KETS, BRAS, AND OPERATORS

In the preceding section we showed how analyses of the Stern-Gerlach experiment lead us to consider a complex vector space.

We first formulate the basic mathematics of vector spaces as used in quantum mechanics employing P. A. M. Dirac.

Ket Space

We consider a complex vector space whose dimensionality is specified according to the nature of a physical system under consideration.

In the case of the silver atoms in the Stern-Gerlach-type experiments, the dimensionality is just two.

Later we consider the case of continuous spectra, e.g., the position (coordinate) or momentum of a particle.

The continuous space is called Hilbert space.

In quantum mechanics a physical state, for example, a silver atom with a definite spin orientation, is represented by a state vector in a complex vector space.

Following Dirac, we call such a vector a ket and denote it by $|\alpha\rangle$.

Two kets can be added:

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

The number c can stand on the left or on the right of a ket.

$$c|\alpha\rangle = |\alpha\rangle c$$

If c=0 results in null ket.

One of the **physics postulates** is that $|\alpha>$ and $c|\alpha>$, with $c\neq0$, represent the same physical state.

In other words, only the "direction" in vector space is of significance.

An observable, such as momentum and spin components, can be represented by an operator, such as A, in the vector space in question.

Quite generally, an operator acts on a ket from the left,

$$A \cdot (|\alpha\rangle) = A|\alpha\rangle$$

which is yet another ket.

There will be more on multiplication operations later.

In general, A|α> is not a constant times |α>.

However, there are particular kets of importance, known as eigenkets of operator A, denoted by

$$|a'\rangle, |a''\rangle, |a'''\rangle, \ldots$$

with the property

$$A|a'\rangle = a'|a'\rangle, \quad A|a''\rangle = a''|a''\rangle, \ldots$$

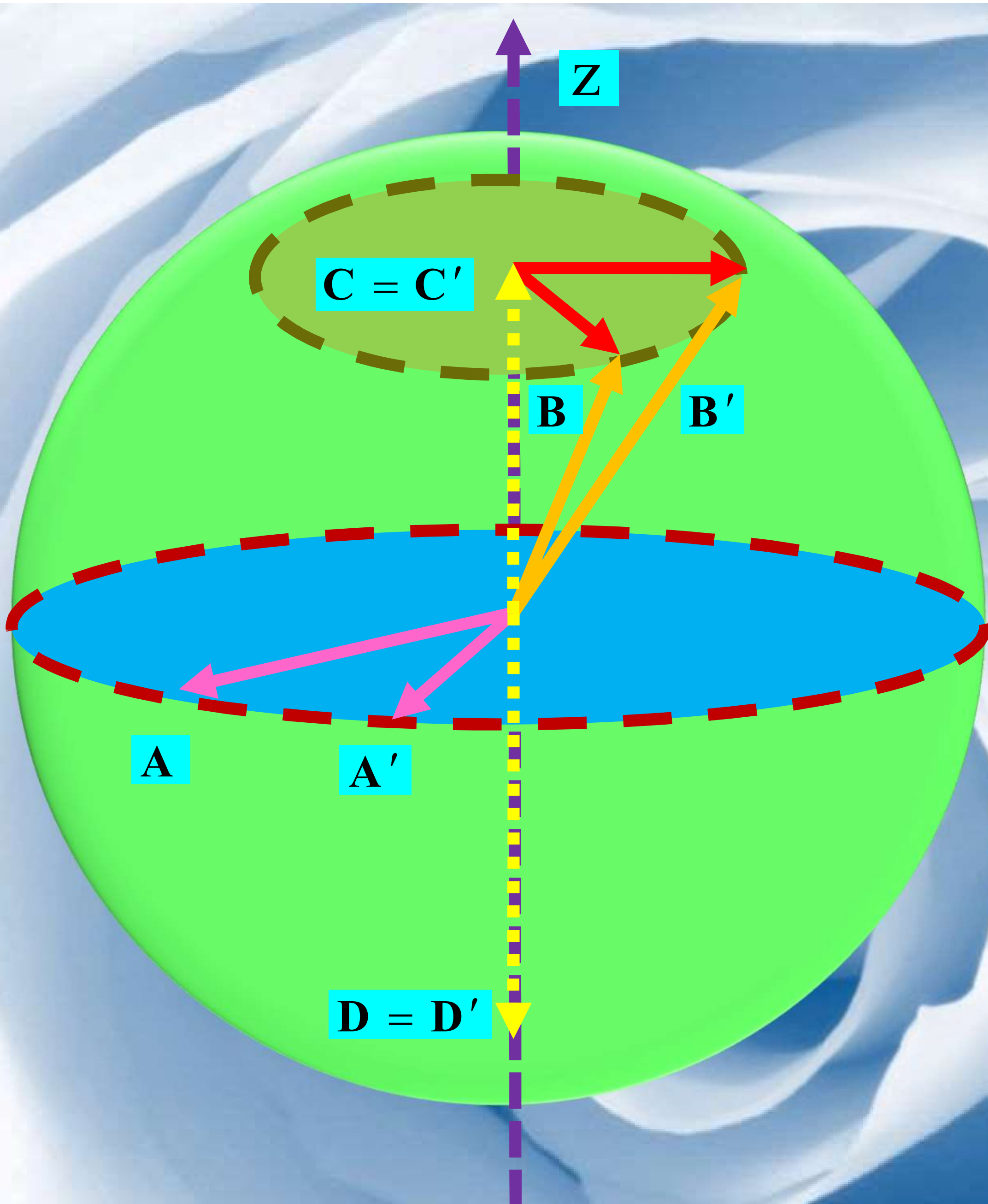
where a', a'', … are just numbers.

Notice that applying A to an eigenket just reproduces the same ket apart from a multiplicative number.

The set of numbers {a, a', a''',...}, more compactly denoted by {a'}, is called the set of eigenvalues of operator A.

When it becomes necessary to order eigenvalues in a specific manner, $\{a^{(1)}, a^{(2)}, a^{(3)} \ldots\}$ may be used in place of {a', a'', a''',...}.

The physical state corresponding to an eigenket is called an eigenstate.



اگر به توابع مانند بردارها نگریسته شود، آنگاه اثر یک عملگر تبدیل یک بردار به بردار دیگری خواهد بود. پس با مطالعه اثر یک عملگر روی یک بردار می توان از اثر آن بر روی بردارهای دیگر نیز اطلاعاتی حاصل کرد.

به عنوان مثال اگر عملگر مورد نظر عملگر دوران به اندازه زاویه 30 درجه حول محور z–ها باشد، آنگاه:

1) بردارهایی از قبیل B به 'B تبدیل می شوند.

2) بردارهایی از قبیل A به 'A تبدیل می شوند.

3) بردارهایی از قبیل C و D به 'C و 'D تبدیل می شوند.

بردارهای مثال 3 بردارهای خاصی هستند که به آنها بردارهای ویژه گویند.

In the simplest case of spin ½ systems, the eigenvalue-eigenket relation is expressed as

$$S_z|S_z;+\rangle = \frac{\hbar}{2}|S_z;+\rangle, \qquad S_z|S_z;-\rangle = -\frac{\hbar}{2}|S_z;-\rangle$$

where $|S_z;\pm\rangle$ are eigenkets of operator S_z with eigenvalues $\pm\hbar/2$. Here we could have used just $|\hbar/2\rangle$ for $|S_z;+\rangle$ in conformity with the notation $|a'\rangle$, where an eigenket is labeled by its eigenvalue, but the notation $|S_z;\pm\rangle$, already used in the previous section, is more convenient here because we also consider eigenkets of S_x:

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

We remarked earlier that the dimensionality of the vector space is determined by the number of alternatives in Stern-Gerlach-type experiments.

More formally, we are concerned with an N-dimensional vector space spanned by the N eigenkets of observable A.

Any arbitrary ket |α> can be written as

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

with $a', a'', \ldots$ up to $a^{(N)}$, where $c_{a'}$ is a complex coefficient.

Bra Space and Inner Products

The vector space we have been dealing with is a ket space.

We now introduce the notion of a bra space, a vector space "dual to" the ket space.

We postulate that corresponding to every ket $|\alpha\rangle$ there exists a bra, denoted by $\langle\alpha|$, in this dual, or bra, space.

The bra space is spanned by eigenbras $\{\langle\alpha'|\}$ which correspond to the eigenkets $\{|\alpha'\rangle\}$.

There is a one-to-one correspondence between a ket space and a bra space:

$$|\alpha\rangle \overset{\text{DC}}{\leftrightarrow} \langle\alpha|$$

$$|a'\rangle, |a''\rangle, \ldots \overset{\text{DC}}{\leftrightarrow} \langle a'|, \langle a''|, \ldots$$

$$|\alpha\rangle + |\beta\rangle \overset{\text{DC}}{\leftrightarrow} \langle\alpha| + \langle\beta|$$

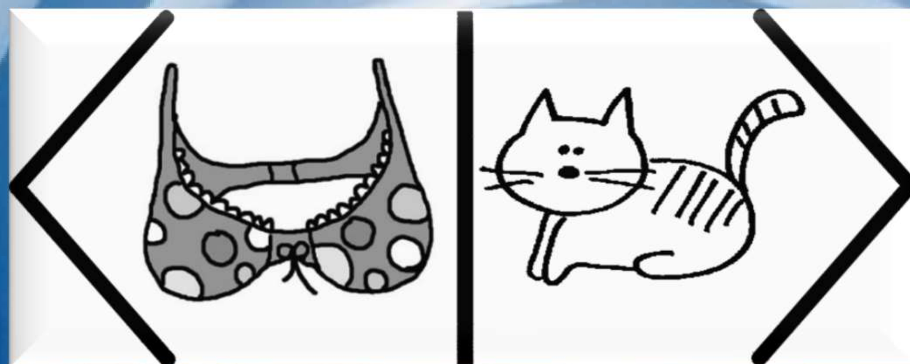
where DC stands for dual correspondence.

Roughly speaking, we can regard the bra space as some kind of mirror image of the ket space.

The bra dual to c|α> is postulated to be c*<α|, not c<α|, which is a very important point.

More generally, we have

$$c_\alpha|\alpha\rangle + c_\beta|\beta\rangle \overset{\text{DC}}{\leftrightarrow} c_\alpha^*\langle\alpha| + c_\beta^*\langle\beta|$$



DC

$$|\alpha\rangle = \begin{pmatrix} 2 \\ 5i+6 \\ 7i \end{pmatrix}_{3\times1} \leftrightarrow \langle\alpha| = \begin{pmatrix} 2 & -5i+6 & -7i \end{pmatrix}_{1\times3}$$

We now define the inner product of a bra and a ket.

The product is written as a bra standing on the left and a ket standing on the right, for example,

$$\langle \beta | \alpha \rangle = \underbrace{(\langle \beta |) \cdot (| \alpha \rangle)}_{\text{bra } (c) \text{ ket}}$$

This product is, in general, a complex number.

Notice that in forming an inner product we always take one vector from the bra space and one vector from the ket space.

We postulate two fundamental properties of inner products.

First,

$$\langle \beta | \alpha \rangle = \langle \alpha | \beta \rangle^*$$

In other words, $\langle\alpha|\beta\rangle$ and $\langle\beta|\alpha\rangle$ are complex conjugates of each other.

Notice that even though the inner product is, in some sense, analogous to the familiar scalar product a.b, $<\alpha|\beta>$ must be clearly distinguished from $<\beta|\alpha>$; the analogous distinction is not needed in real vector space because a.b is equal to b.a.

we can immediately deduce that $<\alpha|\alpha>$ must be a real number.

To prove this just let

$$\langle \beta | \rightarrow \langle \alpha |$$

$$\langle \beta | \alpha \rangle = \langle \alpha | \beta \rangle^*$$

$$\langle \alpha | \alpha \rangle = \langle \alpha | \alpha \rangle^*$$

The second postulate on inner products is

$$\langle \alpha | \alpha \rangle \geq 0$$

where the equality sign holds only if $|\alpha>$ is a null ket.

This is sometimes known as the **postulate of positive definite metric**.

From a physicist's point of view, this postulate is essential for the probabilistic interpretation of quantum mechanics, as will become apparent later.

Two kets $|\alpha\rangle$ and $|\beta\rangle$ are said to be orthogonal if

$$\langle \alpha | \beta \rangle = 0$$

even though in the definition of the inner product the bra $\langle\alpha|$ appears.

$$\langle \beta | \alpha \rangle = 0$$

The orthogonality relation also implies,

$$\langle \beta | \alpha \rangle = \langle \alpha | \beta \rangle^* = 0^* = 0$$

Given a ket which is not a null ket, we can form a normalized ket

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

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

Quite generally, $\sqrt{\langle\alpha|\alpha\rangle}$ is known as the **norm** of $|\alpha\rangle$, analogous to the magnitude of vector $\sqrt{\mathbf{a}\cdot\mathbf{a}} = |\vec{\mathbf{a}}|$ in Euclidean vector space. Because $|\alpha\rangle$ and $c|\alpha\rangle$ represent the same physical state, we might as well require that the kets we use for physical states be normalized in the sense of (1.2.17).†

بردار اصلی

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

بردارهای پایه یا بردارهای یکه

ضرایب بسط یا مولفه های بردار اصلی یا تصویر بردار **|α>** در امتداد بردار پایه **|a’>**

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

$$\langle a|\alpha\rangle = \sum_{a'} c_{a'}\langle a|a'\rangle = \sum_{a'} c_{a'}\delta_{aa'} = c_a$$

$\vec{A}$ $\quad A_x, A_y, A_z \quad \hat{i}, \hat{j}, \hat{k}$

$$\mathbf{A} = A_x\mathbf{i} + A_y\mathbf{j} + A_z\mathbf{k}$$

$$\mathbf{i}.\mathbf{i} = \mathbf{j}.\mathbf{j} = \mathbf{k}.\mathbf{k} = 1 \,\& \qquad \mathbf{i}.\mathbf{j} = \mathbf{i}.\mathbf{k} = \mathbf{j}.\mathbf{k} = 0$$

$$A_x = \mathbf{A}.\mathbf{i} \,\& \quad A_y = \mathbf{A}.\mathbf{j} \,\& \quad A_z = \mathbf{A}.\mathbf{k}$$

Operators

An operator acts on a ket from the left side,

$$X\cdot(|\alpha\rangle) = X|\alpha\rangle$$

and the resulting product is another ket.

Operators X and Y are said to be equal, i.e., X=Y, if

$$X|\alpha\rangle = Y|\alpha\rangle$$

Operator X is said to be the null operator if, for any arbitrary ket |α>, we have

$$X|\alpha\rangle = 0$$

Operators can be added; addition operations are commutative and associative:

$$X + Y = Y + X,$$

$$X + (Y + Z) = (X + Y) + Z$$

With the single exception of the time-reversal operator to be considered in Chapter4, the operators that appear in this book are all linear, that is,

$$X\left(c_\alpha|\alpha\rangle + c_\beta|\beta\rangle\right) = c_\alpha X|\alpha\rangle + c_\beta X|\beta\rangle$$

An operator X always acts on a bra from the right side

$$(\langle\alpha|)\cdot X = \langle\alpha|X$$

The ket X|α> and the bra <α|X are, in general, not dual to each other. We define the symbol X^+ as

$$X|\alpha\rangle \overset{\text{DC}}{\leftrightarrow} \langle\alpha|X^{\dagger}$$

The operator X^+ is called the Hermitian adjoint, or simply the adjoint, of X. An operator X is said to be Hermitian if

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

Multiplication

Operators X and Y can be multiplied. Multiplication operations are, in general, noncommutative, that is,

$$XY \neq YX$$

Multiplication operations are, however, associative:

$$X(YZ) = (XY)Z = XYZ$$

We also have

$$X(Y|\alpha\rangle) = (XY)|\alpha\rangle = XY|\alpha\rangle, \qquad (\langle\beta|X)Y = \langle\beta|(XY) = \langle\beta|XY$$

Notice that

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

Because

$$XY|\alpha\rangle = X(Y|\alpha\rangle) \overset{\text{DC}}{\leftrightarrow} (\langle\alpha|Y^{\dagger})X^{\dagger} = \langle\alpha|Y^{\dagger}X^{\dagger}$$

So far, we have considered the following products: $\langle\beta|\alpha\rangle$, $X|\alpha\rangle$, $\langle\alpha|X$, and XY. Are there other products we are allowed to form? Let us multiply $|\beta\rangle$ and $\langle\alpha|$, in that order. The resulting product

$$(|\beta\rangle)\cdot(\langle\alpha|)=|\beta\rangle\langle\alpha|$$

is known as the **outer product** of $|\beta\rangle$ and $\langle\alpha|$. We will emphasize in a moment that $|\beta\rangle\langle\alpha|$ is to be regarded as an operator; hence it is fundamentally different from the inner product $\langle\beta|\alpha\rangle$, which is just a number.

There are also "illegal products." We have already mentioned that an operator must stand on the left of a ket or on the right of a bra. In other words, $|\alpha\rangle X$ and $X\langle\alpha|$ are examples of illegal products. They are neither kets, nor bras, nor operators; they are simply nonsensical. Products like $|\alpha\rangle|\beta\rangle$ and $\langle\alpha|\langle\beta|$ are also illegal when $|\alpha\rangle$ and $|\beta\rangle$ ($\langle\alpha|$ and $\langle\beta|$) are ket (bra) vectors belonging to the same ket (bra) space.*

The Associative Axiom

As is clear from (1.2.27), multiplication operations among operators are associative. Actually the associative property is postulated to hold quite generally as long as we are dealing with "legal" multiplications among kets, bras, and operators. Dirac calls this important postulate the **associative axiom of multiplication**.

To illustrate the power of this axiom let us first consider an outer product acting on a ket:

$$(|\beta\rangle\langle\alpha|)\cdot|\gamma\rangle$$

Because of the associative axiom, we can regard this equally well as

$$|\beta\rangle\cdot(\langle\alpha|\gamma\rangle)$$

$$|\beta\rangle \cdot (\langle\alpha|\gamma\rangle)$$

where $\langle\alpha|\gamma\rangle$ is just a number. So the outer product acting on a ket is just another ket; in other words, $|\beta\rangle\langle\alpha|$ can be regarded as an operator. Because (1.2.32) and (1.2.33) are equal, we may as well omit the dots and let $|\beta\rangle\langle\alpha|\gamma\rangle$ stand for the operator $|\beta\rangle\langle\alpha|$ acting on $|\gamma\rangle$ *or*, equivalently, the number $\langle\alpha|\gamma\rangle$ multiplying $|\beta\rangle$. (On the other hand, if (1.2.33) is written as $(\langle\alpha|\gamma\rangle)\cdot|\beta\rangle$, we cannot afford to omit the dot and brackets because the resulting expression would look illegal.) Notice that the operator $|\beta\rangle\langle\alpha|$ rotates $|\gamma\rangle$ into the direction of $|\beta\rangle$. It is easy to see that if

$$X = |\beta\rangle\langle\alpha| \quad \Rightarrow \quad X^\dagger = |\alpha\rangle\langle\beta|$$

In a second important illustration of the associative axiom, we note that

$$\underset{\text{bra}}{(\langle\beta|)} \cdot \underset{\text{ket}}{(X|\alpha\rangle)} = \underset{\text{bra}}{(\langle\beta|X)} \cdot \underset{\text{ket}}{(|\alpha\rangle)}$$

Because the two sides are equal, we might as well use the more compact notation

$$\langle\beta|X|\alpha\rangle$$

Recall now that $<\alpha|X^{+}$ is the bra that is dual to $X|\alpha>$, so

$$\langle\beta|X|\alpha\rangle = \langle\beta|\cdot(X|\alpha\rangle)$$

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

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

where, in addition to the associative axiom, we used the fundamental property of the inner product. For a Hermitian X we have

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

BASE KETS AND MATRIX REPRESENTATIONS

Eigenkets of an Observable

Theorem. *The eigenvalues of a Hermitian operator A are real; the eigenkets of A corresponding to different eigenvalues are orthogonal.*

$$A|a'\rangle = a'|a'\rangle$$

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

$$\langle a''|A^{\dagger} = \langle a''|a''^{*}$$

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

$$\langle a''|A = a''^{*}\langle a''|$$

$$A|a'\rangle = a'|a'\rangle \quad\Rightarrow\quad \langle a''|A|a'\rangle = a'\langle a''|a'\rangle$$

$$\langle a''|A = a''^{*}\langle a''| \quad\Rightarrow\quad \langle a''|A|a'\rangle = a''^{*}\langle a''|a'\rangle$$

$$-$$

$$0 = (a' - a''^{*})\langle a''|a'\rangle$$

IF $a' = a''$ $\Rightarrow$ $a' = a'^{*}$

IF $a' \neq a''$ $\Rightarrow$ $\langle a''|a'\rangle = 0$

We expect on physical grounds that an observable has real eigenvalues, a point that will become clearer in the next section, where measurements in quantum mechanics will be discussed. The theorem just proved guarantees the reality of eigenvalues whenever the operator is Hermitian. That is why we talk about Hermitian observables in quantum mechanics.

It is conventional to normalize $|a'\rangle$ so the $\{|a'\rangle\}$ form a **orthonormal** set:

$$\langle a''|a'\rangle = \delta_{a''a'}$$

We may logically ask, Is this set of eigenkets complete? Since we started our discussion by asserting that the whole ket space is spanned by the eigenkets of A, the eigenkets of A must therefore form a complete set by *construction* of our ket space.*

Eigenkets as Base Kets

We have seen that the normalized eigenkets of A form a complete orthonormal set.

An arbitrary ket in the ket space can be expanded in terms of the eigenkets of A.

In other words, the eigenkets of A are to be used as base kets in much the same way as a set of mutually orthogonal unit vectors is used as base vectors in Euclidean space.

Given an arbitrary ket $|\alpha\rangle$ in the ket space spanned by the eigenkets of A, let us attempt to expand it as follows:

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

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

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

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

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \Rightarrow \sum_{a'} |a'\rangle\langle a'| = 1$$

Completeness Relation or Closure

It is difficult to overestimate the usefulness of (1.3.11). Given a chain of kets, operators, or bras multiplied in legal orders, we can insert, in any place at our convenience, the identity operator written in form (1.3.11). Consider, for example $\langle\alpha|\alpha\rangle$; by inserting the identity operator between $\langle\alpha|$ and $|\alpha\rangle$, we obtain

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

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

This, incidentally, shows that if $|\alpha\rangle$ is normalized, then the expansion coefficients in (1.3.7) must satisfy

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

Let us now look at $|a'\rangle\langle a'|$ that appears in (1.3.11). Since this is an outer product, it must be an operator. Let it operate on $|\alpha\rangle$:

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

We see that $|a'\rangle\langle a'|$ selects that portion of the ket $|\alpha\rangle$ parallel to $|a'\rangle$, so $|a'\rangle\langle a'|$ is known as the **projection operator** along the base ket $|a'\rangle$ and is denoted by $\Lambda_{a'}$:

$$\Lambda_{a'} \equiv |a'\rangle\langle a'|$$

The completeness relation (1.3.11) can now be written as

$$\sum_{a'} \Lambda_{a'} = 1$$

Matrix Representations

Having specified the base kets, we now show how to represent an operator, say X, by a square matrix. First, using (1.3.11) twice, we write the operator X as

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

There are altogether N^2 numbers of form $\langle a''|X|a'\rangle$, where N is the dimensionality of the ket space. We may arrange them into an $N \times N$ square matrix such that the column and row indices appear as follows:

$$\langle \underset{\text{row}}{a''}|X|\underset{\text{column}}{a'}\rangle$$

Explicitly we may write the matrix as

$$X \doteq \begin{pmatrix} \langle a^{(1)}|X|a^{(1)}\rangle & \langle a^{(1)}|X|a^{(2)}\rangle & \cdots \\ \langle a^{(2)}|X|a^{(1)}\rangle & \langle a^{(2)}|X|a^{(2)}\rangle & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

where the symbol $\doteq$ stands for "is represented by."

$$\langle a''|X|a'\rangle = \langle a'|X^\dagger|a''\rangle^*$$

If an operator B is Hermitian, we have

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

The way we arranged $\langle a''|X|a'\rangle$ into a square matrix is in conformity with the usual rule of matrix multiplication. To see this just note that the matrix representation of the operator relation

$Z = XY$ reads

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

Let us now examine how the ket relation $|\gamma\rangle = X|\alpha\rangle$ can be represented using our base kets.

$$|\gamma\rangle = X|\alpha\rangle$$

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

But this can be seen as an application of the rule for multiplying a square matrix with a column matrix representing once the expansion coefficients of $|\alpha\rangle$ and $|\gamma\rangle$ arrange themselves to form column matrices as follows:

$$|\alpha\rangle \doteq \begin{pmatrix} \langle a^{(1)}|\alpha\rangle \\ \langle a^{(2)}|\alpha\rangle \\ \langle a^{(3)}|\alpha\rangle \\ \vdots \end{pmatrix}, \qquad |\gamma\rangle \doteq \begin{pmatrix} \langle a^{(1)}|\gamma\rangle \\ \langle a^{(2)}|\gamma\rangle \\ \langle a^{(3)}|\gamma\rangle \\ \vdots \end{pmatrix}$$

Likewise, given $<\gamma| = <\alpha|X$

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

So a bra is represented by a row matrix as follows:

$$\langle\gamma| \doteq (\langle\gamma|a^{(1)}\rangle, \langle\gamma|a^{(2)}\rangle, \langle\gamma|a^{(3)}\rangle, \ldots) = (\langle a^{(1)}|\gamma\rangle^*, \langle a^{(2)}|\gamma\rangle^*, \langle a^{(3)}|\gamma\rangle^*, \ldots)$$

The inner product $<\beta|\alpha>$ can be written as the product of the row matrix representing $<\beta|$ with the column matrix representing $|\alpha>$:

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

$$= (\langle a^{(1)}|\beta\rangle^*, \langle a^{(2)}|\beta\rangle^*, \ldots)\begin{pmatrix}\langle a^{(1)}|\alpha\rangle \\ \langle a^{(2)}|\alpha\rangle \\ \vdots\end{pmatrix}$$

Finally, the matrix representation of the outer product |β><α| is easily seen to be

$$|\beta\rangle\langle\alpha| \doteq \begin{pmatrix} \langle a^{(1)}|\beta\rangle\langle a^{(1)}|\alpha\rangle^* & \langle a^{(1)}|\beta\rangle\langle a^{(2)}|\alpha\rangle^* & \cdots \\ \langle a^{(2)}|\beta\rangle\langle a^{(1)}|\alpha\rangle^* & \langle a^{(2)}|\beta\rangle\langle a^{(2)}|\alpha\rangle^* & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

The matrix representation of an observable A becomes particularly simple if the eigenkets of A themselves are used as the base kets. First, we

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

But the square matrix <a``|A|a`> is obviously diagonal

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

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

Therefore

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

Spin 1/2 Systems

It is here instructive to consider the special case of spin $\frac{1}{2}$ systems.

The base kets used are $|S_z; \pm\rangle$, which we denote, for brevity, as $|\pm\rangle$.

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

$$1 = |+\rangle\langle +| + |-\rangle\langle -|$$

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

$$S_z|\pm\rangle = \pm(\hbar/2)|\pm\rangle$$

$$S_z = (\hbar/2)[(|+\rangle\langle +|) - (|-\rangle\langle -|)]$$

It is also instructive to look at two other operators

$$S_+ \equiv \hbar|+\rangle\langle-|$$

$$S_+^\dagger = \hbar|-\rangle\langle+| = S_- \neq S_+$$

$$S_- \equiv \hbar|-\rangle\langle+|$$

$$S_-^\dagger = \hbar|+\rangle\langle-| = S_+ \neq S_-$$

Which are both non-Hermitian

The physical interpretation of S^+ is that it raises the spin component by one unit of ħ

$$S_+|+\rangle = \hbar|+\rangle\langle-|+\rangle = 0$$

$$S_+|-\rangle = \hbar|+\rangle\langle-|-\rangle = \hbar|+\rangle$$

The physical interpretation of S^- is that it lowers the spin component by one unit of ħ

$$S_-|+\rangle = \hbar|-\rangle\langle+|+\rangle = \hbar|-\rangle$$

$$S_-|-\rangle = \hbar|-\rangle\langle+|-\rangle = 0$$

Matrix Representation of Spin 1/2 Systems

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

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\langle +| = \begin{pmatrix} 1 & 0 \end{pmatrix}$$

$$\langle -| = \begin{pmatrix} 0 & 1 \end{pmatrix}$$

$$S_+ = \hbar|+\rangle\langle -| = \hbar\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \end{pmatrix} = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$S_- = \hbar|-\rangle\langle +| = \hbar\begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$S_z = \frac{\hbar}{2}\left(|+\rangle\langle+| - |-\rangle\langle-|\right)$$

$$= \frac{\hbar}{2}\left(\begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix} - \begin{pmatrix}0\\1\end{pmatrix}\begin{pmatrix}0 & 1\end{pmatrix}\right)$$

$$= \frac{\hbar}{2}\left(\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix} - \begin{pmatrix}0 & 0\\0 & 1\end{pmatrix}\right)$$

$$= \frac{\hbar}{2}\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$$

$$S_+ = \hbar\begin{pmatrix}1 & 0\\0 & 0\end{pmatrix}$$

$$S_- = \hbar\begin{pmatrix}0 & 0\\0 & 1\end{pmatrix}$$

$$S_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$$

We will come back to these explicit expressions when we discuss the Pauli two-component formalism in Chapter 3.

MEASUREMENTS, OBSERVABLES, AND THE UNCERTAINTY RELATIONS

Having developed the mathematics of ket spaces, we are now in a position to discuss the quantum theory of measurement processes.

This is not a particularly easy subject for beginners,

so we first turn to the words of the great master, P. A. M. Dirac, for guidance (Dirac 1958, 36):

"A measurement always causes the system to jump into an eigenstate of the dynamical variable that is being measured."

What does all this mean?

We interpret Dirac's words as follows:

Before a measurement of observable A is made, the system is assumed to be represented by some linear combination

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

When the measurement is performed, the system is "thrown into" one of the eigenstates, say |a`> of observable A.

In other words:

$$|\alpha\rangle \xrightarrow{A \text{ measurement}} |a'\rangle$$

For example, a silver atom with an arbitrary spin orientation will change into either $|S_Z; +\rangle$ or $|S_Z; -\rangle$ when subjected to a SG apparatus of type SGz.

Thus a measurement usually changes the state.

The only exception is when the state is already in one of the eigenstates of the observable being measured:

$$|a'\rangle \xrightarrow{A \text{ measurement}} |a'\rangle$$

When the measurement causes $|\alpha>$ to change into $|a`>$, it is said that A is measured to be a'.

It is in this sense that the result of a measurement yields one of the eigenvalues of the observable being measured.

A state ket of a physical system before the measurement, we do not know in advance into which of the various $|a'>$'s the system will be thrown as the result of the measurement.

We do postulate, however, that the probability for jumping into some particular |a'> is given by

$$\text{Probability for } a' = |\langle a'|\alpha\rangle|^2$$

provided that |α> is normalized.

Although we have been talking about a single physical system, to determine the above probability empirically, we must consider a great number of measurements performed on an ensemble—that is, a collection—of identically prepared physical systems, all characterized by the same ket |α>.

Such an ensemble is known as a **pure ensemble**.

We will say more about ensembles in Chapter 3.

As an example, a beam of silver atoms which survive the first SGz apparatus with the S_Z-component blocked is an example of a pure ensemble because every member atom of the ensemble is characterized by $|S_Z; +>$.

The probabilistic interpretation for the squared inner product $|<a'|\alpha>|^2$ is one of the fundamental postulates of quantum mechanics.

So it cannot be proven.

Let us note, however, that it makes good sense in extreme cases.

Suppose the state ket is |a'> itself even before a measurement is made

Then the probability for getting a'—or, more precisely, for being thrown into |a'>—as the result of the measurement is predicted to be 1, which is just what we expect.

we, of course, get |a'> only; quite generally, repeated measurements of the same observable in succession yield the same result.

If, on the other hand, we are interested in the probability for the system initially characterized by $|a'\rangle$ to be thrown into some other eigenket $|a''\rangle$ with $a'' \neq a'$ then gives zero because of the orthogonality between $|a'\rangle$ and $|a''\rangle$.

From the point of view of measurement theory, orthogonal kets correspond to mutually exclusive alternatives;

for example, if a spin 1/2 system is in $|S_Z; +\rangle$, it is not in $|S_Z; -\rangle$ with certainty.

We define the expectation value of A taken with respect to state |α> as

$$\langle A \rangle \equiv \langle \alpha | A | \alpha \rangle$$

The above equation is a definition; however, it agrees with our intuitive notion of average measured value because it can be written as

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

$$= \sum_{a'} \underset{\text{measured value } a'}{\underset{\uparrow}{a'}} \quad \underbrace{|\langle a' | \alpha \rangle|^2}_{\text{probability for obtaining } a'}$$

It is very important not to confuse eigenvalues with expectation values.

For example, the expectation value of Sz for spin 1/2 systems can assume any real value between $-\hbar/2$ and $+\hbar/2$, say 0.273h; in contrast, the eigenvalue of S_z assumes only two values, h/2 and -h/2.

تست (کنکور کارشناسی ارشد سال 1376): در اندازه گیری یک عملگر، تنها مقادیر ... عملگر اندازه گیری می شود.

1) ارزش انتظاری

2) متوسط

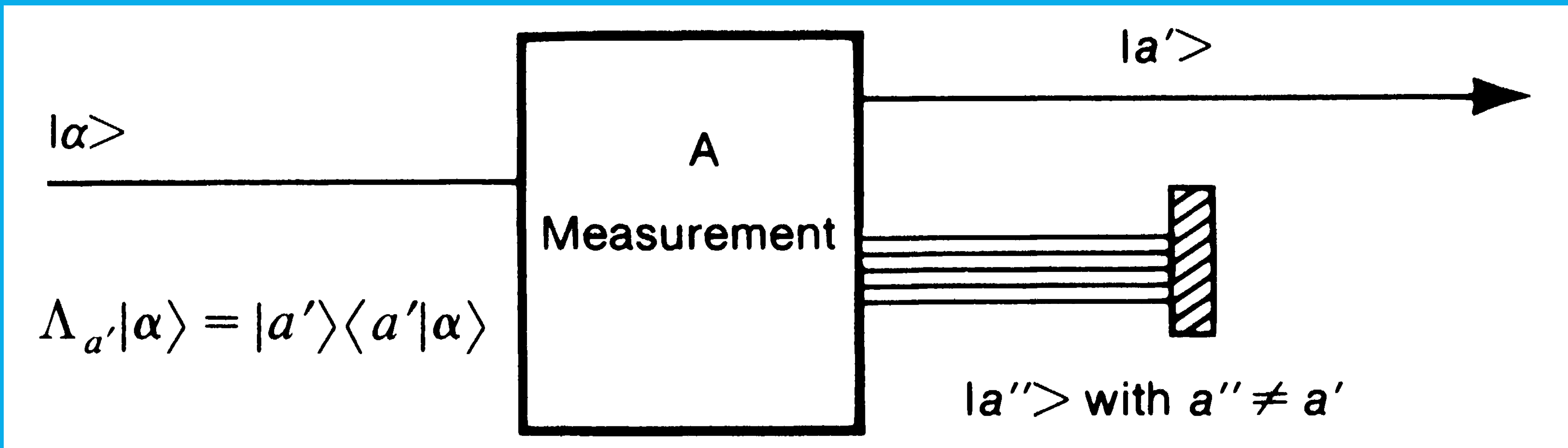
3) نامشخص

4) ویژه

To clarify further the meaning of measurements in quantum mechanics we introduce the notion of a selective measurement, or filtration.

we had considered a Stern-Gerlach arrangement where we let only one of the spin components pass out of the apparatus while we completely blocked the other component.

More generally, we imagine a measurement process with a device that selects only one of the eigenkets of A, say |a'>, and rejects all others.



This is what we mean by a selective measurement; it is also called filtration because only one of the A eigenkets filters through the ordeal.

Spin ½ Systems

This time we show that the results of sequential Stern-Gerlach experiments, when combined with the postulates of quantum mechanics discussed so far, are sufficient to determine not only the $S_{x,y}$ eigenkets, $|S_x;+\rangle$ and $|S_y;+\rangle$, but also the operators S_x and S_y themselves.

First, we recall that when the Sx + beam is subjected to an apparatus of type SGz, the beam splits into two components with equal intensities.

This means that the probability for the Sx + state to be thrown into $|S_Z;\pm\rangle$, simply denoted as $|\pm\rangle$, is 1/2 each; hence,

$$|\langle + | S_x; + \rangle| = |\langle - | S_x; + \rangle| = \frac{1}{\sqrt{2}}$$

We can therefore construct the S_x + ket as follows:

$$|S_x; + \rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}} e^{i\delta_1}|-\rangle$$

The S_x- ket must be orthogonal to the S_x+ ket, which the orthogonality requirement leads to

$$|S_x;-\rangle = \frac{1}{\sqrt{2}}|+\rangle - \frac{1}{\sqrt{2}}e^{i\delta_1}|-\rangle$$

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

$$S_x = \frac{\hbar}{2}\left[\left(|S_x;+\rangle\langle S_x;+|\right) - \left(|S_x;-\rangle\langle S_x;-|\right)\right]$$

$$= \frac{\hbar}{2}\left[e^{-i\delta_1}\left(|+\rangle\langle -|\right) + e^{i\delta_1}\left(|-\rangle\langle +|\right)\right]$$

?

$$|S_x;+\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}e^{i\delta_1}|-\rangle \qquad |S_x;-\rangle = \frac{1}{\sqrt{2}}|+\rangle - \frac{1}{\sqrt{2}}e^{i\delta_1}|-\rangle$$

$$S_x = \frac{\hbar}{2}[(|S_x;+\rangle\langle S_x;+|) - (|S_x;-\rangle\langle S_x;-|)]$$

$$|S_x;+><S_x;+| = \frac{1}{\sqrt{2}}[|+> + e^{i\delta_1}|->]\frac{1}{\sqrt{2}}[<+| + e^{-i\delta_1}<-|]$$

$$= \frac{1}{2}[|+><+| + e^{i\delta_1}|-><+| + e^{-i\delta_1}|+><-| + e^{i\delta_1}e^{-i\delta_1}|-><-|]$$

$$= \frac{1}{2}[|+><+| + e^{i\delta_1}|-><+| + e^{-i\delta_1}|+><-| + |-><-|]$$

$$|S_x;-><S_x;| = \frac{1}{\sqrt{2}}[|+> - e^{i\delta_1}|->]\frac{1}{\sqrt{2}}[<+| - e^{-i\delta_1}<-|]$$

$$= \frac{1}{2}[|+><+| - e^{i\delta_1}|-><+| - e^{-i\delta_1}|+><-| + e^{i\delta_1}e^{-i\delta_1}|-><-|]$$

$$= \frac{1}{2}[|+><+| - e^{i\delta_1}|-><+| - e^{-i\delta_1}|+><-| + |-><-|]$$

$$|S_x;+><S_x;+| = \frac{1}{2}[\cancel{|+><+|} + e^{i\delta_1}|-><+| + e^{-i\delta_1}|+><-| + \cancel{|-><-|}]$$

$$|S_x;-><S_x;-| = \frac{1}{2}[\cancel{|+><+|} - e^{i\delta_1}|-><+| - e^{-i\delta_1}|+><-| + \cancel{|-><-|}]$$

$$S_x = \frac{\hbar}{2}[|S_x;+><S_x;+| - |S_x;-><S_x;|]$$

$$= \frac{\hbar}{2}\left[e^{-i\delta_1}(|+\rangle\langle-|) + e^{i\delta_1}(|-\rangle\langle+|)\right]$$

A similar argument with S_x replaced by S_y leads to

$$|S_y;\pm\rangle = \frac{1}{\sqrt{2}}|+\rangle \pm \frac{1}{\sqrt{2}}e^{i\delta_2}|-\rangle$$

$$S_y = \frac{\hbar}{2}\left[e^{-i\delta_2}(|+\rangle\langle-|) + e^{i\delta_2}(|-\rangle\langle+|)\right]$$

How to determine δ_1 and δ_2?

Suppose we have a beam of spin ½ atoms moving in the z-direction.

We can consider a sequential Stern-Gerlach experiment with SGx followed by SGy.

$$|\langle S_y;\pm|S_x;+\rangle| = |\langle S_y;\pm|S_x;-\rangle| = \frac{1}{\sqrt{2}}$$

$$|S_y;\pm\rangle = \frac{1}{\sqrt{2}}|+\rangle \pm \frac{1}{\sqrt{2}}e^{i\delta_2}|-\rangle$$

$$|S_x;+\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}e^{i\delta_1}|-\rangle$$

$$|S_x;-\rangle = \frac{1}{\sqrt{2}}|+\rangle - \frac{1}{\sqrt{2}}e^{i\delta_1}|-\rangle$$

$$|< S_y;\pm|S_x;+>| = \frac{1}{2}|1 \pm e^{i(\delta_1-\delta_2)}|$$

$$\frac{1}{2}|1 \pm e^{i(\delta_1-\delta_2)}| = \frac{1}{\sqrt{2}}$$

$$\delta_2 - \delta_1 = \pi/2 \quad \text{or} \quad -\pi/2$$

We thus see that the matrix elements of Sx and Sy cannot all be real.

If the Sx matrix elements are real, the Sy matrix elements must be purely imaginary (and vice versa).

Just from this extremely simple example, the introduction of complex numbers is seen to be an essential feature in quantum mechanics.

It is convenient to take the Sx matrix elements to be real and set $\delta_1 = 0$; if we were to choose $\delta_1 = \pi$, the positive x-axis would be oriented in the opposite direction.

The second phase angle δ_2 must then be $-\pi/2$ or $\pi/2$.

The fact that there is still an ambiguity of this kind is not surprising.

Later we will discuss angular momentum as a generator of rotations using the right-handed coordinate system; it can then be shown that $\delta_2 = \pi/2$ is the correct choice.

To summarize, we have:

$$|S_x; \pm\rangle = \frac{1}{\sqrt{2}}|+\rangle \pm \frac{1}{\sqrt{2}}|-\rangle \qquad S_x = \frac{\hbar}{2}\left[(|+\rangle\langle -|) + (|-\rangle\langle +|)\right]$$

$$|S_y; \pm\rangle = \frac{1}{\sqrt{2}}|+\rangle \pm \frac{i}{\sqrt{2}}|-\rangle \qquad S_y = \frac{\hbar}{2}\left[-i(|+\rangle\langle -|) + i(|-\rangle\langle +|)\right]$$

Furthermore, the non-Hermitian S± operators can now be written as

$$S_{\pm} = S_x \pm iS_y$$

The operators Sx and Sy, together with Sz given earlier, can be readily shown to satisfy the commutation relations

$$\left[S_i, S_j\right] = i\varepsilon_{ijk}\hbar S_k$$

and the anticommutation relations

$$\{S_i, S_j\} = \frac{1}{2}\hbar^2\delta_{ij}$$

$$S_x^2 + S_y^2 + S_z^2 = \frac{3}{4}\hbar^2$$

$$[S^2, S_i] = [\frac{3}{4}\hbar^2, S_i] = 0$$

$$S_x^2 + S_x^2 = \frac{1}{2}\hbar^2 \qquad S_y^2 + S_y^2 = \frac{1}{2}\hbar^2 \qquad S_z^2 + S_z^2 = \frac{1}{2}\hbar^2$$

$$S_x^2 = \frac{1}{4}\hbar^2 \qquad S_y^2 = \frac{1}{4}\hbar^2 \qquad S_z^2 = \frac{1}{4}\hbar^2$$

where the commutator [,] and the anticommutator { , } are defined by

$$[A, B] \equiv AB - BA,$$
$$\{A, B\} \equiv AB + BA.$$

We now define the S^2 operator as follows:

$$S^2 = S_x^2 + S_y^2 + S_z^2$$

For spin ½ systems, the S^2 operator is a multiple of the identity operator

$$S^2 = \frac{3}{4}\hbar^2$$

As will be shown in Chapter 3, for spins higher than 1/2, S^2 is no longer a multiple of the identity operator; however, the following relation still holds.

$$[S^2, S_i] = 0$$