Majorana and the path-integral approach to Quantum Mechanics

S. Esposito

Dipartimento di Scienze Fisiche, Università di Napoli "Federico II"
and
I.N.F.N. Sezione di Napoli, Complesso Universitario di M. S. Angelo,
Via Cinthia, 80126 Napoli (`Salvatore.Esposito@na.infn.it`)

ABSTRACT. We report on a manuscript by Ettore Majorana, which probably corresponds to the text for a seminar delivered at the University of Naples in 1938, where he lectured on Theoretical Physics. Some passages reveal a physical interpretation of Quantum Mechanics which anticipates of several years the Feynman approach in terms of path integrals, independently of the underlying mathematical formulation.

1   Introduction

From January to March 1938, Ettore Majorana delivered his only lectures on Quantum Mechanics at the University of Naples, where he obtained a position as a full professor of Theoretical Physics, few months before he mysteriously disappeared. Although the scientific personality of such a physicist is widely recognized, here we only mention that Majorana got that position in the 1937 Italian national competition for three full professorships for "great and well-deserved fame", independently of the competition itself, upon recommendation of the judging committee chaired by Enrico Fermi [1].

The interest in the course on Theoretical Physics, delivered by Ettore Majorana at the University of Naples in 1938, has been recently revived by the discovery of the Moreno Paper [2], which is a faithful transcription of the lecture notes prepared by Majorana himself made by the student Eugenio Moreno. Such a Paper, in fact, includes some previously unknown lecture notes, whose original manuscripts seem to be missing. The handwritten notes by Majorana were reproduced some years ago [3] by including also some papers, probably prepared (by Majorana for his own personal use) for a general seminar or conference held

at the University of Naples, likely at the end of January 1938, soon after the arrival of Majorana in Naples.

The present scientific interest in that dissertation is centered on the interpretation given by Majorana about some topics of the novel, for that time, Quantum Theory (namely, the concept of quantum state) and the direct application of this theory to a particular case (that is, precisely, the molecular bonding). An accurate reading of the manuscript, in fact, not only discloses a peculiar cleverness of the author in treating a pivotal argument of the novel Mechanics, but, keeping in mind that it was written in 1938, also reveals a net advance of at least ten years in the use made of that topic. The last point, however, is quite common for Majorana, and as only one example we refer here to the case of the Thomas-Fermi atomic model [4] (see, however, also Ref. [5]).

This point was already noted some years ago by N. Cabibbo (in Ref. [3]), who saw in the Majorana manuscript a vague and approximate anticipation of the idea underlying the Feynman interpretation of Quantum Mechanics in terms of path integrals. A more analytic study, conducted on the critical edition of that paper [6] which was not available at that time, reveals instead some intriguing surprises, upon which we will here focus on.

In the present work we report an English translation (from the Italian) of the mentioned notes; these are contained into a manuscript kept at the Domus Galilaeana in Pisa. Although the text considered is written in a very simple a clear form (a feature which is very common in the Majorana works [5]), in the next section we give beforehand a brief discussion of the main ideas of the path-integral approach, followed by a simple presentation where the crucial passages in the Majorana paper are pointed out.

2   Quantum Mechanics in the path-integral approach

The general postulate upon which Quantum Mechanics is based tells that the "state" of a certain physical system may be represented with a complex quantity ψ, considered as a (normalized) vector in a given Hilbert space corresponding to the physical system, where all the information on the system is contained [7]. The time evolution of the state vector is ruled by the Schrödinger equation, that may be written in the general form:

$$i\hbar \frac{\mathrm{d}\psi}{\mathrm{d}t} = H\,\psi, \tag{1}$$

where H is the hamiltonian operator of the considered system. The initial state at time t_0 is specified by its choice among the possible eigenstates of a complete set of commuting operators (including, for example, the hamiltonian), while the hamiltonian H itself determines the state of the system at a subsequent time T through Eq. (1). The dynamical evolution of the system is thus completely determined if we evaluate the transition amplitude between the state at time t_0 and that at time t.

Then, as we can easily see, the usual quantum-mechanical description of a given system is strongly centered on the role played by the hamiltonian H and, as a consequence, the time variable plays itself a key role in this description. Such a dissymmetry between space and time variables is, obviously, not satisfactory in the light of the postulates of the Theory of Relativity. This was firstly realized in 1932 by Dirac [8], who put forward the idea of reformulating the whole Quantum Mechanics in terms of lagrangians rather than hamiltonians[1]

The starting point in the Dirac thought is that of exploiting an analogy, holding at the quantum level, with the Hamilton principal function in Classical Mechanics [12]. From this, the transition amplitude from a state in the spatial configuration q_a at time t_a to a state in the spatial configuration q_b at time t_b is written as:

$$\langle q_b | q_a \rangle \sim \mathrm{e}^{\frac{i}{\hbar} S} = \mathrm{e}^{\frac{i}{\hbar} \int_{t_a}^{t_b} L \mathrm{d}t} \qquad (2)$$

where L is the lagrangian of the system and $S[q]$ the action functional defined on the paths from q_a to q_b. The previous relationship, however, cannot be considered as an equality as long as the time interval from t_a to t_b is finite, since it would lead to incorrect results (and Dirac himself was well aware of this; in his paper he introduced several unjustified assumptions in order to overcome such a difficulty). In fact, by splitting the integration field in (2) into N intervals, $t_a = t_0 < t_1 < t_2 < \ldots < t_{N-1} < t_N = t_b$, the transition amplitude could be written as a product of terms,

$$\langle q_b | q_a \rangle = \langle q_b | q_{N-1} \rangle \langle q_{N-1} | q_{N-2} \rangle \cdots \langle q_2 | q_1 \rangle \langle q_1 | q_a \rangle, \qquad (3)$$

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[1]Note, however, that the Quantum Theory of wave fields was already formulated in terms of a variational principle applied to a lagrangian function. As a reference, see the classical book by Heisenberg [9], considered also by Majorana for some works of him as, for example, the development of a relativistic theory of particles with arbitrary spin [10] or the symmetric theory of electron and positron [11].

while it is well known that, by using the completeness relations, the correct formula contains the integration over the intermediate regions:

$$\langle q_b | q_a \rangle = \langle q_b | \int dq_{N-1} | q_{N-1} \rangle \langle q_{N-1} | \ldots \int dq_1 | q_1 \rangle \langle q_1 | q_a \rangle$$

$$= \int dq_1 dq_2 \cdots dq_{N-1} \langle q_b | q_{N-1} \rangle \cdots \langle q_2 | q_1 \rangle \langle q_1 | q_a \rangle. \tag{4}$$

About ten year after the appearance of the Dirac paper, Feynman [13] guessed that the relation in (2) should hold as an equality, up to a constant factor A, only for transitions between states spaced by an *infinitesimal* time interval. In this case, by employing the correct formula in (4), we obtain the well-known Feynman expression for the transition amplitude between two given states:

$$\langle q_b | q_a \rangle = \lim_{\substack{N \to \infty \\ t_b - t_a \text{ finite}}} A^N \int dq_1 dq_2 \cdots dq_{N-1} \, e^{iS/\hbar}$$

$$\equiv \int Dq \, e^{iS/\hbar}. \tag{5}$$

The meaning of the previous formula can be understand as follows. In the integrations present in it, which we have generically denoted with $\int Dq$, the limits t_a and t_b in the integration interval are kept fixed, while we integrate over the space specified by the intermediate points. Since every spatial configuration q_i of these intermediate points corresponds to a given dynamical trajectory joining the initial point t_a with the final one t_b, the integration over all these configurations is equivalent to sum over *all* the possible paths from the initial point to the final one. In other words the Feynman formula with the path integrals points out that the transition amplitude between an initial and a final state can be expressed as a sum of the factor $e^{iS[q]/\hbar}$ over all the paths with fixed end-points. Such a result, on one hand, it is not surprising if we consider that, in Quantum Mechanics, for a given process taking place through different ways, the transition amplitude is given by the sum of the partial amplitudes corresponding to *all* the possible ways through which the process happens. This is particularly evident, for example, in the classical experiment with an electron beam impinging on a screen through a double slit. The interference pattern observed on the screen at a given distance from the slit, should suggest that a single electron has

crossed through both slits. It can be, then, explained by assuming that the probability that has one electron to go from the source to the screen through the double slit is obtained by summing over *all* the possible paths covered by the electron. Thus the fundamental principles of Quantum Mechanics underlie the path-integral approach. However, what is crucial but unexpected in this approach is that the sum is made over the phase factor $e^{iS[q]/\hbar}$, which is generated by the classical action $S[q]$.

One of the major merits of the Feynman approach to Quantum Mechanics is the possibility to get in a very clear manner the classical limit when $\hbar \to 0$ (the other merits being its versatile applicability to field quantization in abelian or non abelian gauge theories, with or without spontaneous symmetry breaking). In fact for large values of S compared to $\hbar$, the phase factor in (5) undergoes large fluctuations and thus contributes with terms which average to zero. From a mathematical point of view, it is then clear that in the limit $\hbar \to 0$ the dominant contribution to Eq. (5) comes out when the phase factor does not varies much or, in other words, when the action S is stationary. This result is precisely what emerges in Classical Mechanics, where the classical dynamical trajectories are obtained from the least action principle. This occurrence was firstly noted by Dirac [8], who realized the key role played by the action functional.

The intuitive interpretation of the classical limit is very simple. Let us consider, in the q, t space, a given path far away from the classical trajectory $q_{\text{cl}}(t)$; since $\hbar$ is very small, the phase $S/\hbar$ along this path will be quite large. For each of such paths there is another one which is infinitely close to it, where the action S will change only for a small quantity, but since this is multiplied by a very large constant $(1/\hbar)$, the resulting phase will have a correspondingly large value. On average these paths will give a vanishing contribution in the sum in Eq. (5). Instead, near the classical trajectory $q_{\text{cl}}(t)$ the action is stationary, so that, passing by a path infinitely close to that classical to this last one, the action will not change at all. Then the corresponding contributions in Eq. (5) will sum coherently and, as a result, the dominant term is obtained for $\hbar \to 0$. Thus, in such approach, the classical trajectory is picked out in the limit $\hbar \to 0$ not because it mainly contributes to the dynamical evolution of the system, but rather because there are paths infinitely close to it that give contributions which sum coherently. The integration region is, actually, very narrow for classical systems, while it becomes wider for quantum ones. As a consequence, the concept of

orbit itself, that in the classical case is well defined, for quantum systems comes to lose its meaning, as for example for an electron orbiting around the atomic nucleus.

3   Majorana contribution

The discussion presented above of the path-integral approach to Quantum Mechanics has been deliberately centered on the mathematical aspect, rather than on the physical one, since the historical process has precisely followed this line, starting from the original Dirac idea in 1932 and arriving at the Feynman formulation in the forties (one can usefully consult the original papers in [8] and [13]). On the other hand, just the development of the mathematical formalism has later led to the impressive physical interpretation mentioned previously.

Coming back to the Majorana paper here considered, we immediately realize that it contains *nothing* of the mathematical aspect of the peculiar approach to Quantum Mechanics. Nevertheless an accurate reading reveals, as well, the presence of the *physical* foundations of it.

The starting point in Majorana is to search for a meaningful and clear formulation of the concept of quantum state. And, obviously, in 1938 the dispute is opened with the conceptions of the Old Quantum Theory.

> According to the Heisenberg theory, a quantum state corresponds not to a strangely privileged solution of the classical equations but rather to a set of solutions which differ for the initial conditions and even for the energy, i.e. what it is meant as precisely defined energy for the quantum state corresponds to a sort of average over the infinite classical orbits belonging to that state. Thus the quantum states come to be the minimal statistical sets of classical motions, *slightly different* from each other, accessible to the observations. These minimal statistical sets cannot be further partitioned due to the uncertainty principle, introduced by Heisenberg himself, which forbids the precise simultaneous measurement of the position and the velocity of a particle, that is the determination of its orbit.

Let us note that the "solutions which differ for the initial conditions" correspond, in the Feynman language of 1948, precisely to the different

integration paths. In fact, the different initial conditions are, in any case, always referred to the same initial time (t_a), while the determined quantum state corresponds to a fixed end time (t_b). The introduced issue of "*slightly different* classical motions" (the emphasis is given by Majorana himself), according to what specified by the Heisenberg's uncertainty principle and mentioned just afterwards, is thus evidently related to that of the sufficiently wide integration region in Eq. (5) for quantum systems. In this respect, such a mathematical point is intimately related to a fundamental physical principle.

The crucial point in the Feynman formulation of Quantum Mechanics is, as seen above, to consider not only the paths corresponding to classical trajectories, but *all* the possible paths joining the initial point with the end one. In the Majorana manuscript, after a discussion on an interesting example on the harmonic oscillator, the author points out:

> Obviously the correspondence between quantum states and sets of classical solutions is only approximate, since the equations describing the quantum dynamics are in general independent of the corresponding classical equations, but denote a real modification of the mechanical laws, as well as a constraint on the feasibility of a given observation; however it is better founded than the representation of the quantum states in terms of quantized orbits, and can be usefully employed in qualitative studies.

And, in a later passage, it is more explicitly stated that the wave function "corresponds in Quantum Mechanics to any possible state of the electron". Such a reference, that only superficially could be interpreted, in the common acceptation, that all the information on the physical systems is contained in the wave function, should instead be considered in the meaning given by Feynman, according to the comprehensive discussion made by Majorana on the concept of state.

Finally we point out that, in the Majorana analysis, a key role is played by the symmetry properties of the physical system.

> Under given assumptions, that are verified in the very simple problems which we will consider, we can say that every quantum state possesses all the symmetry properties of the constraints of the system.

The relationship with the path-integral formulation is made as follows. In discussing a given atomic system, Majorana points out how from one quantum state S of the system we can obtain another one S' by means of a symmetry operation.

> However, differently from what happens in Classical Mechanics for the *single solutions* of the dynamical equations, in general it is no longer true that S' will be distinct from S. We can realize this easily by representing S' with a set of classical solutions, as seen above; it then suffices that S includes, for any given solution, even the other one obtained from that solution by applying a symmetry property of the motions of the systems, in order that S' results to be identical to S.

This passage is particularly intriguing if we observe that the issue of the redundant counting in the integration measure in gauge theories, leading to infinite expressions for the transition amplitudes [14], was raised (and solved) only after much time from the Feynman paper.

Summing up, it is without doubt that no trace can be found of the formalism underlying the Feynman path-integral approach to Quantum Mechanics in the Majorana manuscript (on the contrary to what happens for the Dirac paper of 1933, probably known to Majorana). Nevertheless it is very interesting that the main physical items, about the novel way of interpreting the theory of quanta, were realized well in advance by Majorana. And this is particularly impressive if we take into account that, in the known historical path, the interpretation of the formalism has only followed the mathematical development of the formalism itself.

Furthermore, in the Majorana paper, several interesting applications to atomic and molecular systems are present as well, where known results are deduced or re-interpreted according to the novel point of view. The search for such applications, however, will be left to the reader, who will benefit of the reading of the complete text by Majorana reported in the following.

4   The text by Majorana

The original manuscript by Majorana, as it can be seen from Ref. [3], reports (at the beginning) a sort of table of contents which, however, is only partially followed by the author. For the sake of ease, we have preferred to divide the whole text in some sections, according to the reported table of contents.

1   On the meaning of quantum state

The internal energy of a closed system (atom, molecule, etc.) can take, according to Quantum Mechanics, discrete values belonging to a set $E_0, E_1, E_2, \ldots$ composed of the so-called energy "eigenvalues". To each given value of the energy we can associate a "quantum state", that is a state where the system may remain indefinitely without external perturbations. As an example of these perturbations, we can in general consider the coupling of the system with the radiation field, by means of which the system may loose energy in form of electromagnetic radiation, jumping from an energy level E_k to a lower one $E_i < E_k$. Only when the internal energy takes the minimum value E_0, it cannot be further decrease by means of radiation; in this case the system is said to be in its "ground state" from which it cannot be removed without sufficiently strong external influences, such as the scattering with fast particles or with light quanta of large frequency.

What is the corresponding concept of quantum state in Classical Mechanics? An answer is primarily required to such a question, in order to have a correct representation of the results obtained in our field by Quantum Mechanics, without entering, however, in the complex computational methods adopted by this.

In Classical Mechanics the motion of a system composed of N mass points is entirely determined when the coordinates $q_1 \ldots q_{3N}$ of all the points are known as function of time:

$$q_i = q_i(t) \tag{I}$$

Eqs. (I) give the dynamical equations where all the internal and external forces acting on the system are present, and they can always be chosen in such a way that at a given instant all the coordinates $q_i(0)$ and their time derivatives $\dot{q}_i(0)$ take arbitrarily fixed values. Thus the general solution of the equations of motion must depend $2 \cdot 3N$ arbitrary constants. For system with atomic dimensions the classical representation no longer holds and two successive modifications have been proposed. The first one, due to Bohr and Sommerfeld and that has provided very useful results, has been afterwards completely abandoned with the emerging of the novel Quantum Mechanics, which has been the only one to give an extremely general formalism, fully confirmed by the experiences on the study of the elementary processes. According to the old theory of Bohr-Sommerfeld, Classical Mechanics still holds in describing the atom,

so that the motion of an electron, for example, around the hydrogen nucleus is still described by a solution (I) of the equations of Classical Mechanics; however, if we consider periodic motions, such as the revolution of an electron around the nucleus, not all the solutions of the classical equations are realized in Nature, but only a discrete infinity of those satisfying the so-called Sommerfeld conditions, that is certain cabalistic-like integral relations. For example in every periodic motion in one dimension, the integral of the double of the kinetic energy over the period τ:

$$\int_0^\tau 2T(t)\, \mathrm{d}t = nh$$

must be an integer multiple of the Planck constant ($h = 6.55 \cdot 10^{-27}$). The combination of Classical Mechanics with a principle which is unrelated with it, such as that of the quantized orbits, appears so hybrid that it should be not surprising the complete failure of that theory occurred in the last decade, irrespective of several favorable experimental tests which was supposed to be conclusive.

The novel Quantum Mechanics, primarily due to Heisenberg, is substantially more closed to the classical conceptions than the old one. According to the Heisenberg theory, a quantum state corresponds not to a strangely privileged solution of the classical equations but rather to a set of solutions which differ for the initial conditions and even for the energy, i.e. what it is meant as precisely defined energy for the quantum state corresponds to a sort of average over the infinite classical orbits belonging to that state. Thus the quantum states come to be the minimal statistical sets of classical motions, *slightly different* from each other, accessible to the observations. These minimal statistical sets cannot be further partitioned due to the uncertainty principle, introduced by Heisenberg himself, which forbids the precise simultaneous measurement of the position and the velocity of a particle, that is the determination of its orbit. An harmonic oscillator with frequency ν can oscillate classically with arbitrary amplitude and phase, its energy being given by

$$E = 2\pi^2 m\nu^2 A_0^2$$

where m is its mass and A_0 the maximum elongation. According to Quantum Mechanics the possible values for E are, as well known, $E_0 = \dfrac{1}{2}h\nu,\ E = \dfrac{3}{2}h\nu,\ \dots E_n = \left(n + \dfrac{1}{2}\right)h\nu\ \dots$; in this case we can say that the ground state with energy $E_0 = \dfrac{1}{2}h\nu$ corresponds roughly to

all the classical oscillations with energy between 0 and $h\nu$, the first excited state with energy $E_0 = \dfrac{3}{2}h\nu$ corresponds to the classical solutions with energy between $h\nu$ and $2 \cdot h\nu$, and so on. Obviously the correspondence between quantum states and sets of classical solutions is only approximate, since the equations describing the quantum dynamics are in general independent of the corresponding classical equations, but denote a real modification of the mechanical laws, as well as a constraint on the feasibility of a given observation; however it is better founded than the representation of the quantum states in terms of quantized orbits, and can be usefully employed in qualitative studies.

2 Symmetry properties of a system in Classical and Quantum Mechanics

Systems showing some symmetry property deserve a particular study. For these systems, due to symmetry considerations alone, from one particular solution of the classical equations of motion $q_i = q_i(t)$ we can deduce, in general, some other different ones $q_i' = q_i'(t)$. For example if the system contains two or more electrons or, in general, two or more identical particles, from one given solution we can obtain another solution, which in general will be different from the previous one, just by changing the coordinates of two particles. Analogously if we consider an electron moving in the field of two identical nuclei or atoms (denoted with A and B in the figure), starting from an allowed orbit $q_i = q_i(t)$ described around A with a given law of motion, we can deduce another orbit $q_i' = q_i'(t)$ described by the electron around the nucleus or atom B by a reflection with respect to the center O of the line AB.
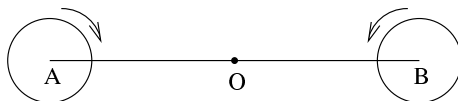
The exchange operations between two identical particles, reflection with respect to one point or other ones corresponding to any symmetry property, keep their meaning in Quantum Mechanics. Thus it is possible to deduce from a state S another one S', *corresponding to the same known value of the energy*, if in the two mentioned examples we exchange two identical particle between them and reflect the system with respect to the point O. However, differently from what happens in Classical Mechanics for the *single solutions* of the dynamical equations, in general

it is no longer true that S' will be distinct from S. We can realize this easily by representing S' with a set of classical solutions, as seen above; it then suffices that S includes, for any given solution, even the other one obtained from that solution by applying a symmetry property of the motions of the systems, in order that S' results to be identical to S.

In several cases, if the system satisfies sufficiently complex symmetry properties, it is instead possible to obtain, by symmetry on a given quantum state, other different states but with the same energy. In this case the system is said to be *degenerate*, i.e it has many states with the same energy, exactly due to its symmetry properties. The study of degenerate systems and of the conditions under which degeneration can take place will bring us too far and, in any case, it is difficult to made such a study in terms of only classical analogies. Then we will leave it completely aside and limit our attention to problems without degeneration. This condition is always satisfied if the symmetry of the mechanical system allows only a so simple transformation that its square, that is the transformation applied twice, reduces to the identity transformation. For example, by a double reflection of a system of mass points with respect a plane, a line or a point, we necessarily recover the same initial arrangement; analogously, the system remains unaltered by changing twice two identical particles. In all these cases we have only simple quantum states, i.e. to every possible value of the energy it is associated only one quantum state. It follows that all the quantum states of system containing two identical particles are symmetric with respect to the two particles, remaining unaltered under their exchange. Thus the states of an electron orbiting around two identical nuclei A and B are symmetric with respect to the middle point O of AB, or remain unaltered by reflection in O, and analogously for other similar cases. Under given assumptions, that are verified in the very simple problems which we will consider, we can say that every quantum state possesses all the symmetry properties of the constraints of the system.

3   *Resonance forces between states that cannot be symmetrized for small perturbations and spectroscopic consequences.   Theory of homeopolar valence according to the method of bounding electrons. Properties of the symmetrized states that are not obtained from non symmetrized ones with a weak perturbation.*

Let us consider an electron moving in the field of two hydrogen nuclei or protons. The system composed by the two protons and the electron

has a net resulting charge of $+e$ and constitutes the simplest possible molecule, that is the positively ionized hydrogen molecule. In such a system the protons are able to move as well as the electron, but due to the large mass difference between the first ones and the second one (mass ratio 1840:1) the mean velocity of the protons is much lower than that of the electron, and the motion of this can be studied with great accuracy by assuming that the protons are at rest at a given mutual distance. This distance is determined, by stability reasons, in such a way that the total energy of the molecule, that at a first approximation is given by the sum of the mutual potential energy of the two protons and the energy of the electron moving in the field of the first ones, and is different for different electron quantum states, is at a minimum.

The mutual potential energy of the protons is given by $\dfrac{e^2}{r}$ if r is their distance, while the binding energy of the electron in its ground state is a negative function $E(r)$ of r that does not have a simple analytic expression, but it can be obtained from Quantum Mechanics with an arbitrary large accuracy. The equilibrium distance r_0 is then determined by the condition that the total energy is at a minimum:

$$W(r_0) = \frac{e^2}{r_0} + E(r_0)$$

The curve $W(r)$ has a behavior like that shown in the figure, if we assume that zero energy corresponds to the molecule which is dissociated into a neutral hydrogen atom and a ionized atom at an infinite distance. The equilibrium distance
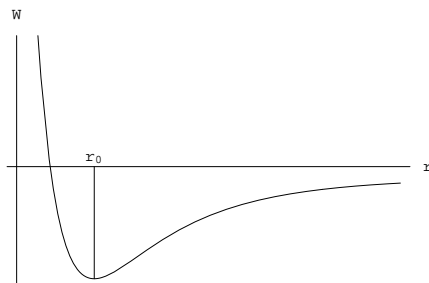
has been theoretically evaluated by Burrau[2] finding $r_0 = 1.05 \cdot 10^{-8}$ cm

[2]Majorana refers here to the paper by Ø. Burrau, *Berechnung des Energiewertes des Wasserstoffmolekel-Ions (H2+) im Normalzustand,* Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **7** (1927) 14.

and, for the corresponding energy, $W(r_0) = -2.75$ electron-volt. Both these results have been fully confirmed by observations on the spectrum emitted by the neutral or ionized molecule, that indirectly depends on them.

What is the origin of the force $F = +\dfrac{\mathrm{d}W}{\mathrm{d}r}$ that tends to get close the two hydrogen nuclei when they are at a distance larger than r_0? The answer given by Quantum Mechanics to this question is surprising since it seems to show that, beside certain polarization forces which can be foreseen by Classical Mechanics, a predominant role is played by a completely novel kind of forces, the so-called *resonance forces.*

Let us suppose the distance r to be large with respect to the radius of the neutral hydrogen atom ($\sim 0.5 \cdot 10^{-8} cm$). Then the electron undergoes the action of one or the other of the two protons, around each of them can classically describe closed orbits. The system composed by the electron and the nucleus around which it orbits forms a neutral hydrogen atom, so that our molecule results to be essentially composed by one neutral atom and one proton at a certain distance from the first. The neutral hydrogen atom in its ground state has a charge distribution with spherical symmetry, classically meaning that all the orientations of the electronic orbit are equally possible, and the negative charge density exponentially decreases with the distance in such a way that the atomic radius can practically be considered as finite; it follows that no electric field is generated outside a neutral hydrogen atom, and thus no action can be exerted on a proton at a distance r which is large compared to the atomic dimensions. However the neutral atom can be polarized under the action of the external proton and acquire an electric moment along the proton-neutral atom direction, and from the interaction of this electric moment with the non uniform field generated by the proton it comes out an attractive force which tends to combine the atom and the ion in a molecular system.

The *polarization forces*, which can be easily predicted with classical arguments, can give origin alone to molecular compounds, that however are characterized by a pronounced fleetingness. More stable compounds can only be obtained if other forces are considered in addition to the polarization ones. In the polar molecules, composed of two ions of different sign charge, such forces are essentially given by the electrostatic attraction between the ions; for example the HCl molecule is kept together essentially by the mutual attraction between the H^+ positive ion and the Cl^- negative one. However in molecule composed by two neutral atoms,

or by a neutral atom and a ionized one, as in the case of the molecular ion H_2^+, the *chemical affinity* is essentially driven by the phenomenon of the resonance, according to the meaning assumed by this word in the novel Mechanics, which has no parallel in Classical Mechanics.

When we study, from the Quantum Mechanics point of view, the motion of the electron in the field of the two protons, assumed to be fixed at a very large mutual distance r, at a first approximation we can determine the energy levels by assuming that the electron should move around the proton A (or B) and neglecting the influence of the other proton in B (or A), which exerts a weak perturbative action due to its distance. For the lowest energy eigenvalue E_0 we thus obtain a state S corresponding to the formation of a neutral atom in its ground state consisting of the electron and the nucleus A, and a state S' corresponding to a neutral atom composed by the electron and the nucleus B. Now if we take into account the perturbation that in both cases is exerted on the neutral atom by the positive ion, we again find, as long as the perturbation is small, not two eigenvalues equal to E_0 but two eigenvalues E_1 and E_2 which are slightly different from E_0 and both close to this value; however the quantum states corresponding to them, let be T_1 and T_2, are not separately close to S e S', since, due to the fact that the potential field where the electron moves is symmetric with respect to the middle point of AB, the same symmetry must be shown, for what said above, by the effective states T_1 and T_2 of the electron, while it is not separately shown by S and S'.

According to the model representation of the quantum states introduced above, S consists of a set of electronic orbits around A, and analogously S' of a set of orbits around B, while the true quantum states of the system T_1 and T_2 each correspond, at a first approximation for very large r, for one half to the orbits in S and for the other half to those in S'. The computations prove, that for sufficiently large nuclear distances, the mean value of the perturbed eigenvalue E_1 and E_2 coincides closely to the single unperturbed value E_0, while their difference is not negligible and has a conclusive importance in the present as well as in infinite other analogous cases of the study of the chemical reactions. We can thus suppose that $E_1 < E_0$ but $E_2 > E_0$, and then T_1 will be the ground state of the electron, while T_2 will correspond to the excited state with a slightly higher energy.

The electron in the T_1 state, as well as in the T_2 state, spends half of its time around the nucleus A and the other half around the nucleus B.

We can also estimate the mean frequency of the periodic transit of the electron from A to B and viceversa, or of the neutral or ionized state exchange between the two atoms, thus finding

$$\nu = \frac{E_2 - E_1}{h}$$

where h is the Planck constant. For large values of r, $E_2 - E_1$ decreases according to an exponential-like curve and thus the exchange frequency rapidly tends to zero, this meaning that the electron which was initially placed around A remains here for an increasingly larger time, as expected from a classical point of view.

If the electron is in the state T_1, that is in its ground state, its energy (E_1) is lower than he would have without the mentioned exchange effect between nuclei A and B. This occurrence gives origin to a novel kind of attractive forces among the nuclei, in addition to the polarization forces considered above, and are exactly the dominant cause of the molecular bonding.

The resonance forces, as said, has no analogy in Classical Mechanics. However, as long as the analogy leading to the correspondence between a quantum state and a statistical set of classical motions can hold, the two states T_1 and T_2, where the resonance forces have opposite sign too, each one result composed identically by half of both the original unperturbed states S and S'. This, however, is true only at a certain approximation, that is exactly at the approximation where we can neglect the resonance forces. For an exact computation taking into account the resonance forces we must necessarily use Quantum Mechanics, and thus find a *qualitative* difference in the structure of the two quantum states that manifest itself mainly in the intermediate region between A and B through which a periodic transit of the electron between one atom and the other takes place, according to a mechanism that cannot be described by Classical Mechanics. Such a qualitative difference is purely formal in nature and we can deal with it only by introducing the wave function $\psi(x, y, z)$ that, as known, corresponds in Quantum Mechanics to any possible state of the electron. The modulus of the square of ψ, which can also be a complex quantity, gives the probability that the electron lies in the volume unit around a generic point x, y, z. The wave function ψ must then satisfy to a linear differential equation and thus we can always multiply ψ in any point by a fixed real or complex number of

modulus 1, this constraint being required by the normalization condition

$$\int |\psi^2| \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z = 1$$

which is necessary for the mentioned physical interpretation of $|\psi^2|$. The multiplication of ψ by a constant of modulus 1 leaves unaltered the spatial distribution of the electronic charge, and has in general no physical meaning. Now we will formally define the reflection of a quantum state with respect to the middle point O between the two nuclei A and B directly on the wave function ψ, by setting

$$\psi(x, y, z) = \psi'(-x, -y, -z)$$

in a coordinate frame with origin in O. If ψ should represent a symmetric quantum states, and thus invariant by reflection in O, the reflected wave function ψ' must have the same physical meaning of ψ and thus differ from ψ, for what said, for a real or complex constant factor of modulus 1. Moreover such a constant factor has to be ± 1, since its square must give the unity, due to the fact that by a further reflection of ψ' with respect to the point O we again obtain the initial wave function ψ. For all the states of the system we than must have:

$$\psi(x, y, z) = \pm \psi(-x, -y, -z)$$

where the $+$ sign holds for a part of them, and the $-$ one for the others. The formal difference between the T_1 and T_2 states considered above consists precisely in the fact that, in the previous equation, the upper sign holds for T_1 while the lower one for T_2. The symmetry with respect to one point and, in general, any symmetry property, determines a formal splitting of the state of the system in two or more sectors, an important property of this splitting being that no transition between different sectors can be induced by external perturbations respecting the symmetries shown by the constraints of the system. Thus in systems containing two electrons, we have two kinds of not combinable states which are determined by the fact that the wave function, which now depends on the coordinates of both the electrons, remains unaltered or changes its sign by exchanging the two identical particles. In the special case of the helium atom this gives rise to the well known spectroscopic appearance of two distinct elements: parahelium and *orthohelium*. The theory of the chemical affinity between the neutral hydrogen atom

and the ionized one, which we have considered until now, can be extended
to the study of the neutral hydrogen molecule and, more in general, of
all the molecules resulting from two equal neutral atoms. Instead of only
one electron moving around two fixed protons, for the neutral hydrogen
molecule we should consider *two* electrons moving in the same field, ne-
glecting at a first approximation their mutual repulsion. The stability
of the molecule can then be understood by assuming that each of the
two electrons lies in the T_1 state, corresponding to attractive resonance
forces. According to F. Hund we can say that the hydrogen molecule
is kept together by two "bounding" electrons. However the interaction
between the two electrons is so large to leave only a qualitative explana-
tion for the schematic theory by Hund, but in principle we could predict
exactly all the properties of the hydrogen molecule, by solving with a
sufficient precision the equations introduced by Quantum Mechanics. In
this way, with appropriate mathematical methods, we can effectively de-
termine the chemical affinity between two neutral hydrogen atoms with
only theoretical considerations, and the theoretical value agrees with
the experimental one, given the precision of the computation imposed
by practical reasons.

For molecules different from the hydrogen one, the theory of the chemi-
cal affinity is considerably more complex, due both to the larger number
of electrons to be considered and to the Pauli principle, forbidding the
simultaneous presence of more than two electrons in the same state;
however the different theories of the chemical affinity proposed in the
last years, each of which has an applicability range more or less large,
practically consist in the search for approximated computation methods
for a mathematical problem that is exactly determined in itself, and not
in the enunciation of novel physical principles.

Then it is possible to bring the theory of the valence saturations back to
more general principles of Physics. Quantum Mechanics opens the road
to the logic unification of all the sciences having the inorganic world as
a common object of study.

Acknowledgments

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