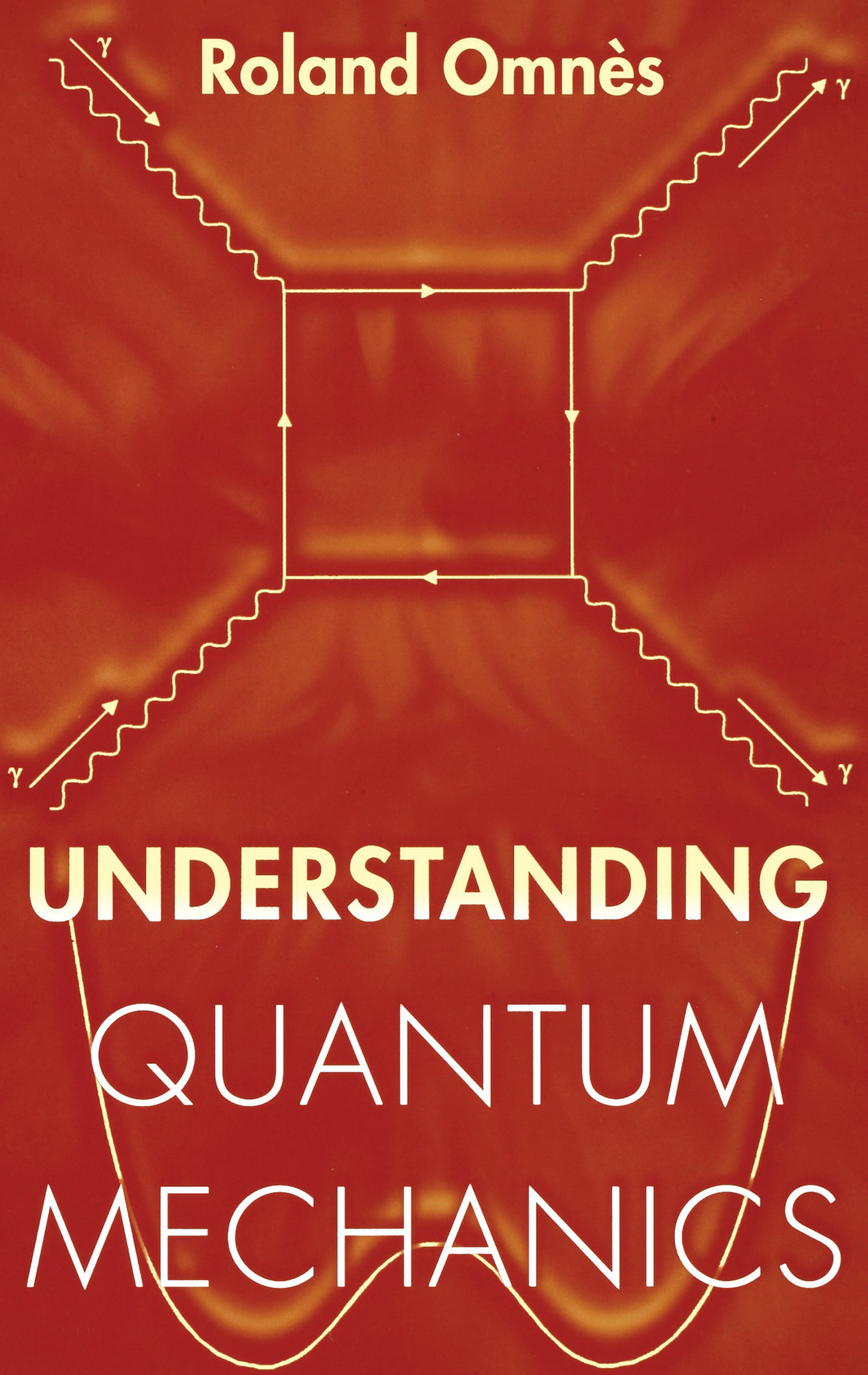

Roland Omnès

UNDERSTANDING QUANTUM MECHANICS

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To Liliane

Contents

Preface

The aim of this book is to explain the interpretation of quantum mechanics, simply and completely if possible. It is addressed to beginners with some elementary knowledge of quantum theory and also to physicists wishing to refresh their memory and see what the present state of interpretation is.

There are many textbooks on quantum mechanics, but most of them do not give much space to interpretation and a book such as this one might be a useful complement to them. One of the meanings of "interpreting" is "understanding," and we all know that this is the main difficulty of quantum mechanics. Can it really be understood ? I think now it can.

Bohr, Heisenberg, and Pauli laid the foundations for interpretation long ago, and nothing that has since been discovered really undermines that groundwork. Some portions of their work have been revised, however, and others were found to be incomplete. Rather than replicate the writings of the founding fathers here, it would certainly be more faithful to their spirit by updating them rather than by repeating them.

Two important discoveries led to a revision of the old interpretation. The first one was the notion of decoherence, an effect explaining why no quantum interference can be seen at a macroscopic level and removing the perennial difficulty known as the Schrödinger cat problem. Decoherence was proposed in 1954 and was seen experimentally in 1996. It is now essential to an understand of quantum measurements. The second advance came in the last two decades from a full insertion of classical physics into the framework of quantum physics. Classical determinism was thereby found to be the direct consequence of a fundamental quantum probabilism, whose only remaining effect at our macroscopic level is that every causal prediction has a tiny probability of error. These results, the outcome of work by many people, shed a completely new light on interpretation.

A third important idea, consistent histories, was put forward in 1984 by Robert Griffiths and was not always clearly understood. Some people believed that it was an attempt (necessarily doomed to failure) for reintroducing a simple-minded realism into the quantum world. Histories have nothing to do with that. They rely directly on the basic principles of the theory and they give us a method, the means for clarifying and organizing interpretation, which can so easily turn into a quagmire, or a maze. Histories are also the foundations of a new language. One can do without them if one does not wish to change old habits, just as one can dig out the foundations of a building with a shovel rather than an excavator.

I wished to provide the reader with a convenient textbook and not a detailed treatise, and this aim entails a few consequences. I avoided difficult proofs and long calculations, replacing them as far as possible, by simple arguments. I refrained from recounting some trends of research, however deep or brilliant, that would be too speculative. The commentaries at the end of the book provide some recommendations for supplementary reading as well as for more technical information.

Physics will remain at the center of this book, but there will be little foray into epistemology. Philosophical issues cannot be completely ignored, however. I will not enter upon the difficult (or perhaps too trivial) question of realism because my emphasis will bear on the pragmatic aspects of physics. Even so, quantum mechanics requires a new way of understanding, as Bohr, Heisenberg, and Pauli knew, and if one is so bold as to take issue with Richard Feynman's famous saying—"nobody understands quantum mechanics!" (1965c, p. 129)—one must say not only how quantum mechanics can be understood, but also why, and what perspectives this understanding reveals.

I wrote another book on a similar topic a few years ago (*The Interpretation of Quantum Mechanics*, Princeton University Press), and I owe the reader an explanation for why a new one is proposed. First, there is a significant difference in emphasis: the present book is much less technical and more explanatory. A fair number of people kindly told me that something more accessible would be useful for students as well as for physicists with a cultural interest in interpretation and I tried to answer the request. A second reason is that research is active in this field and quite several significant results could be added.

Five important new features appear in this new book. The first one originates in a reading of the pioneers of interpretation and their commentators. I learned particularly from Dugald Murdoch and Catherine Chevalley of the inquiries by Bohr, Heisenberg, and Pauli on the language of interpretation. I realized better on this occasion the true nature of consistent histories and the existence of a wider frame for them. They are effectively a language for interpretation. This language has two faces, two versions: a direct one that can be expressed in plain English (or any other vernacular language) and an abstract one relying on mathematics and rooted in the basic principles of quantum mechanics. The second is a universal language: it can deal with atoms, particles, and also with experimental devices as well as with any ordinary object we can see or touch. It is also a rational language with a clear and explicit logical framework. When seen in that light, there is no possible confusion concerning the nature of histories. They are part of the universal language of interpretation. No language defines reality: it can only say what we know of reality. And we know much.

The second feature involves recent progress concerning decoherence. It has been observed, and more powerful theories now exist for it. Decoherence now appears to be an irreversible process, the strongest one in existence, and thus sheds a new light on time, logic, and irreversibility.

The third feature arose from a criticism of decoherence by John Bell and Bernard d'Espagnat. They said that decoherence cannot provide an explanation of the basic problems of interpretation but rather that it hides them by offering an answer valid "for all practical purposes," that is, an answer agreeing with any possible experiment and thereby forbidding us to see more deeply beyond these experiments. I came to the conclusion that these so-called fundamental questions hinge on the meaning of extremely small theoretical probabilities. An interpretation of probability calculus must therefore stand at the entry to an interpretation of quantum mechanics, and the most convenient one was proposed by Émile Borel: an event with too small a probability should be considered as never occurring. From an empirical standpoint, a very small probability is one which cannot be measured by any experimental device that can be realized, or even conceived, in the universe. One can then assert that decoherence cannot be bypassed and is really fundamental.

The fourth feature is also essential. When I wrote *the Interpretation of Quantum Mechanics*, the reader was left with a problem having no solution. This is the so-called *objectification problem*, which concerns the issue of the existence of a unique datum at the end of a quantum measurement. This looked like a big deficiency because many specialists claim that here lies "the" problem of interpretation. When looking at it, thinking of it, dreaming of it, I realized that it might be a false problem. It originates in a traditional line of thought that has no sure logical foundations. When decoherence is taken into account, one finds that the universal language of interpretation cannot encompass anything other than a unique datum, in agreement, of course, with observation. Said otherwise, there is no sound language in which the objectification problem might be stated, so therefore it may very well not exist. I must note that these ideas are an elaboration of previous insights by Robert Griffiths, Murray Gell-Mann, and James Hartle.

The last feature has to do with the meaning of probabilities and the randomness of quantum events. Probabilities enter the language of interpretation by the back door: they are found necessary for providing this language with a logical backbone. The relation with empirical randomness looks rather far-fetched, and it was not clearly explained in my previous book (as a matter of fact, it was not yet clearly understood, either). Here again, one finds that the language we must use cannot deal with anything other than random events. This may be not an explanation, like one could also say of objectification, but it is a logical necessity.

Finally, I may add that no effort has been spared for keeping the present account of interpretation as close as possible to the Copenhagen interpretation. There are four good reasons for doing so. As a complement of standard textbooks, this book would have been useless if it contradicted what one usually learns. It does not. Furthermore, the Copenhagen rules are used everyday in the practice of physics, and because they are correct, my task was to explain why without undue rewriting. It turns out also that histories can be considered as a systematic use of imaginary measurements, as used in Heisenberg's works. As to the last reason, I thought that showing another instance of two approaches, leading to the same conclusions through very different ways, is a beautiful example of the unity of physics.

To make the reader find his or her way more easily through this book, I may say how it is organized. There are three parts. The first one is a brief sketch of the early history of quantum mechanics. I am aware of a fashion in modern books to proceed as if everything worth knowing in science was discovered in the last decade, but it would not work here. On the contrary, I decided to start with a history, because some questions are much better appreciated when one sees them developing from the beginning, as well as how deep they go. There is a strong continuity in quantum mechanics and its interpretation, and I felt that the historical dimension is not only useful but also illuminating. Even if not answering them completely, one cannot ignore such questions as: How came this splendid theory, which needs another theory for being understood? Could it be otherwise? On the other hand, the Einsteinian question, "Should not it be otherwise?" is answered in the two following parts, showing the consistency of interpretation and the completeness of standard quantum mechanics.

The second part of the book is another brief history, this one of interpretation. Interpretation is often confusing and, I tried to provide an orientation.

There are three chapters in this second part. The first one is devoted to the Copenhagen interpretation, a name I propose reserving for the ideas expressed by Bohr, Heisenberg, and Pauli—and of nobody else. The second chapter is a summary of basic contributions, mainly by John von Neumann, that were not integrated in the standard Copenhagen interpretation. The most relevant criticisms by Einstein and Schrödinger are also discussed here. They had an essential role in keeping the question of interpretation alive and pointing out the most important questions. Other proposals and events, particularly around Bell's contributions, are also mentioned, even if very briefly.

The third chapter (Chapter 7 of the book) might be called a keystone, and the reader in a hurry might directly start from it. It is a nontechnical summary of the main aspects of a consistent interpretation of quantum theory establishing its completeness. It cannot be easily condensed, and I therefore will not describe it in this foreword.

The third part of the book is the longest one. It further develops the points indicated at the end of the second part. It does not refer to historical matters and gives a rather detailed and systematic account of interpretation.

The present book relies heavily on essential works, particularly by Murray Gell-Mann, Robert Griffiths, Serge Haroche, James Hartle, Jean-Michel Raimond, Hans Dieter Zeh, and Wojciech Zurek. It also relies on important ideas or advice from Roger Balian, Bernard d'Espagnat, and Lars Hörmander. I benefited immensely from exchanges with these wonderful people. Many others—too many to thank by name—helped me in this enterprise throughout the years.

I also wish to thank the staff of Princeton University Press and Gail Schmitt for her treatment of the manuscript, particularly her improvement of my English.

PART ONE

The Genesis of Quantum Mechanics

1

The Discovery of Planck's Constant

WHY ONE RELIES ON HISTORY

1. There is so wide a chasm between classical and quantum physics that one still marvels that it could be bridged. These two conceptions of the world are almost opposite in every respect. Classical physics relies directly on a reality that one can see and touch, on which one can act. It is basically causal, to the extreme of determinism. On the other hand, quantum physics deals with a world inaccessible to our senses and our common sense, a world that can only be described by abstract mathematics. The most commonplace objects have a shadow of wave functions, simple quantities become matrices, operators, pure constructs of pure mathematics. In place of the excessive certainty of determinism, one is facing absolute randomness. Could there be a more drastic opposition?

These two visions of the world agree, however, and it is now known that classical physics is a consequence of quantum physics. Under everyday circumstances, in our familiar surroundings so far from the atomic scale, quanta become classical. The question of how that happens cannot be separated from a preliminary one, which is how humankind succeeded in bringing to light an atomic world so far from intuition; that is, how its strange concepts were discovered. Our main task in this book will be to understand those concepts, and to do so requires that we look at their origin and make sure of their peremptory necessity.

During the nineteenth century, most chemists had become convinced of the existence of atoms, bound together in molecules and being transferred from one molecule to another during a chemical reaction. Physicists had also understood that the smallness of molecules can explain the laws of thermodynamics. There remained many nagging questions nevertheless. The existence of solid bodies showed that atoms cannot penetrate each other but that they can bind together in a molecule. What kind of force can be responsible for both attraction and repulsion? How can electrons find their way among the compact stack of atoms in a copper wire when there is an electric current? The list of questions was long, so long as to make Nietzsche speak of the existence of atoms as "the most refuted theory," but all the questions boiled down to a unique one: What are the laws of physics in the case of atoms?

The detailed story of the answer, the discovery of quanta, is complicated. It is full of distracting events, with ideas of genius intermingled with errors, and with many forbidding obstacles all along the way. This story holds the key for understanding why a very drastic change had to occur in science. If I were to leave history aside, I could perhaps describe more concisely the present state of knowledge, but with the desire for full understanding, we always need to retrace the old paths and again ask the old questions. The real difficulty in understanding an idea, a vision, or a concept can always be measured by the time it took for humankind to create and master it. This is why there is nothing better than the papers by the pioneers, because nobody else was more oppressed by the anguish of understanding. This is why perhaps understanding with no help from history requires more exertion and cleverness than having the patience to learn from it.

When history is used for the sole purpose of understanding science better, it must not get lost among details and must concern only what is really essential. This is why, while using the rigorous work of historians, I will look at a history of quantum mechanics that has been simplified with the help of later knowledge. This procedure would be a sin for a historian, who must reject anachronisms, but it may be justified when timeless laws (those of nature) are at stake and their existence can shed light on their discovery.

Perhaps the best summary of the story is Einstein's famous sentence: "The Lord is subtle, but He is not wicked." It looks as if there had been privileged pathways offering entries in the maze of atoms, a few fortunately simple and revealing problems, perhaps the only ones that could lead from the clarity of classical thought to the depth of quanta. History took these paths, and even now with our accumulated knowledge, we cannot conceive of other ones that could have been pursued. There were two providential problems: the harmonic oscillator and the hydrogen atom. Planck's constant, the touchstone of quanta, is revealed in its purity by the oscillator. The hydrogen atom is the other "paradigm," whose peculiar virtue is that it shows no essential difference between the deepest energy levels and almost classical ones. These two problems became the keys to quantum physics.

2. The first period in the history of quantum mechanics concerns the problem of the oscillator, which began in the middle of the nineteenth century, reached an apex in 1900, and was practically solved by 1911.

The answer is clear: some subtle laws of physics govern harmonic oscillators. They depend upon only one quantity, Planck's constant h, which is dimensionally an "action" (ML^2T^{-1}). It is extremely small ($6{,}6262 \times 10^{-34}$ joule/second). The only possible values for the oscillator energy are discrete and are given by $n\,h\nu$, n being an integer.

A few comments might be useful before describing how these results were obtained. It was surprising to find action playing a fundamental role in microscopic physics. No experimental device can measure an action. This notion appeared for the first time in mathematical theories with the principle of least action of Lagrange and Hamilton, which had obscure foundations. An oscillator is, on the contrary, a very simple system. It depends on a position variable x, with a kinetic energy $\frac{1}{2}m$ $(dx/dt)^2$ and a potential energy $\frac{1}{2}m\omega^2x^2$ so that x is an oscillating function of time x_o cos (ωt-*constant*) with a frequency $\nu = \omega/(2\pi)$. The coordinate x is not necessarily a length, so that the inertia coefficient m is not always a mass (one may think of x as an electric charge; m is then a self-inductance). This freedom on the dimension of m may partly explain why the properties of a quantum oscillator do not depend much on this parameter.

Three different kinds of oscillators had a role in the story. The first type was abstract: a purely theoretical construct that was used by Max Planck as a tractable model of matter. The second included electromagnetic oscillators, also theoretical notions, which provided a convenient representation of radiation. Their properties were essentially equivalent to Maxwell's equations from the standpoint of dynamics and, when quantized, they became *photons*. The third species of oscillator was the only physically manifest one because it consisted of the elastic vibrations of a crystal. They became *phonons* in their quantum version.

BLACK BODY RADIATION

3. The first chapter of the story began in 1859, when Gustav Kirchhoff tried to explain the thermal radiation coming from the sun, a star, or a fireplace. The only theory at his disposal was thermodynamics, but he was able to apply it to this problem. A body in thermal equilibrium at a temperature T emits radiation through its surface. By $E(\nu)\Delta\nu$ I will denote the energy emitted per unit area and unit time in a frequency range $\Delta\nu$. Kirchhoff took into account the absorption coefficient $a(\nu)$ of the body, which is defined as follows: when the surface of the body receives from outside a radiation with frequency ν and intensity I, it absorbs a fraction $a(\nu)I$ and reflects the fraction $(1 - a(\nu))I$.

Kirchhoff then considered the following situation. Two infinite plates made of different materials are facing each other and are kept at the same temperature T. There is radiation between the plates and it is also in thermal equilibrium. Using simple arguments, Kirchhoff showed that equilibrium requires the ratio $E(\nu)/a(\nu)$ to be the same for all materials, and it must therefore be a universal quantity. For a perfectly black substance (with an absorption $a(\nu) = 1$ for any frequency), the emissivity $E(T, \nu)$ coincides with this universal datum, whence the name of *black-body radiation.*

Later, in 1894, Willy Wien took another important step, again using thermodynamics. He considered a vessel at a temperature T in which there is a perfectly reflecting sphere ($a(\nu) = 0$). The sphere first expands, then contracts, slowly enough for the process to be adiabatic. There is a slight Doppler shift when thermal radiation is reflected on the moving surface of the sphere, and this is enough for producing some energy exchange between neighboring radiation frequencies. Using the reversibility of the complete cycle, Wien found that $E(T, \nu)$ depends on a unique variable. The result is formulated more precisely as Wien's displacement law

$$E(T, \nu) = \nu^3 F(\nu/T). \tag{1.1}$$

The function F appeared to be a fundamental feature of a natural law, and many experiments were conducted to obtain it while many theoretical investigations tried to predict it. I will not recount the difficulties that were encountered nor the necessary advances in measuring techniques that were made but will mention only an important result by Rayleigh, who apparently found the function F in June 1900. He used a standard result from classical statistical physics (the equality, or "equipartition" of energy among all the degrees of freedom) and applied it to the radiation oscillators. He found F to be a constant. The result is perfectly correct from the standpoint of classical physics but at the same time perfectly absurd because his expression predicts that the total radiation energy $\int E(T, \nu)\, d\nu$ is infinite. The prediction had, of course, little to do with experimental data, except at very low frequencies. Therefore, Rayleigh's assumptions, those of well-established classical physics, had to be questioned in this situation. The problem was still more important than had been anticipated.

4. For several years, Planck had been trying to obtain a theory of black-body radiation. He placed special emphasis on the fact that thermal radiation in a vessel does not depend upon which kind of material the vessel walls are made of. Why should one then worry about real matter, so complicated and so little known at that time? Why not use an ideal case? Planck therefore considered an abstract model

consisting of harmonic oscillators with various frequencies. (A model of matter made of oscillators might have been almost realistic. J. J. Thomson proposed soon after—in 1903—a model where each electron behaves like a three-dimensional oscillator.) He had at his disposal a preliminary result, which is clearer when expressed in a later version given by Henri Poincaré: the average energy of an oscillator in matter must be the same as the average energy of an electromagnetic oscillator having the same frequency. This result relied only on the laws of electrodynamics, and the problem of thermal radiation could then be reduced to a single question: what is the average energy U of a single oscillator (U being proportional to νF)?

In October 1900, Planck found an empirical formula that perfectly fitted the data:

$$U = \frac{h\nu}{\exp(h\nu/kT) - 1}, \tag{1.2}$$

where k is Boltzmann's constant. Planck had obtained this formula by trial and error, and one can understand his approach by noting that the function (1.2) is very simple when the ratio $h\nu/kT$ is either large or small. Planck knew how to obtain these limiting expressions by assuming the oscillator entropy S to be proportional to either U or U^2. *Interpolating* between these two expressions of entropy (i.e., setting $S = U^2/(a + bU)$), he had only to solve an elementary differential equation for obtaining U (since $dU = TdS$) to get equation (1.2). The essential novelty of the result is the occurrence of a new constant h, such that the product $h\nu$ is an energy, just like the quantity kT. This empirical approach gave no hint, however, about the meaning of the formula. It said that an energy $h\nu$ is important, but nothing in the known theory of a classical oscillator had anything to do with it. Nevertheless, it must have been the key feature missing in Rayleigh's argument.

Planck then had a stroke of real genius. Could it be that the oscillator energy is not a continuous quantity that changes gradually, as required by classical physics? Could it take only discrete values, integral multiples of $\varepsilon = h\nu$? If so, the calculation is easy. Boltzmann showed that the probability for a system at equilibrium to have an energy E is proportional to $\exp(-E/kT)$. If E can take only the values $nh\nu$ with n an integer, the corresponding probability p_n is proportional to $\exp(-nh\nu/kT)$, and the average energy of the oscillator is given by

$$U = \sum nh\nu p_n \Big/ \left(\sum p_n\right). \tag{1.3}$$

The result is in perfect agreement with equation (1.2) and was published by Planck in December 1900.

As a matter of fact, the calculation I have sketched is not exactly the one Planck made, but his result was immediately reconsidered in many different ways, among which was the one I mentioned. Soon after, Poincaré proved mathematically that the distribution (1.2) cannot be obtained if one does not assume that energy is "quantized."

PHOTONS

5. Planck believed that "matter" oscillators were quantized but that radiation oscillators were not. One may easily understand his standpoint. Soon after Planck's discovery, the most favored models of atoms considered them as a collection of oscillators. So little was known about atoms that they could bear the burden of explanation, whereas on the contrary, radiation was perfectly described by Maxwell's equations and it looked unquestionable. This solution did not convince Einstein. The equal average values for the oscillators in matter and in radiation suggested a bold premise: why not assume that the radiation oscillators are quantized?

This idea was supported by the properties of the photoelectric effect: When visible light or ultraviolet radiation strikes a metal plate, some electrons are extracted from the metal and are seen as an electric current. The number of electrons extracted per unit time is proportional to the radiation intensity, a property that can be attributed to energy conservation. Much more surprising is the all-or-nothing effect that occurs with a change in the radiation frequency. If the frequency is lower than some value ν_o (depending on the material), no current is produced. Above that value, the effect is fully active.

Einstein proposed an explanation for these observations in 1905. If one assumes that in a radiation with frequency ν the energy is carried in "grains" with an energy $h\nu$, then everything becomes clear. From the known electron emissivity of a hot metal plate, one knows that each electron needs a minimal energy W for getting out of the metal. A grain of light must therefore carry an energy larger than W for extracting an electron, wherefrom the threshold effect when W is identified with $h\nu_o$.

The existence of light "grains" or light "quanta," later to be known as *photons*, was much more difficult to accept than Planck's quanta. The community where Einstein's idea was best received, though not fully accepted, was among specialists of X-rays, because hard X-rays can leave straight-line tracks in a photographic emulsion and this is strongly reminiscent of a particle trajectory. The photon hypothesis was not fully supported by experiments until 1923, when Arthur Compton found that X-rays diffracted by electrons show a frequency shift corresponding exactly to a relativistic recoil.

THE SPECIFIC HEAT OF SOLID BODIES

6. The concept of quanta of matter seemed strange, but this could be attributed to the mystery of atoms. Perhaps, after all, they were only accounting for appearances, which might receive a better explanation with further research. As for light quanta, they were almost unbelievable. Yet, by the time of the Solvay Meeting in 1911, everybody, including the foremost physicists of the day, accepted the existence of quanta. One reason for this almost unanimous adoption is that it had been shown there existed real, undeniable oscillators clearly demonstrating energy quantization: the elastic vibrations in a solid body.

X-ray diffraction had shown that the atomic structure of crystals are regular lattices of atoms (or molecules). Every atom has a definite position in the lattice that minimizes the energy of the structure. If an atom is slightly drawn away from its equilibrium position by a small distance a, the change in potential energy is proportional to a^2 (because energy would not be minimal if it contained a term linear in a). It can be shown in these conditions that small collective motions of the atoms are elastic waves with a definite frequency, each wave being mechanically equivalent to an oscillator.

When applying Planck's formula to these oscillators, one easily obtains the average energy of a solid body at thermal equilibrium and, as a consequence, its specific heat. This was shown for the first time by Einstein in 1907, who used a rather crude model in which all the vibrations are given the same frequency. Some time later, Peter Debye improved the model by using a more reliable distribution of frequencies. The results were clear and convincing, and they explained the vanishing of specific heats at low temperatures, which had remained an unsolved puzzle that contradicted classical statistical mechanics.

In a later development in 1916 by Einstein and again concerning thermal radiation, he assumed that the photons can be absorbed *randomly* by an atom. The probability for absorbing a photon in a given mode (i.e., with definite wave-number and polarization), is obviously proportional to the number of photons N in that mode. As for emission, Einstein assumed it to be a kind of decay of an excited state, and he applied the empirical law for the radioactive decay of nuclei, thus obtaining a distribution in time for emission. In order to fall back on Planck's law, one must assume furthermore that the probability of emission is proportional to $(N+1)$. This surprising result can only be understood if one assumes that the $(N+1)$ photons existing after emission are perfectly identical, with no memory of which one of them has just been emitted. Probabilities thereby entered the physics of quanta for the first time, but their subtleties remained hidden behind the poorly understood law of radioactive decay. The idea of indistinguishable particles would remain anyway.

7. It is sometimes said that the early history of quantum physics is obscured by thermodynamics, yet nowadays these questions are approached in the opposite order. Thermodynamics follows from statistical mechanics, which deals with a large number of particles obeying quantum laws.

Harmonic oscillators were central to the first period in the history of quanta. They are so simple that no contradiction of classical physics could have been as clear, and they still remain by now the simplest and most versatile concept in quantum physics. This is because they involve only Planck's constant, and the quantization of energy is as simple as it could be: only integers enter into the calculations. Once it was elaborated, quantum mechanics found that the exact formula for energy is $(n+\frac{1}{2})h\nu$ rather than $nh\nu$, but the correction is of little ado. Discrete energies exist, and their complete disagreement with classical conceptions means that the latter are either incomplete or erroneous. Physics would have to explore the first alternative before being compelled to accept the second.

2

The Bohr Atom

8. The second period in the history of quanta began in 1913. It ended in 1925 when a new theory of quanta, our present quantum mechanics, was taking over. This is the time when the path of physics research is most obscure. The pioneers entered the quantum world with classical minds; they maintained almost all of the classical laws of physics, adding only a few special ones for atoms. It is easy for us now to see how delusive this program was and also how fortunate its final outcome was. It made the failure of classical thought obvious and brought the real difficulties to the surface. Still, it was only a prelude to the advent of a radically new mode of thought.

The overall results at the end of this period were quite valuable. Essential experimental data were obtained, and the mixture of success and failure in explaining them brought imagination and subtlety to the forefront. It is not easy, however, to recount the course of events in a tumultuous period during which ideas came and went. The essential point is perhaps that everything was tried by some of the best people in the entire history of physics to save the classical vision of the world, and yet they failed. Trying to be complete or precise in my narration would be practically impossible given such conditions. I will therefore mention only the main results that survived and try to convey how the search was successful.

THE BOHR MODEL FOR HYDROGEN

The Atom's Nucleus and Rutherford's Model

9. What does an atom look like? For a short time, a model constructed by J. J. Thomson in 1903 was favored. The atom was supposed to be a positively charged, homogeneous sphere inside which electrons moved. The most attractive feature of this model was that an electron behaves in these conditions like a three-dimensional harmonic oscillator and the corresponding frequencies were tentatively identified with the spectral ones.

A quite different structure of atoms resulted from some experiments with radioactivity, that were carried out by Hans Geiger and Ernest Marsden in Thomson's laboratory. In 1909 they observed a remarkable effect: when alpha particles (coming from a radioactive source) cross a thin metal plate, their trajectories can show strong deviations. In 1911 Ernest Rutherford determined the significance of this effect. A strong deviation of the trajectory meant that "something" inside the atom exerts a strong force on the alpha particle, and also that this something is heavy enough for sustaining the recoil. Electrons are too light for that. If the force is electric, it must be exerted at very short distances to be strong enough, so the scattering object must be very small, charged, and heavy, just like an alpha particle. This idea of something at the center of atoms—a nucleus—was checked by Rutherford. After a rather easy calculation of the various deviation probabilities, the agreement between the model and observation was excellent.

The analogy between Coulomb forces and gravitation forces implied strong similarities between an atom and a minute solar system. Nothing could have been simpler, at least at first sight, but hard problems were lurking ahead.

Atomic Spectra

10. Atomic spectroscopy had been the basis of Thomson's model. On the contrary, the one Rutherford proposed was very far from explaining anything in that field. Spectroscopy was nevertheless a well-developed science. The frequencies of emission (and absorption) lines in most atoms were known, at least in the visible domain and its immediate vicinity. Some relationships had also been seen among the data. In 1890 Johannes Rydberg made a discovery that became a principle of spectroscopy: The emission (and absorption) frequencies of an atom can be labelled by two numbers, n and m, and a frequency ν_{nm} can be written as a difference, $\nu_n - \nu_m$, between two reference frequencies in a catalogue $\{\nu_n\}$. In the case of hydrogen, a simple formula had been found by Johann Balmer (and also probably by Rydberg): $\nu_n = R_o/n^2$, n being an integer and R_o the Rydberg constant. But no one could provide an interpretation of these perplexing results.

Bohr's Model

11. The Rutherford model is particularly simple in the case of a hydrogen atom, having a single electron in Keplerian motion. Niels Bohr, a young Dane working in Rutherford's laboratory, however, made

a troubling observation: the electron is accelerated during its motion. According to Maxwell's laws of electromagnetism, an accelerated charged particle should radiate and thereby lose energy. The binding of the electron must increase to compensate for that loss, and as a result the electron will come closer and closer to the nucleus, finally falling onto it. A simple calculation shows that the collapse of the atom must be extremely rapid, almost instantaneous and, moreover, the resulting continuous radiation would have no similarity with the observed line spectrum.

This was not, fortunately, the first instance of a breakdown of classical laws. Planck and Einstein had already found ways out in similar circumstances. Rather than giving up Rutherford's model, Bohr wanted to take into account the existence of Planck's constant. The oscillator example, with its quantized energy levels, suggested that atom energies could also be quantized. Letting E_n denote the energy levels of hydrogen and using an analogy with the photoelectric effect, Bohr assumed that a photon can only be emitted when the atom energy falls from a level E_m to a lower one E_n. Energy conservation requires that the photon energy h_ν be equal to $E_m - E_n$, and one then gets immediately Rydberg's rule:

$$h\nu = (E_m - E_n); \quad \text{with } \nu = \nu_{mn} = \nu_m - \nu_n = E_m/h - E_n/h \qquad (2.1)$$

Because of the reversibility of the basic laws of physics under time reversal, emission is the process inverse of radiation, and the emission lines and absorption lines coincide. There is, therefore, no continuous spectrum, and the atom is stable in its lowest energy state, assuming there is one.

The energy levels E_n were known from the data (up to an additive constant), but the problem was understanding their values. In a classic article published in 1913, Bohr derived them in three different ways. They all yielded the same result, although none of them can be said to be really compelling. In a footnote Bohr mentioned that his results might also be obtained if one assumes that the line integral $\int p\,dl$ along the trajectory (p being the electron momentum and dl an element of length) is a multiple of Planck's constant:

$$\int p\,dl = nh. \qquad (2.2)$$

The result one obtains for the energy levels, using only circular trajectories, is

$$E_n = \frac{me^4}{2\hbar^2 n^2}, \qquad (2.3)$$

where m is the electron mass and e its charge. In the MKSA system of units, which is rather inconvenient for atomic physics, e^2 should be replaced by $e^2/(4\pi\varepsilon_o)$. The modern notation $\hbar = h/(2\pi)$ is also used in this equation.

First Confirmations

12. Bohr's results were in satisfactory agreement with the hydrogen data. The derivation of Rydberg's constant was enough for Einstein to recognize immediately the importance of the new discovery. Two startling events would soon convince most other physicists. First there was the solution of the ζ Puppis enigma. The star ζ Puppis had shown lines very similar to the hydrogen spectrum, except that R_o had to be replaced by $4R_o$. It was easy for Bohr to replace the hydrogen nucleus charge e by $2e$, the charge of a helium nucleus (the factor e^4 in equation (2.3) being replaced by $(Ze)^2e^2$ with $Z = 2$). The spectral lines of ionized helium had not yet been observed under laboratory conditions, but as soon as they were, Bohr's explanation was a complete success.

The other event, which convinced many sceptics, came from highly precise spectroscopic data. Equations (2.2) and (2.3) did not quite agree with the hydrogen data, which contained a slight error of the order of 1/2000. In classical mechanics, however, an electron does not revolve around the center of the nucleus, but around their common center of mass. Inertia is not governed by the electron mass m but by an effective mass $m' = mM/(m + M)$, where M is the nucleus mass. The correction is of the order of m/M, which is 1/1836 for hydrogen. When Bohr made the correction, the agreement with the data became almost perfect.

THE BOHR-SOMMERFELD THEORY

13. The conceptual framework of Bohr's theory had as yet little to do with quantum mechanics as we know it. Classical concepts were still directing the representation of atoms. They involved the electron trajectories, the motion itself, and the expressions giving the kinetic and potential energies. Planck's constant entered only in a supplementary condition, which selected the few permissible trajectories among the many possible ones. One can therefore characterize this kind of physics as classical physics with quantum addenda.

Bohr himself was far from convinced that his solution was akin to a final answer, and he believed that a deeper revision of physics would have to be made. Before doing so, however, the main task was to increase and organize the collection of experimental data, as was done from 1913 to 1925.

The Correspondence Principle

14. In his first paper Bohr had put forward a principle that was to become more and more important. It was the *correspondence principle*, which states that the laws of quantum physics must reduce to those of classical physics when quantum numbers, such as n, become large. As an example, one may consider one of the derivations Bohr had given for equations (2.2) and (2.3), using this principle (it was, by the way, the most convincing one). A charged particle having a classical periodic motion with frequency ν can only emit radiation whose frequencies are multiples of ν. This result follows from the emission theory of Maxwell and Hertz and, more generally, from a Fourier analysis of the motion. It is far from being satisfied by Bohr's model, but when the electron trajectory is big enough to look classical (or n large enough), one can apply the correspondence principle in the following way: The nearest one can approach classical continuous motion is to have the electron jump from a trajectory with a large value of n to the next one with the quantum number $n' = n + 1$. There is emission of a photon during the jump, and according to the principle, the photon frequency should be almost exactly the frequency of classical motion along trajectory number n. This gives equations (2.1–3), although an important proviso must be made: the "proof" is valid for large values of n, but the result is used for any value of it. What luck that it could work!

Sommerfeld's Rules

15. To turn Bohr's discovery into a general theory, it had to be extended to every atom and, in the case of hydrogen, include elliptic trajectories because Bohr had only considered circular ones. Arnold Sommerfeld solved the second problem in 1915 and, for some time, there was hope that the first one, although much more difficult and more general, might also be solved along the same lines.

Sommerfeld considered a physical system and described it in a standard classical manner by general time-dependent coordinates $q_k(t)$. They are not necessarily Cartesian coordinates with the dimension of a length; they can be, for instance, angles (if one thinks of a top, or rigid rotator, in which case Euler angles are the coordinates). Because Planck's constant has the dimension of an action, momenta in equation (2.2) must be replaced by something else having the correct dimension.

What else? Being well aware of classical mechanics, Sommerfeld introduced the Lagrange and Hamilton's conjugates of the coordinates.

Let us recall the principle: The position of a physical system is defined by some variables $q = (q_1, q_2, \ldots, q_N)$, velocities being the time derivatives $\dot{q} = \{\dot{q}_1, \dot{q}_2, \ldots, \dot{q}_N)$. Energy consists of a kinetic energy $T(q, \dot{q})$ (depending generally on q and $\dot{q}$), and a potential energy $V(q)$. The moment conjugate to the position variable q_k is defined by

$$p_k = \frac{\partial T}{\partial \dot{q}_k}. \tag{2.4}$$

It has automatically the right dimension for the product $p_k q_k$ to have the dimension of an action. One can draw from these equations the velocities $\dot{q}$ in terms of the moments $p = (p_1, p_2, \ldots, p_N)$ and the coordinates q. When written as a function $H(q, p)$ of these variables, the total energy $T + V$ is called the *Hamilton function* and the equations for dynamics become the *Hamilton equations*:

$$\frac{dq_k}{dt} = \frac{\partial H}{\partial p_k}; \quad \frac{dp_k}{dt} = -\frac{\partial H}{\partial q_k}. \tag{2.5}$$

This version of classical mechanics, more abstract than Newton's, became thereby more familiar to physicists and would soon become the language of quantum mechanics.

In the case of the hydrogen atom, the most natural position coordinates are the Cartesian coordinates of the electron, the conjugate moments being the components p_k of ordinary momentum. One can also use spherical coordinates (r, θ, ϕ). On an elliptic trajectory, the azimutal angle ϕ varies from 0 to 2π, the angle θ and the radius r oscillate back and forth between some extreme values. Sommerfeld's most important contribution was to notice that one can replace the unique condition (2.2) by a system of three conditions

$$\int p_r \, dr = n_1 h, \quad \int p_\phi \, d\phi = n_2 h, \quad \int p_\theta \, d\theta = n_3 h, \tag{2.6}$$

in which the integration over r and θ are performed on one oscillation (back and forth) of the corresponding variable whereas the integration over ϕ goes from 0 to 2π. The quantities n_j are integers.

These conditions can be combined so as to return to Bohr's condition (2.2) with $n = n_1 + n_2 = n_3$. The other two quantum numbers have a simple interpretation: The number n_3 (usually denoted by m and not to be confused with a mass) is related to the z-component of angular momentum by $L_z = m\hbar$. The quantity $(n_2 + n_3)^2 \hbar^2$ is the square of the angular momentum vector $L^2 = l^2 \hbar^2$. The three quantum numbers (n, l, m), characterize an energy state of hydrogen, and they soon became familiar to everybody.

By introducing elliptical Keplerian trajectories, Sommerfeld had made significant progress. He went further by considering a more general system with coordinates $\{q_k\}$, under the assumption that the kind of oscillatory motion for each coordinate, which is true for hydrogen, is still valid. The quantization rules become in that case

$$\int p_k \, dq_k = n_k h. \tag{2.7}$$

Unfortunately, the assumption of a multiperiodic motion is extremely restrictive and the physical systems for which it holds are quite exceptional. For instance, they do not include an atom with several electrons.[1] They do include, however, most systems for which the motion can be computed explicitly by analytical methods. These systems were the best known ones at that time and gave a temporary illusion that a generalization would be found. As time went on, however, this hope faded until it vanished completely, giving way to the hard truth: Sommerfeld's conditions required assumptions that were too special to be fundamental laws of physics.

LANDÉ'S RULES

16. Two cases in which Sommerfeld's method was successful were its explanations of the Stark and Zeeman effects in hydrogen. The Stark effect is observed when an atom is subjected to an external electric field: spectral lines split and mix. The Zeeman effect occurs in a magnetic field and gives only splitting: a multiplet of spectral lines replace a unique line.

That was the time when Hamilton's formalism took precedence over the Newtonian form of classical dynamics. The choice of variables that allows one to quantize a system under Sommerfeld's rules is rarely given by the ordinary Cartesian coordinates for position and velocity. The Stark effect in hydrogen, for instance, requires parabolic coordinates.

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[1] A precise definition of multiperiodic, or separable, systems relies on the Hamilton-Jacobi equation. It will be more in the spirit of this book to define them by their modern quantum version: they have a basis of energy eigenfunctions $\psi(q)$, each of which can be written as a product $f_1(q_1)f_2(q_2)\ldots f_k(q_k)$.