

Physical and mathematical aspects of quantum theory and the wave function

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Introduction

Quantum mechanics plays a prominent role in modern physics. The development of the quantum theory has had a revolutionary impact on our concepts of the microscopic structure and behavior of matter as well as the fields of chemistry, engineering, and biology.

The basic tool of quantum mechanics is the wave function. The wave function may be visualized as the carrier by means of which the essence of the experimental evidence is conveyed to the human mind or, for that matter, the analytical probe by which the human mind tries to approach the truth of the microcosmos.

In view of the broad scope of quantum mechanics, it is essential to examine the first principles on which the theory is based and to fully understand the meaning of the wave function both from the physical and mathematical standpoints.

This communication is an attempt to summarize the «commonly accepted» interpretation of quantum mechanics and the wave function. By «commonly accepted» one characterizes the interpretation given by the Copenhagen School.

First a historical account of the evolution of quantum mechanics is presented. Then the interpretation of quantum mechanics proposed by the Copenhagen School is discussed and compared to counter proposals that have been suggested by other physicists. A brief outline of some criticisms of quantum theory are included.

The paper is concluded with a restatement of the assumptions on which the derivation of the wave function is based and the adequacy of these assumptions is clarified by an illustrative example.

Throughout the presentation the reader is presumed to have a general knowledge of quantum mechanics.

The evolution of quantum mechanics

The nineteenth century may be considered as the culmination of our understanding of the large scale behavior of matter. During that century, Newtonian mechanics was completed, the electromagnetic theory was formulated and the sciences of thermodynamics and statistical mechanics developed. All the theories were based on the notions of continuum and causality and

many physicists believed that the formalism was so powerful that it had revealed all the laws of nature.

However, at the turn of the century, many experimental observations could not be explained by classical physics and the need for new concepts became imperative. The successful justification of the black body radiation spectrum by Planck (1) in 1900 and the photoelectric effect by Einstein (2) in 1905 through use of the notion of quantized electromagnetic radiation are two cases in point.

Furthermore, the failure of classical physics to account for atomic phenomena was even more accentuated by Rutherford's discovery of the atomic nucleus (3) in 1911 and the work of Frank and Hertz on excitation spectra (4) in 1914. All these experiments involved a denunciation of causality and continuum and indicated the necessity for a probabilistic theory.

In 1917 Einstein showed in one of his famous papers (5) that the postulates which were being suggested in the field of atomic structure were consistent with Planck's theory of thermal radiation. He developed statistical laws regarding the occurrence of radiative transitions and he indicated that causality could be completely ignored.

It is interesting to diverge for a moment and refer to some of Einstein's thoughts on the theories that he himself inspired and developed. He said: «The features of the elementary processes would seem to make the development of quantum treatment of radiation unavoidable. The weakness of the theory lies in the fact that, on the one hand, no closer connection with wave concepts is obtainable and that, on the other hand, it leaves to chance the time and direction of the elementary processes; nevertheless, I have full confidence in the reliability of the way entered upon» (5). These thoughts are important because they represent Einstein's reluctant attitude about admitting the failure of classical physics in the realm of the microcosmos; an attitude that he never changed until he passed away.

However, in spite of Einstein's reluctance, in the following years the yet unformulated quantum theory was gaining more and more momentum while the insufficiency of classical physics increased at a faster rate. The Stern-Gerlach experiment (6) in 1922 on the measurement of angular momenta aroused the interest of many physicists and greatly supported the idea of stationary atomic states and the quantum interpretation of the Zeeman effect developed

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by Sommerfeld (7). Also the Compton electron scattering experiment (8) presented in 1923 afforded a most direct proof based on Einstein's views regarding the quantized transfer of energy and momentum. On the contrary, both experiments created unsurmountable conceptual difficulties when viewed from the standpoint of classical electromagnetic theory or of corpuscular collisions, respectively.

The first attempt to clarify the controversies and to formulate a sound and consistent theoretical frame of reference was made by Louis de Broglie (9) who recognized that the wave-particle duality should not be confined to radiations but should also be extended to material particles as well. De Broglie's idea was proved experimentally a few years later by Davisson and Germer (10) but Einstein recognized immediately its connection with the work of Bohr, Kramers, and Slater (11) on thermal radiations and on gases in the degenerate state.

The new line of thought was successfully pursued by Schrödinger (12) in 1926. He developed a wave equation whose solutions could adequately represent the stationary states of the electronic structure of atoms.

Thus, the creation of the mathematical formalism of the quantum theory was initiated even though the physical significance of the formalism was very obscure. In fact, the horizon of the new theory was so unclear that Schrödinger himself was not aware of the implications of the wave equation. He did not realize that he was dealing with phenomena which were basically discontinuous in nature and entirely outside the realm of the cause-effect line of thinking of classical physics. Characteristic of Schrödinger's attitude is a conversation that he and Bohr had in Copenhagen in 1926. Said Schrödinger: «If we are to stick to this damned quantum jumping, I regret that I ever had anything to do with it». To which Bohr replied: «But the rest of us are thankful that you did, because you have contributed so much to the clarification of the quantum theory» (13).

Nevertheless, the wave equation introduced a new viewpoint and a new element of simplicity into the quantum theory which had to be incorporated into its interpretation. The Copenhagen School undertook the task of unification of all the scattered suggestions and the physical interpretation of the formalism.

The principles of quantum mechanics

The months which followed the development of the wave equation by Schrödinger were a period of intensive work in Copenhagen. The outcome of this work is the orthodox formulation and interpretation of quantum theory.

During this period, Heisenberg was trying

to develop a formalism by means of which one could go from a given experimental observation to its analytical equivalent. The basic hypothesis behind his efforts was that all atomic phenomena must be pictured in a Hilbert space and vice versa: that is, only those states which can be represented by vectors in a Hilbert space can occur in Nature or be realized experimentally.

For the derivation of the mathematical scheme of quantum theory, Heisenberg (14) used two sources. The first was the experimental evidence which brought classical physics to a stall. The second was Bohr's correspondence principle.

That the theory should be consistent with the accumulated experimental evidence is self-explanatory. The correspondence principle on the other hand postulates a detailed analogy between the quantum theory and the classical theory appropriate to the mental picture employed. «This analogy does not merely serve as a guide to the discovery of formal laws; its special value is that it furnishes the interpretation of the laws that are found in terms of the mental picture used» to quote Heisenberg himself (14). In simpler terms, Bohr's correspondence principle states that the motion of a system as described by quantum mechanics and by classical mechanics must agree in the limit in which Planck's constant, h , can be neglected. That is, if the system is large enough and the demand for accurate measurement is not too rigid, classical mechanics should furnish a good approximation to the motion of the system.

In Heisenberg's formalism all the kinematic and dynamic variables of classical mechanics are replaced by symbols subjected to a non-commutative algebra. The symbols are matrices with elements referring to transitions between stationary states. Furthermore Hamilton's canonical equations are kept unaltered and Planck's constant enters only in the rules of commutation. In particular, the non-commutant is:

$$qp - pq = \frac{\hbar}{i} \quad \hbar = \frac{h}{2\pi}$$

and holds for any set of conjugate variables, q and p .

A peculiarity of Heisenberg's formalism is that the knowledge obtainable about the state of an atomic system always involves an «indeterminacy». For example, an experiment, which leads to the determination of the position of an electron, destroys all information about the momentum of this electron. This indeterminacy is the consequence of the non-commutative relationship between conjugate variables as pointed out by Heisenberg (15). In fact, the non-commutant can also be expressed in the form of the uncertainty principle:

$$\Delta q \Delta p \geq \hbar$$

The actual meaning of the uncertainty prin-

ciple was really clarified by Bohr (16) in 1928 when he introduced the complementarity principle. Bohr indicated that even though classical physics cannot explain atomic phenomena, the account of all experimental evidence must be expressed in classical terms. More specifically, in order to describe a particular experiment and certain observations, one has to use non-ambiguous language with the appropriate application of the terminology of classical physics. This implies the impossibility of any sharp separation between the behavior of an atomic object and its interaction with the measuring instruments which serve to define the conditions under which the phenomena appear. Consequently, evidence obtained under different experimental conditions cannot be comprehended within a single picture but must be regarded as complementary. Complementarity is used here in the sense that only the totality of the phenomena exhausts the possible information about the objects.

It is exactly this aspect of experimentation which involves ambiguity in ascribing conventional physical attributes to atomic objects. Such ambiguity should by no means be interpreted as an inherent property of Nature but rather be attributed to the combined observer-object content of the physical theory which, in the case at hand, is man-nature. In the light of this interpretation it can be ascertained that there is no ambiguity or uncertainty if one talks about a phenomenon and the conditions under which it was observed rather than the totality of physical phenomena.

In summary, the orthodox quantum theory is based on the correspondence and complementarity principles and is justified by experimental observations about atomic phenomena. The far-reaching implications of the theory are further exemplified by Jordan, Klein, and Wigner (17) who showed that Schrödinger's three dimensional material waves can be quantized and incorporated into the Hilbert space formalism of Heisenberg. This proof is essential because it emphasizes the equivalence of the wave and particle pictures of the microcosmos on mathematically rigorous grounds. It is needless to repeat that this does not mean either picture is the «true» picture, even though both are indispensable.

Of course the new quantum theory was not accepted unanimously. Several criticisms were raised and a brief account of the most serious objections follows.

Criticisms of quantum theory

The critics of the Copenhagen School interpretation of quantum theory may be divided into three groups.

The first and larger group agrees with the content of the quantum theory proposed by the Copenhagen School but disagrees with the language which is used. Alexandrow (18), Blochinzew (19), Bohm (20), Bopp (21), de Broglie (22), Fenyés (23), and Weizel (24) belong to this group.

The second group attempts to alter the quantum theory. The suggested counter proposals agree only on certain points with the results of the Copenhagen School. The best effort of the group is represented by Janossy (25).

The third group expresses its general dissatisfaction with quantum theory without proposing any other theory which embraces the experimental evidence that classical physics fails to explain. Einstein (26), von Laue (27), Schrödinger (28), and Renninger (29) belong to this group.

The scientists of all three groups have a common desire. They would like to return to the reality concept of classical physics. They favor an objective conception of a real world rather than a formalism which is simply consistent with the experimental evidence.

It is beyond the scope of this communication to discuss all the counter proposals and criticisms of quantum theory. However it is of interest to review some of the ideas that have appeared in the literature.

Bohm (20) tries to relate particle orbits with waves in a configuration space. He postulates that particles represent an objective reality of matter and the waves of configuration space can be interpreted as objective fields; like the electric field, the magnetic field, etc.

It is true that many experiments suggest the particle character of the constituents of matter and therefore it is reasonable to assume that particles represent an objective reality. However Bohm's assumption about the wave fields is as realistic as any other postulate of quantum theory. This is particularly true in view of the fact that there is no tangible proof about the objective existence of the configuration space.

Another conceptual difficulty with Bohm's postulates is that an electron, which is in a stationary state without angular momentum, is always at rest. This is contrary to experimental observations. Bohm overcomes the difficulty by further modifying his theory through the addition of other postulates. In an effort to save physical reality he introduces an «ideological supernature» and he uses a terminology which is more complicated and abstract than the terminology used by quantum theory.

Janossy (25) attacks the orthodox quantum theory entirely on the grounds of physics. His thesis may be summarized as follows: It is well known that, in the Copenhagen theory, a reduction in the wave packet occurs whenever a tran-

sition is completed from the possible to the actual. This reduction is justified by the assumption that the interference terms are removed by the partly undefined interactions of the measuring apparatus with the system under measurement and the rest of the world. Janossy points out that such a reduction cannot be deduced from Schrödinger's equation.

Janossy proposes to alter quantum mechanics by the introduction of damping factors so that the interference terms disappear by themselves after a finite time. However even this proposition is not free of criticisms. One of its alarming consequences is that waves which propagate faster than the speed of light interchange the time sequence of cause and effect. Actually there is no physical experimental reason why such a consequence should be adopted.

Schrödinger (28) denies the existence of quantum jumps altogether. Obviously this is not justifiable since there is a long series of experimental observations which suggest the quantized structure of the microcosmos. Furthermore, what is disappointing with Schrödinger is that he does not make any counter proposal.

Scientists who belong to Einstein's group argue that «God was not playing dice» when he created the world and therefore they cannot accept the formulation and interpretation put forward by the Copenhagen School. They claim the world is an objective reality and no theory can be accepted which denies this fact. However they do not have a counter proposal either.

Now, there can be no doubt that the world is an objective reality which exists regardless of whether physicists attempt to understand the laws of the universe or not. But is it not also true that physical sciences are not Nature itself? Is it not true that physics is an aspect of the relationship between Nature and Man and therefore every natural science is dependent on Man as well as on Nature?

The complementarity principle capitalizes exactly on these facts. Since Man has to learn the physical laws by experiment and visualize them in terms of man made symbols, Man's experimental procedures are bound to disturb the universal order. This is particularly true when one attempts to approach the problems of the microcosmos. Therefore one has either to accept the apparent loss of objectivity in favor of a formalism which is sufficiently consistent with the experimental evidence and itself, or adopt the Greek philosophers' contemptuous standpoint and consider experiment as unworthy of any scientific endeavor. Under the circumstances, there is no choice if another Aristotelian scientific medieval age is to be avoided.

Generally all those who object to the «commonly accepted» interpretation of quantum the-

ory have found themselves compelled to sacrifice essential symmetry properties of the theory in an effort to serve the idea of objective reality. It is questionable whether reality is served when it is forced to sound like superreality. Hence, until further experimental evidence becomes available, the orthodox interpretation of quantum theory is unavoidable.

The wave function

The preceding discussion favors decisively the formalistic conception of quantum theory. This conception is based on the following:

1. Experimental evidence; discrete character of atomic phenomena and their descriptive parameters (depending on the way they are looked at).

2. Schrödinger's equation or matrix formulation of quantum theory.

3. Correspondence principle.

4. Complementarity principle.

The complementarity principle implies that physical phenomena are either described in space and time or conceived in terms of exact mathematical laws with causal relationships. If described in space and time, one has to accept an uncertainty in the determination of any two conjugate variables. If conceived in terms of mathematical laws with causal relationships, the physical description in space and time is impossible. Both implications are equivalent.

Regardless of which attitude is adopted, the basic carrier which conveys the experimental information to the human mind is the wave function.

In the first case the wave function or a set of wave functions form the unitary components of a complete set of vectors in a Hilbert space in which the representation of the physical phenomena takes place. These wave functions can be determined from a unitary transformation. There is no physical reason why the Hilbert space should be considered as real. Consequently the wave function has no physical meaning immediately connected with reality in the sense that such a meaning cannot be experimentally determined.

In the second case, the wave function is considered as a wave associated with matter and can be determined from the solution of Schrödinger's equation. The meaning of the wave function is again one of mental visualization rather than of an objective reality.

The lack of physical meaning attributable to the wave function raises the important question of how the wave function is determined.

Some authors invoke the notion of «common sense» in order to justify certain assumptions or postulates used in the determination of the wa-

ve function. Actually «common sense» is a very unreliable guide to follow in attempting to broaden the understanding of the physical world and particularly of the microcosmos.

In spite of the lack of physical criteria the wave function is uniquely and unambiguously determined by a series of mathematical requirements which are imposed by the very role that the wave function plays in the domain of quantum theory.

First, according to quantum theory all measurable physical quantities are bilinear averages of the symbol associated with the quantity in question. The weighting factors are the wave function and its conjugate. This averaging procedure implies, in general, that the wave function must be square integrable if meaningful results are to be found. In fact, square integrability has also been interpreted by Born in terms of a physical picture. More specifically, Born suggests that the information carried by the wave function is incomplete and permits only statistical predictions concerning aggregates of future events. The statistics are represented by the square of the wave function interpreted as a probability density. If such an interpretation is to be accepted, the wave function must be square integrable in order to ascertain the occurrence of one of the possible events.

Second, the representation of atomic structure by means of waves requires that certain boundary conditions be fulfilled as far as potential levels are concerned. If the boundary conditions are not to be restricted to specific points in phase space, the wave function and its first derivative must be continuous.

Third, Schrödinger's equation is linear. Therefore the principle of superposition is applicable to wave functions.

These are the three requirements which unambiguously determine the wave function. It is evident that the introduction of the requirements needs no new postulates or assumptions but is an immediate consequence of the formalism of quantum theory.

The fact that square integrability, continuity of value and first derivative and superposition are the necessary and sufficient conditions which determine the wave function is illustrated by the following example.

The central field problem

The central field problem is investigated and solved in the light of the principles of quantum theory. The development of the solution proves the consistency of the theory and the sufficiency of the restrictions imposed on the wave function.

More specifically, in a central field problem the Hamiltonian of the system is:

$$H = - \frac{\hbar^2}{2M} \nabla^2 + V(r) \tag{1}$$

where

H=Hamiltonian operator

M=mass

∇^2 =Laplacian operator

V(r)=potential energy of the central field.

For stationary states Schrödinger's equation is:

$$H\psi = E\psi \tag{2}$$

The problem is to determine the axes of the Hilbert space in which the Hamiltonian is diagonal or, in other words to find the eigenvalues of H.

Consider the spherical coordinates system

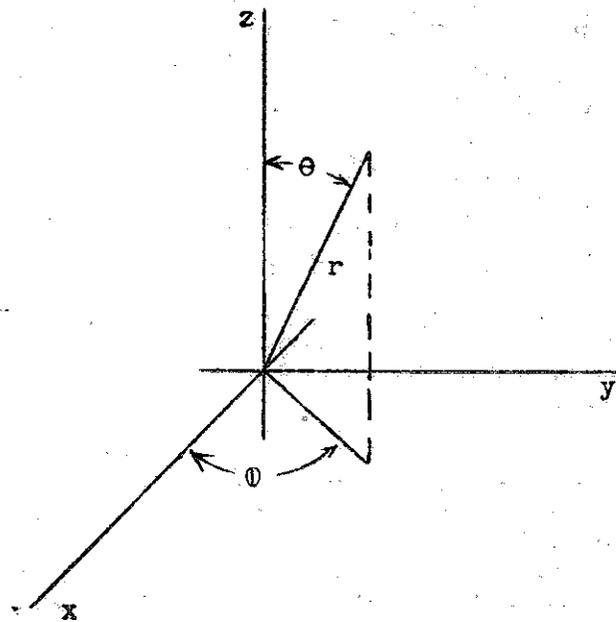


Fig. 1. Spherical coordinates system

shown in Fig. 1. The Laplacian operator can be written as:

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \sin\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right] \tag{3}$$

and thus Schrödinger's equation reduces to:

$$\left[\frac{D_r^2}{2M} + V(r) + \frac{\hbar^2}{2Mr^2} L^2(\theta, \phi) \right] \psi = E\psi \tag{4}$$

where

$$D_r^2 = - \frac{\hbar^2}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}$$

$$L^2 = - \left[\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \sin\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right]$$

The variables of equation (4) are separable, therefore assume:

$$\psi = R(r)Y(\theta, \phi) \tag{5}$$

and thus find:

$$\frac{1}{R} \left[\frac{P_r^2}{2M} + V(r) \right] R + \frac{\hbar^2}{2Mr^2} \frac{1}{Y} \left[L^2 Y \right] = E \quad (6)$$

Since the variables r , θ , ϕ are completely independent, assume:

$$\frac{1}{Y} L^2 Y = \lambda \quad \lambda = \text{const} \quad (7)$$

$$\frac{1}{R} \left[\frac{P_r^2}{2M} + V(r) \right] R + \frac{\hbar^2}{2Mr^2} \lambda = E \quad (8)$$

Next solve equation (7). To this effect, introduce the functions:

$$Y = P(\theta)\Phi(\phi) \quad (9)$$

and reduce equation (7) to:

$$-\frac{1}{P} \frac{1}{\sin\theta} \frac{d}{d\theta} \sin\theta \frac{dP}{d\theta} - \frac{1}{\sin^2\theta} \left[\frac{1}{\Phi} \frac{d^2\Phi}{d\phi^2} \right] = \lambda \quad (10)$$

Notice that for $\theta = \text{constant}$ the second term of equation (10) is constant. Thus assume:

$$\frac{1}{\Phi} \frac{d^2\Phi}{d\phi^2} = -m^2 \quad m^2 = \text{const} \quad (11)$$

The solutions of equation (11) are:

$$\Phi(\phi) = e^{\pm im\phi} \quad (12)$$

Determine the allowable values of m . Note that the values of the probability density cannot depend on the orientation of the zero ϕ -axis. Hence:

$$|\Phi(\phi)|^2 = |\Phi(\phi + 2n\pi)|^2 \quad n = \text{integer} \quad (13)$$

Equation (13) implies that m is real. Then consider the linear combination of two wave functions corresponding to $m = m_1$ and $m = m_2$ respectively. The use of Eq. (13) suggests that $m_1 \pm m_2 = \text{integer}$. Consequently, m is an integer or half integer. It remains to determine whether m can actually be both. This requires some principles of transformation theory which have been purposely omitted in this presentation. In essence, it can be shown that all physical observables are Hermitean in character and furthermore that the Hermitean character of the angular momentum excludes the possibility of $m = \text{half-integer}$ (30).

Now, consider Eq. (10) with $m = \text{integer}$. Introduce the change of variable:

$$\mu = \cos\theta \quad |\mu| \leq 1 \quad (14)$$

and thus find:

$$(1 - \mu^2) \frac{d^2P}{d\mu^2} - 2\mu \frac{dP}{d\mu} + (\lambda - \frac{m^2}{1 - \mu^2}) P = 0 \quad (15)$$

Eq. (15) has singular points at $|\mu| = 1$. This suggests the transformation of variable

$$v = 1 - \mu \quad (16)$$

which yields:

$$\left[1 - \frac{v}{2} \right]^2 \frac{d^2P}{dv^2} + \frac{1}{v} \left[1 - \frac{v}{2} \right] \left[1 - v \right] \frac{dP}{dv} + \frac{1}{v^2} \left[\frac{\lambda(2v - v^2) - m^2}{4} \right] P = 0 \quad (17)$$

The singularity of Eq. (17) is at $v = 0$ and the solutions can be found by the method of Frobenius. In particular, assume:

$$P = v^s \sum_0^{\infty} a_n v^n \quad a_0 \neq 0 \quad (18)$$

Replace Eq. (18) into (17) and find that the indicial equation is:

$$s^2 - \frac{m^2}{4} = 0 \quad \text{or } s = \pm \frac{|m|}{2} \quad (19)$$

Since the wave functions must be square integrable, the only acceptable solution of the indicial equation is:

$$s = \frac{|m|}{2} \quad (20)$$

Thus, conclude that the solutions of Eq. (10) are of the form:

$$P = (1 - \mu^2)^{\frac{|m|}{2}} Q(\mu) \quad (21)$$

$$Q(\mu) = \sum_0^{\infty} b_n \mu^n$$

Replace Eqs. (21) into (10) and find:

$$(1 - \mu^2) \sum_{n=2}^{\infty} b_n n(n-1) \mu^{n-2} - 2(|m| + 1) \mu \sum_{n=1}^{\infty} b_n n \mu^{n-1} + \left[\lambda - |m|(|m| + 1) \right] \sum_{n=0}^{\infty} b_n \mu^n = 0 \quad (22)$$

Eq. (22) is an identity with respect to μ , therefore:

$$b_{n+2} = \frac{(n + |m|)(n + |m| + 1) - \lambda}{(n + 1)(n + 2)} b_n \quad (23)$$

Assign arbitrary values to b_0 and b_1 and admit that the solution of Eq. (10) is an infinite series [Eq. (21)] with two arbitrary constants. Furthermore, admit that the arbitrary series is convergent for $|\mu| < 1$ and divergent for $|\mu| = 1$. The divergence is undesirable if the wave function is to be square integrable. The requirement of square integrability can be fulfilled either if $b_0 = 0$ or $b_1 = 0$ and the series is truncated at μ^{n_1} where n_1 is such that:

$$(n_1 + |m|)(n_1 + |m| + 1) - \lambda = 0 \quad n_1 = \text{integer} \quad (24)$$

Call:

$$n_1 + |m| = 1 \quad (25)$$

and thus find:

$$\lambda = 1(1 + 1) \quad (26)$$

Next admit that if λ is of the form given by Eq. (26) the solutions of Eq. (10) are the associated Legendre polynomials $P_1^m(\mu)$.

In summary, the angular dependence of the solution of the central field problem is given by the spherical harmonics:

$$Y_l^m(\theta, \phi) = e^{im\phi} P_l^m(\theta) \quad (27)$$

The next task is to find the radial dependence of the solution. Assume a coulomb potential.

$$V(r) = -\frac{q^2}{r} \quad (28)$$

and introduce in Eq. (8) the change of variable:

$$R(r) = \frac{1}{r} u(r) \quad (29)$$

Thus find that Eq. (8) reduces to:

$$-\frac{\hbar^2}{2M} \frac{d^2u}{dr^2} - \frac{q^2}{r^2} u + \frac{\hbar^2 l(l+1)}{2Mr^2} u = Eu \quad (30)$$

Introduce the nondimensional constants and variables:

$$r_0 = \frac{\hbar^2}{Mq^2}, E_0 = \frac{q^2}{2r_0}, \sigma = \frac{r}{r_0}, \epsilon^2 = -\frac{E}{E_0}, \epsilon > 0 \quad (31)$$

and reduce Eq. (30) to:

$$\frac{d^2u}{d\sigma^2} + \frac{2}{\sigma} u - \frac{l(l+1)}{\sigma^2} u - \epsilon^2 u = 0 \quad (32)$$

The asymptotic solution of Eq (32) is of the form $e^{\pm\epsilon\sigma}$. However, the plus sign solution is excluded on the basis of square integrability. Therefore, admit that

$$u = u_1 e^{-\epsilon\sigma} \quad (33)$$

where u_1 varies more slowly than $e^{-\epsilon\sigma}$ as $\sigma \rightarrow \infty$. Replace (33) in Eq. (32) and find:

$$\frac{d^2u_1}{d\sigma^2} - 2\epsilon \frac{du_1}{d\sigma} + \left[\frac{2}{\sigma} - \frac{l(l+1)}{\sigma^2} \right] u_1 = 0 \quad (34)$$

Consider the case $l=0$ and try a solution of the form:

$$u_1 = \sigma^k \sum_0^\infty c_j \sigma^j \quad c_0 \neq 0 \quad (35)$$

Following a procedure similar to the one used for Eqs. (10) and (21) admit that:

a. The indicial equation is:

$$k(k-1)=0 \quad k=0 \text{ or } k=1 \quad (36)$$

The value $k=0$ is not acceptable because, if Eq. (21) and $\psi=R(r) Y(\phi, \theta)$ are expressed in terms of cartesian coordinates, it can be easily shown that for $k=0$ the function ψ does not satisfy Eq. (2). Therefore the only appropriate solution is $k=1$. Actually, the value $k=0$ is introduced in the indicial equation through the singular transformation from cartesian to spherical coordinates.

b. The recurrence formula is:

$$c_{j+1} = 2 \frac{(j+1)\epsilon - 1}{(j+1)(j+2)} c_j \quad (37)$$

In particular, for large values of j

$$\frac{c_{j+1}}{c_j} \rightarrow \frac{2\epsilon}{j+1} \quad (38)$$

Therefore, conclude that if the infinite series (35) is not truncated, u_1 will behave like $e^{2\epsilon\sigma}$ for large values of σ . This is again inadmissible on the grounds of square integrability. The infinite series should be terminated by choosing:

$$\epsilon_j = \frac{1}{j+1} \quad (39)$$

Under those conditions Eq. (34), for $l=0$, reduces to:

$$\frac{d^2u_j}{d\sigma^2} - \frac{2}{j+1} \frac{du_j}{d\sigma} + \frac{2}{\sigma} u_j = 0 \quad (40)$$

and admits the general solution (31):

$$u_j = d_j \sigma F(1-j, 2, \frac{2\sigma}{j+1}) \quad (41)$$

where

$d_j = \text{constant}$

$F = \text{confluent hypergeometric function}$

In summary, the radial solution for $l=0$ is:

$$R_j(\sigma) = d_j e^{-\frac{\sigma}{j+1}} F(1-j, 2, \frac{2\sigma}{j+1}) \quad (42)$$

For $l \neq 0$ the procedure is effectively the same. Start with Eq. (32). Replace u by $u_1 e^{-\epsilon\sigma}$ and u_j by series (35). Thus find the indicial equation:

$$k(k-1) = l(l+1) \quad k = l+1 \text{ or } k = -l \quad (43)$$

The value $k = -l$ is excluded because the solution is not square integrable. The only appropriate solution is $k = l+1$,

The recurrence formula is:

$$c_{j+1} = 2 \frac{\epsilon(j+1+1) - 1}{(j+1+1)(j+1+2) - l(l+1)} c_j \quad (44)$$

and must be truncated if the solution is to be square integrable. This is achieved if:

$$\epsilon_j = \frac{1}{j+1+1} \quad (45)$$

and therefore the solution is:

$$u_j = c_0 \sigma^{l+1} F(1+l-j, 2l+2, \frac{2\sigma}{j+1}) \quad (46)$$

In conclusion, the wave functions of the central field problem with a coulomb potential are

$$\psi_{n,l,m} = CY_l^m r^l e^{-\frac{r}{nr_0}} F(2l+2-n, 2l+2, \frac{2r}{nr_0})$$

where $C = \text{normalizing constant}$.

The central field problem can be found in many textbooks on quantum mechanics (32). In most of the cases the solution is established on the basis of unjustified postulates other than square integrability, continuity, and superposition. This is not necessary.

Conclusions

In the preceding discussion the principles of quantum theory have been reviewed and the circumstances which made its formulation imperative outlined. It is evident that the presentation favors the formalistic interpretation of the theory given by Bohr and Heisenberg.

Such a positivistic attitude towards Nature and natural phenomena should not be mistaken as a disregard for mechanistic pictures and realistic explanations. On the contrary, the orthodox quantum theory is adopted because it is believed that the implications of the formalism are far more reaching than the formulae may suggest.

There is no a priori reason why matter should be assumed as made of particles. Such an assumption is a dangerous extrapolation of everyday experience, entirely unjustified and leading to many contradictions. The same comments apply to matter waves.

The fact that some experiments indicate both corpuscular and wave properties of matter proves that the latter is neither the one nor the other. The duality proposed by some authors is unrealistic because it is hard to conceive of a physical entity which behaves tantôt like a particle and tantôt like a wave. On the other hand, the adoption of the complementarity principle frees the theory of such discrepancies. The dualism is the result of the interference of man and his measuring devices with the microcosmos and not a property of matter.

Of course one might ask at this point: «If matter is not made of particles or waves, what is it made of?» It seems that our ignorance on the nature of the exact answer can be expressed by assuming that matter is made of «nephons». A «nephon» is the entity defined by the properties implied by quantum theory. Certainly nothing known in everyday life corresponds to such a nephon. However, this is not a reasonable argument against the acceptance of its existence until further experimental evidence compels us to deny it.

In fact, such an assumption is neither unique nor original. All branches of science have to start from an ultimate postulate and construct their edifice from there on. The need to stop somewhere has been realized ever since Aristotle first stated it explicitly («ἀνάγκη σιῆσαι»).

There is another advantage of quantum theory. The Copenhagen School declares that the theory approaches reality by means of a formalism created by Man. Thus the opportunity is left wide open for further modifications which may be necessary to account for new experimental results. Such modifications would be very

hard to incorporate in the realm of a theory which is based on tangible pictures.

Undoubtedly one might object that quantum theory is nowhere near the absolute truth of the microcosmos since it is based on an abstract formalism. However, is there any physical science which is based on a «real» formalism? Possibly other physical theories are based on formalisms which are more «familiar» but not less «abstract». Furthermore, if quantum theory is nowhere near the absolute truth then this makes it even more interesting. In fact it may be appropriate to conclude this discussion by quoting Poincaré (33). «If God would come in front of me and say: «Well, man, here is the chance of your life. In my left hand I have the absolute truth and in my right hand the lust for the search for the truth which can never be reached. You have your choice. Take the one that you prefer». I would grab his right hand, take its content and make it the goal of my life». Apparently the Copenhagen School has read Poincaré's thoughts and has adopted them.

ΠΕΡΙΛΗΨΙΣ

Φυσική και Μαθηματική Έρμηνεία της Κυματομηχανικής

Υπό

ΗΛΙΑ Π. ΓΥΦΤΟΠΟΥΛΟΥ

Ἡ κυματομηχανική παίζει πρωτεύοντα ρόλο εἰς τὴν σύγχρονον φυσικὴν. Ἡ ἀνάπτυξις τῆς ἔσχεν ἐπαναστατικὸν ἀντίκτυπον, τόσον ἐπὶ τῶν ἀντιλήψεών μας περὶ τῆς δομῆς καὶ συμπεριφορᾶς τῆς ὕλης, ὅσον καὶ εἰς τοὺς κλάδους τῆς χημείας, βιολογίας καὶ τεχνολογίας ἐν γένει.

Βασικὸν ὄργανον τῆς κυματικῆς θεωρίας εἶναι ἡ κυματικὴ συνάρτησις. Αὕτη δύναται νὰ θεωρηθῆ ὡς ὁ φορεὺς διὰ τοῦ ὁποίου τὰ πειραματικὰ δεδομένα μεταφέρονται εἰς τὴν ἀνθρωπίνην σκέψιν, ἢ ὡς τὸ ἀναλυτικὸν δοκίμιον διὰ τοῦ ὁποίου ἡ ἀνθρωπίνη σκέψις προσπαθεῖ νὰ πλησιάσῃ τὴν ἀληθειαν τοῦ μικροκόσμου.

Δοθείσης τῆς εὐρείας σκοπιμότητος τῆς κυματομηχανικῆς, εἶναι ἀπαραίτητον νὰ ὀρίσωμεν ἐπακριβῶς τὰς ἀρχὰς ἐπὶ τῶν ὁποίων αὕτη βασίζεται καὶ νὰ κατανοήσωμεν πλήρως τὴν ἔννοιαν τῆς κυματικῆς συναρτήσεως, τόσον ἀπὸ φυσικῆς, ὅσον καὶ ἀπὸ μαθηματικῆς ἀπόψεως.

Ἡ παρούσα ἐργασία ἐπιχειρεῖ νὰ ἐκπληρώσῃ τὸν σκοπὸν αὐτὸν διὰ μιᾶς συντόμου ἀνασκοπήσεως τῶν ἐρμηνειῶν τῆς κυματομηχανικῆς καὶ τῆς κυματικῆς συναρτήσεως, ὡς αὗται ἐπροτάθησαν ὑπὸ τῆς Σχολῆς τῆς Κοπεγχάγης. Καθ' ὅλην τὴν ἀνάπτυξιν ὁ ἀναγνώστης θεωρεῖται ὡς ἔχων μίαν γενικὴν γνῶσιν τῆς θεωρίας.

Ἡ ἐργασία εἶναι διηρημένη εἰς πέντε κεφάλαια. Εἰς τὸ πρῶτον κεφάλαιον παρουσιάζονται συντόμως αἱ πειραματικαὶ διαπιστώσεις αἱ ὁποιαὶ ὠδή-

γησαν εις την ανάγκην ανάπτυξεως τῆς κυματομηχανικῆς καὶ τὴν ἐγκατάλειψιν τῶν ἀρχῶν τῆς κλασσικῆς φυσικῆς, προκειμένου περὶ ἀτομικῶν φαινομένων. Συγκεκριμένως, αἱ πειραματικαὶ καὶ θεωρητικαὶ ἐργασίαι τῶν Planck (1), Einstein (2, 5), Rutherford (3), Franck - Hertz (4), Stern - Gerlach (6), Sommerfeld (7), Compton (8), de Broglie (9), Davisson - Germer (10), Bohr et al (11) καὶ Schrödinger (12) θεωροῦνται ὡς ἐκ τῶν κυρίως συμβαλοῦσάντων εἰς τὴν καθιέρωσιν στατιστικῶν νόμων διὰ τὴν περιγραφὴν τοῦ μικροκόσμου καὶ τὴν ἀμφισβήτησιν τῆς ἰσχύος τῆς ἀρχῆς τοῦ αἰτίου καὶ αἰτιατοῦ καὶ τῆς ἐννοίας τῆς συνεχείας (continuum) εἰς τὴν περιοχὴν τῆς ἀτομικῆς φυσικῆς.

Εἰς τὸ δεῦτερον κεφάλαιον περιγράφονται τὰ βασικὰ ἀξιώματα τῆς κυματομηχανικῆς ὡς ἀνεπτύχθησαν ὑπὸ τοῦ Heisenberg (14, 15) καὶ ἠρμηνεύθησαν ὑπὸ τῶν Bohr (16), Jordan, Klein καὶ Wigner (17). Αἱ ἀρχαὶ αὗται συνοψίζονται ὡς ἑξῆς:

α. Ἡ θεωρία εἶναι συμβιβαστὴ μετὰ τῶν πειραματικῶν δεδομένων.

β. Ἡ κυματομηχανικὴ περιγραφή ἑνὸς συστήματος τείνει πρὸς τὴν κλασσικὴν περιγραφὴν καθὼς τὸ μέγεθος τοῦ συστήματος αὐξάνει (ἀρχὴ τῆς ἀντιστοιχίας). Μέτρον τῆς συγκρίσεως εἶναι ἡ σταθερὰ τοῦ Planck h .

γ. Αἱ δυναμικαὶ καὶ κινηματικαὶ μεταβληταὶ τῆς κλασσικῆς μηχανικῆς ἀντικαθίστανται ὑπὸ συμβόλων ὑποκειμένων εἰς μὴ ἀντιμεταθετὴν ἀλγεβραν. Συγκεκριμένως, αἱ κανονικαὶ ἐξισώσεις τοῦ Hamilton γράφονται ὡς:

$$qp - pq = -\frac{\hbar}{i}; \quad \hbar = \frac{h}{2\pi}$$

καὶ ἰσχύουν διὰ κάθε ζεύγος συζυγῶν μεταβλητῶν q καὶ p .

Ἡ παραδοχὴ τοῦ ἀνωτέρω συμβολισμοῦ ὁδηγεῖ εἰς τὴν ἀρχὴν τῆς ἀβεβαιότητος

$$\Delta q \Delta p \geq \hbar$$

τῆς ὁποίας ἡ ἐννοια διασαφηνίζεται ὑπὸ τῆς ἀρχῆς τῶν συμπληρωματικῶν μεγεθῶν (complementarity principle).

δ. Ἡ ἀρχὴ τῶν συμπληρωματικῶν μεγεθῶν ἀποσαφηνίζει ὅτι ἡ ἀβεβαιότης ἐπὶ τῶν ἀτομικῶν μετρήσεων δὲν ὀφείλεται εἰς χαρακτηριστικὴν τινα ιδιότητα τῆς φύσεως ἀλλ' εἰς τὸ γεγονός ὅτι ἡ περιγραφή τῶν ἀτομικῶν φαινομένων γίνεται διὰ τῆς χρησιμοποίησεως τῆς ὁρολογίας τῆς κλασσικῆς φυσικῆς.

Εἰς τὸ τρίτον κεφάλαιον περιγράφονται μερικαὶ τῶν ἀντιρρήσεων αἱ ὁποῖαι κατὰ καιροὺς ἐπρόταθον κατὰ τῆς κυματομηχανικῆς καὶ ὑποδεικνύονται οἱ λόγοι διὰ τοὺς ὁποίους αὗται θεωροῦνται ὡς ἀνεδαφικαί. Μεταξὺ τῶν ἐπιστημόνων, τῶν ὁποίων αἱ ἀντιρρήσεις συζητοῦνται, περιλαμβάνονται οἱ Bohm (20), Janossy (25), Schrödinger (28) καὶ Einstein.

Εἰς τὸ τέταρτον κεφάλαιον τονίζεται ἡ ἔλλειψις φυσικῆς σημασίας τῆς κυματικῆς συναρτήσεως καὶ δίδονται αἱ μαθηματικαὶ συνθήκαι αἱ ὁποῖαι καθορίζουν τὴν τελευταίαν μονοσημάντως. Αἱ μαθηματικαὶ συνθήκαι εἶναι:

α. Ὁλοκληρωσιμότης τῆς τετραγωνισμένης κυματικῆς συναρτήσεως.

β. Συνεχεῖα τιμῆς καὶ πρώτης παραγώγου τῆς κυματικῆς συναρτήσεως.

γ. Ἰσχύς τῆς ἀρχῆς τῆς ὑπερθέσεως.

Ἡ ἐπάρκεια τῶν ἀνωτέρω ἀρχῶν, διὰ τὸν πλήρη καθορισμὸν τῆς κυματικῆς συναρτήσεως, ἀποδεικνύεται εἰς τὸ πέμπτον κεφάλαιον, εἰς τὸ ὁποῖον ἐκτίθεται ἡ ἀνάλυσις τοῦ προβλήματος τοῦ κεντρικοῦ πεδίου.

Ἡ ἐργασία κλείεται διὰ μιᾶς γενικῆς ἀνασκοπήσεως τῆς ἀντικειμενικότητος τῆς κυματικῆς θεωρίας. Τονίζεται ὅτι δὲν ὑπάρχει a priori λόγος διὰ τὸν ὁποῖον ἡ ὕλη πρέπει νὰ θεωρηθῆ ὡς ἀποτελουμένη ὑπὸ σωματιδίων ἢ κυμάτων. Προτείνεται ὅπως ἡ ἀδυναμία περιγραφῆς τῆς ὕλης ὑπὸ μοναδικῆς «γνωστῆς» εἰκόνας παρακαμφθῆ διὰ τῆς εἰσαγωγῆς τοῦ ὄρου «νεφόνιον», τοῦ νεφονίου ὀριζομένου ὑπὸ τῶν ιδιοτήτων τῶν περιγραφομένων ὑπὸ τῆς κυματομηχανικῆς.

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