

Reminiscences from Early Quantum Mechanics of Two-Electron Atoms

EGIL A. HYLLERAAS

University of Oslo, Oslo, Norway

MAYBE some of you will be dissatisfied upon learning that I am not going to talk in technical terms of the announced helium problem. I am afraid that, in that way, I should very soon have used up my time in writing equations, which all of you already know, on the blackboard; so I have rather chosen to call my lecture "Reminiscences from early quantum mechanics of two-electron atoms." This sounds like history, and it might well have been a good thing if I had been able to give you a reliable piece of the history of quantum mechanics. But that again is not in accordance with my abilities, nor with my aims. I prefer to talk quite freely of reminiscences coming into my mind. In our language this might be called "å spinne en ende," meaning perhaps something like "spinning a yarn," and is a method supposed to be used by old sailors. Another way of stating this might be to say, "What I am going to tell you might be thought of as 'nearly true.'"

In acting in this way I have, of course, already taken the highest possible advantage of being invited to this symposium as its honorary president. Privately, I am thinking that this must have very much to do with my age, rather than with my achievements, but officially, of course, I will try to behave as though it were otherwise.

For several months now, I have enjoyed myself by being a guest of the University of Wisconsin. The city of Madison should be praised for many things, for example, its beautiful nature and its fairly dense Scandinavian population. But I think that its University of Wisconsin should also be praised for having excellent leaders in scientific research, among whom are found Joe Hirschfelder and Julian Mack, whom, in addition, I have found, from personal experience, to be quite tolerable masters.

As a last step towards happiness, I would like to mention that Professor Löwdin has taken me to Florida for two months in order to save me from the cold winter up in Wisconsin. And now I think I should do my presidential duty by wishing all of you, in the name of Dr. Löwdin, a hearty welcome to this International Symposium on Atomic and Molecular Quantum Mechanics. May you have pleasure in it,

and may you learn from it. Personally, I have already met a number of colleagues here who have proved to be very anxious to come to this meeting or its preceding courses, as well as many who have expressed their great joy and satisfaction in having had the opportunity of joining corresponding courses or symposia in Sweden. The other way, I have also had complaints from European colleagues who, for some reason or other, have been prevented from coming.

For this reason, in addition to his great achievements in the quantum theory of atoms and molecules, we are very proud of Löwdin, not only in Sweden, but all over Scandinavia—a distinction which perhaps means about as much to you as a distinction between Minnesota, Iowa, and Wisconsin.

In the time allowed for this speech, I will choose to concentrate upon a certain period, which I would like to call the Golden Age of atomic physics and which I place in the years 1925–1930, or maybe a year or two more, until the overwhelming discoveries in nuclear physics began to flow. In particular, I shall concentrate upon the Göttingen school under the eminent leadership of Max Born, in a very happy and idyllic period of time, when the disasters of the first World War had begun to be forgotten, and a second one was not yet expected.

In this wonderful period of early quantum mechanics, when old bonds were loosening and things had to be put together in a new and different way, there was no escape from doing some piece of work if you just happened to be present at the right place at the right time, and so I, myself, hit upon the helium atom.

Göttingen was my first visit abroad, where I stayed most of the two years, 1926–1928, and a few weeks in the summer of 1931. Gradually, I became acquainted with, or at least learned to know, a considerable number of already recognized physicists and, even more, the physicists of the coming age. Some short visits to Berlin or other places extended this personal gallery to scientists like Einstein, Schrödinger, von Laue, and other Berlin physicists. In Leipzig I met Heisenberg, Hund, whom I already knew, and, for the first time, Felix Bloch, who is now at Stanford. For some foolish reason, I never came to Munich until long

afterwards, a year or two after the unexpected, accidental death, of Arnold Sommerfeld, whose famous book, *Atombau und Spektrallinien*, had been our student bible and contained the finest outlook to a new world that could ever be given. On the basis of later private correspondence I had come to think of Arnold Sommerfeld as a personal friend, so I regretted sincerely never having met him. Some years later, in 1933, I went to France and England on a rather nonscientific trip, and, while passing through Holland, I met my friend from years ago, H. A. Kramers, and, also, Paul Ehrenfest. In Paris I met both Irene and Frederic Joliot-Curie (Marie Curie had excused herself because of failing health). In England I met only a few of the Cambridge physicists. However, in 1934 at a conference in London and Cambridge, practically all the English physicists whom I knew by name were present, even the "grand old men," J. J. Thomson and Rutherford, together with Dirac, Darwin, Fowler, G. P. Thomson, the two Braggs, and, also D. R. Hartree and J. Lennard-Jones, and a number of French, American, and other scientists. There I also heard and saw for the first time young Fermi, speaking a very melodic Italian-English or maybe French. In France, in 1936, some acquaintances were renewed and some were new. In particular, I remember Bauer, Brillouin, de Broglie, Langevin, and his son-in-law, Solomon, who did not survive the war, and finally my half-Scandinavian friend, Dr. Rosenblum.

Of course, my best source of knowledge of contemporary atomic scientists was in the early thirties and, through the thirties until the war, the yearly meetings at Bohr's institute in Copenhagen. In these meetings you were sure to find colleagues from all parts of Europe and even quite a number from America—too many to be mentioned by name, even though they may have played an important role in the development of atomic (and maybe even more, in nuclear) physics. Even the most outstanding persons like Kramers, Ehrenfest, Pauli, Lise Meitner, and so on, did not come there to prove their prominence, but just to listen and learn.

May I—at the expense of your time—mention an event which has forever made a deep impression upon me, because it illustrates so nicely the role of scientific friendship in general and Niels Bohr's role in particular. For a couple of years the meetings ended up with some humorous performances directed preferably by Delbrück and Weisskopf, among which a new edition of Goethe's "Faust," on occasion of the discovery of the neutron, may have been the most successful; but what I am talking of now came a year

or two later. In the audience there was one person, who, more than any other one, heartily enjoyed the entertainment: this was Ehrenfest. On the final session the next day he gave a serious talk, thanking Providence that, still on earth, a man could be found like Niels Bohr. What I did not know and probably very few did know, was that, at the bottom of his heart, he had a serious grief. Only a few weeks later, his life came to an end.

I am sorry. Up to this point, I have been talking of things around myself, as a means for presenting my connection with science, it is true, but still I have been talking too much of myself. And now I must shock you by telling that I see no other way of expressing what I have in mind than to proceed along the same route and even directly tell of my own life. When I do so, I do it by virtue of my age. I always liked to be young or believe I were so. But now almost all my friends and colleagues at the University of Oslo whom, as a student or even as a member of the Faculty, I looked upon with reverence have retired and, of course, many of them have come to life's end. In this country I have been even more struck by learning how many scientists, well-known to me, whom for their early achievements I have thought of as seniors or my contemporaries, usually prove to be a number of years younger. Looking around in this audience, the majority of faces appear so young, that, quite certainly, their owners have received their education considerably after the period which I have just baptized the Golden Age and even may have been born after that time. Therefore, the few of you who can really claim to have grown up with atomic theory in those years of most intensive new creations are fairly quickly counted.

There is also another thing, quite outside of our subject, which I should like very much to stress on this occasion; that is the unbelievable progress in our century, not only in scientific research, but also in cultural life as a whole, which, of course, is mainly a product of scientific progress. For this purpose I want to make use of myself as a medium; if you like you may think of me as "the missing link." In the art of stretching the time coordinate far back into the past, I wonder whether anybody here could beat me, because I was born in a remote part in the sparsely populated country of Norway. Hence, as an artificial effect, you may perhaps feel rather that I am talking of things from eighty, ninety, or even a hundred years ago. Maybe it is worthwhile to stress first that, in the course of time, things have also changed very much towards the American way of life in our country. And this is caused by the last forty or fifty years

of "automobilism" and equally by lines of electric power stretched, during the last twenty-five years, to every house or hut in the part of our country of which I speak.

However, from my earliest youth, I remember the first very modest roads being built to replace the older trails or paths or water ways in order to make useful the 4000-year old invention of the wheel. The mail came once a week; another means for communication, unknown by earlier generations, was a primitive telephone line. I had not seen a railway train up to the age of seventeen, and many were those who never came to see one.

We lived in a community where nobody was wealthy. Also, fortunately, very few were really poor by our standard. From the age of about ten, youngsters were thought of as useful members of a family, who might, for instance, in summertime watch the cattle up in the mountains (on "fäbovallen" as it is called in Sweden). For this, one should not be pitied. Provided being in good health, which really appeared as a matter of course, I think we were neither more nor less happy than young people are today. In my mind there even is a rosy color now over this life of closest contact with nature. Ten hours a day in rain or sunshine, come what may. However, we learned to make a fire for our comfort, and on bright and warm days we were usually not far away from some small and cooling stream.

In wintertime, two-thirds of the year, we went to school in our homes in the valleys, three weeks in freedom and laziness being interrupted by six weeks at home devoted to what was thought of as useful work. We were also completely happy in the sense that the idea of higher education in the modern sense had no actual reality. Our tools were to be the hands, not the head. Of course, we did not highly regard what we had learned in our school, because that was common to all. Approaching the age of fifteen there might, therefore, be some bright young boys or even girls who were talking of going beyond the borders of our community to some recognized school on a higher level and there, in the course of a year or so, become quite learned people or at least entitled to form some sort of brain trust on their return.

However, this was not a static state of affairs in this century of progress. What applies to my earliest childhood does not apply as well to the end. In particular, the stress on education was an ever growing process all over the country. At the beginning of, and during, the first World War the number of young people who had acquired a fair amount of knowledge beyond that which was taught in the elementary pub-

lic school was steadily increasing, and perhaps it should be said that even our children's school was of a considerably higher quality than you might reasonably guess. And at the end of the war, a considerable number of young people from all parts of our country, coastline and countryside as well, began to invade even our highest center of education, the University of Oslo. In the years 1918-24 I, myself, joined this category of students, whose main activum, as a rule, certainly was their optimism—their firm belief in future success.

Particularly in the field of natural sciences, this was a student's life in the old sense, because unlike doctors and priests and lawyers, and more like the humanists, we were not to be cast in the same form. We could do what we chose to do, and nobody had a responsibility for the result, except ourselves. We thought that what we acquired in mathematics, physics, chemistry, or other fields was solid knowledge, and part of it was. But the top aim of our learning usually was to become useful teachers in our high schools, and none of us, or at least very few, would hit upon the idea of becoming scientists by profession.

Nevertheless, we could not avoid becoming a bit acquainted with scientific work and thoughts, because at the end we had to present a written and, as it was called, scientific paper. For my own part, as an assistant at the department of physics, I was taken away from the first planned studies of pure mathematics into applications which were more to my heart and even into matters of pure physical research. In particular, my field, in cooperation with Professor Vegard to whom I owe the highest gratitude, became that of the inner structure of crystals as explored by means of x-ray technique. Even with poor equipment for x-ray production and other necessities, as for instance an old dental high-voltage generator and self-made Debye-Scherrer cameras, this activity opened my eyes to the beauty of physical research, and the crystals became my first scientific love, besides, of course, applied mathematics in general.

Therefore, upon leaving the university and becoming a school teacher for a year or two and feeling quite happy, also, there among the young boys and girls, I could not forget about many problems of higher interest with which I had become familiar. Being cut off from experimental work, this interest had to be replaced by theoretical studies. Here I had the great luck of being acquainted with a wonderful book by none other than Max Born, professor of theoretical physics at the University of Göttingen.

This book bore the name *Dynamics of Crystal Lattices* or *Atomic Theory of the Solid State*, in either of two editions, and I felt that it crowned the knowledge I might already have acquired from books of such authors as Siegbahn, Ewald, Niggli, Wyckoff, Sommerfeld, and so on. Moreover, this book furnished a basis for actual theoretical work in the field which I loved so much, and, being happily free from much criticism, I even ventured to publish one or two papers based on calculations of double refraction of light in uniaxial crystals in relation to their crystal structures. The basis of this particular part of crystal theory was laid, as you would know, fairly early by P. P. Ewald, still the editor of *Acta Crystallographica*.

This activity was to become my fate. The papers were seized by my friend Professor Vegard, and, attached with some kind acknowledgments from Max Born, they provided me with what was called a Fellowship of the International Education Board from the always helpful United States. This meant that you need not work any more, might go where you liked, and still be paid as though you were of some use. So there was no escape any more. Like Julius Caesar at Rubicon—for nice comparison—I had to say: “*Jacta est alea*” and embark [in September 1926] for Göttingen and Max Born. But you soon will learn just how insufficiently I was prepared for the scientific life in Göttingen at this time.

First of all, I was heartily disappointed when Max Born told me that he was no longer working in the field of crystal lattice theory. His new field of investigation bore the curious name, “Matrix Mechanics,” and, as I understood it, had been invented by himself, or rather by some bright fellows by the names of Werner Heisenberg and Pascual Jordan. The latter was regarded in Göttingen as Born’s most prominent co-worker, the former, away somewhere in Copenhagen or Munich. Moreover, there was much talk of a curious sort of new waves called de Broglie waves. Obviously, they did not exist in the physical sense of the word, since they were running with superlight speed. Nevertheless, people persisted in talking of their wavelengths as something of particular importance, given by a simple formula reminding one of some sort of quantization. Non-existent waves in quantized form—quite a thrilling idea. Should I prefer them to my real crystals?

One day in the institute’s library, Dr. E. H. Kennard from the United States was sitting and reading something, which he told me was the Schrödinger wave equation, and he wondered why I was not doing the same, because that was just what people were

doing now. So you see, there were plenty of new things for me to take care of, and perhaps you may understand that I had more confidence in the real existence of my dear crystals. The shock I had received from Max Born had not quite knocked me down, and so I persisted for some time working in the field of crystal optics. I even succeeded in completing something which I thought of as a very fine piece of work—a calculation of the optical activity of the so-called β quartz, a high-temperature modification of quartz with somewhat simpler crystal structure. A preliminary report, from which I am myself now unable to reconstruct the whole work, was forwarded to *Zeitschrift für Physik*, obviously a compromise in competition with the too fast-running time. The main work, designed for *Zeitschrift für Kristallographie* and which I remember was clear in every detail, appears, however, never to have been forwarded to the *Zeitschrift für Kristallographie*, and the manuscript in the course of time seems to have disappeared. The real cause of this misfortune must have been my deep absorption in studies of the helium atom, but, even with success in this new field, I have never felt fully comforted for the loss of this dear work.

So I betrayed my first love and entered into love with a new one. Later on, I have had several loves, but with moderate success. Obviously, in such matters you must be young, or, as the Germans are singing: “*Das ist nur einmal; es kommt nicht wieder.*”

At this time the basic understanding of the helium atom with its two electrons and its double system of spectral lines or its para- and ortho-states was already established by Heisenberg. Also, a most interesting study of the wave function of the helium atom by Slater appeared fairly early, and I remember learning from it, particularly, I think, with respect to the mutual polarization effect between the two electronic distributions. Also, the wonder of chemical binding forces, as produced by the formerly unknown exchange integrals, was on the way to being understood, thanks to the application of wave mechanics to the hydrogen molecule by the world-renowned firm of Heitler and London. The former was a Göttingen man acting as Born’s assistant, and a not-too-sophisticated person, who was both able and willing to share his knowledge with less experienced people.

You will, I hope, forgive my patriotism when I tell you that Heisenberg’s theory of the helium atom was conceived in Norway. Heisenberg, perhaps the most wonderful of Sommerfeld’s “*Wunderkinder*” had not succeeded in acquiring a doctor’s degree in Munich. The main reason for this misfortune is said to be some unnecessary stubbornness, together with a complete

lack of knowledge of the theory of the lead accumulator. Max Born obviously did not pay so much attention to the lead accumulator, so in a very short time Heisenberg found himself a doctor of the Georgia Augusta University of Göttingen. Then he felt a deep desire for complete freedom and went to Norway, walking in the mountains for several weeks entirely alone and with no connection with his family. This might have cost him his life. One day, when trying to pass a stream, he fell into the water and had a very narrow escape. Back in some hotel he wrote his famous paper. How much the cold bath may have contributed to clearing his mind, I cannot tell.

On the whole, the scientific life in Göttingen appeared somewhat frightening to a newcomer like me. Born's seminars were no children's school. To me all his pupils appeared extremely learned men, using methods which I had not heard of and talking in technical terms whose meaning I did not quite realize. Closest to an exception from this rule was perhaps Max Born himself. At least sometimes in the general physical colloquium, I remember his proving his brilliant faculty for explaining even the deepest mysteries of quantum mechanics in simple words. As a master of teaching, I should also like to remember Friedrich Hund, who was a frequent visitor in Göttingen at that time, and who is now Born's successor there.

As is well known, wave mechanics at once reproduced all correct results obtainable from Bohr's theory, and the use of its much more convenient perturbation theory added considerably more, however, not always in the strict numerical sense. Now, particularly by Max Born, it was argued that the simplest crucial test of the correctness of wave mechanics in general was to be found in its application to the helium atom—in particular to the ground state.

As is well known from Sommerfeld's exposition of the matter in his *Atombau und Spektrallinien*, the Bohr theory, applying a definitely inconsistent *ad hoc* model of the atom with its two electrons in strictly opposite positions with respect to the nucleus, led to a numerical value of about 28 eV for the ionization energy of the first electron. On the other hand, a simple perturbation treatment of the Schrödinger equation, as given by Unsöld, led to a much lower value of about 20.3 eV. The true value of 24.46 eV, as known from spectroscopic measurement, was about in the middle in between. Hence, there was a broad gap of about 4 eV to be filled up.

The reason for the bad results is easily seen. In the Bohr picture, with the electrons held strictly at the

largest possible mutual distance, the interelectronic energy came out too low. In the wave mechanics picture with independent spherical electronic charge distributions, the interelectronic energy would be unreasonably high. About half of the gap might have been filled at once, by letting the two electronic distributions expand to a reasonable degree such that interelectronic repulsion and nuclear attraction would be more balanced. This means a minimization of the total energy and is best known from the use of a scale factor k , which, by the minimization process, also provides for the fulfillment of the virial theorem, which is no less important in quantum theory than in classical mechanics. Finally, if we would think of displacing the electronic charge distributions relative to each other, a bit to either side of the nucleus, remembering the Bohr picture, we would have what is called a polarization effect or correlation energy. But this requires a much more elaborate mathematical treatment.

As to the question of the scale factor or, what amounts to the same thing, a shielding constant or an effective nuclear charge, I remember a very early conversation with Dr. Kellner from Berlin and Professor Born, where I did not fully understand what was meant by something called an arbitrary nuclear charge. Later on, of course, it became clear to me that Born, in arguing for such a freedom in the procedure, was pointing to the use of the variational principle. Hence, the invention of the scale parameter can be traced back to Professor Born, or rather, as I believe, to Dr. Kellner.

A systematic attack on the ground-state problem of the helium atom had been planned by Max Born in cooperation with a pupil, Dr. Biemüller, since Born himself had no preference for numerical work. However, the enterprise came to a stop by the failing health of Dr. Biemüller before his work became particularly useful. If brought to an end, it would at all events have filled only about 2/3 of the gap between simple perturbation theory and spectroscopic measurement. This is an excellent example of the importance of the so-called completeness relation for systems of functions used for the purpose of solving variational problems or equivalent differential equations. Biemüller's use of strict hydrogen wave functions, or rather products of such functions of the two electrons' coordinates, could never have led to a better result. Owing to the existence of a continuous energy spectrum, the hydrogenic functions for the discrete spectrum do not form a complete system, and, even less, do the products of such functions form a complete functional system for the helium atom.

When Professor Born first suggested to me that—as he said—I was the right one to go on with the helium problem, I felt of course greatly flattered. The real cause for my turning that way was, however, that I felt I had gradually acquired some familiarity with the main principles of wave mechanics and, hence, was able to deem the problem as occupying my highest interest, not in the least because of its appealing “anschaulichen” character.

One thing which I noticed fairly soon was that solutions must exist which depend only on three coordinates, instead of the full number of six, and these were the coordinates r_1 , r_2 , ϑ , defining the shape of the electron–nucleus triangle, leaving its orientation in space out of interest. When confronted with this really useful simplification Born asked: “What does that mean? Let us consult Wigner!”

Eugene Wigner was already at that time a central person among the young Göttingen pioneers. He was suspected to be familiar with some kind of black magic, called group theory. This was several years before the culmination of the so-called “Gruppenpest,” when every paper on wave mechanics in order to be taken seriously had to start by stating the “group character” of its subject. Those who know Wigner will not hesitate to guess that he at once gave the correct answer: “Those states,” he said, “are the S states,” i.e., states with zero angular momentum.

Another, and deeper, question was that of the completeness of the functional system from which the wave function had to be built up. This problem was easily solved by removing from the argument of the Laguerre functions the main quantum number n , i.e., replacing r/n simply by r . This, in fact, means a transformation of the discrete eigenvalue spectrum E with series limit at $E = 0$ into that of $1/(-E)^{\frac{1}{2}}$ with series limit at infinity. In this way the continuous eigenvalue spectrum is thrown away, and the functional system becomes complete.

In connection with these mathematical aspects of the theory, it might be just to mention the valuable support for the whole Göttingen school provided by the two famous Göttingen mathematicians, Richard Courant and David Hilbert, and occasionally also Hermann Weyl, a visitor from Zürich. The excellent book by Courant and Hilbert, *Methoden der mathematischen Physik*, may be known to most physicists working in the field of quantum mechanics, and, in those early days, it was of course more badly needed than it ever has been since.

Courant was an excellent lecturer, playing on his audience like an instrument. Hilbert was quite different. As a professor emeritus and “Geheimrat,”

his lectures were given only accidentally and voluntarily, and out of pure interest for the new developments in physics. He never was in a hurry; on the contrary, he rather seemed to like to taste repeatedly on his own sentences. He was extremely popular, and it was a real pleasure to listen to his mild voice and look into his white-bearded gentle face. To him, the inventor of the Hilbert space, the pathways leading from matrix to wave mechanics, and *vice versa*, were of course no secret, and this he expressed in the funny way of shaking his head, saying, “Die Nobel-preise liegen ja auf der Strasse.” Again, talking of spectra and eigenvalue problems, in particular that of the hydrogen atom, he repeatedly murmured: “Runge sagte ja immer, die Eigenwerte müssen sich im endlichen häufen. Ja das sagte er, sie müssen sich im endlichen häufen.”

This brings me to a serious question with respect to the mutual interference of physics and mathematics. If the mathematicians of the eighteenthies or -nineties had been clever enough, or rather, if they had been much more interested in the physical world, why should they have left us merely with the simple acoustic vibrations of finite bodies? Why not extend their investigations to infinite, maybe artificial, bodies as already indicated by mathematical tools like Bessel, Hermite, and Laguerre functions? Finally, why not transform sets of infinite numbers of eigenvalues in a number of different ways and so be able to present before the poor spectroscopists mathematical systems well suited for the classification of spectral lines?

In this way it might well have happened that some bright boy might have hit upon the Schrödinger equation 25 years earlier, and the Thomson and the Bohr theories might never have existed. Admitted, the true nature of atoms and electrons would not have been well understood before the Rutherford disclosure of the smallness of nuclei, but a Schrödinger wave equation might have existed. The conclusion we must draw from this is that the mathematicians as a rule are masters of logic but poor inventors. A mathematician primarily guided by the physical way of thinking, like Erwin Schrödinger, was needed to find the way.

In those days an institute for theoretical physics was not supposed to be in need of any room for its own purposes. It existed as a formal entity in virtue of the presence of a professor or leader, mostly residing at his home. Nevertheless, Born had—apart from his own office—succeeded in acquiring a room for his institute in which I had the opportunity to work when needed, and in his humorous way he told

me how. One day James Franck came to him to explain how badly he needed a room which was just going to be finished at the institute. But now his senior colleague and Director at Ersten Physikalischen Institut, Professor Pohl, considered himself to possess the priority. Next day Pohl also came to Born for support, telling how badly he needed this new room, a matter of course which had now been questioned by their dear colleague, Professor Franck. Then it was Mrs. Born who hit upon the brilliant idea that Professor Born might also have need for it, and with this solution the two colleagues found themselves rather satisfied, seeing that at least the original competitor did not win the prize.

In this room was installed a 10×10 automatic electric desk computer, an excellent Mercedes Euclid, but strong and big as a modern electronic computer and, hence, with the faculty of giving out not only veritable acoustic waves, but even respectable shock waves. Now we all of us know that it does not work very well just to do one's job. In order to gain fame, it may be as important to make some noise about what you are doing, and in this respect the Mercedes Euclid helped me quite excellently. Even Herr Wachtmeister honored me with respect and left me alone in the late afternoons.

The end result of my calculations was a ground-state energy of the helium atom corresponding to an ionization energy of 24.35 eV which was greatly admired and thought of as almost a proof of the validity of wave mechanics, also, in the strict numerical sense. The truth about it, however, was, in fact, that its deviation from the experimental value by an amount of one-tenth of an electron volt was on the spectroscopic scale quite a substantial quantity and might as well have been taken to be a disproof.

The discrepancy continued to bother me for a long time but it was not until a year or so later after my return to Oslo that something began to clear up in my mind, and I think it was the word "completeness" which was constantly ringing in my ears. The inter-electronic term in the Schrödinger equation for two-electron atoms reads, if expanded in terms of Laplace angular functions

$$\frac{1}{r_{12}} = \sum_n \frac{r_1^n}{r_2^{n+1}} P_n(\cos \vartheta), \quad r_2 > r_1.$$

This expression has no close similarity to the fairly civilized terms which so far had been used in the trial wave function, say, powers of,

$$2r_1 r_2 \cos \vartheta = r_1^2 + r_2^2 - r_{12}^2,$$

that is, even powers of any of the three metric ele-

ments in the electronic configuration. Why now, I wondered, shall we have to supplement these expressions with odd powers of r_1 and r_2 and not with odd powers of r_{12} which, moreover, possess expansions similar to the above of $1/r_{12}$ and different in the two half-spaces $r_2 \gtrless r_1$. Obviously, therefore, using both odd and even powers of the quantity

$$u = r_{12},$$

the situation would change fundamentally, so why not try. I could not guess at that time that this should be called an invention and thirty years later still should be termed the Hylleraas method. What I really invented I felt was rather the left-hand side of the equation, the u , together with the $s = r_1 + r_2$ and $t = -r_1 + r_2$, forming the triple s, t, u , of which I am really proud. No hint of a loan from the velocity triple u, v, w of hydrodynamics or from other sources can be traced. The triple is forever reserved for atomic research.

To be just, the r_{12} had already been used in expressions for the wave function a year before in two articles in *The Physical Review* by J. C. Slater. Of these articles I may not have been aware, since only his first one from 1927 is cited in my papers.

This change of coordinates had, to my astonishment and to my great satisfaction as well, almost the effect of a miracle. Already in the third approximation, using only the additional terms u and t^2 , the troublesome discrepancy already told of, disappeared entirely on the electron-volt scale, although still considerable in spectroscopic units. But the tie was loosened and addition of a few more terms made the discrepancy disappear also on the spectroscopic scale within the limits of accuracy of measurements at that time. The rest became a matter of tedious and accurate calculations as improved from time to time by many authors, also myself, and, in particular, Chandrasekhar and Herzberg and their various co-workers. In the most recent time we have to point to the indeed wonderful calculations as performed by Kinoshita and Pekeris.

The result of the new method was published in the first half of 1929, but I was unaware of its recognition until I had presented it myself before Det Skandinaviske Naturforskermøte in Copenhagen in September of the same year. These meetings, at intervals of six years, in 1917 in Oslo, in '23 in Göteborg, and the last one in Helsingfors in '35, were of a most venerable kind as instituted a long time ago by the Danish physicist Hans Christian Oersted. They were always solemnly opened by some member of the royal family and followed by exquisite celebrations

in food and many speeches. Indeed, they were real events, and in particular for me, only a participant in this Naturforskermöte in Copenhagen. There for the first time I obtained the closest contact with most of the physicists and even other scientists from the Nordic countries. Unfortunately, the second World War caused a standstill of the meetings which have never been renewed. It may be feared that the enormously growing number of scientists in all branches of natural sciences would have made them look like a meeting of the American Physical Society, as I remember it from 1947 in Chicago. When going to a lecture, I had to stand outside the door and did not hear, much less see, the speaker. But this may have been an exception, since the lecturer was Enrico Fermi. At all events, even in 1929, since the meeting was held jointly with the Association of Scandinavian Engineers, the number of guests at the celebration dinner, as held in the biggest exhibition hall in Copenhagen, was not less than three thousand.

The number of active physicists, however, was still small enough as to convene in the modest auditorium at Bohr's Institute for Theoretical Physics, so familiar to all physicists. I was somewhat struck by the spontaneous acclamation that followed my report, and in a happy mood I returned to my seat at a peaceful place far back. What the next speaker might be going to say did not hold my interest, so my thoughts went wrong and, in fact, were entirely absent. Then Niels Bohr, himself, thanking the speaker for his nice performance, turned to me and asked for my opinion and wondered whether my method might possibly be applied also to the present case. I felt seriously that my recent nice position was now at stake and, by keeping a bit silent and looking as wise as I possibly could, I tried to master the situation. And now I realized that the speaker, a very young bright-haired Swede, had been telling how to strip off electrons from the lithium atom, having obtained thereby the ionization potential of the positive lithium ion. This, as you may easily guess, was the subsequently very famous spectroscopist Bengt Edlén, whom we are sorry not to see here today.

A most exciting cooperation now started between us. No sooner had I found the energy of the lithium ion lying in between his limits of error than the doubly ionized beryllium ion was on the way, and so it continued with boron 3 plus and carbon 4 plus with me always behind. Suspecting there were no limits to Edlén's power of producing ions I decided to overtake him with a good safety margin by introducing even an infinite nuclear charge. This was the

origin of the energy formula

$$E = -2Z^2 + \frac{5}{4}Z - \epsilon_2 + \epsilon_3/Z - \epsilon_4/Z^2 + \dots$$

as counted in Rydberg units.

Now as things appeared well settled for any high nuclear charge, there came a cry from the lower end. Some time before, a discussion had arisen between the German physicists, Joos and Hüttig, on the one side, and the Russians, Kasarnowsky and Proskurnin, on the other, with respect to the true value of the lattice energy of lithium hydride crystals. In these considerations a so-called Born cycle process relating to the electron affinity of the hydrogen atom interfered. If that was positive, and, hence, the negative hydrogen ion was a stable configuration, Joos and Hüttig would be right and Kasarnowsky and Proskurnin would be wrong.

Some short calculations readily proved that such was the case. Putting the results into *Zeitschrift für Physik* I was shortly afterwards seriously embarrassed by learning that Hans Bethe, the latest wonderchild from Sommerfeld's factory in Munich had, several months earlier, performed almost the same calculations and published them in the very same *Zeitschrift für Physik*. This I think exemplifies neatly the danger of laziness in reading. Of course, I felt ashamed and immediately wrote an article of explanation and excuse together with some more accurate results. But that did not help, so if you read Bethe's article on two-electron atoms in *Handbuch der Physik* you should not trust him. He—not I—is the father of that curious little child, the strange particle H^- , which for a while appeared to be recognized nowhere, neither in heaven nor on earth.

To be very accurate, it was Linus Pauling who, already two years earlier, tried to determine the electron affinity of hydrogen atoms by means of some extrapolation formula. His method would, however, correspond to a first-order perturbation with scale parameter which is known to be insufficient for producing a binding. A year or two later his method would have been successful.

In spite of thus not having the highest responsibility for this new particle, I did my best for it. I put it into the LiH lattice together with positive Li ions, both constituents then being of the same two-electron type. Applying the Pauli principle to all electrons, i.e., by antisymmetrization of the wave function of the whole crystal, I succeeded in stabilizing the lattice against inner collapse and in this way manufactured a crystal, the LiH, purely on the basis of the Schrödinger wave equation. This is the first crystal produced in that way, and to my knowledge

it is so far also the last one. It may be mentioned that the lattice energy came out surprisingly well, and even the lattice constant was not bad, considering that any adjustable parameter was absent. A long time afterwards I planned an attack on the diamond lattice assisted by a clever pupil, but this ended up in difficulties with the atomic wave function of the six-electron carbon atom. Maybe metallic lithium with three-electron lithium atoms should rather be the next.

The rest of the story of the negative hydrogen ion is brief. In 1938 the astrophysicist Wildt procured a nicer place for this particle in heavenly bodies like the sun, suspecting it to be responsible for the opacity or greyness of the sun's atmosphere in the red and infrared region. From that time on, our parentless child was well taken care of by Chandrasekhar and other astrophysicists, and so the story had a very happy ending.

Now, after having taken your time for quite a while, I have scarcely penetrated even the surface of the complex problem I was supposed to explain to you. So I propose that for the time remaining we proceed on the same path of "yarn-spinning." After all, the commonwealth of friendship between scientists may sometimes be as important as the scientific problems themselves.

Therefore, since Göttingen was really an important center of research during the few years of early quantum mechanics, allow me for a short while to return to the idyllic life of this city with its venerable university institutions and traditions. Much may have changed there in the course of some thirty years, but—as I have seen with my own eyes—not at all in any striking way, so visitors might well recognize things I am describing. At all events the university has not, as for example, Munich, developed into the size of an American university.

I shall never forget the charming view of the green slopes of the lower Harz as my wife and I, with eyes wide-open, first approached the city of Göttingen. This was our first journey abroad and we thought it a most remarkable journey. We first found an excellent modern railway station, very much envied by our American friends. It was even whispered that supposed war indemnities went the wrong way to luxury railroad stations in Germany leaving poor legal creditors with their old and ugly ones.

Next to the station at the small river Leine we found a curious little town with a few narrow streets, apparently devoted to the memory of Carl Friedrich Gauss with its Weender- and Prinzenstrasse forming the real and imaginary axis of the Gaussian plane and

an idyllic wall around providing for the unit circle. A Town Hall or Rathaus appeared not to have changed in the course of some hundred years, and in the Rathskeller, of course, students might be sitting drinking beer out of huge glass boots—yes, boots! In front of the Rathaus was the market place with a fine fountain, the Gänselieselbrunnen, with the charming little Lise feeding the goose, and back or to the side old Marien, Nicolai, and Jacobi churches counting the time every hour.

Up along the imaginary axis, on the gentle slopes of the Hainberg there was the "Millionärenviertel" with pretty modern houses where the highly distinguished and well-paid professors and Geheimrats of the former Kaiserly German society were supposed to have their homes. In a castlelike building in the Merckelstrasse, for instance, James Franck could be found, which is easily remembered from an event in a dark evening when the students marched in a torch-light procession, to his house, singing cheerful songs to celebrate Franck's award of the Nobel prize in physics. In those days, the Nobel prizes went to Germany as today they go to America, or rather, half of the prizes in physics and chemistry went there, the other half to England and France.

Around the city, at smaller and greater distances, there were places of interest and beauty which could be reached by walking. In extreme cases you might use the railway. Of course, the "Kleinbahns" to the "Dörfer" were already out of date, but on the real railways there was an excellent choice between "Holz oder Poltz," the first, the second, the third, and the fourth class, of which the last one for obvious reasons was very much preferred. In the city, itself, quite frequently some vehicle might be seen drawn by a pair of milk cows at a speed of approximately one mile per hour. Autocars are quite out of my memory, but they may have been appearing at that time at the railway station. Our best friends, Dr. and Mrs. Hogness from Berkeley, now in Chicago, had two small boys. And whereas the parents neither could nor wanted to care too much about nominative and accusative in the German language, young Johnny, the eldest one, spending much time in the kindergarten, spoke an excellent German. He was lazy too, and walking with his father he might frequently propose: "Vater ich bin so müde, wir nehmen lieber ein Taxi."

To restore the dignity of the Hogness family I should like to add that, on occasion of the Davisson-Germer discovery of electron diffraction in crystals, Dr. Hogness was the first I ever heard to form the historical sentence: "Das Elektron ist eine Welle."

If the word "students" may be used for those staying for a while, there were quite a number of American students and visitors there. From France I remember Brillouin coming repeatedly to give his lectures in German, and from the United States I particularly remember outstanding persons like Irving Langmuir and K. T. Compton. The latter, in congratulating James Franck for his Nobel prize, nicely added that he would not have felt more satisfied "if it had been one of our own." The other Compton, the A. H. or the $h\nu$ Compton as Onsager would call him, I met much later, in London 1934.

Our Chairman today also was a Göttingen man, as may be inferred from the early establishment of the famous Franck-Condon principle. Closing my eyes I believe I see Edward Condon speaking at some colloquium, but that is all, so he may have left too early for me. Even Enrico Fermi is said to have studied in Göttingen, not altogether to his full satisfaction. He may have left too early, or he had problems of his own to be solved somewhere else.

[*Editor's Note:* I was there, in the fall of 1926, but, unfortunately, for only four months, and Hylleraas and I did not become well acquainted until January, 1963.—E.U.C.]

Among the brief visitors I remember a Hungarian nobleman—in wisdom comparable to Wigner—and a very nice-looking man. It made one proud to see him walking on the Weenderstrasse in an elegant summer suit, so I guess this must have been in the summertime in 1928 or in 1931 on my shorter visit there. In 1936 I met him in Paris where we were to give some lectures at the Institut Henri Poincaré, and again he impressed me enormously by his ability in French. With an accurate manuscript supervised by Professor Bauer and backed, for whispering purposes, by my dear French-Scandinavian friend Dr. Rosenblum, I put my tongue in the correct position and received at the end a hearty acclamation from our always gallant French friends. The other lecturer, of course, did not need a manuscript at all and still gave his talks with an eloquence which our friends here, Mr. and Mrs. Pullman, might nearly have envied him. So you may well guess that this was John von Neumann.

Another quite young man of a slender shape and with a good-looking face was frequently seen walking on the wall and sometimes pulling up his pipe. I might sometimes shake hands with him but, unfortunately, never came in closer contact. That was because of my great respect for those belonging to the brain trust, which he obviously did, as inferred from his frequent private conferences with Born. Twenty years later I had, for a shorter time, the

privilege of hospitality at his institute in Princeton. But now he had heavy burdens on his shoulders (he was even well guarded), absorbed in problems outside of my sphere; so you may guess that this was Robert Oppenheimer. Moreover, at that time I was looking more to the side of Wigner and Wheeler at Princeton University. It was however of great interest to meet at the institute mathematicians like von Neumann, Weyl, Siegel, and Oswald Veblen as well as famous visitors like Niels and Harald Bohr and Dirac. Even Albert Einstein might sometimes be seen walking over the green fields between the Institute and his home and always in a nonconventional suit much more in harmony with his prophetic appearance. He also gave a lecture putting, as it appeared to me, a new asterisk to some of his, for me, still incomprehensible tensors. Very modestly he declared himself unable to draw the conclusions except by extensive calculations; it was merely a suggestion he said. Once I met him more head-on and, shaking hands with him, I received a most friendly, however absent, look and I have never guessed what it meant, whether he thought of me as a distinct person or rather only as one of the citizens of the world. And this was my last sight of Albert Einstein.

Back to Göttingen I see an energetic young man with black hair and mighty black eyebrows, also a Hungarian, so I need not hesitate to say that this was Edward Teller, studying under Heitler for his doctoral thesis on the hydrogen molecular ion. At that time it was considered that I knew even a little of the hydrogen molecule and, for that reason, was taken along for joint discussions with both of them. This I tell in order that you may think I have made a little contribution even to the hydrogen bomb.

Finally—and now I mean finally—there was a man from Russia—a stout man with black moustaches and black hair—apart from Edlén it appears that black hair is a good thing for atomic scientists. (Even Weisskopf, you know, is brilliantly black-haired.) I looked up to this distinguished Russian scientist, taking him to be about the age of Professor Born, a recognized colleague from Russia on leave of absence. It was not until two years ago on his visit to Oslo, having much the same appearance as in the Göttingen days, that he revealed that he was a year younger than myself.

For quite a period during the thirties, we had a nice correspondence, and I was frequently pleased by learning of progress in his work, although a little worried about his modest supply of paper. He is, however, now and maybe for some time, of the highest rank as an Academy Professor of Moscow, with

his home and main duties in Leningrad. On presenting me a nice book, he told me that he would be happy to have the privilege of calling me "his old friend," and to this I consented on the condition that this be a reciprocal sort of privilege.

This was V. Fock, the second father of the famous Hartree-Fock method, whose range is far beyond the two-electron problem. The former one, Douglas R. Hartree, I shall never forget, as being one of the kindest persons I ever met, and whose premature death I sincerely regretted. The words he used of his own father, the other Hartree whose name appears in some joint publications, that he was the most wonderful artist in numerical calculations he ever know, may well be turned toward himself.

It is a sad thing to observe friends and colleagues and pioneers of the Atomic Age passing away. Among the nearly half a hundred persons I have touched upon in this review half of them are no longer alive and quite a number of them did not reach the normal length of a life. The latest, fairly normal cases, I know of are those of Niels Bohr and Charles Darwin.

In this sense my review, although unintentionally, may still be called a little piece of history.

Above all we have to remember the giants of early atomic research in our century like Planck, Einstein, Rutherford, Bohr, and Sommerfeld, to mention only a few, and to these I should like to add as one of the most venerable representatives still alive from that time, Max Born of Göttingen, now, after twenty years of exile, living peacefully in the nearby Bad Pyrmont. His eightieth birthday was recently celebrated at the Physics Institute in Göttingen, on which occasion I had letters from him. Although his health is perhaps not the strongest, his mind is unusually active, and, in his memory, as I personally have learned from him, he holds a store of valuable reminiscences, particularly from early days in Berlin together with Albert Einstein.

You will forgive me that, if my lecture has turned too much towards early days in Göttingen, it has been rather to the honor of my dear friend and first teacher in theoretical atomic physics, Max Born.

Two-Electron Atoms

II. A Perturbation Study of Some Excited States*

ROBERT E. KNIGHT AND CHARLES W. SCHERR

Department of Physics, The University of Texas, Austin 12, Texas

I. INTRODUCTION

THE first paper of the present series,¹ hereafter referred to as I, investigated the ground state (1^1S) of the two-electron atomic species via a perturbational approach. The calculations have now been extended to include the 2^1S , 2^3S , 2^1P , and 2^3P states of the same system.

For purposes of definition, let the Hamiltonian H be written as

$$H = H_0 + \lambda H'$$

When the Hamiltonian for the N -electron atom is written in appropriate units,² it is of this form with λ

equal to the reciprocal nuclear charge Z^{-1} , and H' to the electron interaction terms. Thus, the atomic wave function for a given state is obtained as an expansion in inverse powers of the nuclear charge Z :

$$\psi = \sum_n \psi_n Z^{-n}, \tag{1}$$

where summation to a particular n is called the n th-order wave function. Similarly, the energy is given by

$$E = \sum_n \epsilon_n Z^{-n}, \tag{2}$$

where ϵ_n is referred to as the n th-order perturbation energy coefficient. For each state of an N -electron system, ϵ_0 , ϵ_1 , and ψ_0 are known exactly. The procedure used in the present series is a variational perturbation procedure due to Hylleraas.³ It fur-

* This work was supported by a grant from the National Aeronautics and Space Administration.

¹ R. E. Knight and C. W. Scherr, *Phys. Rev.* **128**, 2675 (1962).

² Units of length, Za_0 ; units of energy $2RhcZ^2$ are used unless it is explicitly indicated that atomic units are being used. These latter are units of length a_0 , units of energy $2Rhc$.

³ E. Hylleraas, *Z. Physik* **65**, 209 (1930); also see H. A. Bethe and E. E. Salpeter, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. 35, Part 1, p. 208ff.