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JOHN CLARKE SLATER

*1900—1976*

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*A Biographical Memoir by*

PHILIP M. MORSE

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*Biographical Memoir*

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John C. Slater

## JOHN CLARKE SLATER

*December 22, 1900–July 25, 1976*

BY PHILIP M. MORSE

JOHN C. SLATER merits commemoration for several reasons. He contributed significantly to the start of the quantum revolution in physics; he was one of the very few American-trained physicists to do so. He was exceptional in that he persisted in exploring atomic, molecular, and solid state theory, 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 1940's and 1950's.\*

Slater's background was academic. His father, born in Virginia, was an undergraduate at Harvard, a doctoral student at the University of Chicago, and head of the English Department at the University of Rochester. John enjoyed literature, history, and music throughout his life, but his youthful preoccupations were with things mechanical, chemical, and electrical. His goal was set when a family helper, a college girl, put a name to his interests—physics.

He took a course in high school physics the next year, which he found pedestrian except for the laboratory. Never-

\* See J. C. Slater, *Solid-State and Molecular Theory: A Scientific Biography* (New York: Wiley-Interscience, 1975) for a more detailed account of Slater's life than is possible in this short memoir.

theless, when he entered the University of Rochester in 1917 he took physics courses as well as a curriculum of chemistry and mathematics. As a senior he assisted in the physics laboratory and did his first independent research for a special honors thesis, a measurement of the dependence on pressure of the intensities of the Balmer lines of hydrogen. The curriculum in those days did not extend to modern physics, but he was referred to Bohr's 1913 paper. From it he was able to devise a bit of theory that partially explained his observations.

His thesis must have had some merit, for it helped to get him into Harvard graduate school, with the choice of a fellowship or assistantship. He chose the assistantship, during which he worked for P. W. Bridgeman, collecting data from equipment designed by Bridgeman. He was happy at Harvard, where he found great intellectual stimulation from his teachers and fellow students. He followed Bridgeman's courses in fundamental physics and launched into the new quantum physics with the courses of E. C. Kemble. He completed the work for the Ph.D. in three years by publishing his (1924)\* paper "Compressibility of the Alkali Halides," which embodied the thesis work he had done under Bridgeman.

His longtime friend J. H. Van Vleck remembers those days:

Neither Slater nor I have ever written any papers concerning the relation of philosophy and physics, but I have the feeling that both of us were influenced by Bridgeman. The essence of his philosophy, which is basically pragmatic, is that research physicists should not be distracted to the realm of metaphysics or politics, but should concentrate on explaining observable facts. In practically all of Slater's papers, except for the experimental ones, the emphasis is on making calculations or developing theories that explain observed phenomena.

We both had the benefit of what I call "operation head start," inasmuch

\*The dates in parentheses or brackets refer to the bibliography appended.

as in 1920–1921 Kemble gave the most mature and sophisticated course in quantum theory given in the United States. Slater has said that the training at that time at Harvard was fully the equal of that in English and European universities. By the summer of 1922 he was thoroughly indoctrinated in the successes and failures of the then quantum theory. One historian of science has referred to that period as the crisis in quantum theory. Slater and I lived in the same dormitory and he and I had many talks about the crisis. Like most American theoretical physicists of his generation, Slater wrote an experimental thesis. However his real heart was in theory and his first publication was not his doctor's thesis, but a note [1924] to *Nature* on "Radiation and Atoms."

Life for a graduate student at that time was in some ways harder, in some ways easier than now. Hardly any graduate student had a car or a wife. There was practically no secretarial help for anyone except senior faculty. Most of the books and journals were in the central [Widener] library rather than the physics building. To work in the laboratory at night required special permission and I remember Slater telling how he had to use a flashlight to get to the fuse box to make his apparatus functional. The respects in which life was better were that there were maids who cleaned the rooms and made up the beds, and especially that there was a dining hall in Memorial Hall with full waiter service three meals a day. The days that Bridgeman had classes were grim, as he insisted on beginning his lectures at 8:40 so he could lecture twice a week for eighty minutes instead of the customary three fifty-minute sessions. Little did Slater or I realize that the particular table of the group to which we belonged would have so many distinguished alumni—among others the mathematicians Franklin (at MIT), Walsh and Widder (at Harvard), the economists Ellis and Chamberlain, Woodward of the Harvard Music Department, and Paul Buck, Pulitzer Prize winner and longtime provost of Harvard.

After receiving his Ph.D., Slater held a Harvard Sheldon Fellowship for study in Europe. He spent a period in Cambridge, England, before going to Copenhagen. In spite of these influences Slater's ideas were very much his own, what formal training he had was in America. His concept of virtual oscillators germinated while he was still here. When Slater reached Copenhagen he explained to Bohr and Kramers his idea that classical radiation fields guided the light quanta, a sort of forerunner of the duality principle. The result of Slater's conversations was the celebrated paper [1924] on "The Quantum Theory of Radiation" in the *Philosophical Magazine*, listed as by Prof. Bohr, Dr. Kramers, and Mr. Slater (actually John already had his Ph.D.). With the prestige of the senior author and the interesting

character of the subject matter, this paper produced quite a splash; Slater suddenly became an internationally known name. Interest in the paper subsided with the arrival of quantum mechanics but in recent years it has been recognized that the correct ideas in the article are those of Slater.

It was natural that the Harvard Physics Department annexed Slater to its staff when he returned to America. Though all papers written by theoretical physicists on the eve of the quantum mechanical breakthrough were speculative in nature, two of Slater's speculations were essentially correct. One [1925] was the correlation of the width of a spectral line with the reciprocal lifetime of a stationary state, a sort of precursor of a 1930 paper of Weisskopf and Wigner that demonstrated this quantum mechanically. The other [1925] was concerned with the interpretation of the spectra of hydrogen and ionized helium. In the early days it was customary to use four quantum numbers for the valence electron in the alkali and but three for the hydrogen and ionized helium atoms. The additional quantum number in the alkalis was ascribed to the interior electron shells, something obviously lacking in hydrogenic atoms, where there is only one electron. Uhlenbeck and Goudsmit, in a note to *Naturwissenschaften*, suggested that there were really four quantum numbers in hydrogen but that a fortuitous degeneracy made things look like there are only three. Independently and practically simultaneously, Slater had the same idea. In a second paper Uhlenbeck and Goudsmit suggested that the fourth quantum number be attributed to electron spin, with a gyromagnetic ratio of twice the classical value. Had Slater terminated his paper with a similar suggestion, which could have been made in a sentence, Slater would have shared their honors with them. Instead of talking about a spin doublet, however, he simply spoke abstractly in terms of the duality of states found in the Pauli exclusion principle—perhaps a reflection of Slater's pragmatic approach. His papers of the period, though theoretical, sometimes did not contain a single equation, a reflection of the fact that quantum mechanics had not then achieved analytic form.

The advent of the true quantum mechanics, with the miraculous near simultaneity of the matrix and wave forms, brought a whole new world to the theoretical physicist. Slater, despite being at somewhat of a geographical disadvantage on account of being in America, rapidly absorbed the content of the new discoveries. His first quantum mechanical paper [1927] was one on "Radiation and Absorption on Schroedinger's Theory." Slater preferred to make most of his analyses by means of the Schroedinger wave equation; for that reason he was able to use a variational procedure

[1928], essentially equivalent to that of Hyleraas, to show that quantum mechanics gives the proper binding energy for the normal helium atom.

In 1929 Slater published what I regard as his greatest paper, "The Theory of Complex Spectra," which he wrote just before going to Europe on a Guggenheim Fellowship. In this he introduced the Slater determinants, now universally named for him. Heisenberg and Dirac had independently shown that the complete wave function, inclusive of spin factors, must be antisymmetric if both spin and orbit are permuted, and Pauli had shown how to interpret spin in terms of a factor in the wave function which had only two values. However no one had proposed constructing in explicit detail a determinant whose individual entries included the Pauli spin factor. In retrospect it seems an obvious thing to do, as the determinantal form automatically insures the proper antisymmetry. The fact is that almost two years elapsed between the appearance of Pauli's paper and Slater's. In this article Slater also introduced the so-called Slater F and G parameters, integrals describing the energies of all the states arising from a given configuration as long as *interconfiguration interaction* is neglected.

In addition to other notable papers which Slater wrote in the late 1920's, on such subjects as Hartree's self-consistent field, the quantum mechanical derivation of the Rydberg formula and the best values of atomic shielding constants, he wrote a seminal paper on directing valence. It was published in 1931 but he had been working and talking about the subject before 1930. The idea of directed valence is that by using proper linear combinations of s and p wave functions one can construct wave functions that project out in particular directions like the horns of a cow. From  $sp^3$  hybridization one can, for example, construct the tetrahedral valence properties of the carbon atom so dear to the organic chemist. Linus Pauling had the same idea about the same time; his paper and Slater's were practically simultaneous.

These were some of the achievements that resulted in his being elected to the National Academy at the almost unprecedented age of thirty-one. He played a key role in lifting American theoretical physics to high international standing for the first time since Willard Gibbs.\*

The writer of the present memoir first met Slater in the late spring of 1930. The occasion was the installation of Karl

\*J. H. Van Vleck, remarks, Slater Memorial Session, American Physical Society, Chicago, 7 February 1977.

Compton as president of MIT. John had just been appointed the new chairman of the Institute's Physics Department; I had just accepted an offer of an assistant professorship in that department. Slater impressed me. Though there was a difference of only three years in our ages, and though at that time he looked more like a freshman than a department head, there seemed to me a decade's difference between us in regard to knowledge and experience in physics. John had twice spent time in Europe, taking significant part in hammering out the implications of the new quantum mechanics, whereas I was scheduled to make my first pilgrimage to Europe in the next year.

It is hard for this generation to appreciate the feeling of inferiority we then, in this country, felt for pure science in Europe. Europe was where new physics was being made and one's ambition was to finish one's education there. A few active centers were being started in this country: Harvard, Princeton, Caltech and Berkeley, as well as a few others. We were just beginning to catch up. What impressed me most, in my first meeting with Slater, was his determination to recast the physics curriculum at MIT so the young physicist would not need to go abroad to finish his education, though he would be able to go abroad to work with equals. We did not know then how important this goal was to be ten years later.

When I came back from my year abroad, things were already well under way. With Slater's active support, N. H. Frank was busy recasting the freshman-sophomore course in physics that every MIT undergraduate had to take. It was a tough course for the time, using calculus from the start. But it meant that, by the end of the senior year, the physics majors would be at least the equals of most graduate students after a year of graduate study. Slater himself concentrated on the senior course in theoretical physics. His text, written with

Frank, *Introduction to Theoretical Physics* (1933), became a classic. The whole inventory of graduate courses was also reorganized and the system of general examinations was restructured to give the student more freedom for research—and Slater inseminated much of that research. Many outstanding theoretical physicists of the 1940's and 1950's got their start from him in the 1930's.

His most tangibly lasting contribution was his books. Between 1933 and 1968 he wrote fourteen books—on chemical physics, on microwaves, and on the quantum theory of atoms, molecules, and solids—an average of one weighty tome every two-and-a-half years. Even the oldest of these is still worth reading. The style of all of them is businesslike and simple, though the subject matter may be complex. Apparently, to John, writing was as easy as breathing. While most of the rest of us had to struggle through successive drafts, Slater typed out his first draft himself; as far as I know it needed little revision. In his office, in the few pauses between administrative duties, he would turn to his typewriter to complete another page or two that he had been mentally composing earlier. Administration of the department took up a good deal of time, more time than he would have preferred. John was a good department head.

In spite of the administrative load, Slater continued to write books, to teach and supervise student research, and to do his own research. During the 1930's his research interests shifted from atomic structure to molecular and solid state structure, as is illustrated by a sampling of his publications. In 1931 he wrote on directed valence and on the quantum theory of the equation of state, in 1934 there was a paper on energy bands in metals, and in 1936 one on ferromagnetism in nickel. In 1937 he was writing on the structure of alloys and on the superconductive state, in 1938 on the structure of

insulating crystals. All this while he was building, from scratch, one of the most prestigious physics departments in the country.

Through most of this decade he looked more like an undergraduate than a department head. Many secretaries made that mistake once; they did not do so a second time. But those of us who knew him in the 1930's remember him as friendly, stimulating, never dictatorial but inspirational in his own unique and quiet way. He was entertaining, too, if he was so minded. Some of us still remember how he could render his guests weak with laughter simply by counting, slowly and solemnly, up to forty in Danish.

In 1940 the beginning of World War II disrupted all research, but gave the newly trained American physicists a chance to show that their education could be put to practical use. Compton, with Vannevar Bush's National Defense Research Committee's financing, set up the Radiation Laboratory at MIT to develop microwave radar. At these high frequencies the electromagnetic fields had more in common with sound waves than with the usual wire-borne currents, and those familiar with theoretical physics were better acquainted with their behavior than were the electrical engineers of that era. Slater soon joined the staff of the Radiation Laboratory. To quote from his 1975 autobiography:

I. I. Rabi, one of the moving spirits of the Radiation Laboratory, asked my help in understanding the theory of the magnetron, the power oscillator whose development by the British had made microwave radar practical, but whose workings were very poorly understood. I told Rabi I also didn't know, but would try to find out.

The problem is analogous to that of the self-consistent field in an atom, one in which we study the motion of an electron in the presence of the space charge produced by all the other electrons and of the nuclei (which take the place of the electrodes in the magnetron). This problem is too hard to solve all in one step. One proceeds instead by iteration, assuming a form for the space charge, solving for the motion of an electron in that field,

studying the space charge produced by all the electrons moving in the way just described and demanding that the final space charge be identical with that originally assumed. I resolved to try to carry through such an iterative calculation for the magnetron and see if the result would include not only a time independent space charge, but more interesting, an oscillating, or rather rotating, space charge which would produce the oscillating or rotating electromagnetic field which corresponds to the radio-frequency output of the magnetron. I set to work and after a few weeks I had a satisfactory answer.

But it was necessary to go further. The behavior of a magnetron depended very profoundly on the impedance of the output circuit, and yet this was not an ordinary lumped circuit, but a set of wave guides. I had been dealing with the microwave cavity as a real cavity, rather than as a circuit element, and it was clear that the same thing had to be done for the rest of the microwave circuit.\*

Based on this work, Slater was able to write the book *Microwave Transmission*, which was the bible of the radar designers for a long time.

In the fall of 1941, John arranged to transfer his work to the Bell Telephone Laboratories (at that time in Manhattan), where an MIT graduate, Jim Fisk, was doing fundamental work on magnetrons. Slater stayed with Fisk's team throughout the war, doing experimental as well as theoretical work on magnetron design. Mervin Kelley, then head of Bell Labs, has stated that John had done more than any other person to provide the understanding requisite to progress in the microwave field.

As the war came to an end, the problems of reconverting laboratories and people to peacetime pursuits loomed large. Slater shared his time between finishing the tasks at Bell Labs and planning the postwar Physics Department at MIT. As he put it:

\*J. C. Slater, *Solid-State and Molecular Theory: A Scientific Biography* (New York: Wiley-Interscience, 1975), p. 212.

During the war practically every member of the MIT Physics Department had been associated with war work one way or another. As the end of the war approached many of them turned back to Cambridge, as I did, full of new plans for the development of physics at the Institute. The war had brought physics to the attention of the public, of industry and government, as had never happened before. In particular, the fields of electronics, as exemplified in radar, and of nuclear structure, as applied in the atomic bomb, were bound to lead to greatly accelerated research and application and greatly increased numbers of students and opportunities for their employment.

Important was the matter of having different fields of physics represented in the department. We had never believed in the extreme concentration in one or two specialities which some departments have chosen. We could afford to diversify, partly on account of the large size of the department made necessary by the large teaching load, and partly because we felt it a duty in a technical institution to carry on work in applications of physics which do not attract interest in an arts college. Our work in electronics, X-rays, optics and acoustics was in each case in a field pursued in only a few institutions. Our department was often looked down on by those who felt that no physicist of any imagination would be in any field except nuclear and high-energy physics. And yet in each of these less popular fields our department was looked up to by the industrial leaders as the best department in the country, and we were constantly urged to turn out more students in each of these fields. After the war I felt firmly that this diversity was a good thing and that we should not alter it.\*

As a result the Radiation Laboratory was transformed into a peacetime Research Laboratory of Electronics; a Laboratory of Nuclear Science and Engineering was established and the wartime work in acoustics was transferred to a smaller but active Acoustics Laboratory.

John's own research returned to molecular and solid state theory. As the postwar department began to take form, he was able to spend more time in this field. By 1951 he was ready to take a number of important steps. A year earlier he had organized a small research group, called the Solid State

\**Ibid.*, p. 217.

and Molecular Theory Group (SSMTG), which was the forerunner of the interdepartmental Center for Materials Science and Engineering, established ten years later. "As he put it, 'Our purpose is to take the quantum theory of atoms, molecules and solids out of the semi-empirical form which it has largely followed since the development of wave mechanics and to proceed as rapidly as possible to put it on a quantitative basis.'"\*

Having served as departmental head for twenty-one years, he was ready to give up administration and become an Institute Professor, able to devote his energies to research and teaching. For the year 1951-1952 he decided to accept the invitation of Brookhaven National Laboratory on Long Island, taking some of the SSMTG with him.

As a starting point for the work of the group, Slater wrote two papers, into which he distilled his wide experience with the Hartree self-consistent field method as applied to the structure of atoms, molecules, and solids. The first paper (1951), entitled "A Simplification of the Hartree-Fock Method," suggested a way whereby the complications produced by electron exchange can be somewhat simplified. This later came to be called the  $X\alpha$  method. The relationship between this exchange term and the magnetic properties of the material was the subject of the second (1951) paper, "Magnetic Effects and the Hartree-Fock Method."

At the time these papers were written, the  $X\alpha$  method was far too complicated for one to expect to find solutions by the laborious use of desk calculators, as was done in the 1930's. But John could see that the new digital computers, just beginning to be developed, would eventually be able to carry out the needed calculations in a time short enough to make

\*G. Koster, remarks, Slater Memorial Session, American Physical Society, Chicago, 7 February 1977.

the method practical. Professor George Koster has outlined the history of the work:

I was with the group from the beginning. From the start we worked closely together, discussing the problems we were working on. Slater's object in this intense communication was in part educational. He wanted to teach us the developments in our field before World War II.

The attention from the outset was about equally divided between atoms, molecules, and solids, not only because the mathematical methods are closely related but because the physical problems are practically indistinguishable. Slater felt that a calculation of electronic structure should be based on the Hartree-Fock method. This does not give an exact ground state for a system, but one can improve on the Hartree-Fock wave function by taking a linear combination of the ground state and excited states in the form of Slater determinants and varying the coefficients.

George Pratt used an early IBM card programmed calculator for his  $X\alpha$  method on the  $\text{Cu}^+$  ion. From this small beginning our computer use increased until we had our own IBM 709 computer in the 1960's. The greatest activity on atoms came in the late 1950's and early 1960's, with extensive Hartree-Fock calculations, that were applied to the computation of X-ray form factors, hyperfine interaction constants and other properties of interest.\*

Work on molecules did not progress as rapidly because of the inherently greater difficulties in computation. With atoms, the Hartree-Fock-Slater potential is spherically symmetrical, but with molecules the potential involves two or more centers; the interaction integrals between wave functions far exceeded the computational capabilities of the time. With the advent of the Whirlwind computer, Alvin Meckler was able to do a landmark calculation of the states of the  $\text{O}_2$  molecule from infinite atomic separation to the equilibrium separation. To quote Koster again:

As our computational prowess increased and our programming of more sophisticated computers became better, we were able to use more realistic molecular wave functions and work was done on diatomic mole-

\**Ibid.*

cules such as LiH, OH and HF; by the early 1960's work was done on H<sub>2</sub>O, NH<sub>3</sub>, CH<sub>4</sub> and others. It was in the field of solids that the greatest activity was centered, but the overall approach was to be the same, though the approach is more difficult. First, it is well-nigh impossible to obtain a completely self-consistent field, both in the region near a nucleus and in the nearly field-free region between nuclei. Second, the wave function has a quite different form in the two regions. The first attempts neglected self-consistency; they gave satisfactory results for energy bands, but were not adequate in other respects. By about 1965 the method was made self-consistent. It was one of the outstanding accomplishments of the group.

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. He was part of every aspect of the group's research efforts. But one contribution was solely his. During this period he wrote five books on the quantum theory of atoms, molecules and solids, which have become standard references in the field.\*

In 1964 John and his ninety-two-year-old father were both awarded honorary degrees by the University of Rochester.

By 1965 Slater had reached retirement age at MIT. He was offered and accepted a position of research professor at the University of Florida, where the retirement age is seventy. He joined the Quantum Theory Project there, which had been set up by Professor Per-Olov Löwdin, who had been an occasional member of the SSMTG during the late 1950's. As Slater has written: "The Florida Physics Department was a congenial one, with main emphasis on solid state physics, statistical physics and related fields. 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."†

\**Ibid.*

†J. C. Slater, *Solid-State and Molecular Theory: A Scientific Biography*, p. 275.

In the friendly and relaxing atmosphere of Gainesville he was able to carry forward his objective of understanding the mechanical, electromagnetic, and chemical properties of matter. Back in the 1920's he had read the prophesy of P. A. M. Dirac, "quantum mechanics can explain most of the phenomena of physics and all of the phenomena of chemistry," and, alone of all the theory's pioneers, he continued to demonstrate its validity in ever greater detail and accuracy. Together with Löwdin and an active group of graduate students and postdoctoral assistants, he extended and perfected the methods he devised in the 1950's and 1960's, using more and more powerful computer programs.

He and his colleagues calculated the compressibilities of various solids (thus coming full circle from his doctoral thesis), the magnetic properties of ferromagnetic and anti-ferromagnetic materials, the binding energies and magnetic properties of various polyatomic molecules, X-ray absorption in molecules and solids, the relationship between the  $X\alpha$  method and the virial theorem and the use of the  $X\alpha$  method in understanding the catalytic process. He continued to publish books and important papers right up to his death.

Slater married Helen Frankenfeld in 1926. They had three children: Louise Chapin, John Frederick, and Clarke Rothwell. All of them are following academic careers. John was divorced and in 1954 he married Dr. Rose Mooney, a physicist, who moved to Florida with him.

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