## Chapter 5

# The Structure of Quantum Mechanics

In these pages we will outline the basics for the structure of wave mechanics on which Schrodinger and Heisenberg quantum mechanics is based. We will use the wave vector analogy at first to establish the formulation and will go through the rest of the topic smoothly.

The most important items of wave mechanics are

- 1. **The wave function**: it describes the state of the system. Different wave functions describe different states of the system.
  - 2. Uncertainty principle.
  - 3. The probabilities
  - 4. The expectation values

The most important of the structural elements of quantum mechanics are

- 1. The Eigenvalue equation: it is the equation of motion
- 2. The boundary condition
- 3. The commutation relations
- 4. Orthagonality relations
- 5. The expansion postulate

#### I. LINEAR VECTOR SPACES

A linear vector space  $\vartheta$  can be constructed once we define a set of basis (unit vectors)  $\{\mathbf{e}_i\}$  such that any vector  $\mathbf{V}$  can be expanded in term of these bases. This expansion is given by

$$\mathbf{V} = \sum_{i} \mathbf{e}_{i} v_{i} \tag{1}$$

The sum will run over all the allowed values. Obviously the number of values will correspond to the dimensionality of the space.  $v_i$  are the components of  $\mathbf{V}$ .

#### Scalar product

The scalar product of two vectors V and U is defined by

$$\mathbf{V} \cdot \mathbf{U} = VU \cos \theta \tag{2}$$

Note that the scalar product on one vector with another is the projection of one vector onto the other. If the two vectors are represented by areas then the scalar product is the *union* between the two areas.

The basis are always assumed to be orthonormal such that

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} \tag{3}$$

Using the expansion in (1) and the definition of the scalar product (2), and the orthonormality condition 3, the components of V are given by

$$\mathbf{e}_j \cdot \mathbf{V} = \sum_i (\mathbf{e}_j \cdot \mathbf{e}_i) v_i = \sum_i v_i \delta_{ij} = V_j \tag{4}$$

So that

$$V_1 = \mathbf{e}_1 \cdot V$$
,  $V_2 = \mathbf{e}_2 \cdot V$ ,  $V_3 = \mathbf{e}_3 \cdot V$ , .....  $etc$ 

All vectors and basis do satisfy the conditions of linearity.

#### II. WAVEFUNCTIONS AS STATE VECTORS

Wave functions can be treated as *vectors* in an n-dimensional linear vector space whose basis are complex functions of space and time. Customary an infinite-dimensional space of this sort is called *Hilbert space*.

Linear vector spaces of this sort can be constructed once we have a well-defined complete set of basis (state vectors). In order to differentiate these from ordinary vectors we denote a vector by  $|\psi\rangle$  or  $|\phi\rangle$  or  $|\chi\rangle$  and would call it ket-vector. Also we will define the symbols  $\langle\psi|, \langle\phi|$  and  $\langle\chi|$  to be the conjugates of the ket-vectors, and we call them bra-vectors. The relation between the vector and its conjugate is given by

$$\langle \psi | = |\psi \rangle^{\dagger} = (|\psi \rangle^*)^{\top} \tag{5}$$

 $|\psi\rangle$  is called the Hermitian conjugate of  $<\psi|$ .

#### A. Scalar Product

The scalar product of two state vectors  $<\psi|$  and  $<\phi|$  is defined as

$$<\psi|\phi> = <\phi|\psi>^{\dagger}$$
 (6)

## B. The Expansion Postulate

If we have available a complete set of state vectors say  $\{|i\rangle\}$ , and that this set is orthonormal, i.e.,

$$\langle i|j \rangle = \delta_{ij}$$
 (7)

then this set can be used to construct a linear vector space such that any other state vector can be expanded in terms of these basis as

$$|\psi\rangle = \sum_{i} \psi_i |i\rangle \tag{8}$$

where  $\psi_i$  are the components of  $|\psi>$  . To find these components multiply both sides of (7) by < j|

$$\langle j|\psi \rangle = \sum_{i} \langle j|\psi_{i}|i \rangle = \sum_{i} \psi_{i} \langle j|i \rangle = \sum_{i} \psi_{i} \delta_{ji} = \psi_{j}$$
 (9)

so that

$$\psi_i = \langle i|\psi \rangle \tag{10}$$

Substituting (10) in (8) we get

$$|\psi\rangle = \sum_{i} |i\rangle\langle i|\psi\rangle \tag{11}$$

Since  $|\psi\rangle$  is arbitrary, therefore we can write

$$\sum_{i} |i\rangle \langle i| = 1 \tag{12}$$

this is called the completeness condition.

## C. The Eigenvalue equation

The general eigenvalue equation is given by

$$A|\psi\rangle = \alpha|\psi\rangle \tag{13}$$

where A is an operator and  $\alpha$  is the corresponding eigenvalue. The eigenvalue correspond to the value that would be obtained once we perform a measurement of the observable corresponding to the operator in question. The expectation value of many measurements of the effect of the operation A is given by

$$\langle A \rangle = \langle \psi | A | \psi \rangle = \alpha \langle \psi | \psi \rangle$$
 (14)

If the measurement is performed between two different states of  $|\psi\rangle$  say  $|\psi_n\rangle$  and  $|\psi_m\rangle$  the we have

$$<\psi_n|A|\psi_m>=\alpha\delta_{nm}$$
 (15)

The quantities

$$<\psi_n|A|\psi_m> = A_{nm} = \alpha\delta_{nm}$$
 (16)

are called *Matrix Elements* of A.

Equation (13) can be solved both for the eigenvalues  $\alpha$  and for the eigenvectors  $|\psi\rangle$ . This can be easily realized once we know that the operator A is a square matrix and the eigenvectors  $|\psi\rangle$  are column matrix. i.e.,

$$A_{nm} = \begin{pmatrix} A_{11} & A_{12} & . & A_{1m} \\ A_{21} & A_{22} & & & \\ & & . & & \\ A_{n1} & & A_{nn} \end{pmatrix}$$

$$(17)$$

and

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \cdot \\ \cdot \\ \psi_n \end{pmatrix} \tag{18}$$

Obviously  $\langle \psi |$  is a row matrix

$$\langle \psi | = \left( \psi_1^* \dots \psi_n^* \right) \tag{19}$$

So that  $\langle \psi_n | A | \psi_m \rangle$  and is, generally a complex-number and

$$\langle \psi | \psi \rangle = \begin{pmatrix} \psi_1^* \dots \psi_n^* \end{pmatrix} \begin{pmatrix} \psi_1 \\ \vdots \\ \vdots \\ \psi_n \end{pmatrix} = |\psi_1|^2 + \dots + |\psi_n|^2$$

$$(20)$$

Note that

$$<\psi|A|\psi> = < A\dagger\psi|\psi> = <\alpha\psi|\psi> = \alpha^* <\psi|\psi>$$

The eigenvectors contains all the information needed about the system it describes.

Also note that the eigenvalues of the Hamiltonian are always real, since they represent the possible values of the energy. Also this applies to the eigenvalues of the momentum operator.

Now we can then understand the meaning of the expansion coefficients (or components) of  $|\psi\rangle$  better. It is clear that if a measurement on  $|\psi\rangle$  is made then the value of such a measurement would yield one of the eigenvalues. The probability of getting this eigenvalue is  $|\psi_n|^2$ .

$$|\psi_i|^2 = |\langle i|\psi\rangle|^2 \tag{21}$$

Note that once  $|\psi\rangle$  is normalized then we should have the total probability equal 1.

$$<\psi|\psi> = |\psi_1|^2 + \dots + |\psi_n|^2$$
 (22)

So each of the  $|\psi_n|^2$  represent a portion of the total probability to get the specified eigenvalue in a measurement. This is part of the beauty of quantum mechanics

#### III. CONTINUOUS SYSTEMS

The above treatment assumed a discete value for the possible stes of the system, this applies, for example, to the energy states of a bound system. But if the values were continuous then the Hilbert space is an infinite dimensional linear vector space and the formulation will change so that summations will become integrals. The formulation goes as follows:

The scalar product in (6) is then defined by

$$<\psi|\phi> = \int \psi^*\phi dv$$
 (23)

where dv is the volume element and the integral is over all the covered space.

Obviously  $\psi(x)$  is said to square integrable which means that

$$\int_{-\infty}^{\infty} |\psi|^2 dx < \infty$$

The expansion postulate is given by

$$\psi(x) = \int_{-\infty}^{\infty} \phi(p) u_p(x) dp$$

Note that what we called earlier as the wave function in momentum space is really just an expansion coefficient, and with our interpretation, its absolute square  $|\phi(p)|^2 dp$  gives us the probability that a momentum measurement on the system described by  $\psi(x)$  will yield a value in the range (p, p + dp).

The orthonormality relationships for the basis vectors  $u_p(x)$  becomes

$$\int_{-\infty}^{\infty} u_{p_1}(x)u_{p_2}(x)dx = \delta(p_1 - p_2)$$
(24)

where  $\delta(p_1 - p_2)$  is the Dirac delta function.

the expectation value of an operator is

$$\langle A \rangle = \langle \psi | A | \psi \rangle = \int_{-\infty}^{\infty} \psi^*(x) A \psi(x) dx$$
 (25)

If we need to get the probability of obtaining a given state of the system say  $|\psi_1\rangle$  in one certain measurement we have to calculate

$$|\langle \psi_1 | \psi \rangle|^2 = |\int_{-\infty}^{\infty} \psi_1^*(x) \psi(x) dx|^2$$
 (26)

For discrete systems mostly we do not need to calculate the integrals.

## IV. HERMITIAN OPERATORS

If an operator A satisfy the relation

$$<\psi|A|\psi> = <\psi|A^{\dagger}|\psi> =$$
 (27)

then A is called Hermitian operator.

In matrix form

$$(A_{nm}) = (A_{mn}^*)$$

#### 1. Theorem1

Eigenvalues of Hermitian operators must be real.

*Proof:* Let A be a Hermitian operator such that

$$A|\psi>=\alpha|\psi>$$

then according to the definition of the Hermitain operator we must have

$$<\psi|A|\psi> = < A\psi|\psi>$$

that is,

$$<\psi|\alpha|\psi>=\alpha<\psi|\psi>=<\alpha\psi|\psi>=\alpha^*<\psi|\psi>$$

which means that

$$\alpha = \alpha^* \tag{28}$$

that is the eigenvalues are real

## 2. Theorem2

Eigenvectors belonging to the same Hermitian operator but with different eigenvalues must be orthogonal.

*Proof:* Let A be a Hermitian operator, and let  $|\psi_1\rangle$  and  $|\psi_2\rangle$  be two different eigenvectors belonging to A such that

$$A|\psi_1\rangle = \alpha_1|\psi_1\rangle \tag{29}$$

$$A|\psi_2\rangle = \alpha_2|\psi_2\rangle$$

with  $\alpha_1 \neq \alpha_2 \neq 0$ . then since A is assumed to be Hermitian then,

$$<\psi_2|A|\psi_1> = < A\psi_2|\psi_1>$$

This means that

$$\alpha_2 < \psi_2 | \psi_1 > = \alpha_1^* < \psi_2 | \psi_1 > = \alpha_1 < \psi_2 | \psi_1 >$$

which implies that

$$(\alpha_2 - \alpha_1) < \psi_2 | \psi_1 > = 0$$

This means that

$$\langle \psi_2 | \psi_1 \rangle = 0 \tag{30}$$

which implies orthogonality.

## V. SIMULTANEOUS EIGENVECTORS AND DEGENERACY

#### A. Simultaneous Eigenvectors

If an eigenvector belongs to two different operators like A and B, then this eigenvector is said to be simultaneous for A and B. The general condition for this to happen is that both A and B should commute. To see this let  $|u_a\rangle$  be an eigenvector belonging to A and B such that

$$A|u_a\rangle = a|u_a\rangle. \tag{31}$$

$$B|u_a\rangle = b|u_a\rangle.$$

Now

$$AB|u_a> = ab|u_a>$$
  
 $BA|u_a> = ba|u_a> = ab|u_a>$ .

This means that

$$(AB - BA)|u_a> = 0,$$

which means that

$$AB - BA = [A, B] = 0,$$
 (32)

therefore both operators commute.

Conversily if we have two operators A and B such that [A, B] = 0, then we can find an eigenvector that will belong to both A and B simultaneously. This is seen as follows:

If

$$AB|u_a> = aB|u_a>$$

then this means that  $B|u_a>$  is an eigenvector of A therefore we can say it is proportional to  $|u_a>$  say  $b|u_a>$ . So that

$$AB|u_a>=ab|u_a>.$$

## B. Degenerate states

These are different states that belong to the same operator A but with the same eigenvalue, i.e.,

$$A|u_a^{(1)}\rangle = a|u_a^{(1)}\rangle$$

$$A|u_a^{(2)}\rangle = a|u_a^{(2)}\rangle$$
(33)

Now for the operator B we expect that

$$B|u_a^{(1)}\rangle = b_{11}|u_a^{(1)}\rangle + b_{12}|u_a^{(2)}\rangle$$
  
 $B|u_a^{(2)}\rangle = b_{21}|u_a^{(1)}\rangle + b_{22}|u_a^{(2)}\rangle$ 

So that

$$B(|u_a^{(1)}\rangle + \lambda |u_a^{(2)}\rangle) = (b_{11} + \lambda b_{12})|u_a^{(1)}\rangle + (b_{21} + \lambda b_{22})|u_a^{(2)}\rangle$$
$$= b_{\pm}(|u_a^{(1)}\rangle + |u_a^{(2)}\rangle).$$

provided that

$$\lambda = \frac{b_{12} + \lambda b_{22}}{b_{11} + \lambda b_{21}} \tag{34}$$

This is a quadratic equation that one can solve for  $\lambda$  to get  $b_+$  and  $b_-$ .

## C. Uncertainty Relations

The uncertainty of an observable A is defined by

$$(\Delta A)^2 = \langle (A - \langle A \rangle)^2 = \langle A^2 - 2A \langle A \rangle + \langle A \rangle^2 \rangle$$

$$= \langle A^2 \rangle - \langle A \rangle^2$$
(35)

If A and B are two operators such that

$$[A, B] = iC (36)$$

then

$$(\Delta A)^2 (\Delta B)^2 \geqslant \frac{\langle C \rangle^2}{4} \tag{37}$$

Observables obeying the above relationship are called complementary.

Example

We know that

$$[x,p] = i\hbar$$

then

$$(\Delta x)^2 (\Delta p)^2 \geqslant \frac{\hbar^2}{4} \tag{38}$$

x and p are called *complementary observables*.

## VI. TIME DEPENDENCE AND THE CLASSICAL LIMIT

The time-dependent expectation value of an operator A is given by

$$\langle A \rangle_t = \langle \psi | A | \psi \rangle$$
 (39)

and

$$\frac{d}{dt} \langle A \rangle_{t} = \frac{i}{\hbar} \langle H\psi | A | \psi \rangle + \langle \frac{dA}{dt} \rangle - \frac{i}{\hbar} \langle \psi | AH | \psi \rangle$$
$$= \langle \frac{dA}{dt} \rangle + \frac{i}{\hbar} \langle \psi | [H, A] | \psi \rangle$$

If A itself is time-independent, then

$$\frac{d}{dt} \langle A \rangle_t = \frac{i}{\hbar} \langle \psi | [H, A] | \psi \rangle \tag{40}$$

where H is the Hamiltonian operator given by

$$H = \frac{p^2}{2m} + V(x) \tag{41}$$

Equation (40) is normaly called the Equation of Motion.

Examples:

Take A = x

Show that

$$\frac{d}{dt} \langle x \rangle = \langle \frac{P}{m} \rangle \tag{42}$$

Take A = p

Show that

$$\frac{d}{dt} = -\langle \frac{dV(x)}{dx} \tag{43}$$

So that from (42) and (43) we get

$$m\frac{d^2 < x >}{dt^2} = -\langle \frac{dV(x)}{dx} \rangle \tag{44}$$

This is similar to the classical equation of motion.

We cannot claim that

$$\langle x \rangle = x_{cl}$$

because

$$\langle \frac{dV}{dx} \rangle \neq \frac{d}{d < x >} V(< x >)$$

Only in case that V(x) is a very slowly varying function of x that we can make such approximation.

## VII. SOLUTION OF THE EIGENVALUE EQUATION

Now that we have understood that A is a square matrix, then by (15) it is clearly realized that we can solve for the eigenvalues of A through solving the secular equation

$$\det |A_{mn} - \alpha \delta_{mn}| = 0 \tag{45}$$

from this equation we should obtain enough number of algebraic equations that would be solved to find the different eigenvalues. Then we can substitute these eigenvalues in the matrix representation of A and operate on  $|\psi\rangle$  assuming that, for example

$$|\psi\rangle = \begin{pmatrix} a \\ b \\ . \\ . \\ g \end{pmatrix} \tag{46}$$

and then solve for  $a, b, \dots, g$ , to find the different eigenvalues.

## VIII. CHANGE OF BASIS AND THE UNITARY TRANSFORMATION

A state vector  $|\psi\rangle$  that is expanded in a Hilbert space having complete set of basis  $|i\rangle$  can be also expanded in another set of basis say  $|i'\rangle$  such

$$|\psi>=\sum_{i}|i\rangle >\psi_{n}'$$

where

$$\psi_n = \langle i' | \psi \rangle$$

The relation between |i> and |i|'> is given by

$$|i\>'>=U^\dagger|i>$$

Such a transformation is called Unitary (or Similarity) transformation where U is a unitary matrix satisfying

$$U^{\dagger}U = I$$

The expansion in another basis can be used to diagonalize a given matrix. This is useful when calculationg the eigenvalues for a given Hamiltonian. If the Hamiltonian matrix is diagonal then we can take the diagonal elements as eigenvalues. But if the matrix is not diagonal we can diagonalize it using the unitary matrix U by constructing

$$H^{'}=U^{\dagger}HU$$

The method to construct U is to take the column eigenvectors for H and set them as a square matrix. This will be shown toward the end of the following example.

# Example

Given that

$$M = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{47}$$

Find the eigenvalues and the normalized eigenvectors of M. Solution

$$M |\psi> = \lambda |\psi>$$

In matrix form

$$\begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = \lambda \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix}$$

The secular equation is

$$\det \begin{pmatrix} -\lambda & -i & 0 \\ i & -\lambda & 0 \\ 0 & 0 & -\lambda \end{pmatrix} = 0$$

This gives

$$-\lambda \begin{vmatrix} -\lambda & 0 \\ 0 & -\lambda \end{vmatrix} - (-i) \begin{vmatrix} i & 0 \\ 0 & -\lambda \end{vmatrix} + 0 = 0 \implies -\lambda^3 + \lambda = 0 \implies \lambda^2 - 1 = 0 \implies \lambda = \pm 1 \text{ and } \lambda = 0$$

The corresponding Eigenvectors can be obtained by substituting for each of these eigenvalues.

For  $\lambda = 1$ :

$$\begin{pmatrix} -1 & -i & 0 \\ i & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = 0$$

This matrix equation gives

$$-\psi_1 - i\psi_2 = 0$$
$$i\psi_1 - \psi_2 = 0$$
$$\psi_3 = 0$$

If we assume that  $\psi_1 = 1$ , then  $\psi_2 = i$  and  $\psi_3 = 0$ . The eigenvector will be then

$$|u_1>=c_1\begin{pmatrix}1\\i\\0\end{pmatrix}$$

 $c_1$  is a normalization constant. Normalization means that

$$< u_1 | u_1 > = 1 \implies c_1^* c_1 \left( 1 - i \ 0 \right) \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix} = 1 \implies |c_1|^2 = \frac{1}{2} \implies c_1 = \frac{1}{\sqrt{2}}$$

Therefore

$$|u_1> = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\i\\0 \end{pmatrix}$$

For  $\lambda = 0$ :

$$\begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = 0$$

This matrix equation gives

$$-i\psi_2 = 0$$
$$i\psi_1 = 0$$
$$\psi_3 = 1$$

so that

$$|u_2>=c_2\begin{pmatrix}0\\0\\1\end{pmatrix}$$

to find  $c_2$ 

$$< u_2 | u_2 > = 1 \implies c_2^* c_2 \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 1 \implies |c_2|^2 = 1 \implies c_2 = 1$$

For  $\lambda = -1$ :

$$\begin{pmatrix} 1 & -i & 0 \\ i & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = 0$$

This matrix equation gives

$$\psi_1 - i\psi_2 = 0$$
$$i\psi_1 + \psi_2 = 0$$
$$\psi_3 = 0$$

so that

$$|u_3>=c_3\begin{pmatrix}1\\-i\\0\end{pmatrix}$$

It is easy to see that  $c_3 = \frac{1}{\sqrt{2}}$  so that

$$|u_3> = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\ -i\\ 0 \end{pmatrix}$$

In order to diagonal the matrix M we construct first the unitary matrix U

$$U = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & 0 & \frac{-i}{\sqrt{2}} \\ 0 & 1 & 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ i & 0 & -i \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

The conjugate matrix is

$$U^{\dagger} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & i & 0 \end{pmatrix}$$

It is clear that

$$U \ ^{\dagger}U = \left( \begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right)$$

Now the new matrix is

$$\begin{split} M &' = U^{\dagger} M U \\ &= \frac{1}{2} \begin{pmatrix} 1 & -i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & i & 0 \end{pmatrix} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 1 \\ i & 0 & -i \\ 0 & \sqrt{2} & 0 \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \end{split}$$

This complete the solution.