Chapter 1 : Holdings : Quantum theory of matter | York University Libraries

First published in , written by John C. Slater, who was a Professor of Physics at MIT. This book lays the groundwork for our current understanding of Quantum Mechanics and Quantum Physics.

The very nature of the quantum theory thus forces us to regard the space-time co-ordination and the claim of causality, the union of which characterises the classical theories, as complementary but exclusive features of the description, symbolising the idealisation of observation and definition respectively. Just as the relativity theory has taught us that the convenience of distinguishing sharply between space and time rests solely on the smallness of the velocities ordinarily met with compared to the velocity of light, we learn from the quantum theory that the appropriateness of our usual causal space-time description depends entirely upon the small value of the quantum of action as compared to the actions involved in ordinary sense perceptions. The quantum mechanics of particles and the competing "wave mechanics" had just been developed. Bohr saw these as complementary, the waves in space-time, the particles needing causal interactions This view is already clearly brought out by the much-discussed question of the nature of light and the ultimate constituents of matter. As regards light, its propagation in space and time is adequately expressed by the electromagnetic theory. Especially the interference phenomena in vacuo and the optical properties of material media are completely governed by the wave theory superposition principle. Nevertheless, the conservation of energy and momentum during the interaction between radiation and matter, as evident in the photoelectric and Compton effect, finds its adequate expression just in the light quantum idea put forward by Einstein. As is well known, the doubts regarding the validity of the superposition principle on one hand and of the conservation laws on the other, which were suggested by this apparent contradiction, have been definitely disproved through direct experiments. This situation would seem clearly to indicate the impossibility of a causal space-time description of the light phenomena. On one hand, in attempting to trace the laws of the time-spatial propagation of light according to the quantum postulate, we are confined to statistical considerations. On the other hand, the fulfilment of the claim of causality for the individual light processes, characterised by the quantum of action, entails a renunciation as regards the space-time description. Once again, space-time and causality are complementary views of classical concepts. Of course, there can be no question of a quite independent application of the ideas of space and time and of causality. The two views of the nature of light are rather to be considered as different attempts at an interpretation of experimental evidence in which the limitation of the classical concepts is expressed in complementary ways. The problem of the nature of the constituents of matter presents us with an analogous situation. The individuality of the elementary electrical corpuscles is forced upon us by general evidence. Nevertheless, recent experience, above all the discovery of the selective reflection of electrons from metal crystals, requires the use of the wave theory superposition principle in accordance with the original ideas of L. Just as in the case of light, we have consequently in the question of the nature of matter, so far as we adhere to classical concepts, to face an inevitable dilemma, which has to be regarded as the very expression of experimental evidence. Waves of radiation in free space and individual material particles are complementary Isolation is impossible. Property definitions and their observations require interactions. In fact, here again we are not dealing with contradictory but with complementary pictures of the phenomena, which only together offer a natural generalisation of the classical mode of description. In the discussion of these questions, it must be kept in mind that, according to the view taken above, radiation in free space as well as isolated material particles are abstractions, their properties on the quantum theory being definable and observable only through their interaction with other systems. Nevertheless, these abstractions are, as we shall see, indispensable for a description of experience in connexion with our ordinary space-time view. The difficulties with which a causal space-time description is confronted in the quantum theory, and which have been the subject of repeated discussions, are now placed into the foreground by the recent development of the symbolic methods. The "symbolic methods" are Heisenberg-Born-Jordan "quantum mechanics. An important contribution to the problem of a consistent application of these methods has been made lately by Heisenberg Zeitschr. In particular, he has stressed the peculiar reciprocal uncertainty which affects all measurements of atomic quantities. Before we enter upon his results it will be advantageous to show how the complementary nature of the description appearing in this uncertainty is unavoidable already in an analysis of the most elementary concepts employed in interpreting experience. The fundamental contrast between the quantum of action and the classical concepts is immediately apparent from the simple formulas which form the common foundation of the theory of light quanta and of the wave theory of material particles. In these formulae the two notions of light and also of matter enter in sharp contrast. While energy and momentum are associated with the concept of particles, and hence may be characterised according to the classical point of view by definite space-time co-ordinates, the period of vibration and wave-length refer to a plane harmonic wave train of unlimited extent in space and time. Only with the aid of the superposition principle does it become possible to attain a connexion with the ordinary mode of description. Indeed, a limitation of the extent of the wave-fields in space and time can always be regarded as resulting from the interference of a group of elementary harmonic waves. Now according to the relativity theory we have for a particle with the velocity v: The circumstance that the former is in general greater than the velocity of light emphasises the symbolic character of these considerations. At the same time, the possibility of identifying the velocity of the particle with the group-velocity indicates the field of application of space-time pictures in the quantum theory. The use of a wave description reduces sharpness in definitions Here the complementary character of the description appears, since the use of wave-groups is necessarily accompanied by a lack of sharpness in the definition of period and wave-length, and hence also in the definition of the corresponding energy and momentum as given by relation 1. They may be regarded also as signifying that the group as a whole has no phase in the same sense as the elementary waves. From equation 1 we find thus: In general, the conditions for attributing an energy and a momentum value to a wave-field by means of formula 1 are much less favourable. Even if the composition of the wave-group corresponds in the beginning to the relations 2 , it will in the course of time be subject to such changes that it becomes less and less suitable for representing an individual. It is this very circumstance which gives rise to the paradoxical character of the problem of the nature of light and of material particles. For a general definition of these concepts we are confined to the conservation laws, the rational formulation of which has been a fundamental problem for the symbolical methods to be mentioned below. In the language of the relativity theory, the content of the relations 2 may be summarised in the statement that according to the quantum theory a general reciprocal relation exists between the maximum sharpness of definition of the space-time and energy-momentum vectors associated with the individuals. Bohr may still hope to "reconcile" conservation laws by claiming space-time points are "unsharp" reminiscent of his BKS statistical conservation ideas. This circumstance may be regarded as a simple symbolical expression for the complementary nature of the space-time description and the claims of causality. At the same time, however, the general character of this relation makes it possible to a certain extent to reconcile the conservation laws with the space-time coordination of observations, the idea of a coincidence of well-defined events in a space-time point being replaced by that of unsharply defined individuals within finite space-time regions. This circumstance permits us to avoid the well-known paradoxes which are encountered in attempting to describe the scattering of radiation by free electrical particles as well as the collision of two such particles. Bohr-Kramers-Slater failed to combine instantaneous and discontinuous electron jumps with continuous radiation. Here Bohr hopes the electron can be spread out in a finite space-time region just as the radiation is? According to the classical concepts, the description of the scattering requires a finite extent of the radiation in space and time, while in the change of the motion of the electron demanded by the quantum postulate one seemingly is dealing with an instantaneous effect taking place at a definite point in space. Just as in the ease of radiation, however, it is impossible to define momentum and energy for an electron without considering a finite space-time region. Furthermore, an application of the conservation laws to the process implies that the accuracy of definition of the energy momentum vector is the same for the radiation and the electron. In consequence, according to relation 2 , the associated space-time regions can be given the same size for both individuals in interaction. A similar remark applies to the collision between two material particles, although the significance of the quantum postulate for this phenomenon was disregarded before the necessity of the wave concept was realised. Here this postulate does indeed represent the idea of the individuality of the particles which, transcending the space-time description, meets the claim of causality. While the physical content of the light quantum idea is wholly connected with the conservation theorems for energy and momentum, in the case of the electrical particles the electric charge has to be taken into account in this connexion. It is scarcely necessary to mention that for a more detailed description of the interaction between individuals we cannot restrict ourselves to the facts expressed by formulae 1 and 2 , but must resort to a procedure which allows us to take into account the coupling of the individuals, characterising the interaction in question, where just the importance of the electric charge appears. As we shall see, such a procedure necessitates a further departure from visualisation in the usual sense. In his investigations already mentioned on the consistency of the quantum theoretical methods, Heisenberg has given the relation 2 as an expression for the maximum precision with which the space-time co-ordinates and momentum-energy components of a particle can be measured simultaneously. His view was based on the following consideration: On one hand, the coordinates of a particle can be measured with any desired degree of accuracy by using, for example, an optical instrument, provided radiation of sufficiently short wave-length is used for illumination. According to the quantum theory, however, the scattering of radiation from the object is always connected with a finite change in momentum, which is the larger the smaller the wave-length of the radiation used. The momentum of a particle, on the other hand, can be determined with any desired degree of accuracy by measuring, for example, the Doppler effect of the scattered radiation, provided the wave-length of the radiation is so large that the effect of recoil can be neglected, but then the determination of the space co-ordinates of the particle becomes correspondingly less accurate. The essence of this consideration is the inevitability of the quantum postulate in the estimation of the possibilities of measurement. A closer investigation of the possibilities of definition would still seem necessary in order to bring out the general complementary character of the description. Indeed, a discontinuous change of energy and momentum during observation could not prevent us from ascribing accurate values to the space-time co-ordinates, as well as to the momentum-energy components before and after the process. The reciprocal uncertainty which always affects the values of these quantities is, as will be clear from the preceding analysis, essentially an outcome of the limited accuracy with which changes in energy and momentum can be defined, when the wave-fields used for the determination of the space-time co-ordinates of the particle are sufficiently small. Ironically, Max Born My Life, p. Heisenberg looked up the answers to all the questions he could not answer, and the optical formula for resolution became the basis for his most famous work just a few years later. Heisenberg says he was "brought to tears. The product of the least inaccuracies with which the positional co-ordinate and the component of momentum in a definite direction can be ascertained is therefore just given by formula 2. One might perhaps expect that in estimating the accuracy of determining the position, not only the convergence but also the length of the wave-train has to be taken into account, because the particle could change its place during the finite time of illumination. Due to the fact, however, that the exact knowledge of the wave-length is immaterial for the above estimate, it will be realised that for any value of the aperture the wave-train can always be taken so short that a change of position of the particle during the time of observation may be neglected in comparison to the lack of sharpness inherent in the determination of position due to the finite resolving power of the microscope. In measuring momentum with the aid of the Doppler effectâ€”with due regard to the Compton effectâ€”one will employ a parallel wave-train. For the accuracy, however, with which the change in wave-length of the scattered radiation can be measured the extent of the wave-train in the direction of propagation is essential. For simplicity, we here have regarded the velocity of light as large compared to the velocity of the particle. Indeed, the general theory of the Compton effect allows us to compute the momentum components in the direction of the radiation before and after the recoil from the wavelengths of the incident and scattered radiation. Even if the positional co-ordinates of the particle were accurately known in the beginning, our knowledge of the position after observation nevertheless will be affected by an uncertainty. Here, too, the product of the inaccuracies in the measurement of position and momentum is thus given by the general formula 2. Just as in the case of the determination of position, the time of the process of observation for the determination of momentum may be made as short as is desired if only the wavelength of the radiation used is sufficiently small. The fact that the recoil then gets larger does not, as we have seen, affect the accuracy of measurement. It should further be mentioned, that in referring to the velocity of a particle as we have here done repeatedly, the purpose has only been to obtain a connexion with the ordinary space-time description convenient in this ease. As it appears already from the considerations of de Broglie mentioned above, the concept of velocity must always in the quantum theory be handled with- caution. It will also be seen that an unambiguous definition of this concept is excluded by the quantum postulate. This is particularly to be remembered when comparing the results of successive observations. Indeed, the position of an individual at two given moments can be measured with any desired degree of accuracy; but if, from such measurements, we would calculate the velocity of the individual in the ordinary way, it must be clearly realised that we are dealing with an abstraction, from which no unambiguous information concerning the previous or future behaviour of the individual can be obtained. According to the above considerations regarding the possibilities of definition of the properties of individuals, it will obviously make no difference in the discussion of the accuracy of measurements of position and momentum of a particle if collisions with other material particles are considered instead of scattering of radiation. In both cases we see that the uncertainty in question equally affects the description of the agency of measurement and of the object. In fact, this uncertainty cannot be avoided in a description of the behaviour of individuals with respect to a co-ordinate system fixed in the ordinary way by means of solid bodies and unperturbable clocks. The experimental devicesâ€"opening and closing of apertures, etc. In tracing observations back to our sensations, once more regard has to be taken to the quantum postulate in connexion with the perception of the agency of observation, be it through its direct action upon the eye or by means of suitable auxiliaries such as photographic plates, Wilson clouds, etc. It is easily seen, however, that the resulting additional statistical element will not influence the uncertainty in the description of the object. It might even be conjectured that the arbitrariness in what is regarded as object and what as agency of observation would open up a possibility of avoiding this uncertainty altogether. In connexion with the measurement of the position of a particle, one might, for example, ask whether the momentum transmitted by the scattering could not be determined by means of the conservation theorem from a measurement of the change of momentum of the microscope â€" including light source and photographic plate â€" during the process of observation. Bohr famously defended the uncertainty principle against criticisms by Einstein in his " discussion with Einstein " at the Solvay conference. A closer investigation shows, however, that such a measurement is impossible, if at the same time one wants to know the position of the microscope with sufficient accuracy. In fact, it follows from the experiences which have found expression in the wave theory of matter, that the position of the centre of gravity of a body and its total momentum can only be defined within the limits of reciprocal accuracy given by relation 2. Strictly speaking, the idea of observation belongs to the causal space-time way of description.

Chapter 2 : BKS theory - Wikipedia

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While Europe dominated quantum theory, pragmatic American universities like Caltech excelled in experimental physics [3]. In the late s, however, the growing American appetite and capacity for theory heralded a shift in the quantum center of gravity. Before the s, U. Top American universities such as Caltech and the University of Chicago boasted adept laboratory physicists, having collectively housed three Nobel Prize winners in a span of just over two decades [4]. In contrast, nurturing theorists of a similar caliber faced logistical obstacles, among them a lack of funding, geographic isolation from European hubs of quantum theory, and professors who garnered respect as teachers but not research scientists. Additionally, reputation was at stake: The surge of interest in quantum theory among American physicists prompted new research funding that enabled institutional changes, such as postdoctoral fellowships and the creation of research centers like the Institute for Advanced Study that could attract a critical mass of theorists together to collaborate. The Rockefeller and Guggenheim Foundations gave funds for prestigious fellowships that gave newly minted, competitively selected American physicists the opportunity to tackle open research problems immediately upon earning their degrees [1]. On account of these funds and the departure from the strictly practical culture of pres experimental physics, American theoretical physics became a viable career for the first time. Physicists made effective use of this new funding by traveling between the U. For those who did not leave the U. Pioneers of quantum theory visited the Pasadena campus so that Caltech physicists could stay apprised of key developments in atomic theory and radiation. Even Einstein, who by the s was already a celebrity, lectured at Caltech during the winter terms from [6]. Similarly, on the other coast, Max Born lectured at MIT from and kept its physicists abreast of the ongoing developments [2]. Werner Heisenberg himself even came to America in as a missionary for the gospel of the Copenhagen geist, though he did not sway many Americans from their focus on phenomenology [7]. Underpinning the modernization of American theoretical physics research were scholar-politicians, reputable intellectuals who brought foreign research talent to the American academic job market and created a comprehensive quantum mechanics curriculum. In doing so, they restructured American universities to foster discoveries in quantum theory. Each leading American institution had its champion for the development of competitive theory departments: Some academic leaders exploited the free flow of physicists between Europe and the U. These foreign physicists were often compelled to leave their home countries to avoid persecution, although it should be noted that the U. Nonetheless, physics department leaders and administrators persistently recruited top foreign talent to their departments. The influx of stalwart theorists to the U. Among the emigrants that improved the standing of American theoretical physics were Samuel Goudsmit and George Uhlenbeck, who came to the University of Michigan. The Dutchmen had famously discovered electron spin, a property that had at first been misunderstood by even Wolfgang Pauli [1]. Wigner later won the Nobel Prize in Physics for, inter alia, his study of the strong nuclear force and quantum mechanical symmetries, which he carried out shortly after coming to the U. Scholar-administrators also created original coursework in quantum mechanics so that their students could graduate with a working knowledge of modern developments, and thus paved the way for comprehensive American theoretical physics training. Slater created MIT Course 8, developing lecture notes on atomic spectra and spin physics. A decade later, the prominent physicists of the day started to generate new pedagogy in earnest, creating extensive graduate courses on quantum mechanics and shortly thereafter on the early results in quantum field theory. With this curriculum, American-trained physicists were equipped to make original contributions to quantum theory. These American theorists thus not only sowed the seeds of theoretical physics institutions in the U. American theoretical physics was born out of the quantum revolution that began in Europe, but has now lived and thrived in the United States for almost a century. The author is a senior studying physics, mathematics, and computer science at the Massachusetts Institute of Technology. American Historical Review A History of Physics in the Twentieth Century. Historical Studies in the Physical and Biological Sciences Institute for Advanced Study. Accessed 19 April Fast Facts About Caltech History. The Earliest Missionaries of the Copenhagen Spirit. Office of the Historian. The Back Page is a forum for member commentary and opinion. The views expressed are not necessarily those of APS. Responses may be sent to: David Voss Staff Science Writer: Leah Poffenberger Contributing Correspondent: Levine Publication Designer and Production:

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Wave-Particle Duality of Matter Wave-like Behavior of Matter In , Louis DeBroglie hypothesized that if light, which everyone thought for so long was a wave, is a particle, then perhaps particles like the electron, proton, and neutron might have wave-like behaviors. For example, an electron with a velocity of 5. So, matter and light are composed of particles that have wave-like properties. The wave-like behavior is only observed on the subatomic length scales where the masses are small enough for the wavelengths to be detectable. Quantized States You may be wondering how does all this about wave-particle duality relates to the electronic structure of the atom. When the ends are fixed only certain discrete wavelengths frequencies are allowed which depend on the length of the string. The lowest frequency is called the fundamental or first harmonic and has no nodes. The next frequency is the second harmonic and has one node; it is twice the fundamental frequency. You can keep going, increasing the number of nodes, and increasing the frequency in multiples of the fundamental frequency. Now we use the analogy of the standing waves of a string because the wavefunction of an electron trapped between two walls would in the same way be constrained to be a standing wave with only discretely allowed wavelengths. That is, an electron trapped between two walls has its wavelength determined by the distance between the walls and the number of nodes. As in the case of the photon, the energy of the trapped electron is proportional to its frequency. The lowest energy is called the ground state and it has the fundamental frequency. The higher energy states are called the excited states and occur at harmonics multiples of the fundamental frequency. As you can see, the energy states of the trapped electron, just like its frequency, are discrete or quantized. Quantized means that there are only certain "allowed" energy levels or frequencies, and nothing in between. Trapped electrons have quantized energy levels for the same reason that the standing wavelengths we set up with our string are quantized What is the physical reality behind this wavefunction? So we have this picture where electrons, protons, neutrons, and photons are all particles with a wave-like behavior that causes them to constructively and destructively interfere with themselves, and to set up standing waves when confined within boundaries. But what is the physical meaning of this wavefunction that is associated with these subatomic particles? One interpretation is that the square of the wave function tells us the probability of finding an electron at that point x in space. Notice how the probability equals zero at the nodes, since the wave function is always zero at those points.

Chapter 4 : Quantum Theory of Matter | Grandinetti Group

John Clarke Slater (December 22, - July 25,) was a noted American physicist who made major contributions to the theory of the electronic structure of atoms, molecules and solids.

In further comments, [18] John Van Vleck pays particular attention to 1 the study of the spectra of hydrogen and ionized helium, [23] that J. He played a key role in lifting American theoretical physics to high international standing. Research during the war and the return to peace time activities[edit] Slater, in his experimental and theoretical work on the magnetron key elements paralleled his prior work with self-consistent fields for atoms [1] and on other topics at the Radiation Laboratory and at the Bell Laboratories did "more than any other person to provide the understanding requisite to progress in the microwave field", in the words of Mervin Kelley, then head of Bell Labs, quoted by Morse. Among these, George H. Vineyard received his Ph. This was in part to serve as a balance for electronic physics to survive the overwhelming growth of nuclear physics following the war". He wrote "During the fifteen-year life of the group some sixty persons were members and thirty-four took doctoral degrees with theses connected with its work. In my report I have been unable to separate the work of Slater from that of the group as a whole. Every member of the group was expected to contribute a summary of his own work and ideas to the Quarterly Progress Report". They were quoted widely for scientific and biographical content, in journal articles and government reports and libraries are starting to put them online. An early paper on augmented plane waves [57] used an IBM card programmed calculator. Molecular and atomic calculations also flourished in the hands of Fernando J. This initial work followed lines largely set by Slater. Michael Barnett came in He and John Wood were given faculty appointments. Robert Nesbet, Brian Sutcliffe, Malcolm Harrison and Levente Szasz brought in a variety of further approaches to molecular and atomic problems. Major pieces of work which he did coauthor dealt with applications of 1 group theory in band structure calculations [58] and 2 equivalent features of linear combination of atomic orbital LCAO , tight binding and Bloch wave approximations, to interpolate results for the energy levels of solids, obtained by more accurate methods, [59] People[edit] A partial list of members of the SSMTG Ph. Toronto, ab initio calculations, drug design. Kleiner, solid state physics, continued at Lincoln Laboratory. Parmenter, later Professor of Physics, U. Arizona, crystal properties and superconductivity. Slater has taken primary responsibility for planning the facilities in the new Center for Materials. These include a new Cooperative Computing Laboratory completed this year and equipped with an I. It embodied the ethos of interdepartmental research and teaching that Slater had espoused throughout his career. By , two years after Slater left, the MIT Physics Department "had a very, very small commitment to condensed matter physics" because it was so "heavily into high energy physics. Rose Mooney, a physicist, who moved to Florida with him in In , in his scientific autobiography, he wrote: It reminded me of the MIT department in the days when I had been department head there. It was a far cry from the MIT Physics Department which I was leaving; by then it had been literally captured by the nuclear theorists. Slater was also Committee Member for Dr. He and Rose said to Ravi that he had lost his books and research papers when the truck carrying his belongings overturned while moving from MIT to Gainesville. It took place at the end of his undergraduate days at MIT, when he wanted to stay on to do a Ph. You should find out how the rest of the world is. And I often advise my students the same way. Learn what the rest of the world is like. The variety is worth while. He was exceptional in that he persisted in exploring atomic, molecular and solid state physics, while many of his peers were coerced by war, or tempted by novelty, to divert to nuclear mysteries. Not least, his texts and his lectures contributed materially to the rise of the illustrious American generation of physicists of the s and s. The new generation that Slater launched from the SSMTG and the QTP took knowledge and skills into departments of Physics and Chemistry and Computer Science, into industrial and government laboratories and academe, into research and administration. They have continued and evolved his methodologies, applying them to an increasing variety of topics from atomic energy levels to drug design, and to a host of solids and their properties. Slater imparted knowledge and advice, and he recognized new trends, provided financial support from his grants, and motivational support by sharing the enthusiasms of the protagonists. In a slight paraphrase of a recent and forward looking comment of John Connolly, [86] it can be said that the contributions of John C. Slater and his students in the SSMTG and the Quantum Theory Project laid the foundations of density functional theory which has become one of the premier approximations in quantum theory today. These are available in several major research libraries. Introduction to Theoretical Physics. Introduction to Chemical Physics. Quantum Theory of Atomic Structure. Quantum Theory of Matter 2nd ed. Quantum Theory of Molecules and Solids, Vol. Electronic Structure of Molecules. Symmetry and Energy Bands in Crystals. Insulators, Semiconductors, and Metals. Solid-State and Molecular Theory:

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