FORMULATION OF QUANTUM MECHANICS

Gautam Kumar

Assistant Teacher, Govt. of Bihar.

Abstract : The paper proposes to study the mathematical formulation of quantum mechanics. The foundations of quantum mechanics are concerned more or less with Hilbert space; the theory of which furnishes the mathematical by ground for the application of lattice theory in quantum. The main concepts of states, observables and propositions in quantum mechanical formalism, three approaches to quantum mechanics have evolved – (i) the basic notions of states and observables; (ii) takes the observables as the basic concept, and (iii) draws it authority directly from experiment. This paper is devoted to the study of the first two formulations of quantum mechanics and to show that the latter, both from foundational as well as technical point of view, is preferable to the former.

Keywords : Hilbert space, Abstruct lattice, Entity, Quantum mechanics, Orthocomplementation.

0. Introduction

The paper proposes to study the mathematical formulation of quantum mechanics. Several models to describe a quantum system have been introduced so for but it was never claimed to be unique although more than hundred research papers have been written and also there are several books related to this subject. The foundations of quantum mechanics are concerned more or less with Hilbert space; the theory of which furnishes the mathematical by ground for the application of lattice theory in quantum. Antoine, J. P. [1] and Maderid, R. de la [16] who studied quantum mechanics beyond Hilbert space have had to be considered Rigged Hilbert space instead of Hilbert space.

Considering the main concepts of states, observables and propositions in quantum mechanical formalism, three approaches to quantum mechanics have evolved. The first approach due to Dirac [8], Jordan, Neumann and Wigner [14] takes the basic notions of states and observables; the second due to Segal [19-21] alone takes the observables as the basic concept, whereas the third due to von Neumann [5, 25], Birkhoff and von Neumann [6], Birkhoff [5], Mackey [15], Varadrajan [23, 24], Srinivas [22], Gudder [11, 12], Ferroer [10], Gleason [11], Barbara [2, 3], Boris Ischi [7], Navara [17], Randall and Foulis [18], Bell [4], Dirk Aerts [9] and others.

This paper is devoted to the study of the first two formulations of quantum mechanics and to show that the latter, both from foundational as well as technical point of view, is preferable to the former. Let us begin with the classical postulates for quantum mechanics mainly due to Dirac [8].

Postulate 1.2.1. Each eigenstate of a quantum system at any particular time is represented by a state function Ψ_α or by a ket vector $|\alpha\rangle$, which may be looked upon as a ray in a complex Hilbert space. Any given state can always be represented as a linear combination of eigenstates of the system. A ket vector corresponding to a state as well as its multiple represents the some state. The hermitian adjoint of Ψ_α or of $|\alpha\rangle$ corresponds to $\Psi_\alpha^\uparrow$ or a bra vector $\langle\alpha|$. The inner product of two state vectors is written as :

$$\Psi_\alpha^\uparrow\Psi_\beta = \int \Psi_\alpha^*(r)\Psi_\beta(r)d^3r = \langle\alpha|\beta\rangle;\quad \text{where } \Psi^*(r) \tag{1.1}$$

denotes the complex conjugate of $\Psi_\alpha(r)$.

$$\begin{aligned}(\Psi_\alpha^\uparrow\Psi_\beta)^* &= \int(\Psi_\alpha^*(r)\Psi_\beta(r))^* d^3r \\ &= \int(\Psi_\beta^*(r)\Psi_\alpha(r))^* d^3r \\ &= \Psi_\beta^\uparrow\psi_\alpha = \langle\beta|\alpha\rangle.\end{aligned} \tag{1.2}$$

If $|\alpha\rangle$ is a representative of a state, then its normalization conditions can be expressed as:

$$\langle\alpha|\alpha\rangle = 1 \text{ and } \langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*, \tag{1.3}$$

where $\langle\beta|\alpha\rangle^*$ denotes the complex conjugate of $\langle\beta|\alpha\rangle$; and the condition of orthogonality of $\langle\alpha|$ and $|\beta\rangle$ or of $|\alpha\rangle$ and $|\beta\rangle$ or of $\langle\alpha|$ and $|\beta\rangle$ can be expressed by relation:

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

An operator $\chi = ||\chi_{\alpha\beta}||$ is defined on a set of kets as will as on that of bras by setting:

$$\chi\,\Psi_\beta = \chi\,|\beta\rangle = |\beta'\rangle = \Psi_{\beta'}; \tag{1.5}$$

$$\Psi_\alpha^\uparrow\chi = \langle\alpha|\chi = \langle\chi^\uparrow\alpha| = (\chi^\uparrow\Psi_\alpha)^\uparrow = \langle\alpha''|, \tag{1.6}$$

where the matrix element $\chi_{\alpha\beta}$ associated between two states $\langle\alpha|$ and $|\beta\rangle$ is giving by in any of the three equivalent form:

$$\begin{aligned}\chi_{\alpha\beta} &= \Psi_\alpha^\uparrow\chi\Psi_\beta \\ &= \int\Psi_\alpha^*(r)(\chi\Psi_\beta(r))d^3r \\ &= \langle\alpha|\beta\rangle && (I) \\ &= \int(\chi^\uparrow\Psi_\alpha(r)^*\Psi_\beta(r)d^3r \\ &= \int\Psi_\alpha^*(r)\Psi_\beta(r)d^3r \\ &= \langle\alpha''|\beta\rangle && (II) \\ &= \langle\alpha|\chi|\beta\rangle && (III)\end{aligned} \tag{1.7}$$

of which $\langle\alpha|\chi|\beta\rangle$ is the most commonly used notation.

The matrix element $\chi_{\alpha\beta}^\uparrow$ of the hermitian adjoint operator $\chi^\uparrow$ is given by:

$$\chi_{\alpha\beta}^\uparrow = \langle\alpha|\chi|\beta\rangle = \langle\alpha|\chi|\beta\rangle^* = \langle\beta|\chi|\alpha\rangle. \tag{1.8}$$

The inner product $\langle\alpha|\beta\rangle$ of bra $\langle\alpha|$ and ket $|\beta\rangle$ can easily be seen to satisfy the following conditions:

$$\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*. \tag{1.9}$$

$$\begin{aligned}&\text{(a) } \langle\alpha|\lambda_1\beta_1 + \lambda_2\beta_2\rangle = \lambda_1\langle\alpha|\beta_1\rangle + \lambda_2\langle\alpha|\beta_2\rangle \\ &\text{(b) } \langle\lambda_1\alpha_1 + \lambda_2\alpha_2|\beta\rangle = \lambda_1^*\langle\alpha_1|\beta\rangle + \lambda_2^*\langle\alpha_2|\beta\rangle;\end{aligned} \tag{1.10}$$

where $\lambda_i^*(i=1,2)$ is the complex conjugate of λ_i

$$\langle\alpha|\alpha\rangle \geq 0 \tag{1.11}$$

$$\langle\alpha|\beta\rangle = 0 \text{ for all } \beta \text{ iff } <\alpha| = 0 \tag{1.12}$$

It follows from the superposition principal that the system of states of a quantum system form a linear manifold which with the above four conditions is a complex Hilbert space. This is the fundamental principle of the quantum mechanics.

Postulate 1.2.2. An observable (i.e. measurable property) of a quantum system corresponds to a self–adjoint (or hermitian) operator $\chi = \chi^{\uparrow}$ with a complete set of orthonormal eigenkets and real eigen values χ', i.e.,

$$\chi|\chi'\rangle = \chi'|\chi'\rangle\,; \tag{1.13}$$

$$\chi'|\chi''\rangle = \delta\,\chi'|\chi''\rangle\,; \tag{1.14}$$

$$\sum_{\chi'}\chi'\rangle|\langle\chi'| = | \tag{1.15}$$

where the symbol δ is to be understood as the Kronecker symbol if χ' and χ'' lie in the discrete spectrum and the Dirac delta function $\delta(\chi'-\chi'')$ if either or both lie in the continuous spectrum. Similarly the summation in the completeness relation (equation (1.15)) is to be regarded as an integration over the continuous spectrum.

It can be easily shown that the collection of all self–adjoint operators on a Hilbert space form a real Banach space which can be partially ordered. As a matter of fact this collection is about as far being a lattice as a partially ordered set can be, for it can be shown that two operators in the set have a infimum iff they are comparable. This whole situation is intimately related to the quantum of commutatively for the algebra of operators and is too complicated for us to explore here.

Postulate 1.2.3. If the measurement is performed on a system to determine the value of the observable χ, the probability of finding the system, described by the state vector $|\alpha\rangle$, to have χ with eigen value χ' is given by

$$|\langle\chi'|\alpha\rangle|^2$$

In other words, $\langle\chi'|\alpha\rangle$ is the probability amplitude of observing the value χ'.

If a system is in the state defined by one of the eigenkets say $|\alpha\rangle$, of a self adjoint operator χ and not in any other state defined by any ket then the state is a pure state and the probability of finding the system in that state is one similarly, if the system is in the another state defined by another ket $|\beta\rangle$ and not in any other state, then it is in the pure state. If the system is described by a number of kets with different probabilities, then the system is in the mixed state.

Postulate 1.2.4. The position and momenta operators of a quantum particle obey the following rule :

$$[q_i, p_j] = i\hbar\delta ij \ \ (i, j = 1,2,3) \tag{1.16}$$

where q and p are cononical co-ordinates and momenta; the symbol [,] is to be understood as Poisson bracket; ђ, the Planck constant and δij, the Kronecker delta.

All the previous postulates are concerned with relations between states and observables of a quantum mechanical system at a given instant of time, i.e. they are the postulates of quantum static. Therefore to get complete theory we must consider the connection between different instants of time leading to quantum dynamics.

Postulate 1.2.5. The dynamical beheviour of a quantum system is described by the Schrödinger equation

$$\frac{1}{i}\hbar\frac{\partial}{\partial t}|\alpha_s(t)\rangle + H|\alpha_s(t)\rangle = 0 \tag{1.17}$$

where the subscript identifies the Schrödinger picture [8, p. 111] according to which it varies in time in conformity with the above differential equation and H, the Hamiltonian operator of the system, corresponds to the translation operator of the system, corresponds to the translation operator for infinitesimal time translations. By this is meant the following :

Suppose the time evaluation of the state vector can be obtained by thy action of an operation $\chi(t,t_0)$ on the initial state $|\alpha_s(t_0)\rangle$ such that

$$|\alpha_s(t)\rangle = \chi(t,t_0)|\alpha_s(t_0)\rangle; \tag{1.18}$$

$$\chi(t,t_0) = 1 \tag{1.19}$$

Conversation of probability requires that the norm vector $|\alpha_s(t)\rangle$ be constant in time :

$$\begin{aligned}\langle\alpha_s(t)|\alpha_s(t)\rangle &= \langle\alpha_s(t_0)|\alpha_s(t_0)\rangle \\ &= \langle\alpha_s(t_0)|\chi^{\uparrow}(t,t_0)\chi(t,t_0)|\alpha_s(t_0)\rangle;\end{aligned} \tag{1.20}$$

and therefore

$$\chi^{\uparrow}(t,t_0)\chi(t,t_0) = 1 \tag{1.21}$$

This dose not yet guarantee that χ is unitary. For this to be the case, the following equation must hold :

$$\chi(t,t_0)\chi^{\uparrow}(t,t_0) = 1 \tag{1.22}$$

This condition will hold of χ satisfies the group property :

$$\chi(t,t_1)\chi(t_1,t_0) = \chi(t,t_0) \tag{1.23}$$

If, in the above equation, we set $t = t_0$ and assume its validity for $t_0 < t_1$, we then obtain

$$\chi(t_0,t_1)\chi(t_1,t_0) = 1 \quad (1.24)$$

whence $$\chi(t_0,t_1) = \chi^{-1}(t_1,t_0) \quad (1.25)$$

Multiplying (1.24) on left by $\chi^{\uparrow}$ and using (1.21), we have

$$\chi(t_1,t_0) = \chi(t_0,t_1) = \chi^{-1}(t_1,t_0) \quad (1.26)$$

Hence χ is unitary.

If we let t be infinitesimal close to t_0 with $t - t_0 = \delta t$, then to first order in δt, we may write

$$\chi(t_0+\delta t,t_0) = 1 - \frac{i}{\hbar}H\delta t \quad (1.27)$$

In order that χ be unitary, H must be Hamiltonian. The dimension of H is that of an energy. Equation (1.18) for infinitesimal case thus reads

$$|\alpha_s(t_0+\delta t)\rangle - |\alpha_s(t_0)\rangle = -\frac{i}{\hbar}H\delta t|\alpha_s(t_0)\rangle \quad (1.28)$$

which in limit $\delta t \to 0$ becomes the equitation (1.17), since by definition

$$\lim_{\delta t\to 0}(\delta t)^{-1}\left(|\alpha_s(t+\partial t)\rangle - |\alpha_s(t)\rangle\right) = \frac{\partial}{\partial t}|\alpha_s(t)\rangle \quad (1.29)$$

These postulates of quantum mechanics are effective only in the case of the system of a finite number of degrees of freedom. Moreover, they involve the concepts of states and observables separately, where as in quantum mechanics, it appears mathematically as well as physically that observables play a fundamental role. Observables are considered to behave as self-adjoint operators on a Hilbert space, which are not necessarily bounded, in which simple algebraic operations on non-cummulative self-adjoint operators together with various possibilities for treating unbounded in terms of bounded operators strongly suggests the limitation to bounded ones. Considering the above mentioned facts Segal [19, 20] has studied a closed system of observables $\mathcal{U}$ isomorphic to the system of all bounded self-adjoint operators on a Hilbert space for describing a quantum mechanical system for its secureness. In this connection he propounded the following postulates :

A closed system of bounded observables $\mathcal{U}$ is a quantum mechanical system if it is a real Banach space in which squares exist and which satisfies :

(i) $\|X^2\| = \|X\|^2$ for all $X \in \mathcal{U}$

(ii) X^2 is a continuous function of X.

(iii) $\|X^2 - X^2\| \le \max [\|X^2\|, \|Y^2\|]$

Form an empirical point of view, a state exists only as a rule which assigns to each bounded observable its expectation value in the state. A state of $\mathcal{U}$ is defined as a real valued function m on $\mathcal{U}$ such that

(iv) $m(X + Y) = m(X) + m(Y)$

$m(\lambda X) = \lambda m(X)$, for real λ

(v) $m(X^2) \ge 0$

(vi) $m(I) = 0$, where I is the unit observable.

Thus a state must be some observable sort of normalised positive linear functional on the observables. A pure state is one which is not a linear combination with positive co-efficients of two states, on the other hands, if it is so, this state is called mixed state. In the state m, $m(X)$ is called the expectation value of m. A collection of states of $\mathcal{U}$ is full if for every two observables there is a state in the collection in which the observables have different expectation values. For any two observables X and Y the pseudo-product $X \circ Y$ is defined by the equation

(vii) $X \circ Y = \frac{1}{4}[(X+Y)^2 - (X-Y)^2]$

If the pseudo-product satisfies the following laws for all $x, y, z \in \mathcal{U}$ and for any real number λ

(viii) $(X \circ Y)\circ Z = X \circ (Y \circ Z)$

(ix) $(X+Y)\circ Z = X\circ Z + Y\circ Z$

(x) $(\lambda X)\circ Y = \lambda(X \circ Y)$

then $\mathcal{U}$ is said to be commutative system.

An observable of $\mathcal{U}$ is called non-negative if it is a sum of squares and if for any two observables X and Y, $X - Y$ is non-negative, then X is said to greater then Y and is written as $X \ge Y$. It can be easily seen that with this ordering the system can be partially ordered but, in general, it can't be a lattice relative to the partial ordering [19].

Let B_C be a collection of commutative observables in $\mathcal{U}$ and B_g, a system generated by the elements of B_C. Then it can be shown that B_g is isomorphic to the system of all real valued continuous functions on a compact Hausdorff space X_C. The spectral value of an observable are the values of the function corresponding to the observable in the isomorphism. Moreover it follows that for any arbitrary state m there exists a regular probability measure μ on X_C such that

(xi) $m(x) = \int_{\chi_C} X(\delta)\, d\mu(\delta), \quad x \in B_g.$

where $X(\delta)$ is a function on X_C corresponding to X. Hence the condition that a set of observables will be in a given set of real numbers is given by the probability. That an observables X lies in a Borel set E of real numbers for all X in the subset B_{C_1} of B_C is $\mu(\Delta)$, where $\mu(\Delta) = \bigcap_{X\in B_{C_1}} X_X$ and $X_X = \{\delta : X(\delta) \in E\}$.

Here either E is closed or B_{C_1} is countable.

The notion of simultaneous measurability of observables is introduced with the help of their definite values.

An observable X is said to have a definite value in a state m if any of the following equivalent conditions is satisfied :

(xii) the spectral values of X about its expectation values is zero.
(xiii) m is pure on the subsystem generated by X
(xiv) $m(X^2) = (m(X))^2$

A collection of observables is simultaneously measurable if the system which they generate has a full set of states in each of which every observable in B_C has a definite value. It is easy to see that a collection of observables is simultaneously measurable iff it is commutative. This fact establishes a coincidence of simultaneous measurability with commutatively.

On the strength of these postulates, all of the physically plausible and conventionally accepted principle of quantum phenomenology may be established. The proofs are based on the familiar results and method of abstruct analysis.

We have seen that Segal [19-21] has considered a non-commutative structure of bounded observables rather than lattice structure. Such a structure is then equipped with a linear functional which is interpreted as expectation value; but the connection with the lattice theory is then lost.

The connecting link between the lattice and the observables and their expectation values can be established explicitly by important theorem of Gleason [11] only for conventional quantum mechanics.

References

[1] Antonine, J. P. (1966) : Quantum Mechanics beyond Hilbert Space, Springer-Verlag, Berlin, ISBN 3-540-64305-2.
[2] Barbara, J. (1972) : J. of Sym Logic, Vol. 37, 642-645.
[3] ——— (1973) : Indiana Univ. Math. Journal, Vol. 23, 369-376.
[4] Bell, J. L (1986) : Brit. J. Phil. Sci. Vol. 37, 83-99 (Printed in Great Britain).
[5] Birkhoff, G. (1961) : Proc. Sym. in Pure Math., Vol. II, Amer. Math. Soc., 155-184.
[6] Birkhoff, G. and von Neumann, J. (1936) : Ann. of Math., Vol. 37, 823-843.
[7] Boris, Ischi (2004) : Orthocomplementation and Compound System : Proceedings of QSA. Conference, Denver, 2004.
[8] Dirac, P. A. M. (1958) : The Principle of Quantum Mechanicas, Oxford Univ. Press, London.
[9] Dirk, Aerts (1982) : Foundation of Physics, Vol. 12, No. 12, 1131-1170.
[10] Ferrier, P. (1959) : Logical Structure of Physical Theories, Proc. Int. Sym. Axiomatic Method, Amsterdam, 376-389.
[11] Gleason, A. M. (1957) : J. of Math. Mach., Vol. 6, 885-895.
[12] Gudder, S.P. (1967) : J. Math. Anal. Appl., Vol. 20, 1848-1858.
[13] ——— (1970): Axomatic Quantum Mechanics and Generalised Probability Theory. Probabilitic Methods in Applied Mathematics, Edited by Barucha-Reid, A.T., Acad. Press, New York, Vol. 2.
[14] Jordon, P.; von Neumann, J. and Wigner, E. (1974) : Annals of Math., Vol. 33, 29-64.
[15] Mackey G. M. (1963) : Mathematical Foundation of Quantum Mechanics, Bengamin, New York.
[16] Madrid, R. de la (2005) : Eur. J. Phy., 26, 287, Quant. Ph/0502053.
[17] Navara, M. (2008) : Int. J. Theoret. Phys., 47, No. 1, 36-43.
[18] Randall, C. H. and Foulis, D. J. (1970) : An Approach to Empirical Logic, Amer. Math. Monthly, Vol. 1970, 363-374.
[19] Sagal, J. E. (1947) : Ann. of Math, Vol. 48, 930-948.
[20] ——— (1959) : Proc. Int. Sym. Axiomatic Method, 341-352.
[21] ——— (1963) : Mathematical Problems of Relativistic Physics, Amer. Math. Soc. Providence.
[22] Srinivas, M. D. (1975) : J. of Math. Phy. Vol. 16, 1672-1685.
[23] Varadarajan, V. S. (1962) : Comm. Pure Appl. Math., Vol. 15, 189 -217.
[24] ——— (1968) : Geometry of Quantum Theory. D. Van Nastrand Company, INC, Princeton, New Jersey, Toronto, London, Melbourne, Volume I.
[25] von Neumann, J. (1949) : Annals of Mathematics, 50, 401-485.