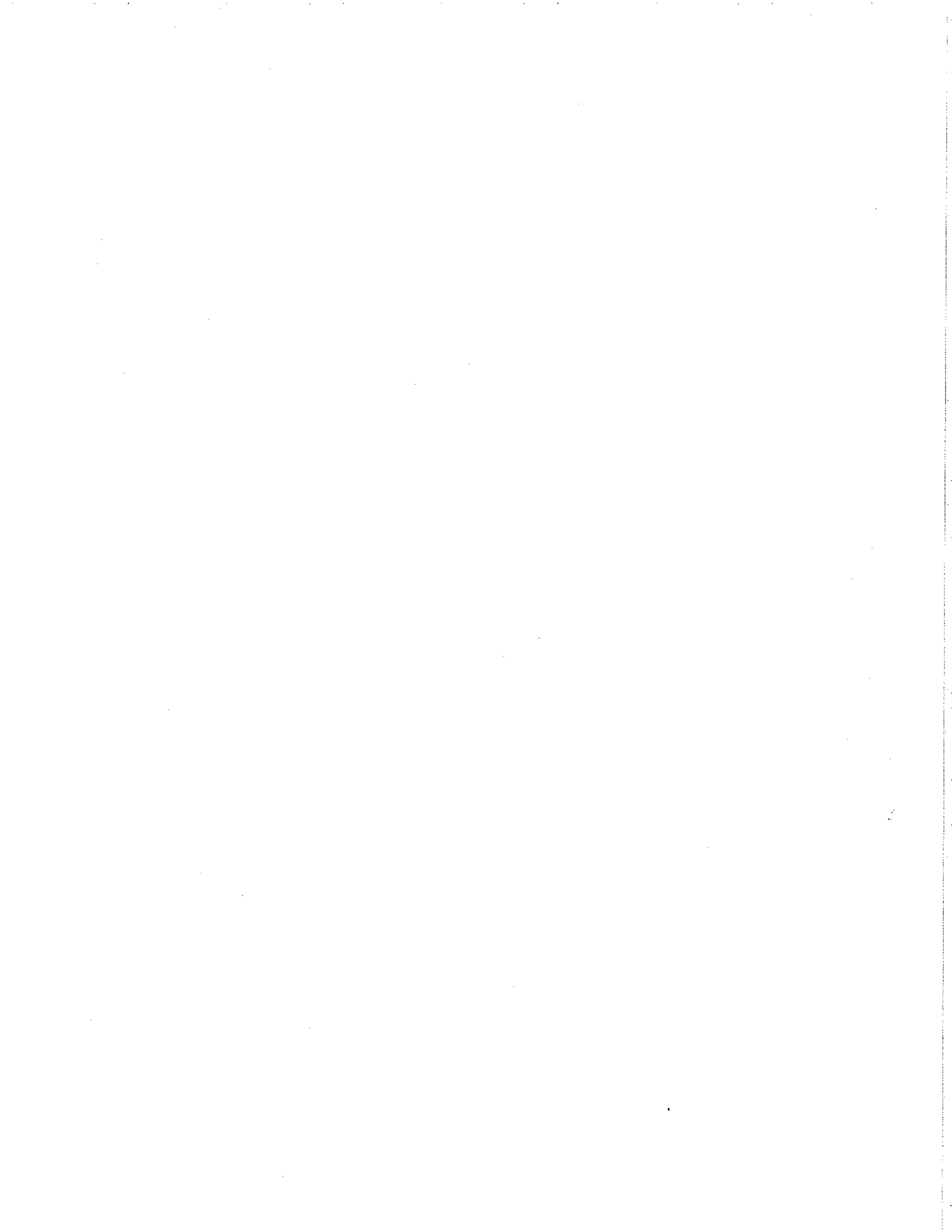
It follows from (5.79), (5.80) and (5.83) that

$$p_k = \frac{e^{-\beta \epsilon_k}}{Z} \quad (5.84)$$

$$Z = \sum_{k=1}^n e^{-\beta \epsilon_k} = \text{Tr } e^{-\beta H} \quad (5.85)$$

It follows from (5.15), (5.82) and (5.84) that

$$\Psi = \sum_{k=1}^n |\epsilon_k \rangle \frac{e^{-\beta \epsilon_k}}{Z} \langle \epsilon_k| = \frac{e^{-\beta H}}{Z} \quad (5.86)$$



6.1 Introductory remarks

The quantum mechanics of a Lorentz invariant single particle with arbitrary spin is discussed in *QLB: Some Lorentz Invariant Systems* Chapter 3. Included in that chapter are expressions for the Poincare generators for the system and a discussion of the coordinate-space and momentum-space wave functions for the particle.

In this chapter, we describe the spin states of a spin $\frac{1}{2}$ particle. Our purpose is to discuss the quantum mechanics of spin more fully than is given in *QLB: Some Lorentz Invariant Systems* Chapter 3. We consider the simplest nontrivial example of spin and, for simplicity, we disregard entirely any change in position or momentum of the particle. The spin states of a spin 1 particle are discussed in Chapter 7.

Pure spin states are described in Section 6.2. This section includes a discussion of the preparation of pure states using a Stern-Gerlach apparatus and the measurement of the components of spin using a Stern-Gerlach apparatus. The density operator corresponding to a pure state is also discussed. The density operator is characterized by the orientation of the unit length polarization vector for the particle which vector also characterizes the orientation of the Stern-Gerlach apparatus used for preparing the state of the particle.

Mixed states of the particle are described in Section 6.3. The density operator for a mixed state has the same form as the density operator for a pure state: for the mixed state, the length of the polarization vector is less than unity. The spin temperature for the particle is discussed in Topic 6.3.2.

6.2 Description of pure states

Let $| + \rangle, | - \rangle$ be a set of orthonormal vectors which span the 2-dimensional vector space for a spin $\frac{1}{2}$ particle. That is,

$$1 = | + \rangle \langle + | + | - \rangle \langle - | \quad (6.1)$$

$$\langle + | + \rangle = \langle - | - \rangle = 1 \quad (6.2)$$

$$\langle + | - \rangle = \langle - | + \rangle = 0 \quad (6.3)$$

Pauli operators are defined by

$$\sigma^1 = | + \rangle \langle - | + | - \rangle \langle + | \quad (6.4)$$

$$\sigma^2 = -i | + \rangle \langle - | + i | - \rangle \langle + | \quad (6.5)$$

$$\sigma^3 = | + \rangle \langle + | - | - \rangle \langle - | \quad (6.6)$$

Comments

1. Eigenvalue decomposition of σ^3

$| \pm \rangle$ are eigenvectors of σ^3 belonging to eigenvalues ± 1 .

(6.6) is the eigenvalue decomposition of σ^3 .

2. Pauli matrices

The matrix representation of $\sigma^1, \sigma^2, \sigma^3$ with respect to $|\pm\rangle$ are the Pauli matrices (A.62) to (A.64).

3. Expressions for operators

Every operator in the vector space can be written as a linear combination of the unit operator (6.1) and the three Pauli operators (6.4) to (6.6).

4. Spin

The spin \vec{S} of the particle is defined as

$$\vec{S} = \frac{1}{2}\hbar\vec{\sigma} \quad (6.7)$$

$$\vec{\sigma} = \sigma^1\vec{i} + \sigma^2\vec{j} + \sigma^3\vec{k} \quad (6.8)$$

where $\vec{i}, \vec{j}, \vec{k}$ are unit vectors along the coordinate axes.

5. Commutation relations

It follows from (6.4) to (6.6) that

$$[S^j, S^k] = i\hbar\epsilon_{jkl}S^l \quad (6.9)$$

$$\vec{S} \cdot \vec{S} = s(s+1)\hbar^2 \quad (6.10)$$

where $s = \frac{1}{2}$.

6. Eigenvalue decomposition of $\vec{\sigma} \cdot \vec{m}$

Let \vec{m} be a unit vector whose spherical polar coordinates are (θ, φ) .

$$\vec{m} = \sin \theta \cos \varphi \vec{i} + \sin \theta \sin \varphi \vec{j} + \cos \theta \vec{k} \quad (6.11)$$

The vectors

$$|m+\rangle = \cos \frac{\theta}{2} |+\rangle + e^{i\varphi} \sin \frac{\theta}{2} |-\rangle \quad (6.12)$$

$$|m-\rangle = -e^{-i\varphi} \sin \frac{\theta}{2} |+\rangle + \cos \frac{\theta}{2} |-\rangle \quad (6.13)$$

are eigenvectors of $\vec{\sigma} \cdot \vec{m}$ belonging to eigenvalues $+1$ and -1 , respectively.

The eigenvalue decomposition of $\vec{\sigma} \cdot \vec{m}$ is

$$\vec{\sigma} \cdot \vec{m} = |m+\rangle \langle m+| - |m-\rangle \langle m-| \quad (6.14)$$

$|m\pm\rangle$ are a complete set of orthonormal vectors which span the vector space.

$$1 = |m+\rangle \langle m+| + |m-\rangle \langle m-| \quad (6.15)$$

$$\langle m+ | m+ \rangle = \langle m- | m- \rangle = 1 \quad (6.16)$$

$$\langle m+ | m- \rangle = \langle m- | m+ \rangle = 0 \quad (6.17)$$

It follows from (6.12) and (6.13) that

$$| + \rangle = \cos \frac{\theta}{2} | m+ \rangle - e^{i\varphi} \sin \frac{\theta}{2} | m- \rangle \quad (6.18)$$

$$| - \rangle = e^{-i\varphi} \sin \frac{\theta}{2} | m+ \rangle + \cos \frac{\theta}{2} | m- \rangle \quad (6.19)$$

7. Rotation of \vec{k} to \vec{m}

Let

$$R = | m+ \rangle \langle + | + | m- \rangle \langle - | \quad (6.20)$$

Then R is unitary

$$RR^\dagger = R^\dagger R = 1 \quad (6.21)$$

and

$$|m+\rangle = R |+\rangle \quad (6.22)$$

$$|m-\rangle = R |-\rangle \quad (6.23)$$

$$R\sigma^3 R^\dagger = \vec{\sigma} \cdot \vec{m} \quad (6.24)$$

R corresponds to the rotation of \vec{k} to \vec{m} .

8. Exponential form of rotation operator

(6.20) can be written in the form

$$R = e^{-iS^3\varphi/\hbar} e^{-iS^2\theta/\hbar} e^{iS^3\varphi/\hbar} \quad (6.25)$$

which corresponds to a rotation by $-\varphi$ about the z -axis followed by a rotation by θ about the y -axis followed by a rotation by φ about the z -axis.

In general, the rotation of \vec{k} to \vec{m} is described by the unitary operator

$$e^{-iS^3\varphi/\hbar} e^{-iS^2\theta/\hbar} e^{-iS^3\eta/\hbar} \quad (6.26)$$

where

$$e^{-iS^3\eta/\hbar} \quad (6.27)$$

corresponds to an arbitrary initial rotation by η about the z -axis. Specifying η (e.g., $\eta = -\varphi$) corresponds to specifying the overall phase of the two eigenvectors of $\vec{\sigma} \cdot \vec{m}$.

9. Matrix representation

The matrix representation of R with respect to $|\pm\rangle$ is

$$\begin{aligned} (R) &= \begin{pmatrix} \langle + | R | + \rangle & \langle + | R | - \rangle \\ \langle - | R | + \rangle & \langle - | R | - \rangle \end{pmatrix} \\ &= \begin{pmatrix} \cos \frac{\theta}{2} & -e^{-i\varphi} \sin \frac{\theta}{2} \\ e^{i\varphi} \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix} \end{aligned} \quad (6.28)$$

(6.28) is the rotation matrix $D_{m,\lambda}^{\frac{1}{2}}(\varphi, \theta, 0)$ which appears in the discussion of the helicity states of a spin $\frac{1}{2}$ particle in *QLB: Some Lorentz Invariant Systems* Chapter 3.

10. Polarization vector

The polarization vector for a state of a spin $\frac{1}{2}$ particle is the average value of $\vec{\sigma}$ for the state.

The polarization vectors for the states $|m_{\pm}\rangle$ are

$$\langle m_{\pm} | \vec{\sigma} | m_{\pm} \rangle = \pm \vec{m} \quad (6.29)$$

11. Preparation by a Stern-Gerlach apparatus

The states $|m_{\pm}\rangle$ may be thought of as being prepared by a Stern-Gerlach apparatus whose inhomogeneous magnetic field is in direction \vec{m} .

We call such an apparatus an mSG apparatus.

An mSG apparatus measures $\vec{S} \cdot \vec{m}$. The possible results of a measurement of $\vec{S} \cdot \vec{m}$ are $\pm \frac{1}{2}\hbar$.

The states $|\pm\rangle$ may be thought of as being prepared by a kSG apparatus. A kSG apparatus measures $\vec{S} \cdot \vec{k} = S^3$. The possible results of a measurement of S^3 are $\pm \frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$.

The unitary operator R (6.20) corresponds to rotating a Stern-Gerlach apparatus whose inhomogeneous magnetic field is in the \vec{k} -direction such that the inhomogeneous magnetic field after the rotation is in \vec{m} -direction. That is, it corresponds to rotating a kSG apparatus so that it becomes an mSG apparatus.

12. Probabilities

We consider states prepared by an mSG apparatus and measured by a kSG apparatus.

If the system is known to be in the state $|m+\rangle$ then

$$|\langle + | m+\rangle|^2 = \cos^2 \frac{\theta}{2} \quad (6.30)$$

$$|\langle - | m+\rangle|^2 = \sin^2 \frac{\theta}{2} \quad (6.31)$$

are the probabilities that on measurement of S^3 the system be found in the states $|\pm\rangle$.

If the system is known to be in the state $|m-\rangle$ then

$$|\langle + | m- \rangle|^2 = \sin^2 \frac{\theta}{2} \quad (6.32)$$

$$|\langle - | m- \rangle|^2 = \cos^2 \frac{\theta}{2} \quad (6.33)$$

are the probabilities that on measurement of S^3 the system be found in the states $|\pm\rangle$.

13. Density operator for a pure state

The density operator corresponding to a pure state of a system is given by (5.1). The density operators for the states $|m_{\pm}\rangle$ may be written in the form

$$|m_{\pm}\rangle\langle m_{\pm}| = \frac{1}{2}(1 \pm \vec{\sigma} \cdot \vec{m}) \quad (6.34)$$

where \vec{m} is the polarization vector for the state.

(6.34) illustrates an important feature of the density operator formalism: in contradistinction to (6.12) and (6.13), (6.34) is expressed explicitly in terms of the polarization vector \vec{m} which characterizes the state, which vector also describes the orientation of the Stern-Gerlach apparatus used to prepare the state.

We note also that (6.34) is characterized by two real numbers, as opposed to three which characterize a general pure state as described by a state vector (the third corresponding to the overall phase of the vector).

14. Density operators and rotations

It follows from (6.22) and (6.23) that the density operators for the states

$|m_{\pm}\rangle$ and $|\pm\rangle$ are related by

$$|m_{\pm}\rangle\langle m_{\pm}| = R|\pm\rangle\langle\pm|R^{\dagger} \quad (6.35)$$

$$\frac{1}{2}(1 \pm \vec{\sigma} \cdot \vec{m}) = R\frac{1}{2}(1 \pm \vec{\sigma} \cdot \vec{k})R^{\dagger} \quad (6.36)$$

where R is given by (6.20).

That is, the effect on the density operator by R is simply, of course, to change the polarization vector from \vec{k} to \vec{m} .

6.3 Description of mixed states

So far in this chapter, we have only considered pure states of a spin $\frac{1}{2}$ particle. We consider mixed states of a spin $\frac{1}{2}$ particle in this section.

It is shown in Topic 6.3.1 that the density operator for a mixed state has the same form as the density operator for a pure state, the only difference being that the polarization vector for a mixed state is shorter than unity. Thus, a mixed state of a spin $\frac{1}{2}$ particle is characterized by three parameters which are the length and orientation of the polarization vector for the particle. The spin temperature for the particle is discussed in Topic 6.3.2.

Polarization vector

We recall from Section 6.2 that the states $|m_{\pm}\rangle$ of a spin $\frac{1}{2}$ particle may be thought of as being prepared by a Stern-Gerlach apparatus whose inhomogeneous magnetic field is in the \vec{m} -direction (that is, by an mSG apparatus). An mSG

apparatus prepares pure states of the system: one can decide with certainty whether an mSG apparatus has prepared the state $|m_+\rangle$ or the state $|m_-\rangle$.

We now imagine preparing a state of the system with an inefficient mSG-like apparatus which does not allow one to decide with certainty whether the apparatus has prepared the state $|m_+\rangle$ or the state $|m_-\rangle$. This will be the case if the gradient of the inhomogeneous magnetic field in the Stern-Gerlach apparatus is not sufficiently strong. We call such an inefficient mSG—like apparatus an mFSG apparatus (F for fuzzy).

We can only assign probabilities for preparing the state $|m_+\rangle$ or the state $|m_-\rangle$ with an mFSG apparatus. These probabilities are specified by the characteristics of the mFSG apparatus.

Let p_{m_\pm} be the probabilities for preparing the states $|m_\pm\rangle$ with an mFSG apparatus. Then

$$0 \leq p_{m_+} \leq 1 \quad \text{and} \quad 0 \leq p_{m_-} \leq 1 \quad (6.37)$$

$$p_{m_+} + p_{m_-} = 1 \quad (6.38)$$

As given by (5.15), the state prepared by the mFSG apparatus is represented by the density operator

$$\Psi = |m_+\rangle p_{m_+} \langle m_+| + |m_-\rangle p_{m_-} \langle m_-| \quad (6.39)$$

Measurement of $\vec{S} \cdot \vec{m}$ with an mSG apparatus for the system in the state Ψ yields the values $+\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$ with probabilities p_{m_+} and p_{m_-} , respectively.

It follows from (6.34) that (6.39) can be written in the form

$$\Psi = \frac{1}{2} (1 + \vec{\sigma} \cdot \vec{m}) \quad (6.40)$$

where

$$\vec{m} = (p_{m+} - p_{m-}) \vec{n} \quad (6.41)$$

It follows from (6.40) that

$$\vec{m} = \text{Tr} (\vec{\sigma} \Psi) \quad (6.42)$$

\vec{m} is the polarization vector for the state Ψ . It follows from (6.41) that

$$|\vec{m}| \leq 1 \quad (6.43)$$

That is, a mixed state is characterized by a polarization vector with length less than unity.

Measurement of S^3 with a KSG apparatus for the system in the state Ψ yields the values $+\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$ with probabilities

$$p_{m+} \cos^2 \frac{\theta}{2} + p_{m-} \sin^2 \frac{\theta}{2} \quad (6.44)$$

$$p_{m+} \sin^2 \frac{\theta}{2} + p_{m-} \cos^2 \frac{\theta}{2} \quad (6.45)$$

For example, if the polarization vector for the state Ψ is $0.6\vec{k}$, then the above probabilities are 80% and 20%, respectively.

If the state Ψ is unpolarized, that is,

$$p_{m+} = p_{m-} = \frac{1}{2} \quad (6.46)$$

$$\vec{m} = 0 \quad (6.47)$$

$$\Psi = \frac{1}{2} \quad (6.48)$$

then each of the above probabilities is 50%.

Spin temperature

In Section 5.5 we determined the state (5.38) of a system which had been prepared such that only its average energy is specified. In this topic, we specialize (5.38) for a spin $\frac{1}{2}$ particle prepared in a constant, homogeneous magnetic field \vec{B} . We show that (5.38) may be written in the form (6.40) where the polarization vector is

$$\vec{m} = \tanh\left(\frac{1}{2}\beta\hbar\omega_0\right)\vec{b} \quad (6.49)$$

where, as in (5.40),

$$\beta = \frac{1}{\kappa T} \quad (6.50)$$

and ω_0 is the Larmor precession frequency (8.1), κ is Boltzmann's constant and \vec{b} is a unit vector in the direction of \vec{B} .

Comments

1. Stationary state

(5.38) is a stationary state of the system.

The polarization vector (6.49) is constant in time; it is parallel to the magnetic field \vec{B} and does not precess.

2. Spin temperature

The parameter T in (6.49) is the spin temperature for the state (5.38).

T is not the temperature of the surroundings.

The state of the particle is specified by its spin temperature.

3. Ranges of parameters

The ranges of β , T and $\tanh\left(\frac{1}{2}\beta\hbar\omega_0\right)$ are

$$-\infty < \beta \leq 0 \quad 0 \leq \beta < +\infty \quad (6.51)$$

$$0 > T > -\infty \quad +\infty > T > 0 \quad (6.52)$$

$$-1 \leq \tanh\left(\frac{1}{2}\beta\hbar\omega_0\right) \leq +1 \quad (6.53)$$

In particular, the system has a positive spin temperature when its polarization vector points along the direction of the magnetic field and a negative spin temperature when its polarization vector points opposite to the direction of the magnetic field.

Derivation of (6.49)

The Hamiltonian for the particle is given by (8.7). It follows that

$$e^{-\beta H} = \cosh a + \vec{\sigma} \cdot \vec{b} \sinh a \quad (6.54)$$

where

$$a = \frac{1}{2}\beta\hbar\omega_0 \quad (6.55)$$

It follows from (6.54) that

$$\text{Tr } e^{-\beta H} = 2 \cosh a \quad (6.56)$$

$$\text{Tr } (\vec{\sigma} e^{-\beta H}) = 2 \sinh a \vec{b} \quad (6.57)$$

(6.49) follows from (6.41), (6.56) and (6.57).

A second derivation of (6.49)

We assume that the fixed Cartesian reference frame in the laboratory is defined such that $\vec{B} = B\vec{k}$ in which case the Hamiltonian is given by (8.16) and the eigenvalues and eigenvectors are given by (8.23) and (8.24).

(6.49) follows using (5.81) and (5.86) and the density operators for the states $|\pm\rangle$ as given by (6.34).

7.1 Introductory remarks

In this chapter we describe the spin states of a spin 1 particle. As in Chapter 6, our purpose is to discuss the quantum mechanics of spin more fully than is given in *QLB: Some Lorentz Invariant Systems* Chapter 3. The mathematical description and the physics of a spin 1 particle is richer than that of a spin $\frac{1}{2}$ particle discussed in Chapter 6. As in Chapter 6, for simplicity we disregard entirely any change in position or momentum of the particle.

Spin operators and pure states are described in Section 7.2 and spherical tensor operators are discussed in Section 7.3. The density operator corresponding to a pure state and to a mixed state is described in Section 7.4. The characterization of a state of a spin 1 particle in terms of a polarization vector and a polarization ellipsoid is also discussed in Section 7.4.

7.2 Spin operators and pure states

The spin \vec{S} of a spin 1 particle is defined as

$$\vec{S} = S^1 \vec{i} + S^2 \vec{j} + S^3 \vec{k} \quad (7.1)$$

where $\vec{i}, \vec{j}, \vec{k}$ are unit vectors along the coordinate axes and where

$$S^j = -i\hbar \epsilon_{jab} |a\rangle\langle b| \quad (7.2)$$

where $|1\rangle, |2\rangle, |3\rangle$ are a set of orthonormal vectors which span a

3-dimensional vector space. That is,

$$\sum_{a=1}^3 |a\rangle\langle a| = 1 \quad (7.3)$$

$$\langle a | b \rangle = \delta_{ab} \quad (7.4)$$

Comments

1. Commutation relations

It follows from (7.2) that

$$[S^j, S^k] = i\hbar\epsilon_{jkl}S^l \quad (7.5)$$

$$\vec{S} \cdot \vec{S} = s(s+1)\hbar^2 \quad (7.6)$$

where $s = 1$.

2. Matrix representation of S^j

It follows from (7.2) that the matrix elements of S^j with respect to $|1\rangle$, $|2\rangle$, $|3\rangle$ are

$$\langle a | S^j | b \rangle = S_{ab}^j = -i\hbar\epsilon_{jab} \quad (7.7)$$

That is,

$$(S_{ab}^1) = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad (7.8)$$

$$(S_{ab}^2) = \hbar \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \quad (7.9)$$

$$(S_{ab}^3) = \hbar \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (7.10)$$

(7.8) to (7.10) are identical to the matrices S_j given by (5.42), Rose (1957).

3. Products of spin operators

It follows from (7.2) that¹

$$S^j S^k = \delta_{jk} - |j\rangle\langle k| \quad (7.11)$$

$$S^j S^k S^l = -i\delta_{kl}\epsilon_{jab} |a\rangle\langle b| + i\epsilon_{jak} |a\rangle\langle l| \quad (7.12)$$

¹ In the following we often set $\hbar = 1$.

$$\begin{aligned}
 & S^j S^k S^l S^m \\
 & = \delta_{jk}(\delta_{lm} - |l\rangle\langle m|) - \delta_{lm} |j\rangle\langle k| + \delta_{kl} |j\rangle\langle m|
 \end{aligned}
 \tag{7.13}$$

A special case of (7.12) is

$$(S^j)^3 = S^j
 \tag{7.14}$$

It follows from (6.9) that $|1\rangle, |2\rangle, |3\rangle$ are simultaneous eigenvectors of $(S^1)^2, (S^2)^2$ and $(S^3)^2$.

4. Traces of products of spin operators

It follows from (7.2) and (7.11) to (7.13) that

$$\begin{aligned}
 \text{Tr} S^j & = 0 & (7.15) \\
 \text{Tr} S^j S^k & = 2\delta_{jk} & (7.16) \\
 \text{Tr} S^j S^k S^l & = -i\epsilon_{jkl} & (7.17) \\
 \text{Tr} S^j S^k S^l S^m & = \delta_{jk}\delta_{lm} + \delta_{jm}\delta_{kl} & (7.18)
 \end{aligned}$$

It follows from (7.18) that

$$\text{Tr} \left[(S^j)^2 (S^k)^2 \right] = \text{Tr} \left[S^j (S^k)^2 S^j \right] = 1 + \delta_{jk} \quad (7.19)$$

and that all other traces (7.18) vanish.

5. Rotations about the coordinate axes

The operator $R^j(\theta)$ corresponding to a rotation by θ about the j -axis is

$$\begin{aligned} R^j(\theta) &= e^{-iS^j\theta} = 1 - iS^j \sin \theta + (S^j)^2 (\cos \theta - 1) \\ &= \cos \theta + (1 - \cos \theta) |j\rangle\langle j| - \epsilon_{jab} |a\rangle\langle b| \sin \theta \end{aligned} \quad (7.20)$$

with the second and third equalities following using (7.14) and (7.2).

It follows from (7.2) that the matrix elements of $R^j(\theta)$ with respect to $|1\rangle, |2\rangle, |3\rangle$ are

$$\begin{aligned} \langle a | R^j(\theta) | b \rangle &= R_{ab}^j(\theta) \\ &= \delta_{ab} \cos \theta + \delta_{ja} \delta_{jb} (1 - \cos \theta) - \epsilon_{jab} \sin \theta \end{aligned} \quad (7.21)$$

That is,

$$(R_{ab}^1(\theta)) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta \\ 0 & \sin \theta & \cos \theta \end{pmatrix} \quad (7.22)$$

$$(R_{ab}^2(\theta)) = \begin{pmatrix} \cos \theta & 0 & \sin \theta \\ 0 & 1 & 0 \\ -\sin \theta & 0 & \cos \theta \end{pmatrix} \quad (7.23)$$

$$(R_{ab}^3(\theta)) = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (7.24)$$

(7.23) and (7.24) are the transpose of (A.55) and (A.56), respectively.

6. Rotation of \vec{k} to \vec{m}

The unitary operator

$$R = e^{-iS^3\varphi/\hbar} e^{-iS^2\theta/\hbar} \quad (7.25)$$

corresponds to a rotation of \vec{k} to a vector \vec{m} (6.11) which has spherical polar coordinates (θ, φ) . It follows from (7.2) and (7.20) that

$$RS^3R^\dagger = \vec{S} \cdot \vec{m} \quad (7.26)$$

The corresponding equation for a spin $\frac{1}{2}$ particle is (6.24).

7. Matrix representation of R

We denote the matrix elements of the rotation operator R (7.25) with respect to $|1\rangle, |2\rangle, |3\rangle$ by

$$\langle a | R | b \rangle = R_{ab} \quad (7.27)$$

It follows from (7.20) that

$$(R_{ab}) = \begin{pmatrix} \cos \theta \cos \varphi & -\sin \varphi & \sin \theta \cos \varphi \\ \cos \theta \sin \varphi & \cos \varphi & \sin \theta \sin \varphi \\ -\sin \theta & 0 & \cos \theta \end{pmatrix} \quad (7.28)$$

(7.28) is a special case of (4.43), Rose (1957),

8. Eigenvectors of S^3

It follows from (7.14) that the eigenvalues of S^j are $\pm 1, 0$. We denote the corresponding eigenvectors of S^3 by $|\pm\rangle, |0\rangle$. Solving the eigenvalue problem for S^3 yields

$$|\pm\rangle = \frac{1}{\sqrt{2}} e^{i\delta_{\pm}} (|1\rangle \pm i |2\rangle) \quad (7.29)$$

$$|0\rangle = e^{i\delta_0} |3\rangle \quad (7.30)$$

It follows from (7.29) and (7.30) that

$$|1\rangle = \frac{1}{\sqrt{2}} \left(e^{-i\delta_+} |+\rangle + e^{-i\delta_-} |-\rangle \right) \quad (7.31)$$

$$|2\rangle = \frac{i}{\sqrt{2}} \left(-e^{-i\delta_+} |+\rangle + e^{-i\delta_-} |-\rangle \right) \quad (7.32)$$

$$|3\rangle = e^{-i\delta_0} |0\rangle \quad (7.33)$$

The usual choice for the phase factors, which we use from now on, is

$$e^{i\delta_{\pm}} = \mp 1 \quad e^{i\delta_0} = 1 \quad (7.34)$$

(7.29) and (7.30) are a set of orthonormal vectors which span the vector space, that is,

$$\sum_{\mu=\pm,0} |\mu\rangle \langle \mu| = 1 \quad (7.35)$$

$$\langle \mu | \mu' \rangle = \delta_{\mu\mu'} \quad (7.36)$$

9. Another form for S^j

It follows from (7.2) and (7.31) to (7.33) that

$$S^1 = \frac{1}{\sqrt{2}}(|+\rangle\langle 0| + |0\rangle\langle +| + |0\rangle\langle -| + |-\rangle\langle 0|) \quad (7.37)$$

$$S^2 = \frac{i}{\sqrt{2}}(-|+\rangle\langle 0| + |0\rangle\langle +| - |0\rangle\langle -| + |-\rangle\langle 0|) \quad (7.38)$$

$$S^3 = |+\rangle\langle +| + |-\rangle\langle -| \quad (7.39)$$

(7.39) is the eigenvalue decomposition of S^3 .

10. Another matrix representation of S^j

We denote the matrix elements of S^j with respect to $|\pm\rangle, |0\rangle$ by

$$\langle \mu | S^j | \mu' \rangle = S_{\mu\mu'}^j \quad (7.40)$$

It follows from (7.37) to (7.39) that

$$(S_{\mu\mu'}^1) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad (7.41)$$

$$(S_{\mu\mu'}^2) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad (7.42)$$

$$(S_{\mu\mu'}^3) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad (7.43)$$

(7.41) to (7.43) are identical to the matrices S^j given by (5.52), Rose (1957).

11. Another matrix representation of R

We denote the matrix elements of the rotation operator R (7.25) with respect to $|\pm\rangle, |0\rangle$ by

$$\langle \mu | R | \mu' \rangle = R_{\mu\mu'} \quad (7.44)$$

It follows from (7.20) and (7.31) to (7.33) that

$$(R_{\mu\mu'}) = \begin{pmatrix} e^{-i\varphi} \cos^2 \frac{\theta}{2} & -\frac{1}{\sqrt{2}} e^{-i\varphi} \sin \theta & e^{-i\varphi} \sin^2 \frac{\theta}{2} \\ \frac{1}{\sqrt{2}} \sin \theta & \cos \theta & \frac{1}{\sqrt{2}} \sin \theta \\ e^{i\varphi} \sin^2 \frac{\theta}{2} & \frac{1}{\sqrt{2}} e^{i\varphi} \sin \theta & e^{i\varphi} \cos^2 \frac{\theta}{2} \end{pmatrix} \quad (7.45)$$

(7.45) is a special case of the rotation matrix $D^1(\alpha\beta\gamma)$ given by (4.46), Rose (1957).

12. Eigenvectors of $\vec{S} \cdot \vec{m}$

It follows from (7.26) that the eigenvalues of $\vec{S} \cdot \vec{m}$ are $\pm 1, 0$. We denote the corresponding eigenvectors of $\vec{S} \cdot \vec{m}$ by $|m\pm\rangle, |m0\rangle$. It follows from (7.26) and the eigenvalue problem for $\vec{S} \cdot \vec{m}$ that

$$|m\mu\rangle = R |\mu\rangle \quad (7.46)$$

where $|\pm\rangle, |0\rangle$ are the eigenvectors of S^3 and R is given by (7.25). It follows using (7.45) that

$$|m+\rangle = e^{-i\varphi} \cos^2 \frac{\theta}{2} |+\rangle + \frac{1}{\sqrt{2}} \sin \theta |0\rangle + e^{i\varphi} \sin^2 \frac{\theta}{2} |-\rangle \quad (7.47)$$

$$|m0\rangle = -\frac{1}{\sqrt{2}} e^{-i\varphi} \sin \theta |+\rangle + \cos \theta |0\rangle + \frac{1}{\sqrt{2}} e^{i\varphi} \sin \theta |-\rangle \quad (7.48)$$

$$|m-\rangle = e^{-i\varphi} \sin^2 \frac{\theta}{2} |+\rangle + \frac{1}{\sqrt{2}} \sin \theta |0\rangle + e^{i\varphi} \cos^2 \frac{\theta}{2} |-\rangle \quad (7.49)$$

(7.47) to (7.49) are a set of orthonormal vectors which span the vector space,

that is,

$$\sum_{\mu=\pm,0} |m\mu\rangle\langle m\mu| = 1 \quad (7.50)$$

$$\langle m\mu | m\mu' \rangle = \delta_{\mu\mu'} \quad (7.51)$$

13. Preparation by a Stern-Gerlach apparatus

The states $|m\mu\rangle$ may be thought of as being prepared by a Stern-Gerlach apparatus with inhomogeneous magnetic field in direction \vec{m} .

As in Chapter 6, we call such an apparatus an mSG apparatus.

An mSG apparatus measures $\vec{S} \cdot \vec{m}$. The possible results of a measurement of $\vec{S} \cdot \vec{m}$ are $\mu\hbar$ where $\mu = \pm 1, 0$.

The states $|\mu\rangle$ may be thought of as being prepared by a kSG apparatus. A kSG apparatus measures $\vec{S} \cdot \vec{k} = S^3$. The possible results of a measurement of S^3 are $\mu\hbar$ where $\mu = \pm 1, 0$.

The unitary operator (7.25) corresponds to rotating a Stern-Gerlach apparatus with inhomogeneous magnetic field in the \vec{k} —direction such that the inhomogeneous magnetic field after the rotation is in \vec{m} —direction. That is, it corresponds to rotating a kSG apparatus so that it becomes an mSG apparatus.

14. Probabilities

We consider states prepared by an mSG apparatus and measured by a kSG apparatus.

If the system is known to be in the state $|m+\rangle$ then

$$|\langle + | m+ \rangle|^2 = \cos^4 \frac{\theta}{2} \quad (7.52)$$

$$|\langle 0 | m+ \rangle|^2 = \frac{1}{2} \sin^2 \theta \quad (7.53)$$

$$|\langle - | m+ \rangle|^2 = \sin^4 \frac{\theta}{2} \quad (7.54)$$

are the probabilities that on measurement of S^3 the system be found in the states $|\pm\rangle, |0\rangle$.

If the system is known to be in the state $|m0\rangle$ then

$$|\langle \pm | m0 \rangle|^2 = \frac{1}{2} \sin^2 \theta \quad (7.55)$$

$$|\langle 0 | m0 \rangle|^2 = \cos^2 \theta \quad (7.56)$$

are the probabilities that on measurement of S^3 the system be found in the states $|\pm\rangle, |0\rangle$.

If the system is known to be in the state $|m-\rangle$ then

$$|\langle + | m- \rangle|^2 = \sin^4 \frac{\theta}{2} \quad (7.57)$$

$$|\langle 0 | m- \rangle|^2 = \frac{1}{2} \sin^2 \theta \quad (7.58)$$

$$|\langle - | m- \rangle|^2 = \cos^4 \frac{\theta}{2} \quad (7.59)$$

are the probabilities that on measurement of S^3 the system be found in the states $|\pm\rangle, |0\rangle$.

7.3 Spherical tensors

As shown in Chapter 6, every operator in the spin $\frac{1}{2}$ vector space can be written as a linear combination of the unit operator (6.1) and the three Pauli operators (6.4) to (6.6). The corresponding statement for the spin 1 vector space is more complicated: there are nine basic operators for the space as opposed to four for the spin $\frac{1}{2}$ vector space.

For example, it follows from (7.35) that a hermitian operator A in the spin 1 vector space can be written in the form

$$A = \sum_{\mu, \mu' = \pm 1, 0} |\mu\rangle a_{\mu\mu'} \langle \mu'| \quad (7.60)$$

where

$$a_{\mu\mu'} = \langle \mu | A | \mu' \rangle = \langle \mu' | A | \mu \rangle^* = a_{\mu'\mu}^* \quad (7.61)$$

where $|\pm\rangle, |0\rangle$ are the eigenvectors of S^3 belonging to eigenvalues $\pm, 0$.

Expansion (7.60) in terms of the nine operators $|\mu\rangle\langle\mu'|$ may be convenient in many instances; it is not particularly convenient, however, when the effect of rotations is to be considered.

We construct a set of eight spherical tensor operators T_{lm} which, in addition to the unit operator, are appropriate for expanding an arbitrary operator in the spin 1 vector space. The T_{lm} are constructed in order that they transform simply under rotations.

We define the operators T_{lm} as follows:

$$T_{1\pm 1} = \mp \frac{1}{\sqrt{2}} (S^1 \pm iS^2) \quad (7.62)$$

$$T_{10} = S^3 \quad (7.63)$$

$$T_{2\pm 2} = \frac{1}{2} (S^1 \pm iS^2)^2 \quad (7.64)$$

$$T_{2\pm 1} = \mp \frac{1}{2} \{ S^1 \pm iS^2, S^3 \} \quad (7.65)$$

$$T_{20} = \sqrt{\frac{3}{2}} \left[(S^3)^2 - \frac{2}{3} \right] \quad (7.66)$$

where S^1, S^2, S^3 are the spin operators discussed in Section 7.2.

Properties

1. Adjoint

It follows from (7.62) to (7.66) that

$$T_{lm}^\dagger = (-)^m T_{l-m} \quad (7.67)$$

2. Matrix elements

It follows from (7.62) to (7.66) that

$$\langle \mu | T_{lm} | \mu' \rangle = c_l (1l\mu'm | 1\mu) \quad (7.68)$$

$$c_1 = \sqrt{\frac{5}{6}} c_2 = \frac{1}{\sqrt{2}} \quad (7.69)$$

where $|\mu\rangle$ is the eigenvector of S^3 belonging to eigenvalue $\mu\hbar$ and $(j_1 j_2 m_1 m_2 | j_3 m_3)$ is a Clebsch-Gordon coefficient.

(7.68) is an example of the Wigner-Eckart theorem: the dependence of $\langle \mu | T_{lm} | \mu' \rangle$ on μ, m, μ' resides entirely in the Clebsch-Gordon coefficient $(1l\mu'm | 1\mu)$.

3. Traces

It follows from (7.62) to (7.66) that

$$\text{Tr } T_{lm} = 0 \quad (7.70)$$

$$\text{Tr} \left(T_{lm} T_{l'm'}^\dagger \right) = n_l \delta_{ll'} \delta_{mm'} \quad (7.71)$$

$$\frac{1}{2} n_1 = n_2 = 1 \quad (7.72)$$

4. Commutation relations

It follows from (7.62) to (7.66) that

$$[S^1 \pm iS^2, T_{lm}] = \sqrt{(l \mp m)(l \pm m + 1)} T_{lm \pm 1} \quad (7.73)$$

$$[S^3, T_{lm}] = m T_{lm} \quad (7.74)$$

5. Transformation under rotations

It is shown in Chapter V, Rose (1957) that it follows from (7.73) and (7.74) that

$$R(\alpha, \beta, \gamma)T_{lm}R^\dagger(\alpha, \beta, \gamma) = \sum_{m'=-l}^{+l} D_{m'm}^l(\alpha, \beta, \gamma)T_{lm'} \quad (7.75)$$

where

$$R(\alpha, \beta, \gamma) = e^{-iS^3\alpha}e^{-iS^2\beta}e^{-iS^3\gamma} \quad (7.76)$$

and where

$$D_{m'm}^l(\alpha, \beta, \gamma) \quad (7.77)$$

is a rotation matrix. In particular,

$$RT_{l0}^\dagger R^\dagger = \sqrt{\frac{4\pi}{2l+1}} \sum_{m=-l}^{+l} Y_{lm}(\theta, \varphi)T_{lm}^\dagger \quad (7.78)$$

where $Y_{lm}(\theta, \varphi)$ is a spherical harmonic and

$$R = R(\varphi, \theta, 0) = e^{-iS^3\varphi}e^{-iS^2\theta} \quad (7.79)$$

R corresponds to the rotation of \vec{k} to a vector which has spherical polar

coordinates (θ, φ) .

In view of (7.75), the T_{1m} are called spherical tensors of rank l .

6. Spin operators

It follows from (7.62) and (7.63) that

$$S^1 = \frac{1}{\sqrt{2}}(-T_{11} + T_{1-1}) \quad (7.80)$$

$$S^2 = \frac{i}{\sqrt{2}}(T_{11} + T_{1-1}) \quad (7.81)$$

$$S^3 = T_{10} \quad (7.82)$$

7. Scalar product of spin operators

Let $\vec{a} = a^1\vec{i} + a^2\vec{j} + a^3\vec{k}$. It follows from (7.80) to (7.82) that

$$\vec{a} \cdot \vec{S} = \sum_{m=-1}^{+1} a_{1m} T_{1m}^\dagger = \sqrt{\frac{4\pi}{3}} a \sum_{m=-1}^{+1} Y_{1m}(\theta, \varphi) T_{1m}^\dagger \quad (7.83)$$

where

$$a_{1\pm 1} = \mp \frac{1}{\sqrt{2}}(a^1 \pm ia^2) \quad (7.84)$$

$$a_{10} = a^3 \quad (7.85)$$

are the spherical components of \vec{a} and (a, θ, φ) are the spherical polar coordinates of \vec{a} .

8. Products of spin operators

It follows from (7.5) and (7.6) and (7.62) to (7.66) that

$$(S^1)^2 = \frac{2}{3} - \frac{1}{\sqrt{6}}T_{20} + \frac{1}{2}(T_{22} + T_{2-2}) \quad (7.86)$$

$$(S^2)^2 = \frac{2}{3} - \frac{1}{\sqrt{6}}T_{20} - \frac{1}{2}(T_{22} + T_{2-2}) \quad (7.87)$$

$$(S^3)^2 = \frac{2}{3} + \sqrt{\frac{2}{3}}T_{20} \quad (7.88)$$

$$S^1 S^2 = \frac{i}{2}(T_{10} - T_{22} + T_{2-2}) \quad (7.89)$$

$$S^1 S^3 = \frac{1}{2\sqrt{2}}(T_{11} + T_{1-1}) + \frac{1}{2}(-T_{21} + T_{2-1}) \quad (7.90)$$

$$S^2 S^3 = \frac{i}{2\sqrt{2}}(-T_{11} + T_{1-1}) + \frac{i}{2}(T_{21} + T_{2-1}) \quad (7.91)$$

9. Operators $|\mu\rangle\langle\mu'|$

The operators $|\mu\rangle\langle\mu'|$ which appear in (7.60) may be written in terms of the operators $|a\rangle\langle b|$ which appear in (7.2) using (7.29) and (7.30). These latter operators may be written in terms products of spin operators using (7.5) and in terms of the T_{lm} using (7.86) to 7.91). Finally, then, the operators $|\mu\rangle\langle\mu'|$ may be written in terms of the T_{lm} as follows:

$$|+\rangle\langle+| = \frac{1}{3} + T_{10} + \frac{1}{\sqrt{6}} T_{20} \quad (7.92)$$

$$|0\rangle\langle 0| = \frac{1}{3} - T_{10} + \frac{1}{\sqrt{6}} T_{20} \quad (7.93)$$

$$|-\rangle\langle-| = \frac{1}{3} - \sqrt{\frac{2}{3}} T_{20} \quad (7.94)$$

$$|+\rangle\langle 0| = \frac{1}{2} T_{11} - \frac{1}{\sqrt{2}} T_{21} \quad (7.95)$$

$$|0\rangle\langle-| = -\frac{1}{2} T_{11} - \frac{1}{\sqrt{2}} T_{21} \quad (7.96)$$

$$|+\rangle\langle-| = T_{22} \quad (7.97)$$

10. General hermitian operator

A hermitian operator A is expressed in terms of the operators $|\mu\rangle\langle\mu'|$ by (7.60); it may be written equivalently in terms of the spherical tensor operators T_{lm} as follows:

$$A = \frac{1}{3} \text{Tr}A + \sum_{l=1,2} \sum_{m=-l}^l a_{lm} T_{lm}^\dagger \quad (7.98)$$

where

$$a_{lm}^* = (-)^m a_{l-m} \quad (7.99)$$

and where, using (7.71),

$$a_{lm} = \frac{1}{n_l} \text{Tr} (T_{lm} A) \quad (7.100)$$

$\text{Tr}A$ and the a_{lm} are expressed in terms of the $a_{\mu\mu'}$ as follows:

$$\text{Tr}A = \sum_{\mu=\pm,0} a_{\mu\mu} \quad (7.101)$$

$$a_{11} = \frac{1}{2}(a_{0+} - a_{-0}) \quad (7.102)$$

$$a_{10} = a_{++} - a_{--} \quad (7.103)$$

$$a_{22} = a_{-+} \quad (7.104)$$

$$a_{21} = -\frac{1}{\sqrt{2}}(a_{0+} + a_{-0}) \quad (7.105)$$

$$a_{20} = \frac{1}{\sqrt{6}}(a_{++} + a_{--} - 2a_{00}) \quad (7.106)$$

A general operator on the spin 1 vector space is specified by nine complex numbers: its trace and the coefficients of the eight T_{lm}^\dagger . For a hermitian operator on the space, the trace is real and the coefficients satisfy the eight conditions (7.99).

Accordingly, (7.98) expresses a general hermitian operator A in terms of nine real numbers: its trace, three real numbers related to the coefficients of the rank one tensor T_{1m}^\dagger and five real numbers related to the coefficients of the rank two tensor T_{2m}^\dagger .

7.4 Density operators

We recall from Topic 5.3 that the general state of a system is represented by a unit trace hermitian density operator. It follows from (7.98) that the general state of a spin 1 system is represented by the density operator

$$\Psi = \frac{1}{3} + \sum_{l=1,2} \sum_{m=-l}^{+l} a_{lm} T_{lm}^\dagger \quad (7.107)$$

where a_{lm} satisfies (7.99) and

$$a_{lm} = \frac{1}{n_l} \text{Tr} (T_{lm} \Psi) \quad (7.108)$$

Density operator for a pure state

The density operator for a pure state is discussed in Section 5.2. In this topic we apply the formalism to pure states of a spin 1 particle prepared and measured by a Stern-Gerlach apparatus.

Density operator corresponding to $|\mu\rangle$

It follows from (5.1) that the density operator Ψ^μ corresponding to the eigenvector $|\mu\rangle$ of S^3 belonging to eigenvalue $\mu\hbar$ is

$$\Psi^\mu = |\mu\rangle\langle\mu| \quad (7.109)$$

It follows from (7.92) to (7.94) that

$$\Psi^\mu = \frac{1}{3} + \sum_{l=1,2} a_l^\mu T_{l0}^\dagger \quad (7.110)$$

where

$$a_1^+ = -a_1^- = 1 \quad (7.111)$$

$$a_1^0 = 0 \quad (7.112)$$

$$a_2^+ = a_2^- = -\frac{1}{2}a_2^0 = \frac{1}{\sqrt{6}} \quad (7.113)$$

Density operator corresponding to $|m_\mu\rangle$

It follows from (5.1) that the density operator Ψ^{m_μ} corresponding to the eigenvector $|m_\mu\rangle$ of $\vec{S} \cdot \vec{m}$ belonging to eigenvalue $\mu\hbar$ is

$$\Psi^{m_\mu} = |m_\mu\rangle\langle m_\mu| \quad (7.114)$$

It follows from (7.78) and (7.110) that

$$\Psi^{m_\mu} = \frac{1}{3} + \sum_{l=1,2} \sum_{m_l=-l}^{+l} a_{lm_l}^\mu T_{lm_l}^\dagger \quad (7.115)$$

where

$$a_{lm_l}^\mu = \sqrt{\frac{4\pi}{2l+1}} a_l^\mu Y_{lm_l}(\theta, \varphi) \quad (7.116)$$

where (θ, φ) are the spherical polar coordinates of the unit vector \vec{m} .

The pure state (7.115) is labelled by four real parameters $(a_1^\mu, a_2^\mu, \theta, \varphi)$. The geometrical interpretation of these parameters is given below.

Probabilities

As given by (5.3), the probability $P(\mu, \Psi^{m\mu'})$ that the system be found in the state $|\mu\rangle$ when it is known to be in the state $\Psi^{m\mu'}$ is

$$P(\mu, \Psi^{m\mu'}) = \langle \mu | \Psi^{m\mu'} | \mu \rangle \quad (7.117)$$

It follows using (7.68) and (7.115) that

$$P(\mu, \Psi^{m\mu'}) = \frac{1}{3} + \sum_{l=1,2} \sqrt{\frac{4\pi}{2l+1}} a_l^{\mu'} c_l \sum_{m_l=-l}^{+l} (1, l, \mu, m_l | 1, \mu) Y_{lm_l}^*(\theta, \varphi) \quad (7.118)$$

(7.118) is identical to (7.52) to (7.59).

Polarization vector

As given by (5.9), the average $\overline{S}^{m\mu}$ of the spin \vec{S} for the system in the state $\Psi^{m\mu}$ is

$$\overline{S}^{m\mu} = \text{Tr} (\vec{S} \Psi^{m\mu}) \quad (7.119)$$

$\overline{S}^{m\mu}$ is the polarization vector for the system in the state $\Psi^{m\mu}$.

It follows using (7.80) to (7.82) with (7.108) that

$$\overline{S^1}^{m\mu} = a_1^\mu \sin \theta \cos \varphi \quad (7.120)$$

$$\overline{S^2}^{m\mu} = a_1^\mu \sin \theta \sin \varphi \quad (7.121)$$

$$\overline{S^3}^{m\mu} = a_1^\mu \cos \theta \quad (7.122)$$

That is, $(a_1^\mu, \theta, \varphi)$ are the spherical polar coordinates of the polarization vector $\overline{S}^{m\mu}$. The polarization vector is directed along the inhomogeneous magnetic field of the mSG apparatus which prepared the state $\Psi^{m\mu}$.

Polarization ellipsoid

As given by (5.9), the average of $(S^j)^2$ for the system in the state $\Psi^{m\mu}$ is

$$\overline{[(S^j)^2]}^{m\mu} = \text{Tr} [(S^j)^2 \Psi^{m\mu}] \quad (7.123)$$

It follows using (7.86) to (7.88) with (7.108) that

$$\overline{[(S^1)^2]}^{m\mu} = \frac{2}{3} + \frac{1}{\sqrt{6}} a_2^\mu (3 \sin^2 \theta \cos^2 \varphi - 1) \quad (7.124)$$

$$\overline{[(S^2)^2]}^{m\mu} = \frac{2}{3} + \frac{1}{\sqrt{6}} a_2^\mu (3 \sin^2 \theta \sin^2 \varphi - 1) \quad (7.125)$$

$$\overline{[(S^3)^2]}^{m\mu} = \frac{2}{3} + \frac{1}{\sqrt{6}} a_2^\mu (3 \cos^2 \theta - 1) \quad (7.126)$$

In particular,

$$\overline{[(S^1)^2]}^{k\mu} = \overline{[(S^2)^2]}^{k\mu} = \frac{2}{3} - \frac{1}{\sqrt{6}} a_2^\mu \quad (7.127)$$

$$\overline{[(S^3)^2]}^{k\mu} = \frac{2}{3} + \sqrt{\frac{2}{3}} a_2^\mu \quad (7.128)$$

and

$$\overline{[(S^1)^2]}^{k\pm} = \overline{[(S^2)^2]}^{k\pm} = \frac{1}{2} \quad (7.129)$$

$$\overline{[(S^3)^2]}^{k\pm} = 1 \quad (7.130)$$

$$\overline{[(S^1)^2]}^{k0} = \overline{[(S^2)^2]}^{k0} = 1 \quad (7.131)$$

$$\overline{[(S^3)^2]}^{k0} = 0 \quad (7.132)$$

Comments

1. Semiaxes of the polarization ellipsoid

The above results correspond to an ellipsoid (the polarization ellipsoid) centred at the origin of the coordinate system. The semiaxes $(c^{1m\mu}, c^{2m\mu}, c^{3m\mu})$ along the coordinate axes of the polarization ellipsoid for the system in the state $\Psi^{m\mu}$ are defined by

$$c^{jm\mu} = \left(\overline{[(S^j)^2]}^{m\mu} \right)^{\frac{1}{2}} \quad (7.133)$$

(7.133) involves the parameters $(a_2^\mu, \theta, \varphi)$.

In particular, (7.127) and 7.128) correspond to an ellipsoid of revolution about the z -axis: (7.129) and 7.130) correspond to a prolate ellipsoid; (7.131) and 7.132) correspond to an extreme oblate ellipsoid (a disc).

2. Stern-Gerlach apparatuses in series

The observable $\vec{S} \cdot \vec{m}$ is measured by a Stern-Gerlach apparatus with inhomogeneous magnetic field in direction \vec{m} (an mSG apparatus).

The observable $(S^j)^2$ is measured by two jSG apparatuses in series: that is, by two jSG apparatuses such that the entire output from the first jSG apparatus is the input to the second jSG apparatus. The output from the first jSG apparatus is not observed.

Density operator for a mixed state

The density operator for a mixed state is discussed in Section 5.3. In this topic we apply the formalism to a mixed state of a spin 1 particle prepared by a fuzzy Stern-Gerlach apparatus and measured by efficient Stern-Gerlach apparatuses.

We recall from Item 13 in Section 7.2 that the states $|m\mu\rangle$ of a spin 1 particle may be thought of as being prepared by a Stern-Gerlach apparatus whose inhomogeneous magnetic field is in the \vec{m} -direction (an mSG apparatus). An mSG apparatus prepares pure states of the system: one can decide with certainty whether an mSG apparatus has prepared the state $|m+\rangle$ or the state $|m0\rangle$ or the state $|m-\rangle$.

We now imagine preparing a state of the system with an inefficient mSG-like apparatus which does not allow one to decide with certainty whether the apparatus has prepared the state $|m+\rangle$ or the state $|m0\rangle$ or the state $|m-\rangle$. This will be the case if the gradient of the inhomogeneous magnetic field in the Stern-Gerlach apparatus is not sufficiently strong. As in Chapter 6, we call such an inefficient mSG-like apparatus an mFSG apparatus (F for fuzzy).

We can only assign a probability for preparing the state $| m\mu \rangle$ which probability is specified by the characteristics of the mFSG apparatus.

Let $p_{m\mu}$ be the probability for preparing the state $| m\mu \rangle$ with an mFSG apparatus. Then

$$0 \leq p_{m\mu} \leq 1 \quad (7.134)$$

$$\sum_{\mu=\pm,0} p_{m\mu} = 1 \quad (7.135)$$

As given by (5.15), the state prepared by the mFSG apparatus is represented by the density operator

$$\Psi^m = \sum_{\mu=\pm,0} p_{m\mu} \Psi^{m\mu} \quad (7.136)$$

It follows from (7.115) and (7.116) that the mixed state (7.136) is labelled by the four real parameters $(a_1, a_2, \theta, \varphi)$ where

$$a_l = \sum_{\mu=\pm,0} p_{m\mu} \alpha_l^\mu \quad (7.137)$$

(θ, φ) specify the direction of the inhomogeneous magnetic field of the mFSG apparatus which prepared the state Ψ^m ; (a_1, θ, φ) are the spherical polar components of the polarization vector for the state; (a_2, θ, φ) determine the semiaxes of the polarization ellipsoid for the state.

Measurement of $\vec{S} \cdot \vec{n}$ with an mSG apparatus for the system in the state Ψ^m yields the value $\mu\hbar$ with probability $p_{m\mu}$.

Measurement of S^3 with a kSG apparatus for the system in the state Ψ^m yields the value $\mu\hbar$ with probability

$$P(\mu, \Psi^m) = \sum_{\mu'=\pm,0} p_{m\mu'} P(\mu, \Psi^{m\mu'}) \quad (7.138)$$

Unpolarized state

If the state Ψ^m is unpolarized, that is, if

$$p_{m+} = p_{m0} = p_{m-} = \frac{1}{3} \quad (7.139)$$

then

$$\Psi^m = \frac{1}{3} \quad (7.140)$$

$$a_l = 0 \quad (7.141)$$

It follows from (7.141) that, not unexpectedly, the polarization vector for the unpolarized state vanishes and the polarization ellipsoid is a sphere with radius $\sqrt{s(s+1)}$ where $s = 1$.

Chapter 8 PARTICLE IN A MAGNETIC FIELD

8.1 Introductory remarks

In this chapter, we describe interaction of a particle with spin with a magnetic field. Our purpose is to apply the methods of quantum mechanics to the important processes of spin precession and magnetic resonance.

We consider the interaction of a particle with spin with a constant, homogeneous magnetic field in Section 8.2. We show that the average magnetic moment of the particle precesses about the direction of the magnetic field with the Larmor frequency. The phenomenon of magnetic resonance is discussed in Section 8.3. Magnetic resonance of a spin $\frac{1}{2}$ particle and of a spin 1 particle are discussed in detail.

8.2 Particle in a constant magnetic field

Observation

A particle with spin is subjected to a constant, homogeneous magnetic field \vec{B} . It is observed that the average magnetic moment of the particle precesses about \vec{B} with angular frequency

$$\omega_0 = \frac{geB}{2mc} \quad (8.1)$$

g is the gyromagnetic ratio of the particle, m is its rest mass, e is the charge of a proton and c is the speed of light.

ω_0 is the Larmor precession frequency. For a proton in a one Tesla field, $\omega_0/2\pi = 42$ MHz; for a proton in the Earth's magnetic field, $\omega_0/2\pi = 850$ Hz.

Analysis

We describe the quantum mechanics of the system. We work in the Schrodinger picture as described in Section 4.2.

We characterize a fixed Cartesian reference frame in a laboratory by unit vectors $\vec{i}, \vec{j}, \vec{k}$ along the coordinate axes. We disregard any change in position of the particle. The fundamental dynamical variables are the three Cartesian components S^1, S^2, S^3 of the spin \vec{S} of the particle.

$$\vec{S} = S^1\vec{i} + S^2\vec{j} + S^3\vec{k} \quad (8.2)$$

The fundamental algebra is given by

$$[S^j, S^k] = i\hbar\epsilon_{jkl}S^l \quad (8.3)$$

$$\vec{S} \cdot \vec{S} = s(s+1)\hbar^2 \quad (8.4)$$

where s is the spin of the particle.

Since change in position of the particle is disregarded, the angular momentum \vec{J} of the particle is

$$\vec{J} = \vec{S} \quad (8.5)$$

The magnetic moment $\vec{\mu}$ of the particle is

$$\vec{\mu} = \frac{ge}{2mc} \vec{S} \quad (8.6)$$

The Hamiltonian H for the particle in the magnetic field \vec{B} is

$$H = -\vec{\mu} \cdot \vec{B} \quad (8.7)$$

The state of the particle at time t is $|\psi(t)\rangle$ as given by (4.3).

Comments

1. Precession of the polarization vector

The particle experiences a torque \vec{T} due to the magnetic field \vec{B} . The torque on the particle is the time rate of change of its angular momentum, that is,

$$\vec{T}(t) = \frac{d}{dt} \vec{J}(t) \quad (8.8)$$

where $\vec{T}(t)$ and $\vec{J}(t)$ are the torque and angular momentum in the Heisenberg picture. It follows from (4.8) that

$$\vec{T}(t) = U^\dagger(t)\vec{T}U(t) \quad (8.9)$$

$$\vec{J}(t) = U^\dagger(t)\vec{J}U(t) \quad (8.10)$$

On carrying out the differentiation in (8.8) , it follows using (4.4), (8.9) and (8.10) that

$$i\hbar\dot{\vec{T}} = [\vec{J}, H] \quad (8.11)$$

Substitution of (8.5) and (8.7) into (8.11) yields

$$\dot{\vec{T}} = \vec{\mu} \times \vec{B} \quad (8.12)$$

As given by (4.5), the average torque $\overline{\vec{T}}(t)$ acting on the particle in the state $|\psi(t)\rangle$ is

$$\overline{\vec{T}}(t) = \langle \psi(t) | \vec{T} | \psi(t) \rangle \quad (8.13)$$

It follows from (8.12) that

$$\dot{\overline{\vec{T}}}(t) = \overline{\vec{\mu}}(t) \times \vec{B} \quad (8.14)$$

where

$$\bar{\mu}(t) = \langle \psi(t) | \vec{\mu} | \psi(t) \rangle \quad (8.15)$$

$\bar{\mu}(t)$ is the average magnetic moment of the particle in the state $|\psi(t)\rangle$.

(8.14) states that the average torque acting on the particle is perpendicular to the average magnetic moment and the magnetic field. Accordingly, the torque causes a precession of $\bar{\mu}(t)$ about \vec{B} as is observed.

2. Precession frequency

To determine the precession frequency, we take $\vec{B} = B\vec{k}$ in which case

$$H = -\omega_0 S^3 \quad (8.16)$$

where ω_0 is given by (8.1).

It follows from (4.7) that

$$\bar{\mu}^1(t) = \bar{\mu}^1 \cos \omega_0 t + \bar{\mu}^2 \sin \omega_0 t \quad (8.17)$$

$$\bar{\mu}^2(t) = -\bar{\mu}^1 \sin \omega_0 t + \bar{\mu}^2 \cos \omega_0 t \quad (8.18)$$

$$\bar{\mu}^3(t) = \bar{\mu}^3 \quad (8.19)$$

We assume that the average magnetic moment at time zero lies in the

$\vec{j}\vec{k}$ -plane and makes an angle θ with the magnetic field. That is,

$$\vec{\mu} = [\sin \theta \vec{j} + \cos \theta \vec{k}] \bar{\mu} \quad (8.20)$$

where $\bar{\mu} = \sqrt{\vec{\mu} \cdot \vec{\mu}}$. It follows that

$$\vec{\mu}(t) = [\sin \theta \vec{j}(t) + \cos \theta \vec{k}] \bar{\mu} \quad (8.21)$$

where

$$\vec{j}(t) = \sin \omega_0 t \vec{i} + \cos \omega_0 t \vec{j} \quad (8.22)$$

(8.22) defines a vector which rotates about the \vec{k} -axis with angular frequency ω_0 .

Thus, $\vec{\mu}(t)$ precesses about \vec{B} with angular frequency (8.1) as is observed.

3. Average energy and uncertainty for a spin $\frac{1}{2}$ particle

For a spin $\frac{1}{2}$ particle, the eigenvalues and corresponding eigenvectors of (8.16) are

$$\epsilon_2 = +\frac{1}{2}\hbar\omega_0 \quad |\epsilon_2\rangle = |-\rangle \quad (8.23)$$

$$\epsilon_1 = -\frac{1}{2}\hbar\omega_0 \quad |\epsilon_1\rangle = |+\rangle \quad (8.24)$$

where $|\pm\rangle$ are the eigenvectors of σ^3 as discussed in Section 6.2.

The evolution operator (4.4) may be written in the form

$$U(t) = \cos \frac{\omega_0 t}{2} + i\sigma^3 \sin \frac{\omega_0 t}{2} \quad (8.25)$$

The average energy \bar{E} and the uncertainty in energy ΔE for the particle in the state

$$|\psi(t)\rangle = U(t) |m+\rangle \quad (8.26)$$

are

$$\bar{E} = \langle \psi(t) | H | \psi(t) \rangle = -\frac{1}{2}\hbar\omega_0 \cos \theta \quad (8.27)$$

$$\Delta E = \| (H - \bar{E}) | \psi(t) \rangle \| = \frac{1}{2}\hbar\omega_0 \sin \theta \quad (8.28)$$

It follows from (8.27) and (8.28) that

$$-\frac{1}{2}\hbar\omega_0 \leq \bar{E} \leq +\frac{1}{2}\hbar\omega_0 \quad (8.29)$$

$$0 \leq \Delta E \leq \frac{1}{2}\hbar\omega_0 \quad (8.30)$$

It follows from (8.30) and the time-energy uncertainty relation (3.26) that

$$\Delta t_{min}(t) \geq \frac{1}{\omega_0} \quad (8.31)$$

That is, it takes a time interval of at least $\frac{1}{\omega_0}$ to measure a change in the state of the particle.

For example,

$$\frac{1}{\omega_0} \simeq 1 \text{ ns} \quad (8.32)$$

for a proton in a 4 T magnetic field.

Since the speed of light $c = 30 \text{ cm/ns}$, it follows that a fast moving proton must travel of the order of 30 cm in a constant, homogeneous 4 T magnetic field in order to have its polarization vector rotated by an observable amount.

The magnet used for rotating the polarization vector of the proton beam at TRIUMF is a one-metre long superconducting solenoid which produces a magnetic field of the order of 4 T.

8.3 Magnetic resonance

Observation

A particle with spin is subjected to a magnetic field \vec{B} which is a superposition of a constant, homogeneous field \vec{B}_0 and a rotating field \vec{B}_1 which is perpendicular to \vec{B}_0 .

It is observed that the rotating field causes the average spin vector of the particle to change sign. The probability of this “spin flip” can be made equal to

one when the frequency of the rotating field is equal to the Larmor precession frequency of the particle in the field \vec{B}_0 . This is the phenomenon of magnetic resonance.

Analysis

We describe the quantum mechanics of the system. We set up the quantum mechanics in the Schrodinger picture as described in Section 4.2 and solve the equation of motion in the interaction picture as described in Section 4.4.

The physical system is characterized as in Section 8.2. The Hamiltonian is given by (8.7) where, in this case, the magnetic field \vec{B} acting on the particle is

$$\vec{B} = \vec{B}_0 + \vec{B}_1 \quad (8.33)$$

where

$$\vec{B}_0 = B_0 \vec{k} \quad (8.34)$$

$$\vec{B}_1 = B_1 (\cos \omega t \vec{i} - \sin \omega t \vec{j}) \quad (8.35)$$

B_0 , B_1 and ω are constants. ω is the angular rotation frequency of \vec{B}_1 .

The Hamiltonian for the particle in the magnetic field (8.33) is

$$H = H_0 + H_1 \quad (8.36)$$

where

$$H_0 = -\omega_0 S^3 \quad (8.37)$$

$$H_1 = -\omega_1 (S^1 \cos \omega t - S^2 \sin \omega t) \quad (8.38)$$

where ω_0 is the Larmor frequency (8.1) and

$$\omega_1 = \frac{geB_1}{2mc} \quad (8.39)$$

To determine the time evolution of the system in the magnetic field, in view of (4.11), we solve the equation of motion in the interaction picture.

We recall from Section 4.4 that in the interaction picture the state of the system $|\psi'(t)\rangle$ satisfies (4.17), that is,

$$i\hbar \frac{d}{dt} |\psi'(t)\rangle = H_1'(t) |\psi'(t)\rangle \quad (8.40)$$

where

$$H_1'(t) = e^{+iH_0 t/\hbar} H_1 e^{-iH_0 t/\hbar} \quad (8.41)$$

Evaluating the right side of (8.41) using (8.37) to (8.39) yields

$$H_1'(t) = -\omega_1 [S^1 \cos(\omega_0 - \omega)t + S^2 \sin(\omega_0 - \omega)t] \quad (8.42)$$

We solve the equations of motion for a spin $\frac{1}{2}$ particle and a spin 1 particle in the following topics.

Spin $\frac{1}{2}$ particle

The eigenvalues and corresponding eigenvectors of H_0 (8.37) are given by (8.23) and (8.24).

We take the initial state $|\psi(0)\rangle$ of the system to be ground state of H_0 . That is,

$$|\psi(0)\rangle = |+\rangle \quad (8.43)$$

To solve (8.40) we use (6.1) to write

$$|\psi'(t)\rangle = \sum_{\mu=\pm} a_{\mu}(t) |\mu\rangle \quad (8.44)$$

where

$$a_{\mu}(t) = \langle \mu | \psi'(t) \rangle \quad (8.45)$$

$$\sum_{\mu=\pm} |a_{\mu}(t)|^2 = 1 \quad (8.46)$$

It follows from (8.43) that

$$a_{\mu}(0) = \delta_{\mu+} \quad (8.47)$$

$|a_{\mu}(t)|^2$ is the probability that the polarization vector of the particle at time t is $\mu \frac{1}{2} \vec{k}$.

$|a_{-}(t)|^2$ is the probability of a “spin flip”.

Substituting (8.44) into (8.40) yields two coupled first-order differential equations for $a_{+}(t)$ and $a_{-}(t)$. Solving these equations subject to the initial conditions (8.47) yields

$$|a_{+}(t)|^2 = \left(\frac{\omega_1}{\Omega}\right)^2 \cos^2 \frac{\Omega t}{2} + \frac{\delta^2}{\Omega^2} \quad (8.48)$$

$$|a_{-}(t)|^2 = \left(\frac{\omega_1}{\Omega}\right)^2 \sin^2 \frac{\Omega t}{2} \quad (8.49)$$

where

$$\Omega = \sqrt{\omega_1^2 + \delta^2} \quad (8.50)$$

$$\delta = \omega - \omega_0 \quad (8.51)$$

Comments

1. Resonance function

The function

$$\left(\frac{\omega_1}{\Omega}\right)^2 = \frac{\omega_1^2}{(\omega - \omega_0)^2 + \omega_1^2} \quad (8.52)$$

in (8.48) and (8.49) characterizes a resonance; it is symmetric about $\omega = \omega_0$, has a maximum equal to unity when $\omega = \omega_0$ and drops to half-maximum when $\omega = \omega_0 \pm \omega_1$.

ω_1 characterizes the width of the resonance. There is a sharp resonance if $\omega_1 \ll \omega_0$, that is, $B_1 \ll B_0$.

When $\omega = \omega_0$,

$$|a_+(t)|^2 = \cos^2 \frac{\omega_1 t}{2} \quad (8.53)$$

$$|a_-(t)|^2 = \sin^2 \frac{\omega_1 t}{2} \quad (8.54)$$

2. Magnetic resonance

It follows from (8.54) that

$$\left| a_{-} \left(\frac{\pi}{\omega_1} \right) \right|^2 = 1 \quad (8.55)$$

That is, a spin flip is certain when the angular frequency ω of the rotating magnetic field \vec{B}_1 (8.35) is equal to the Larmor precession frequency ω_0 (8.1) and the particle is subjected to the rotating magnetic field for the time π/ω_1 .

The particle absorbs energy $\hbar\omega_0$ from the magnetic field \vec{B}_1 in making a transition from the ground state $| + \rangle$ to the excited state $| - \rangle$.

This is the phenomenon of magnetic resonance.

3. Applications of magnetic resonance

Magnetic resonance was first used in the 1940's to determine gyromagnetic ratios of nuclei.

It has since become one of the most widely-used diagnostic tools in all of science.

One reason for this wide range of applicability lies in the fact that, as seen from (8.1) and (8.39), the resonance parameters ω_0 and ω_1 depend upon a number of other parameters (B_0, B_1, g, m) which can be controlled or varied depending upon the application under consideration.

Spin 1 particle

The eigenvalues and corresponding eigenvectors of H_0 (8.37) are

$$\epsilon_3 = +\hbar\omega_0 \quad | \epsilon_3 \rangle = | - \rangle \quad (8.56)$$

$$\epsilon_2 = 0 \quad | \epsilon_2 \rangle = | 0 \rangle \quad (8.57)$$

$$\epsilon_1 = -\hbar\omega_0 \quad | \epsilon_1 \rangle = | + \rangle \quad (8.58)$$

where $| \pm \rangle, | 0 \rangle$ are the eigenvectors of S^3 as discussed in Section 7.2.

We take the initial state $| \psi(0) \rangle$ of the system to be ground state of H_0 . That is,

$$| \psi(0) \rangle = | + \rangle \quad (8.59)$$

To solve (8.40) we use (7.35) to write

$$| \psi'(t) \rangle = \sum_{\mu=\pm,0} a_{\mu}(t) | \mu \rangle \quad (8.60)$$

where

$$a_{\mu}(t) = \langle \mu | \psi'(t) \rangle \quad (8.61)$$

$$\sum_{\mu=\pm,0} |a_{\mu}(t)|^2 = 1 \quad (8.62)$$

It follows from (8.59) that

$$a_{\mu}(0) = \delta_{\mu+} \quad (8.63)$$

$|a_{\mu}(t)|^2$ is the probability that the polarization vector of the particle at time t is $\mu\vec{k}$.

$|a_{-}(t)|^2$ is the probability of a "spin flip".

Substituting (8.44) into (8.40) yields three coupled first-order differential equations for $a_{+}(t)$, $a_0(t)$ and $a_{-}(t)$. Solving these equations subject to the initial conditions (8.63) yields

$$|a_{+}(t)|^2 = \left(\frac{\omega_1}{\Omega}\right)^4 \left(\cos^2 \frac{\Omega t}{2} + \frac{\delta^2}{\omega_1^2}\right)^2 \quad (8.64)$$

$$|a_0(t)|^2 = 2\left(\frac{\omega_1}{\Omega}\right)^4 \sin^2 \frac{\Omega t}{2} \left(\cos^2 \frac{\Omega t}{2} + \frac{\delta^2}{\omega_1^2}\right) \quad (8.65)$$

$$|a_{-}(t)|^2 = \left(\frac{\omega_1}{\Omega}\right)^4 \sin^4 \frac{\Omega t}{2} \quad (8.66)$$

where Ω and δ are given by (8.50) and (3.28).

Comments

1. Resonance function

The resonance function

$$\left(\frac{\omega_1}{\Omega}\right)^4 = \left(\frac{\omega_1^2}{(\omega - \omega_0)^2 + \omega_1^2}\right)^2 \quad (8.67)$$

in (8.64) to (8.66), because of the higher power, characterizes a sharper resonance than (8.52) which appears in the spin $\frac{1}{2}$ equations (8.48) and (8.49).

When $\omega = \omega_0$,

$$|a_+(t)|^2 = \cos^4 \frac{\omega_1 t}{2} \quad (8.68)$$

$$|a_0(t)|^2 = \frac{1}{2} \sin^2 \omega_1 t \quad (8.69)$$

$$|a_-(t)|^2 = \sin^4 \frac{\omega_1 t}{2} \quad (8.70)$$

2. Magnetic resonance

It follows from (8.70) that

$$\left|a_-\left(\frac{\pi}{\omega_1}\right)\right|^2 = 1 \quad (8.71)$$

That is, a spin flip is certain when the angular frequency ω of the rotating magnetic field \vec{B}_1 (8.35) is equal to the Larmor precession frequency ω_0 (8.1) and the particle is subjected to the rotating magnetic field for the time π/ω_1 . This is the phenomenon of magnetic resonance.

3. Energy transitions

The interaction of the magnetic moment of the particle with the magnetic field \vec{B}_1 (8.35) does not cause a direct transition from the ground state $| + \rangle$ to the second excited state $| - \rangle$; the Hamiltonian H_1 (8.38) does not connect these states directly. The particle absorbs energy $\hbar\omega_0$ from the magnetic field \vec{B}_1 in making a transition from $| + \rangle$ to the first excited state $| 0 \rangle$; it then absorbs further energy $\hbar\omega_0$ in making a transition from $| 0 \rangle$ to the second excited state $| - \rangle$.

The probability $| a_0(t) |^2$ (8.69) that the particle is in the first excited state $| 0 \rangle$ has a maximum equal to $\frac{1}{2}$: there is leakage to the second excited state $| - \rangle$ during the energy absorption process and leakage to the ground state $| + \rangle$ during the energy emission process.

Chapter 9

OBSERVABLES WITH CONTINUOUS SPECTRA

9.1 Introductory remarks

In this chapter we consider the description of a physical system whose observables have continuous values. Such a system is described in an infinite-dimensional separable Hilbert space. An example of such a system is the single spinless particle discussed in *QLB: Some Lorentz Invariant Systems* Chapter 2. The position and momentum of the particle have continuous values.

The Dirac method for handling an observable with continuous values is used throughout *QLB*. The Dirac method introduces the notion of an eigenket of an operator and defines a complex function (wave function) of a real variable associated with a vector in the infinite-dimensional separable Hilbert space.

Our purpose in this chapter is to discuss the Dirac method more fully than is given in other parts of *QLB*. The spectral theorem for Hermitian operators is discussed in Section 9.2 and the Dirac method is discussed in Section 9.3.

The particular case of the position and momentum of a spinless particle confined to move in one dimension is considered in Chapter 10.

9.2 Spectral theorem

Central to the description and analysis of a physical system whose observables have continuous values is:

Spectral Theorem for Hermitian Operators

For each Hermitian operator A defined on a separable Hilbert space there is a unique family of operators $E(a)$ such that

$$A = \int_{-\infty}^{+\infty} a dE(a) \quad (9.1)$$

$$1 = \int_{-\infty}^{+\infty} dE(a) \quad (9.2)$$

$$E(-\infty) = 0 \quad (9.3)$$

$$E(+\infty) = 1 \quad (9.4)$$

$$E(a)E(a') = E(a')E(a) = E(\text{minimum of } a \text{ and } a') \quad (9.5)$$

Comments

1. Nomenclature

(9.1) is the spectral decomposition of A .

The value a in the integrand in (9.1) is a spectral value of A .

The spectrum of A is continuous in the range $(-\infty, +\infty)$.

(9.2) is the resolution of the identity.

In view of (9.5), the family of operators $E(a)$ is a family of projection operators.

2. Stieltjes integral

The integral in (9.1) and (9.2) is a Stieltjes integral.

The Stieltjes integral of $f(x)$ with respect to $g(x)$

$$\int_{\alpha}^{\beta} f(x) dg(x) \tag{9.6}$$

is defined as

$$\int_{\alpha}^{\beta} f(x) dg(x) = \lim_{n \rightarrow \infty} \sum_{k=1}^n f(\xi_k) [g(x_k) - g(x_{k-1})] \tag{9.7}$$

where

$$\alpha = x_0 < x_1 < \cdots < x_n = \beta \quad (9.8)$$

$$x_{k-1} \leq \xi_k \leq x_k \quad (9.9)$$

3. Riemann integral and Stieltjes integral

The Riemann integral of $f(x)$

$$\int_{\alpha}^{\beta} f(x) dx \quad (9.10)$$

is the special case of the Stieltjes integral (9.6) when

$$g(x) = x \quad (9.11)$$

4. Stieltjes integral with respect to a discontinuous function

The Stieltjes integral (9.6) of $f(x)$ with respect to $g(x)$ can be defined for a discontinuous function $g(x)$.

For example,

$$\int_{-\infty}^{+\infty} f(x) d\theta(x) = f(0) \quad (9.12)$$

$$\int_{-\infty}^{+\infty} d\theta(x) = 1 \quad (9.13)$$

where $\theta(x)$ is defined by

$$\begin{aligned} \theta(x) &= +1 \quad \text{if } x \geq 0 \\ &= 0 \quad \text{if } x < 0 \end{aligned} \quad (9.14)$$

5. Eigenvalue Decomposition Theorem

The Eigenvalue Decomposition Theorem given in Section 3.2 is a special case of the Spectral Decomposition Theorem when A is defined on an n -dimensional vector space:

Let $|a_1\rangle, |a_2\rangle, \dots, |a_n\rangle$ be the eigenvectors of A belonging to eigenvalues a_1, a_2, \dots, a_n of A defined on an n -dimensional vector space.

The eigenvectors $|a_1\rangle, |a_2\rangle, \dots, |a_n\rangle$ may be chosen to satisfy $\langle a_k | a_{k'} \rangle = \delta_{kk'}$.

We label the eigenvalues such that $-\infty < a_1 \leq a_2 \leq \dots \leq a_n < +\infty$.

(3.1) and (3.2) follow from (9.1) to (9.5) when

$$E(a) = \sum_{a_k \leq a} |a_k\rangle\langle a_k| \quad (9.15)$$

9.3 Dirac method

Dirac invented a method for handling an observable with a continuous spectrum which does not explicitly involve the Stieltjes integral. The Dirac method replaces the Stieltjes integral by the Riemann integral and uses the Dirac δ -function.

For example, the Dirac method replaces the Stieltjes integrals (9.12) and (9.13) by Riemann integrals by writing

$$d\theta(x) = dx\delta(x) \quad (9.16)$$

where $\delta(x)$ is the Dirac δ -function.

Regarding the Spectral Theorem, the Dirac method takes

$$dE(a) = da |a\rangle\langle a| \quad (9.17)$$

which equation introduces the eigenket $|a\rangle$ of A .

Using (9.17) in (9.1) and (9.2) yields

$$A = \int_{-\infty}^{+\infty} da | a \rangle \langle a | \quad (9.18)$$

$$1 = \int_{-\infty}^{+\infty} da | a \rangle \langle a | \quad (9.19)$$

It follows from (9.3) and (9.17) that

$$E(a) = \int_{-\infty}^a da' | a' \rangle \langle a' | \quad (9.20)$$

(9.20) is the generalization of (9.15) for a Hermitian operator with a continuous spectrum.

(9.4) follows from (9.20) and (9.5) holds provided

$$\langle a | a' \rangle = \delta(a - a') \quad (9.21)$$

(9.18), (9.19) and (9.21) give the Dirac method for handling an observable A with a continuous spectrum.

(9.18), (9.19) and (9.21) are the continuous spectrum analogs of (3.1) to (3.3).

Comments

1. The eigenket $|a\rangle$

$|a\rangle$ is the eigenket of A belonging to spectral value a of A .

$|a\rangle$ is not a vector in the Hilbert space because $\langle a|a\rangle$ is not finite.

2. Notation for vectors and eigenkets

Throughout *QLB* we use lower case Greek letters $|\psi\rangle, |\phi\rangle, \dots$ to denote vectors and lower case Roman letters $|x\rangle, |p\rangle, \dots$ to denote eigenkets.

3. Wave functions

It follows using (9.19) that

$$|\psi\rangle = \int_{-\infty}^{+\infty} da |a\rangle \psi(a) \quad (9.22)$$

$$\psi(a) = \langle a|\psi\rangle \quad (9.23)$$

(9.23) defines a complex function $\psi(a)$ of the real variable a .

$\psi(a)$ is the A -wave function for the vector $|\psi\rangle$.

Now

$$\langle \psi | a \rangle = \langle a | \psi \rangle^* = \psi^*(a) \quad (9.24)$$

so

$$\begin{aligned} 1 = \langle \psi | \psi \rangle &= \int_{-\infty}^{+\infty} da \langle \psi | a \rangle \langle a | \psi \rangle \\ &= \int_{-\infty}^{+\infty} |\psi(a)|^2 da \end{aligned} \quad (9.25)$$

(9.22) provides a correspondence between a vector $|\psi\rangle$ in the Hilbert space of states and a function $\psi(a)$ in the Hilbert space of square-integrable wave functions.

(9.22) provides a representation of the vector $|\psi\rangle$ by the square-integrable function $\psi(a)$.

4. Probabilities

The probability $P(a)da$ of obtaining a value in the range a to $a + da$ on measurement of A for the system in the state $|\psi\rangle$ is

$$P(a)da = \langle \psi | a \rangle \langle a | \psi \rangle da = |\psi(a)|^2 da \quad (9.26)$$

It follows that

$$\int_{-\infty}^{+\infty} P(a) da = \int_{-\infty}^{+\infty} |\psi(a)|^2 da = 1 \quad (9.27)$$

5. Averages

The average \bar{A} of the results obtained on measurement of A for the system in the state $|\psi\rangle$ is

$$\begin{aligned} \bar{A} = \langle \psi | A | \psi \rangle &= \int_{-\infty}^{+\infty} \langle \psi | a \rangle a \langle a | \psi \rangle da \\ &= \int_{-\infty}^{+\infty} a |\psi(a)|^2 da \end{aligned} \quad (9.28)$$

Chapter 10

SPINLESS PARTICLE IN ONE DIMENSION

10.1 Introductory remarks

QLB: Some Lorentz Invariant Systems Chapter 2 gives a description of a single relativistic spinless particle of rest mass m . Proofs of some results stated there are given in this chapter for a particle confined to move in one dimension.

Position and momentum eigkets and the relationship between them are given in Section 10.2 and coordinate- and momentum-space wave functions are defined in Section 10.3. The optimum state of position and momentum is given in Section 10.4 and the partial differential Schrodinger equation for the wave function of a nonrelativistic particle moving in a central potential is derived in Section 10.5. Some other derivations are given in Section 10.6.

10.2 Position and momentum

Fundamental dynamical variables for a spinless particle confined to move in one dimension are the Cartesian coordinate X and momentum P of the particle. These variables satisfy the fundamental quantum condition

$$[X, P] = i\hbar \quad (10.1)$$

X and P are each a complete set of compatible observables; the spectrum of X and the spectrum of P are both continuous in the range $(-\infty, \infty)$.

We use the Dirac method as given in Section 9.3 for handling these observables. We denote the eigenkets of X and P by

$$|x\rangle \quad \text{and} \quad |p\rangle \quad (10.2)$$

respectively. These eigenkets may be used as bases for the Hilbert space. That is,

$$X = \int_{-\infty}^{+\infty} dx |x\rangle x \langle x| \quad (10.3)$$

$$P = \int_{-\infty}^{+\infty} dp |p\rangle p \langle p| \quad (10.4)$$

where

$$1 = \int_{-\infty}^{+\infty} dx |x\rangle \langle x| = \int_{-\infty}^{+\infty} dp |p\rangle \langle p| \quad (10.5)$$

and

$$\langle x | x' \rangle = \delta(x - x') \quad (10.6)$$

$$\langle p | p' \rangle = \delta(p - p') \quad (10.7)$$

where $\delta(x - x')$ and $\delta(p - p')$ are Dirac delta functions.

We show in Section 10.6 that it follows from (10.1), (10.3) and (10.4) that

$$\langle x | P | x' \rangle = -i\hbar\delta^1(x - x') \quad (10.8)$$

$$\langle p | X | p' \rangle = i\hbar\delta^1(p - p') \quad (10.9)$$

$$\langle x | p \rangle = \left(\frac{1}{2\pi\hbar}\right)^{\frac{1}{2}} e^{ipx/\hbar} \quad (10.10)$$

where

$$\delta^1(x) = \frac{d\delta(x)}{dx} \quad (10.11)$$

10.3 Wave functions

The state $|\psi(t)\rangle$ of the particle at time t is

$$|\psi(t)\rangle = U(t) |\psi\rangle \quad (10.12)$$

where $U(t)$ is the evolution operator for the particle and $|\psi\rangle$ is the state of the particle at time zero.

The coordinate-space wave function for the particle is

$$\psi(x, t) = \langle x | \psi(t) \rangle \quad (10.13)$$

and

$$\psi^*(x, t)\psi(x, t)dx \quad (10.14)$$

is the probability that the position of the particle is between x and $x + dx$ at time t .

The momentum-space wave function for the particle is

$$\psi(p, t) = \langle p | \psi(t) \rangle \quad (10.15)$$

and

$$\psi^*(p, t)\psi(p, t)dp \quad (10.16)$$

is the probability that the momentum of the particle is between p and $p + dp$ at time t .

It follows using (10.5), (10.8) and (10.9) that

$$\langle x | P^n | \psi(t) \rangle = (-i\hbar)^n \frac{\partial^n}{\partial x^n} \psi(x, t) \quad (10.17)$$

$$\langle p | X^n | \psi(t) \rangle = (i\hbar)^n \frac{\partial^n}{\partial p^n} \psi(p, t) \quad (10.18)$$

where n is a positive integer.

It follows using (10.5), (10.10), (10.13) and (10.15) that

$$\psi(x, t) = \left(\frac{1}{2\pi\hbar} \right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} dp e^{ipx/\hbar} \psi(p, t) \quad (10.19)$$

$$\psi(p, t) = \left(\frac{1}{2\pi\hbar} \right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} dx e^{-ipx/\hbar} \psi(x, t) \quad (10.20)$$

Comments

1. Fourier transforms

(10.19) and (10.20) show that the coordinate-space and momentum-space wave functions of the particle are Fourier transforms of each other.

This remarkable result is a direct consequence of the fundamental quantum

condition (10.1).

It follows using (10.5) that

$$\int_{-\infty}^{+\infty} dx \psi^*(x, t) \psi(x, t) = \int_{-\infty}^{+\infty} dp \psi^*(p, t) \psi(p, t) \quad (10.21)$$

which is Parseval's theorem on Fourier transforms.

10.4 Optimum state of position and momentum

In this section we specialize the material of Section 3.4 to consider the optimum state $|\psi_{opt}\rangle$ of position and momentum.

It follows from (3.16) and (10.1) that the uncertainties ΔX and ΔP in the position and momentum of the particle in the state $|\psi_{opt}\rangle$ satisfy

$$(\Delta X)(\Delta P) = \frac{\hbar}{2} \quad (10.22)$$

It follows from (2.13) that $|\psi_{opt}\rangle$ satisfies

$$\left(\frac{X - \bar{X}}{\Delta X} + i \frac{P - \bar{P}}{\Delta P} \right) |\psi_{opt}\rangle = 0 \quad (10.23)$$

where \bar{X} and \bar{P} are the average position and momentum of the particle in the state $|\psi_{opt}\rangle$.

We show in Section 10.6 that it follows from (10.23) that the coordinate-space and momentum-space wave functions for $|\psi_{opt}\rangle$ are

$$\psi_{opt}(x) = \left[\frac{1}{2\pi(\Delta X)^2} \right]^{\frac{1}{4}} e^{-i\bar{P}\bar{X}/2\hbar} e^{i\bar{P}x/\hbar} e^{-[(x-\bar{X})/2\Delta X]^2} \quad (10.24)$$

$$\psi_{opt}(p) = \left[\frac{1}{2\pi(\Delta P)^2} \right]^{\frac{1}{4}} e^{i\bar{P}\bar{X}/2\hbar} e^{-i\bar{X}p/\hbar} e^{-[(p-\bar{P})/2\Delta P]^2} \quad (10.25)$$

where

$$\psi_{opt}(x) = \langle x | \psi_{opt} \rangle \quad (10.26)$$

$$\psi_{opt}(p) = \langle p | \psi_{opt} \rangle \quad (10.27)$$

Comments

1. Gaussian wave functions

(10.24) and (10.25) are gaussian wave functions.

(10.24) gives a coordinate-space probability function centred at the average position \bar{X} of the particle with width dependent on the position uncertainty ΔX .

(10.25) gives a momentum-space probability function centred at the average momentum \bar{P} of the particle with width dependent on the momentum uncertainty ΔP .

(10.24) and (10.25) are consistent with the fact that the Fourier transform of a gaussian function is another gaussian function.

The phase factors in (10.24) and (10.25) have been chosen in order that (10.24) and (10.25) are related by the replacements

$$x \leftrightarrow p \quad \bar{X} \leftrightarrow \bar{P} \quad i \leftrightarrow -i \quad (10.28)$$

as implied by (10.1) and (10.23).

2. Another form for $|\psi_{opt}\rangle$; the state $|\psi_0\rangle$

We show in Section 10.6 that $|\psi_{opt}\rangle$ may be written in the form

$$|\psi_{opt}\rangle = e^{i(\bar{P}X - \bar{X}P)/\hbar} |\psi_0\rangle \quad (10.29)$$

where $|\psi_0\rangle$ satisfies

$$A |\psi_0\rangle = 0 \quad (10.30)$$

where

$$A = \frac{1}{2} \left(\frac{X}{\Delta X} + i \frac{P}{\Delta P} \right) \quad (10.31)$$

It follows from (10.30) that

$$\langle \psi_0 | X | \psi_0 \rangle = \langle \psi_0 | P | \psi_0 \rangle = 0 \quad (10.32)$$

That is, $|\psi_0\rangle$ is the optimum state of position and momentum with average position and momentum both equal to zero.

3. Ladder operator

A defined by (10.31) is a ladder operator (lowering operator); that is, it obeys (11.1).

(10.31) may be written as

$$A = \frac{1}{\sqrt{2}} \left(\frac{X}{\hbar/mc} + i \frac{P}{mc} \right) \quad (10.33)$$

where the constant c is defined by

$$\Delta X = \frac{1}{\sqrt{2}} \frac{\hbar}{mc} \quad (10.34)$$

$$\Delta P = \frac{1}{\sqrt{2}} mc \quad (10.35)$$

Choosing c by (11.14) and (11.15) corresponds to regarding the particle as a nonrelativistic harmonic oscillator. $|\psi_0\rangle$ in this case is the ground state of the oscillator.

10.5 Partial differential Schrodinger equation

For a nonrelativistic particle moving in a potential $V(X)$, the evolution operator is

$$U(t) = e^{-iHt/\hbar} \quad (10.36)$$

and the Hamiltonian H is

$$H = \frac{P^2}{2m} + V(X) \quad (10.37)$$

Differentiating (10.12) with respect to t yields the Schrodinger equation

$$H | \psi(t) \rangle = i\hbar \frac{\partial}{\partial t} | \psi(t) \rangle \quad (10.38)$$

the coordinate representative of which

$$\langle x | H | \psi(t) \rangle = i\hbar \frac{\partial}{\partial t} \langle x | \psi(t) \rangle \quad (10.39)$$

using (10.17), becomes

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + V(x)\psi(x, t) = i\hbar \frac{\partial}{\partial t} \psi(x, t) \quad (10.40)$$

(10.40) is the partial differential Schrodinger equation for the coordinate-space wave function $\psi(x, t)$.

10.6 Some derivations

Derivation of (10.8) and (10.9)

It follows from (10.1) that

$$\langle x | (XP - PX) | x' \rangle = i\hbar \langle x | x' \rangle \quad (10.41)$$

which, using (10.3) and (10.6), becomes

$$(x - x') \langle x | P | x' \rangle = i\hbar \delta(x - x') \quad (10.42)$$

It follows using (A.32) that (10.42) is solved by

$$\langle x | P | x' \rangle = -i\hbar \delta^1(x - x') \quad (10.43)$$

which is (10.8). (10.9) follows similarly.

(10.43) is a particular solution of (10.42); it follows using (A.31) that the most general solution of (10.42) is

$$-i\hbar \delta^1(x - x') + a\delta(x - x') \quad (10.44)$$

where a is real. Now

$$\begin{aligned} & -i\hbar \delta^1(x - x') + a\delta(x - x') \\ &= -i\hbar \left[1 - \frac{i(x - x')a}{\hbar} \right] \delta^1(x - x') = e^{-i(x-x')a/\hbar} [-i\hbar \delta^1(x - x')] \quad (10.45) \\ &= \langle x | P | x' \rangle_a \end{aligned}$$

where

$$|x\rangle_a = e^{ixa/\hbar} |x\rangle \quad (10.46)$$

The most general solution of (10.42) therefore corresponds to a choice of phase factor in the position ket. The choice $a = 0$ is standard and can be made without loss of generality.

Derivation of (10.10)

It follows from (10.4) that

$$\langle x | P | p \rangle = p \langle x | p \rangle \quad (10.47)$$

which, using (10.5) and (10.8), becomes

$$-i\hbar \frac{\partial}{\partial x} \langle x | p \rangle = p \langle x | p \rangle \quad (10.48)$$

Similarly, it follows from (10.3) that

$$i\hbar \frac{\partial}{\partial p} \langle p | x \rangle = x \langle p | x \rangle \quad (10.49)$$

Integrating (10.48) and (10.49) yields

$$\langle x | p \rangle = c_1(p) e^{ipx/\hbar} \quad (10.50)$$

and

$$\langle p | x \rangle = c_2(x) e^{-ipx/\hbar} \quad (10.51)$$

Now

$$\langle p | x \rangle = \langle x | p \rangle^* \quad (10.52)$$

so

$$c_2(x) = c_1^*(p) = \text{constant} = c \quad (10.53)$$

and

$$\delta(x - x') = \langle x | x' \rangle = \int_{-\infty}^{+\infty} dp \langle x | p \rangle \langle p | x' \rangle \quad (10.54)$$

$$= cc^* \int_{-\infty}^{+\infty} dp e^{ip(x-x')/\hbar} = cc^* 2\pi\hbar \delta(x - x')$$

Choosing c positive real yields (10.10).

Derivation of (10.24) and (10.25)

It follows using (10.17) and (10.22) that the coordinate-space representative of (10.23) is

$$\left(\frac{\partial}{\partial x} + \frac{x - \bar{X}}{2(\Delta X)^2} - \frac{i\bar{P}}{\hbar} \right) \psi_{opt}(x) = 0 \quad (10.55)$$

Solving (10.55) yields (10.24). (10.25) follows similarly or using (10.20).

Derivation of (10.30)

(10.30) follows from (10.23) and the identities

$$X - \bar{X} = DXD^\dagger \quad (10.56)$$

$$P - \bar{P} = DPD^\dagger \quad (10.57)$$

where

$$D = e^{i(\bar{P}X - \bar{X}P)/\hbar} \quad (10.58)$$



11.1 Introductory remarks

Ladder operators are referred to in *QLB: Some Lorentz Invariant Systems* Chapter 2 with reference to countable bases for the Hilbert space for a single spinless particle. In this chapter we give a more complete discussion of ladder operators and we derive properties of these operators which are stated in *QLB: Some Lorentz Invariant Systems* Chapter 2.

Ladder operators were introduced by Dirac to determine the energy eigenvalues of the nonrelativistic harmonic oscillator and they subsequently provided an important bridge in the development of relativistic quantum mechanics.

Dirac's method for determining the eigenvalues of the ladder operator number operator is given in Section 11.2.

Ladder operators are used in Section 11.3 to determine eigenvalues of angular momentum operators. The method is due to J. Schwinger; see J. Schwinger, *On Angular Momentum* (1952) in L.C. Biedenharn and H. van Dam (1965).

Some derivations are given in Section 11.4.

11.2 One pair of ladder operators

We consider an operator A which with its adjoint A^\dagger obeys

$$\boxed{[A, A^\dagger] = 1} \quad (11.1)$$

We define a Hermitian operator N by

$$N = A^\dagger A \quad (11.2)$$

We show in Section 11.4 that it follows from (11.1) and (11.2) that the eigenvalues of N are the nonnegative integers and the corresponding eigenvectors are obtained by operating with powers of A^\dagger on the eigenvector belonging to eigenvalue zero.

More specifically,

$$N |n\rangle = n |n\rangle \quad (11.3)$$

where

$$|n\rangle = \frac{1}{\sqrt{n!}} (A^\dagger)^n |0\rangle \quad (11.4)$$

and

$$\langle n | n' \rangle = \delta_{nn'} \quad (11.5)$$

$$n = 0, 1, 2, \dots \quad (11.6)$$

Furthermore,

$$A^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \quad (11.7)$$

$$A |n+1\rangle = \sqrt{n+1} |n\rangle \quad (11.8)$$

and

$$A |0\rangle = 0 \quad (11.9)$$

$$\langle 0 | A^\dagger = 0 \quad (11.10)$$

Comments

1. Nomenclature

In view of (11.7) and (11.8), A^\dagger and A are called ladder operators; A^\dagger is a raising operator and A is a lowering operator.

N is the ladder operator number operator.

2. Comparison with boson operators

A^\dagger and A bear some formal similarity to creators and annihilators defined in *QLB: Quantum Mechanics in Fock Space* Chapter 6 for a system of identical bosons. Indeed, the harmonic oscillator ladder operators discussed in Topic 11.2.1 historically provided a bridge to the description of a system of identical bosons.

The similarity between boson operators and ladder operators is only apparent however: creators and annihilators change the number of particles in a system; ladder operators do not.

One-dimensional harmonic oscillator

We show in this topic that the vectors $|n\rangle$ defined by (11.4) are eigenvectors of the Hamiltonian for a one-dimensional nonrelativistic harmonic oscillator.

The nonrelativistic harmonic oscillator is discussed in depth in all standard books on nonrelativistic quantum mechanics and these books should be consulted for further details. Our purpose here is simply to define ladder operators in terms of particle position and momentum and to relate the ladder operator number operator to the harmonic oscillator Hamiltonian.

The description of particle of rest mass m confined to move in one dimension is given in Chapter 10. When the particle is subjected to a force

$$F = -kX \quad (11.11)$$

where k is a constant, the Hamiltonian for the particle, in the Galilei approximation, is

$$H = \frac{P^2}{2m} + \frac{1}{2}kX^2 \quad (11.12)$$

On defining A by

$$A = \frac{1}{\sqrt{2}} \left(\frac{X}{\hbar/mc} + i \frac{P}{mc} \right) \quad (11.13)$$

where c is defined by

$$\hbar\omega = mc^2 \quad (11.14)$$

$$\omega = \sqrt{\frac{k}{m}} \quad (11.15)$$

it follows from (10.1) that (11.1) holds. A defined by (11.13) is a ladder operator.

It follows from (11.13) that

$$X = \frac{\hbar}{\sqrt{2}mc} (A^\dagger + A) \quad (11.16)$$

$$P = \frac{imc}{\sqrt{2}} (A^\dagger - A) \quad (11.17)$$

and

$$X^2 = \frac{1}{2} \left(\frac{\hbar}{mc} \right)^2 \left[1 + 2A^\dagger A + (A^\dagger)^2 + A^2 \right] \quad (11.18)$$

$$P^2 = \frac{1}{2} (mc)^2 \left[1 + 2A^\dagger A - (A^\dagger)^2 - A^2 \right] \quad (11.19)$$

and therefore

$$H = \hbar\omega \left(N + \frac{1}{2} \right) \quad (11.20)$$

where N is given by (11.2).

The eigenvectors of H span the Hilbert space, that is,

$$N = \sum_{n=0}^{\infty} |n\rangle \langle n| \quad (11.21)$$

$$H = \hbar\omega \sum_{n=0}^{\infty} |n\rangle \left(n + \frac{1}{2} \right) \langle n| \quad (11.22)$$

$$1 = \sum_{n=0}^{\infty} |n\rangle \langle n| \quad (11.23)$$

Comments

1. Countable set of basis vectors

As given by (11.23), the eigenvectors of N are a countable set of vectors which span the Hilbert space.

This contrasts with the eigenkets of X and P which are labelled by a continuous variable and are not vectors in the Hilbert space but which nevertheless which may be used as bases for the Hilbert space as expressed by (10.5).

The eigenvectors of N are used in *QLB: Some Lorentz Invariant Systems* Chapter 2 to provide a countable basis for the Hilbert space for a single spinless particle.

They are also used in *QLB: Quantum Mechanics in Fock Space* Chapter 3 to provide a countable set of basis vectors for a one-particle system which is appropriate for developing the occupation number representation for a system of identical particles.

2. Normal order

(11.1) has been used to write (11.18) and (11.19) in normal order, that is, with raising operators written to the left of lowering operators.

3. Ladder operator method

We determine the average and uncertainty of position and momentum for the oscillator in the ground state $|0\rangle$ to illustrate the ladder operator method.

Using (11.9) and (11.10) with (11.16) to (11.19) immediately yields

$$\overline{X} = \overline{P} = 0 \quad (11.24)$$

$$\Delta X = \frac{1}{\sqrt{2}} \frac{\hbar}{mc} \quad (11.25)$$

$$\Delta P = \frac{1}{\sqrt{2}} mc \quad (11.26)$$

$$(\Delta X)(\Delta P) = \frac{\hbar}{2} \quad (11.27)$$

According to (10.22), $|0\rangle$ is an optimum state of position and momentum.

Indeed, (11.9) is a special case of (10.30).

4. Coordinate-space wave functions

It follows from (10.24) that the coordinate-space ground state wave function $\psi_0(x) = \langle x | 0 \rangle$ is

$$\psi_0(x) = \left(\frac{mc}{\sqrt{\pi\hbar}} \right)^{\frac{1}{2}} e^{-\hat{x}^2/2} \quad (11.28)$$

where

$$\hat{x} = \frac{x}{\hbar/mc} \quad (11.29)$$

It follows from (11.7), (11.13) and (10.17) that

$$\psi_n(x) = \frac{1}{\sqrt{n!}} \left[\frac{1}{\sqrt{2}} \left(\hat{x} - \frac{d}{d\hat{x}} \right) \right]^n \psi_0(x) \quad (11.30)$$

where $\psi_n(x) = \langle x | n \rangle$ is the coordinate-space wave function for the state $| n \rangle$.

(11.30) allows $\psi_n(x)$ to be determined from $\psi_0(x)$. $\psi_n(x)$ involves the Hermite polynomial

$$H_n(\hat{x}) = e^{\hat{x}^2/2} \left(\hat{x} - \frac{d}{d\hat{x}} \right)^n e^{-\hat{x}^2/2} \quad (11.31)$$

11.3 Ladder operators and angular momentum

We consider operators A_u, A_d which with their adjoints A_u^\dagger, A_d^\dagger obey

$$[A_\alpha, A_\beta] = 0 \quad (11.32)$$

$$[A_\alpha, A_\beta^\dagger] = \delta_{\alpha\beta} \quad (11.33)$$

We define mutually commuting Hermitian operators N_u, N_d, N by

$$N_u = A_u^\dagger A_u \quad (11.34)$$

$$N_d = A_d^\dagger A_d \quad (11.35)$$

$$N = N_u + N_d \quad (11.36)$$

It follows from an analysis similar to that given in Section 11.4 that

$$N_u |n_u n_d\rangle = n_u |n_u n_d\rangle \quad (11.37)$$

$$N_d |n_u n_d\rangle = n_d |n_u n_d\rangle \quad (11.38)$$

$$N |n_u n_d\rangle = n |n_u n_d\rangle \quad (11.39)$$

where

$$|n_u n_d\rangle = \frac{1}{\sqrt{n_u! n_d!}} (A_u^\dagger)^{n_u} (A_d^\dagger)^{n_d} |00\rangle \quad (11.40)$$

and

$$n_u + n_d = n \quad (11.41)$$

$$n_u, n_d = 0, 1, 2, \dots \quad (11.42)$$

Furthermore,

$$A_u^\dagger |n_u n_d\rangle = \sqrt{n_u + 1} |n_u + 1 n_d\rangle \quad (11.43)$$

$$A_u |n_u n_d\rangle = \sqrt{n_u} |n_u - 1 n_d\rangle \quad (11.44)$$

$$A_d^\dagger |n_u n_d\rangle = \sqrt{n_d + 1} |n_u n_d + 1\rangle \quad (11.45)$$

$$A_d |n_u n_d\rangle = \sqrt{n_d} |n_u n_d - 1\rangle \quad (11.46)$$

and

$$A_u |0 n_d\rangle = 0 \quad (11.47)$$

$$A_d |n_u 0\rangle = 0 \quad (11.48)$$

We define

$$J^1 = \frac{1}{2} \left(A_d^\dagger A_u + A_u^\dagger A_d \right) \quad (11.49)$$

$$J^2 = \frac{i}{2} \left(A_d^\dagger A_u - A_u^\dagger A_d \right) \quad (11.50)$$

$$J^3 = \frac{1}{2} \left(A_u^\dagger A_u - A_d^\dagger A_d \right) \quad (11.51)$$

and

$$\left(\vec{J} \right)^2 = \vec{J} \cdot \vec{J} = (J^1)^2 + (J^2)^2 + (J^3)^2 \quad (11.52)$$

It follows from (11.32) to (11.36) that

$$\left[J^a, J^b \right] = i \epsilon_{abc} J^c \quad (11.53)$$

$$\left[\left(\vec{J} \right)^2, J^1 \right] = \left[\left(\vec{J} \right)^2, J^2 \right] = \left[\left(\vec{J} \right)^2, J^3 \right] = 0 \quad (11.54)$$

and

$$\left(\vec{J}\right)^2 = \frac{N}{2} \left(\frac{N}{2} + 1\right) \quad (11.55)$$

$$J^3 = \frac{1}{2}(N_u - N_d) = (N - 2N_d) \quad (11.56)$$

It follows from (11.37) to (11.42) that the eigenvalues of $\left(\vec{J}\right)^2$ and J^3 are, respectively,

$$j(j+1) \quad \text{where} \quad j = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots \quad (11.57)$$

$$m \quad \text{where} \quad m = j, j-1, \dots, -j \quad (11.58)$$

On writing

$$n_u = j + m \quad (11.59)$$

$$n_d = j - m \quad (11.60)$$

it follows from (11.37) to (11.42) that

$$(\vec{J})^2 |jm\rangle = j(j+1) |jm\rangle \quad (11.61)$$

$$J^3 |jm\rangle = m |jm\rangle \quad (11.62)$$

$$J^+ |jm\rangle = \sqrt{j(j+1) - (m+1)} |jm+1\rangle \quad (11.63)$$

$$J^- |jm\rangle = \sqrt{j(j+1) - (m-1)} |jm-1\rangle \quad (11.64)$$

where

$$|jm\rangle = \frac{1}{\sqrt{(j+m)!(j-m)!}} (A_u^\dagger)^{j+m} (A_d^\dagger)^{j-m} |00\rangle \quad (11.65)$$

$$J^+ = J^1 + iJ^2 = A_u^\dagger A_d \quad (11.66)$$

$$J^- = J^1 - iJ^2 = A_d^\dagger A_u \quad (11.67)$$

Comments

1. Commutation relations

(11.53) and (11.54) are the standard commutation relations satisfied by the Cartesian components of angular momentum.

2. Eigenvalues

(11.57) and (11.58) are standard results for the eigenvalues of $(\vec{J})^2$ and J^3 .

3. Angular momentum ladder operators

(11.66) and (11.67) define angular momentum ladder operators.

(11.63) and (11.64) are standard results for angular momentum ladder operators.

4. Generators of $SU(3)$

The discussion of this section can be extended to include any number of ladder operators.

The generators of $SU(3)$ can be defined in terms of three ladder operators A_u, A_d, A_s similarly to the above definition of $SU(2)$ generators in terms of A_u, A_d .

11.4 Some derivations

Derivation of (11.3)

The eigenvalue problem for N is to solve

$$N |\lambda\rangle = \lambda |\lambda\rangle \quad (11.68)$$

for nonzero vector $|\lambda\rangle$ and constant λ .

It follows from (11.1) and (11.2) that

$$[N, A] = -A \quad (11.69)$$

$$[N, A^\dagger] = A^\dagger \quad (11.70)$$

and therefore

$$NA | \lambda \rangle = (\lambda - 1)A | \lambda \rangle \quad (11.71)$$

$$\langle A\lambda | A\lambda \rangle = \lambda \langle \lambda | \lambda \rangle \geq 0 \quad (11.72)$$

and

$$NA^\dagger | \lambda \rangle = (\lambda + 1)A^\dagger | \lambda \rangle \quad (11.73)$$

$$\langle A^\dagger \lambda | A^\dagger \lambda \rangle = (\lambda + 1) \langle \lambda | \lambda \rangle \geq 0 \quad (11.74)$$

It follows from (11.71) and (11.72) that

$$\lambda \geq 0 \quad (11.75)$$

$$A | 0 \rangle = 0 \quad (11.76)$$

It follows also from (11.73) that $| 0 \rangle$, $A^\dagger | 0 \rangle$, $(A^\dagger)^2 | 0 \rangle$, \dots are eigenvectors of N belonging to eigenvalues $0, 1, 2, \dots$, respectively.

That there are no eigenvalues between 0 and 1 follows from (11.71) and (11.75). That there are no eigenvalues between 1 and 2 and between 2 and 3 etc. follows from (11.73).

The norm of the vectors $A^\dagger | 0 \rangle$, $(A^\dagger)^2 | 0 \rangle$, \dots is expressed in terms of the norm of $| 0 \rangle$ by (11.74).

This completes the proof of (11.3).

Appendix: Mathematical Preliminaries

A.1 Some properties of operators

Jordan (1969) should be consulted for the mathematics of linear and antilinear operators for quantum mechanics. We give a few properties of these operators below.

Linear operators

A linear operator A satisfies

$$Aa = aA \quad (\text{A.1})$$

for any constant a . The adjoint A^\dagger of a linear operator A is defined by

$$\langle \psi | A^\dagger = \langle A\psi | \quad (\text{A.2})$$

Antilinear operators

An antilinear operator A satisfies

$$Ai = -iA \quad (\text{A.3})$$

The adjoint A^\dagger of an antilinear operator A is defined by

$$\langle \psi | A^\dagger | \phi \rangle = \langle A\psi | \phi \rangle^* \quad (\text{A.4})$$

Linear unitary and antilinear antiunitary operators

Linear unitary operators and antilinear antiunitary operators preserve the norms of states. They satisfy

$$UU^\dagger = U^\dagger U = 1 \quad (\text{A.5})$$

Notation for the inverse of an operator

$$\frac{1}{A} = A^{-1} \quad (\text{A.6})$$

$$\frac{A}{B} = AB^{-1} = B^{-1}A \quad \text{when} \quad [A, B] = 0 \quad (\text{A.7})$$

A.2 Commutator and anticommutator identities

The commutator $[A, B]$ and anticommutator $\{A, B\}$ of linear operators A and B are defined as

$$[A, B] = AB - BA \quad (\text{A.8})$$

$$\{A, B\} = AB + BA \quad (\text{A.9})$$

It follows that

$$[A^\dagger, B^\dagger] = -[A, B]^\dagger \quad (\text{A.10})$$

$$\{A^\dagger, B^\dagger\} = \{A, B\}^\dagger \quad (\text{A.11})$$

$$\left[\frac{1}{A}, B \right] = -\frac{1}{A} [A, B] \frac{1}{A} \quad (\text{A.12})$$

$$\left\{ \frac{1}{A}, B \right\} = \frac{1}{A} \{A, B\} \frac{1}{A} \quad (\text{A.13})$$

$$[A, BC] = [A, B]C + B[A, C] = \{A, B\}C - B\{A, C\} \quad (\text{A.14})$$

$$[AB, C] = A[B, C] + [A, C]B = A\{B, C\} - \{A, C\}B \quad (\text{A.15})$$

$$\begin{aligned}
[AB, CD] &= A[B, C]D + C[A, D]B + [A, C]BD + CA[B, D] \\
&= A[B, C]D + C[A, D]B + [A, C]DB + AC[B, D] \\
&= A\{B, C\}D - C\{A, D\}B - \{A, C\}BD + CA\{B, D\} \\
&= A\{B, C\}D - C\{A, D\}B + \{A, C\}DB - AC\{B, D\}
\end{aligned} \tag{A.16}$$

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0 \tag{A.17}$$

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A, B]} \quad \text{if} \quad [A, [A, B]] = [B, [A, B]] = 0 \tag{A.18}$$

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \dots \tag{A.19}$$

A.3 Summation conventions

Repeated Roman indices

We use the convention that repeated Roman indices are summed 1, 2, 3. That is,

$$A^j B^j \quad \text{implies} \quad \sum_{j=1}^3 A^j B^j \tag{A.20}$$

Repeated Greek indices

We use the Einstein summation convention that repeated Greek indices are summed 0, 1, 2, 3. That is,

$$A^\mu B^\mu \text{ implies } \sum_{\mu=0}^3 A^\mu B^\mu \quad (\text{A.21})$$

A.4 Miscellaneous symbols

Kronecker delta δ_{jk}

$$\delta_{11} = \delta_{22} = \delta_{33} = 1$$

$$\delta_{jk} = 0 \quad (j \neq k) \quad (\text{A.22})$$

Kronecker delta δ^μ_ν

$$\delta^0_0 = \delta^1_1 = \delta^2_2 = \delta^3_3 = 1$$

$$\delta^\mu_\nu = 0 \quad (\mu \neq \nu) \quad (\text{A.23})$$

Dirac delta $\delta(x)$ and $\delta^m(x)$

$\delta(x)$ and $\delta^m(x)$ are defined by

$$\begin{aligned}\delta(x) &= 0 & \text{if } x &\neq 0 \\ &= \infty & \text{if } x &= 0\end{aligned}\tag{A.24}$$

$$\int_{-\infty}^{+\infty} \delta(x) dx = 1\tag{A.25}$$

$$\delta^m(x) = \frac{d^m \delta(x)}{dx^m}\tag{A.26}$$

It follows that

$$\int_{-\infty}^{+\infty} \delta(a-b) f(b) db = f(a)\tag{A.27}$$

$$\int_{-\infty}^{+\infty} \delta^m(a-b) f(b) db = \frac{d^m f(a)}{da^m}\tag{A.28}$$

$$\delta(-x) = \delta(x)\tag{A.29}$$

$$\delta^m(-x) = (-)^m \delta^m(x)\tag{A.30}$$

$$x\delta(x) = 0 \quad (\text{A.31})$$

$$x\delta^1(x) = -\delta(x) \quad (\text{A.32})$$

$$\delta(ax) = \frac{1}{|a|}\delta(x) \quad (\text{A.33})$$

$$\delta(x^2 - a^2) = \frac{1}{2|a|}[\delta(x + a) + \delta(x - a)] \quad (\text{A.34})$$

$$\delta(f(x)) = \sum_n \frac{1}{\left| \frac{df(x_n)}{dx} \right|} \delta(x - x_n) \quad \left\{ f(x_n) = 0; \frac{df(x_n)}{dx} \neq 0 \right\} \quad (\text{A.35})$$

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ikx} dk \quad (\text{A.36})$$

$$\delta^1(x) = \frac{i}{2\pi} \int_{-\infty}^{+\infty} k e^{ikx} dk \quad (\text{A.37})$$

$$\delta(k - k') = \frac{2k^2}{\pi} \int_0^{\infty} dr r^2 j_1(kr) j_1(k'r) \quad (\text{A.38})$$

Levi-Civita permutation symbol ϵ_{jkl}

ϵ_{jkl} is defined as the totally antisymmetric quantity with

$$\epsilon_{123} = 1 \quad (\text{A.39})$$

It follows that

$$\epsilon_{jkl}\epsilon_{jmn} = \delta_{km}\delta_{ln} - \delta_{kn}\delta_{lm} \quad (\text{A.40})$$

Permutation symbol $\epsilon^{\mu\nu\sigma\tau}$

$\epsilon^{\mu\nu\sigma\tau}$ is defined as the totally antisymmetric quantity with

$$\epsilon^{0123} = 1 \quad (\text{A.41})$$

Metric tensor $g^{\mu\nu}$

$g^{\mu\nu}$ is defined by

$$g^{00} = -g^{11} = -g^{22} = -g^{33} = 1 \quad (\text{A.42})$$

$$g^{\mu\nu} = 0 \quad (\mu \neq \nu)$$

$$g_{\mu\nu} = g^{\mu\nu} \quad (\text{A.43})$$

It follows that

$$g^{\mu\sigma} g_{\sigma\nu} = \delta^{\mu}_{\nu} \quad (\text{A.44})$$

A.5 Raising and lowering indices

$$A_{\mu} = g_{\mu\nu} A^{\nu} \quad (\text{A.45})$$

$$A^{\mu} = g^{\mu\nu} A_{\nu} \quad (\text{A.46})$$

$$A_{\mu}{}^{\nu} = g_{\mu\sigma} A^{\sigma\nu} \quad (\text{A.47})$$

$$A_{\mu\nu} = g_{\mu\sigma} g_{\nu\tau} A^{\sigma\tau} \quad (\text{A.48})$$

A.6 Dot and cross products of operators

We define

$$\vec{A} \cdot \vec{B} = A^j B^j \quad (\text{A.49})$$

$$A \cdot B = A_{\mu} B^{\mu} = A^{\mu} B_{\mu} = A^0 B^0 - \vec{A} \cdot \vec{B} \quad (\text{A.50})$$

$$(\vec{A} \times \vec{B})^j = \epsilon_{jkl} A^k B^l \quad (\text{A.51})$$

Then

$$\vec{A} \cdot (\vec{A} \times \vec{B}) = 0 \quad \text{if} \quad [A^j, A^k] = 0 \quad (\text{A.52})$$

We write

$$\vec{A} \cdot \vec{A} = A^2 \quad (\text{A.53})$$

The superscript 2 thus refers both to the 2-component of a triad and to $\vec{A} \cdot \vec{A}$. Which meaning of A^2 pertains will always be clear from the context.

The dot and cross products (A.49) to (A.51) are only used for operators which transform like vectors under rotations.

A.7 Rotation matrices

Rotation matrices $r^1(\theta), r^2(\theta), r^3(\theta)$ are defined by

$$r^1(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & \sin \theta \\ 0 & -\sin \theta & \cos \theta \end{pmatrix} \quad (\text{A.54})$$

$$r^2(\theta) = \begin{pmatrix} \cos \theta & 0 & -\sin \theta \\ 0 & 1 & 0 \\ \sin \theta & 0 & \cos \theta \end{pmatrix} \quad (\text{A.55})$$

$$r^3(\theta) = \begin{pmatrix} \cos \theta & \sin \theta & 0 \\ -\sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (\text{A.56})$$

That is,

$$r_{ab}^j(\theta) = \delta_{ab} \cos \theta + \delta_{ja} \delta_{jb} (1 - \cos \theta) + \epsilon_{jab} \sin \theta \quad (\text{A.57})$$

(A.54) to (A.56) are involved in coordinate transformations under rotations.

$r^2(\beta)$ and $r^3(\gamma)$ are identical to $M(\beta)$ and $M(\gamma)$, respectively, on page 65, Rose (1957).

A.8 Lorentz transformation matrices

Lorentz transformation matrices $l^1(u), l^2(u), l^3(u)$ are defined by

$$l^1(u) = \begin{pmatrix} \cosh u & -\sinh u & 0 & 0 \\ -\sinh u & \cosh u & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{A.58})$$

$$l^2(u) = \begin{pmatrix} \cosh u & 0 & -\sinh u & 0 \\ 0 & 1 & 0 & 0 \\ -\sinh u & 0 & \cosh u & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{A.59})$$

$$l^3(u) = \begin{pmatrix} \cosh u & 0 & 0 & -\sinh u \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\sinh u & 0 & 0 & \cosh u \end{pmatrix} \quad (\text{A.60})$$

That is,

$$l^j{}^\mu{}_\nu(u) = \delta^\mu{}_\nu + \left(\delta^\mu{}_0 \delta^\nu{}_0 + \delta^\mu{}_j \delta^\nu{}_j \right) (\cosh u - 1) - \left(\delta^\mu{}_0 \delta^\nu{}_j + \delta^\mu{}_j \delta^\nu{}_0 \right) \sinh u \quad (\text{A.61})$$

μ labels the rows and ν labels the columns of $l^j(u)$.

(A.58) to (A.60) are involved in coordinate transformations under Lorentz boosts.

A.9 Pauli matrices

Pauli matrices $\sigma_x, \sigma_y, \sigma_z$ are defined by

$$\sigma_x = \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (\text{A.62})$$

$$\sigma_y = \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (\text{A.63})$$

$$\sigma_z = \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\text{A.64})$$

It follows that

$$\sigma^j \sigma^k = \delta_{jk} + i\epsilon_{jkl}\sigma^l \quad (\text{A.65})$$

$$(\vec{\sigma} \cdot \vec{A})(\vec{\sigma} \cdot \vec{B}) = \vec{A} \cdot \vec{B} + i\vec{\sigma} \cdot (\vec{A} \times \vec{B}) \quad (\text{A.66})$$

$$(\vec{\sigma} \cdot \vec{A})^2 = A^2 \quad \text{if} \quad [A^j, A^k] = 0 \quad (\text{A.67})$$

$$e^{a\sigma^j} = \cosh a + \sigma^j \sinh a \quad (\text{A.68})$$

A.10 Dirac matrices

Dirac matrices $\alpha^1, \alpha^2, \alpha^3, \beta$ satisfy

$$\{\alpha^j, \alpha^k\} = 2\delta_{jk} \quad (\text{A.69})$$

$$\{\alpha^j, \beta\} = 0 \quad (\text{A.70})$$

$$\beta^2 = 1 \quad (\text{A.71})$$

Dirac representation:

$$\alpha^j = \begin{pmatrix} 0 & \sigma^j \\ \sigma^j & 0 \end{pmatrix} \quad (\text{A.72})$$

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\text{A.73})$$

Each element in the matrices on the right side of (A.72) and (A.73) is a 2×2 matrix.

A.11 γ -matrices

γ -matrices $\gamma^0, \gamma^1, \gamma^2, \gamma^3, \gamma^5$ are related to Dirac matrices $\alpha^1, \alpha^2, \alpha^3, \beta$ by

$$\gamma^0 = \beta \quad (\text{A.74})$$

$$\gamma^j = \beta \alpha^j \quad (\text{A.75})$$

$$\gamma^5 = \gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3 \quad (\text{A.76})$$

It follows that

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} \quad (\text{A.77})$$

$$\{\gamma^5, \gamma^\mu\} = 0 \quad (\text{A.78})$$

$$(\gamma^0)^2 = -(\gamma^1)^2 = -(\gamma^2)^2 = -(\gamma^3)^2 = (\gamma^5)^2 = 1 \quad (\text{A.79})$$

$$\gamma^{\mu\dagger} = \gamma^0 \gamma^\mu \gamma^0 \quad (\text{A.80})$$

$$\gamma^{0\dagger} = \gamma^0 \quad (\text{A.81})$$

$$\gamma^{j\dagger} = -\gamma^j \quad (\text{A.82})$$

$$\gamma^{5\dagger} = \gamma^5 \quad (\text{A.83})$$

Dirac representation

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\text{A.84})$$

$$\gamma^j = \begin{pmatrix} 0 & \sigma^j \\ -\sigma^j & 0 \end{pmatrix} \quad (\text{A.85})$$

$$\gamma^5 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (\text{A.86})$$

Weyl representation

$$\gamma^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (\text{A.87})$$

$$\gamma^j = \begin{pmatrix} 0 & \sigma^j \\ -\sigma^j & 0 \end{pmatrix} \quad (\text{A.88})$$

$$\gamma^5 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad (\text{A.89})$$

Chiral representation

$$\gamma^0 = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \quad (\text{A.90})$$

$$\gamma^j = \begin{pmatrix} 0 & \sigma^j \\ -\sigma^j & 0 \end{pmatrix} \quad (\text{A.91})$$

$$\gamma^5 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (\text{A.92})$$

Comments

1. Notation

Each element in the matrices on the right side of (A.84) to (A.92) is a 2×2 matrix.

2. Unitary transformations

Let

$$U_{\pm} = \frac{1}{\sqrt{2}}(1 \pm \gamma^5 \gamma^0) \quad (\text{A.93})$$

$$V_{\pm} = U_{\pm}^2 = \pm \gamma^5 \gamma^0 \quad (\text{A.94})$$

Then

$$U_{\pm}^{\dagger} = \frac{1}{\sqrt{2}}(1 \mp \gamma^5 \gamma^0) \quad (\text{A.95})$$

$$V_{\pm}^{\dagger} = \mp \gamma^5 \gamma^0 = -V_{\pm} \quad (\text{A.96})$$

$$U_{\pm} \gamma^0 U_{\pm}^{\dagger} = \pm \gamma^5 \quad (\text{A.97})$$

$$U_{\pm} \gamma^j U_{\pm}^{\dagger} = \gamma^j \quad (\text{A.98})$$

$$U_{\pm} \gamma^5 U_{\pm}^{\dagger} = \mp \gamma^0 \quad (\text{A.99})$$

$$U_{\pm} \gamma^5 \gamma^0 U_{\pm}^{\dagger} = \gamma^5 \gamma^0 \quad (\text{A.100})$$

$$V_{\pm} \gamma^0 V_{\pm}^{\dagger} = -\gamma^0 \quad (\text{A.101})$$

$$V_{\pm} \gamma^j V_{\pm}^{\dagger} = \gamma^j \quad (\text{A.102})$$

$$V_{\pm} \gamma^5 V_{\pm}^{\dagger} = -\gamma^5 \quad (\text{A.103})$$

$$V_{\pm} \gamma^5 \gamma^0 V_{\pm}^{\dagger} = \gamma^5 \gamma^0 \quad (\text{A.104})$$

3. Dirac, Weyl and chiral representations

The Dirac, Weyl and chiral representations are related as follows:

$$U_+ \gamma_{\text{dirac}}^\mu U_+^\dagger = \gamma_{\text{weyl}}^\mu \quad (\text{A.105})$$

$$U_- \gamma_{\text{dirac}}^\mu U_-^\dagger = \gamma_{\text{chiral}}^\mu \quad (\text{A.106})$$

$$V_\pm \gamma_{\text{weyl}}^\mu V_\pm^\dagger = \gamma_{\text{chiral}}^\mu \quad (\text{A.107})$$

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