

My Life as a Physicist: Memories and Perspectives

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This paper constitutes a brief personal history from my beginnings as a physicist through the period of my discovery and consolidation of what has since become the self-consistent field theory of molecular structure. My career as a molecular theorist began only a few short years after the most traumatic experiences of my life took place during World War II. My growth as a scientist did not stop during those difficult years, but proceeded as if driven by forces independent of the surrounding events.

It is only during the last decade or so that I have spoken somewhat more freely about the painful experiences described below. However, those events were always vividly present in my mind. I hope that sharing those memories with my friends and colleagues will help them to understand me better, and perhaps also the human condition. And since my training in the fundamentals of physics occurred during those years, my account may also offer some insight into how learning can, and does, occur under improbable circumstances.

But first I like to turn back to my childhood, when I experienced the earliest stirrings of scientific curiosity. I am certain that my interest in science began when I was three years old. I did not understand how toasters, lamps and irons depended on a wire coming out of the wall. In those days, wall outlets were surface mounted and covered by porcelain caps. One day I found an outlet whose cap had crumbled. I began to put my finger systematically on the various exposed parts, intent on getting some response from this mysterious gadget. I finally did, in the form of an electric shock that made me withdraw my finger abruptly, and imbued me with great respect for the mysterious force I had just experienced.

This was one experiment that I reported to no one; I was brought up in a proper home and had sense enough to know that, whatever I had done, it was wrong. The experience increased my prudence but in no way diminished my curiosity. By the age of seven, I was conducting less dangerous experiments with batteries, lights, switches and electric bells. Radio broadcasting was just beginning around that time. At the age of ten, I built my first crystal receiver and, throughout my teens, I continued experimenting with radio reception to the extent that my meager budget allowed.

During my last two years at the gymnasium (high school), I elected the mathematical-scientific curriculum. After graduation, I enrolled at the Technical University of Delft in the Department of Electrical Engineering.

Class attendance at Delft was optional; to satisfy requirements, one only had to pass yearly examinations. During my first two years there, I spent my afternoons in the shops and laboratories, but rarely attended lectures; I preferred to study textbooks and the required literature on my own. The extensive language training mandated in Dutch gymnasia made this self-study possible, since by the time we graduated, we were able to read the scientific literature in French, German and English.

During my third year—it was now 1938–1939—I became dissatisfied with my academic program. The electrical engineering curriculum in Delft was a two-track program, one with emphasis on electric power (transformers, transmission lines, electric motors), the other emphasizing electronics and acoustics. I had a strong interest in the latter, but could not avoid a number of mandatory courses in the former, which interested me very little. I had heard that in the German technical institutes, it was possible to take a program in which one could concentrate fully on electronics and acoustics. To explore this option, I spent the spring of 1939 auditing classes at the Technical University of Karlsruhe.

During the summer of 1939, which I spent at my parental home in Nijmegen, all hope for peace in Europe evaporated. Events moved swiftly. In July, the Hitler–Stalin pact was signed. By mid-August, it was clear that Poland would not yield, that Germany would attack and that France and England would be brought into the war. On August 29, 1939, the Netherlands government declared a general mobilization in order to defend its neutrality as it had successfully done during World War I.

During peacetime, Dutch university students were always permitted, and indeed encouraged, to complete their academic studies before fulfilling their military obligation. These deferrals were now revoked and, on my 21st birthday, which coincided with the date of the mobilization, I was inducted into the Royal Engineers Regiment of the Netherlands Army.

The officer corps of that regiment consisted almost exclusively of graduates of the University of Delft. The army now faced a dilemma: the students from Delft who had been inducted should be given officers training, but a prerequisite for the latter was prior graduation from the university.

After about six weeks, during which we were billeted in Rotterdam basically doing nothing, the army resolved its dilemma by sending the entire student contingent of the Royal Engineers back to school in uniform. We were billeted in one of the university buildings requisitioned for the purpose. After an hour of drill in the morning, we attended classes and laboratories as normal students for the rest of the day.

Having concluded earlier that year that I did not want to continue with the electrical engineering program at Delft, half of which did not turn me on, I decided to become a physicist. So, while the world situation around us became more ominous all the time, I eagerly devoured all the physics I could absorb.

The Physics Department at Delft had recently acquired R. Kronig as its resident theoretician. Kronig's lectures, together with lectures by H. A. Kramers, who came

in once a week from neighboring Leiden for that purpose, opened up the world of physics for me. I also learned differential geometry and its relation to relativity and quantum mechanics from J. A. Schouten, who had pioneered a very original approach to those subjects.

Our lives were rudely interrupted in the early morning hours of May 10, 1940, when the German attack on the Netherlands and Belgium was launched—as was Nazi custom, with no declaration of war. The only declaration of war by Germany in World War II was against the United States after Pearl Harbor, direct invasion not being an option.

Our group of student soldiers, who had had no more training than morning drills for about six months, and who had never fired a gun, was now deployed around Delft to cope with German paratroopers and glider convoys descending on an airfield a few kilometers out of town close to The Hague, the seat of the government. I was assigned to guard one of the canal bridges on the outskirts of Delft. Quaking in my boots one night, I fired my only shot of the war, missing a moving shadow that later turned out to be a goat grazing in a nearby meadow. The paratroopers were contained by more experienced forces, thereby permitting the Dutch government to escape to England.

After four days, The Netherlands was crushed by the overwhelming military might of Germany. It was utterly depressing. Nevertheless, despite our defeat, we believed in an ultimate allied victory, and continued to believe so even after the narrow escape of the British Expeditionary Forces from Dunkirk and the subsequent fall of France.

Initially, the German occupation of the Netherlands was relatively benign. Upon demobilization, the Dutch army was allowed to return to civilian life rather than being interned in POW camps. Thus, in the fall of 1940, I returned to Delft as a civilian graduate student in physics.

The Physics Department had recently begun to use teaching assistants, and I had the good fortune to be selected to assist in an advanced laboratory where several classical experiments were set up for student training. Among these were the determination of e/m by subjecting an electron beam to balancing electrostatic and magnetic deflections, and the famous Milliken oil drop experiment for the determination of e . The laboratory was directed by a distinguished lady, Dr. H. van Leeuwen, who had been a student and research assistant with H. A. Lorentz. In today's academic environment, Miss van Leeuwen would undoubtedly occupy a prestigious chair.

Gradually the German occupiers tightened the noose and began to interfere in virtually every aspect of life. The food stores that had been stockpiled by the Dutch government to be prepared for a blockade were now carted off to Germany. The first measures against Jews were instituted, beginning with registration, followed by restriction of movement and exclusion from gainful employment. In the spring of 1941, university students were required to sign a loyalty oath stating that they would not undertake any acts of resistance or sabotage against the occupier.

We students considered it dishonorable to sign such a declaration and—perhaps

naively—decided to register a protest by boycotting classes. In retaliation, the German authorities closed down the universities of Leiden and Delft. Leiden remained closed during the entire war, but Delft was allowed to reopen a few months later.

Once again, after a relatively brief interruption, I was able to resume my studies and to continue as a student and teaching assistant in physics for about two more years. Fortunately, the physics faculty remained intact and library resources were more than adequate despite the absence of new acquisitions.

By late 1942, the allies were gaining strength and we were heartened by news of major German defeats in North Africa and Stalingrad. However, the occupation itself was becoming increasingly oppressive. Dutch resistance gradually stiffened, culminating in a series of strikes during the month of April, 1943.

The Germans responded by declaring martial law. Young men were now grabbed off the streets, routinely and at random, to be carted off as slave labor in German factories. Since university communities would be prime targets for this practice, I decided to clear out of Delft for a while and lie low at my family's home in Nijmegen. For the same reason, my youngest brother John returned from Groningen where he was a medical student; Victor, our middle brother, was still living in Nijmegen where he was studying sociology.

When the three of us were together, Victor informed us that he was engaged with a group of friends in underground activities. Shortly thereafter, on April 30, 1943, he received a phone call alerting him that several members of his group had been arrested by the security police (Sicherheitsdienst or SD).

Victor promptly took off on his bicycle. John and I reasoned that the SD did not have anything on us; foolishly, we decided to stay put. A few hours later, the SD, reinforced by collaborationist Dutch Police, showed up. Unimpressed by our declarations of non-involvement, they immediately placed us under arrest. They never found Victor, who managed to remain in hiding throughout the war.

John and I spent the night in the police lockup in Nijmegen. At dawn we were put on an army truck to take us to a military court in Hengelo, about 90 km away. On the truck we met four of Victor's co-conspirators—one laborer, Marinus, and three university students. Later that afternoon, the three students were sentenced to the firing squad (they were shot the next morning), and Marinus was given a long term in concentration camp, while John and I were relegated to the police lockup in Hengelo.

We stayed in that police lockup for three and a half months. We managed to get books sent to us from our respective university libraries, and tried to keep our minds focused on our studies. I remember struggling through Hermann Weyl's "Raum, Zeit und Materie".

We became relatively permanent fixtures in the lockup; most "guests", comprising common criminals, black marketeers, political dissenters, and Jews who had been flushed out of hiding, stayed only a few days. I remember seven Jews who came in during that period. Three managed to commit suicide in their cells: John and I carried out their bodies.

On August 13, 1943, John and I were suddenly removed from the lockup and transferred to the concentration camp at Vught (between 'sHertogenbosch and Eindhoven). We were never convicted of anything—this was simply "Schutzhaft" (protective custody). We were to stay there until September 5, 1944.

In Vught, we found new opportunities to keep our academic interests alive. John, as a medical student, managed to capture the much-coveted position of hospital orderly. Miraculously, I got back into physics.

Vught is not far from Eindhoven, which was then, as it is now, the company town of the electronics giant N. V. Philips. The top management, including the son-in-law of the company founder, had been evacuated by the Dutch army to England, where they could continue to direct Philips' worldwide operations for the benefit of the allied cause. However, other managers—including the founder's son—had been left behind in Eindhoven. Now they were forced by the Germans to produce electronic components and devices for the German war effort. At the same time, the ranks of Philips employees were repeatedly subjected to arbitrary drafts of personnel to serve as slave labor in German factories.

The executives of Philips then suggested to their German overlords that they be permitted to tap the pool of labor in the nearby camp of Vught. This proposal was received favorably, and thus Philips was encouraged to set up manufacturing facilities inside the camp. Working in the "Philips Commando" was considered a great privilege.

Although the Philips Commando employed only a small fraction of the camp population, its mere presence improved the ambiance of the camp significantly. Each morning a group of Philips managers came into the camp to direct the manufacturing operations, namely of electric razors and short-wave radios. The radios also had to be tested at the end of the assembly line, providing us with an excellent source of "forbidden" news on a daily basis.

For the academically inclined, the Philips management created the "Computation Chamber" in which about two dozen professors, students, and scientists from industry got various research assignments. I was invited to join that group.

My first assignment, as a member of the Chamber, was to carry out a Kronig-Penney calculation of the Schroedinger equation for a one-dimensional finite crystal. This constituted in a sense my first experience as a practising quantum theoretician. When that was finished, complete with beautifully drawn graphs of wavefunctions and charge densities, I was given a much more ambitious project, consisting of a calculation of elastic constants in a classical crystal, where the interaction between lattice sites consisted of central as well as non-central forces.

This problem had been formulated by Dr. Druivesteyn of Philips, who had consulted with my professors in Delft to give me a project that would further my academic program. To learn the field, I struggled through Max Born's monograph "Dynamik der Kristallgitter". My assignment was completed, and a final report transmitted to the Philips Management in Eindhoven, a few days before the camp was evacuated on September 5, 1944. After the war, this work was accepted in Delft as my master's thesis.

The evacuation of camp Vught conformed to standard Nazi practice that no concentration camp inmates should ever be liberated. The allied armies were poised for a push northward just a few dozen kilometers to the south of us. Unfortunately for us, that push occurred 12 days later.

On the day of the evacuation, about 500 prisoners who had been in solitary confinement were executed. The remaining few thousand "less dangerous" inmates were crammed into railroad cattle cars, and began a three-day journey which ended on September 8, 1944 at the camp "Sachsenhausen", also called "Oranienburg" after the nearby Berlin suburb of that name.

The world of concentration camps reminds me of Dante's description of the seven levels of Hell. At the deepest level were the extermination camps with gas chambers, and also some camps nicknamed "Nacht und Nebel" (Night and Fog) from which virtually no-one came out alive. Sachsenhausen—like Dachau and Buchenwald—was somewhere in the middle; I estimate the survival rate at 15–20%. Vught had been comparatively benign, due in no small part to the presence of the Philips civilians.

In Sachsenhausen I had to suspend my pursuit of physics and focus every ounce of energy on survival. Bruno Bettelheim attributed his own survival to his will to live and to his understanding of the sociology of the camp structure. I concur that these were necessary prerequisites, but they were by no means sufficient; in order to survive one also needed a good deal of luck.

I judged that being a university student would be of little value in landing a good job. Thus, at intake registration I declared that I was an electrician. My brother John professed to be a medical orderly. After a short while, I landed a good job with a "Baukommando" (construction commando), where I started as a draftsman and later served as an electrician. Unfortunately, John ended up in menial work.

The winter of 1944–1945 was harsh. Every morning at 4:00 a.m., we had to brave the elements standing at attention for about one and a half hours at "Appell" (roll call), wearing no more than flimsy indoor clothing. After roll call, the prisoners regrouped to march off to arrive at 6:00 a.m. at their regular work assignments.

By the end of January 1945 the Russian army was on German soil, less than 60 km from Berlin and our camp. The German army dug in for a tenacious defense of their capital and, on February 1, 1945, camp officials began a gradual evacuation of Sachsenhausen, moving inmates to the north and west in order to prevent liberation of the prisoners by the advancing Russians. My brother John went with one of these transports to the infamous camp Bergen-Belsen, where he perished from deprivation and typhoid in late March.

I stayed in Sachsenhausen until the final evacuation on April 20 when, guarded by SS troops, with the Russian army at our heels, we began a forced march which lasted 12 days and covered 160 km. The SS had made no provision for feeding or billeting the tens of thousands of undernourished miserable victims whom they were now driving like a herd of cattle to nowhere, either to die along the road or, probably, be drowned in the Baltic Sea. Anyone whose strength gave out and sat down was promptly shot. I have made a rough guess that at least one-third of us perished. My own life was saved in large measure by a fellow prisoner who, as a

long-time inmate of Sachsenhausen, had been better connected than I and had thus been able to acquire a stockpile of food which he generously shared with me.

After about one week of this life-and-death struggle, small rays of hope began to break through. Swiss staffers from an International Red Cross depot in the Baltic port of Lübeck courageously took matters in their own hands. They loaded their trucks with food parcels which had been destined for POW camps, and supplied any prisoners they could find on the roads with their precious life-saving gifts.

The Red Cross representatives also convinced our SS guards—who had by now been abandoned by their officers, and were quite demoralized—to let collapsing prisoners be taken on the Red Cross trucks. Fearful of retribution by the prisoners, who at this point outnumbered the guards about fifty to one, our remaining guards gradually disappeared from sight. Many were Eastern Europeans who had been forced into service and who were eager to return to their homelands. As we now continued on our own, we were joined by a new group: German soldiers desperately rushing to the West to avoid capture by the Russians. Our march ended about halfway between Berlin and Denmark in Schwerin, the regional capital of Mecklenburg, where we met American troops. It was May 2, 1945.

I was repatriated to the Netherlands in late May—I do not remember the exact date. After resting up for a few weeks, I returned to Germany to see if I could find some trace of my brother John. After arrival in the Bergen-Belsen area, it became obvious to me that he could not possibly have survived. Later investigation turned up testimony from a few survivors that he had indeed succumbed about five weeks before war's end.

I returned to Delft about September 1, 1945, and was officially granted my diploma of "Ingenieur", roughly equivalent to a Master's degree, on October 15. I had by then applied for, and obtained, a postgraduate fellowship at the University of Chicago. I arrived in Chicago on January 6, 1946.

Chicago was then the most exciting place to be for a young physicist. It boasted the famous site of the first self-sustaining nuclear chain reaction; among the physics faculty were Enrico Fermi, Edward Teller, Maria Goeppert-Mayer, and Robert Mulliken. Nuclear research was of course *de rigueur*. However, since nuclear research was then still cloaked in heavy secrecy, I concluded that as an alien I would be better off in a program that was not encumbered by government-imposed restrictions. I applied to and was accepted by Robert Mulliken as a research student to pursue the study of molecular structure and spectra.

My studies at Delft had given me an excellent foundation in mechanics, electricity and magnetism, thermodynamics and statistical mechanics, and of course advanced calculus and other subjects in mathematics. However, I had not learned much about nuclear physics, quantum mechanics and, in modern mathematics, linear algebra and group theory. I spent the period between January 1946 and June 1947 filling in some of these gaps, as well as carrying out semiempirical molecular orbital calculations on several simple organic molecules with "alphas and betas".

I passed the Ph.D. candidacy examination in physics in June 1947. Shortly thereafter Professor Mulliken suggested semiempirical MO calculations on substituted

benzenes as my thesis subject. Through the good offices of Maria Mayer, I also received at that time an offer from Professor Karl Herzfeld of the Catholic University of America in Washington, DC, to join the physics faculty as an instructor. I accepted that offer and spent the next two years teaching in Washington while working on my thesis, making frequent trips to Chicago to confer with Mulliken.

I began with summarizing the theoretical foundations of the calculations I was to perform. Mulliken expressed his approval and praise for the first account he received. However, I was not satisfied with the current state of the art. All MO calculations started with a "one-electron Hamiltonian", but I could not find a definition of the latter anywhere in the literature.

I realized that a similar problem had been faced for atoms by Hartree and Fock [1]. At least for closed-shell atoms, there was a clear definition of the one-electron Hartree-Fock Hamiltonian: it emerged in the process of applying the N -electron variation principle to a Slater determinant of orbitals which had to be optimized. Furthermore, F. Seitz and others had extended the model to deal with solids, albeit again limited to a closed-shell system [2]. Clearly, the model was also applicable to molecules, most of which are, conveniently, closed-shell systems. The difficulty with standard MO theory was that a mystical one-electron Hamiltonian was adopted before anything at all could be written down.

The solution to the puzzle came to me in June 1948. I had returned from Washington to Chicago for the summer to work intensively on my thesis. I went with a group of friends, including my future wife, to a concert by the Chicago Symphony Orchestra at its open-air summer home in Ravinia Park, north of Chicago. Lying in the grass, listening to the music and looking at the stars, it suddenly flashed through my head that standard MO theory did not start with the right question. Just like Hartree, Fock and Seitz had applied the variation principle to an N -electron Slater determinant of yet to be determined orbitals, one should start the same way with molecules, with the additional constraint that the MOs are constructed as linear combinations of atomic orbitals (LCAO). Nowadays we prefer to say that the MOs are constructed from a predetermined basis set.

The LCAO approximation for the MOs was of course not new; it had been used for years by Mulliken, Lennard-Jones and others in semi-empirical calculations. However, entering this approximation formally into the N -electron variation principle provided a new and much better mathematical point of departure for electronic structure calculations on molecules.

When I communicated my insight to Mulliken, he fully understood its significance. It is a testimony to his stature as a scientist and human being that he wholeheartedly supported that I would now dedicate myself primarily to working out the details of what I then called the LCAO-SCF theory, rather than the thesis topic originally assigned.

Having returned to Washington in the fall of 1948, I continued working out the details of the LCAO-SCF theory during the following Academic year. The first three chapters were completed in late 1948, consisting, respectively, of an introduction, a derivation of the closed-shell molecular Hartree-Fock-SCF equations,

and the analogous derivation of the LCAO-SCF equations [3]. Publication in a journal had to be postponed until after the Ph.D. degree was granted and the Ph.D. committee had approved the final version of my dissertation.

In June 1949 I returned to Chicago, this time as a research associate, for a full year. That period in Chicago proved even more stimulating and exciting than my earlier stays in Mulliken's laboratory. I had the privilege of interacting with many young physicists and theoretical chemists who came to quench their thirst at this watering hole. I recall many stimulating discussions with Jake Bigeleisen, Mike Kasha, Christopher Longuet-Higgins, Al Matsen, Harden McConnell, Bob Parr, and Bill Price. I thank them for the many good conversations we had.

During that year, the remaining four chapters of my thesis were completed [4]. These four chapters covered, respectively, ionization and excitation processes, the use of symmetry in the Hartree-Fock-SCF model, the use of symmetry in the LCAO-SCF model, and an LCAO-SCF calculation of the benzene molecule. The thesis was accepted and approved by the committee in June 1950.

The last chapter of my thesis, the LCAO-SCF calculation of benzene, constituted only a crude and approximate application of the new theoretical framework. This was, however, all that could be done within a reasonable time frame, due to the unavailability of adequate computational tools in those days. The inclusion of this last chapter also put to rest the reservations as expressed by one of the committee members, "never mind all those beautiful formalities—what can you really calculate?" In the published version of my thesis [5] I decided to omit this last chapter, since I was convinced that much better and more interesting and convincing calculations would be carried out within a few years.

While our work in Chicago was available prior to official publication to our colleagues worldwide through our Technical Reports [5a], we were not always informed about developments in other laboratories as they were occurring. Thus, while I was working out the LCAO-SCF theory, I was not aware of the parallel development in Cambridge, England, by Lennard-Jones and Hall [6-9]. A comparison between these two separate developments seems in order.

The two developments show a great deal of similarity, both in subject matter and in methodology. This is evidenced in particular by the adoption of a single Slater determinant to describe the ground state of a closed-shell molecule; the transformability of the one-electron functions; the application of the N -electron variation principle to derive the molecular Hartree-Fock-SCF equations as well as the LCAO-SCF equations; the exploitation of symmetry; and the treatment of ionization and excitation processes.

The most significant difference between the two developments is in the interpretation and exploitation of the LCAO-SCF equations. Hall observed that these equations simplify considerably if M , the number of atomic orbitals, equals N , the number of occupied molecular orbitals [9]. Restricting himself to that special case, $M = N$, he then derived useful relations between ionization potentials of related chemical compounds. On the other hand, dealing with the general case where $M > N$, I noted that these equations exhibit a striking resemblance to the Hartree-Fock equations. I proposed that these equations be adopted to calculate wavefunc-

tions for molecules in actual practice, using an iterative procedure, henceforth to be called the "LCAO-SCF method" [3].

After obtaining my degree, I was invited to join the faculty of the Physics Department of the University of Chicago, and I accepted. With strong support from Robert Mulliken and his junior colleague John R. Platt, I now embarked on a broad-based program, using my thesis as a blueprint, to develop the tools necessary for calculating all-electron wavefunctions of atoms and molecules routinely and accurately. Henceforth, the work of Mulliken, Platt and myself would be conducted under the auspices of the "Laboratory for Molecular Structure and Spectra" (LMSS).

My first major task was to systematize the calculation of one- and two-electron integrals over the basis functions from which the MOs are constructed. This work got a significant boost when I was joined by Klaus Rüdenberg, who had come to Chicago from Zürich with his mentor, Professor Gregor Wentzel, who had joined our physics faculty in 1948.

A comprehensive integrals project which would cover polyatomic molecules made up of any atoms in the periodic table was clearly too ambitious. Thus we settled for diatomic molecules consisting of atoms in the first two rows of the periodic table. We furthermore adopted the Slater-type basis functions as the most suitable building blocks for the construction of MOs. Klaus tackled the mathematically most demanding class of these integrals, namely the two-center two-electron exchange integrals; I dedicated myself to the remaining types.

A second major task was to prepare ourselves to use digital computers, first for calculating the integrals we were working on, and later for developing programs implementing other mathematical procedures which crop up in calculations on atoms and molecules. This was no small undertaking, since the first computers available to us had no floating point hardware, while the systems software consisted of binary input and output routines only; compilers, and even assemblers, were still in the future.

Many of the tools needed by LMSS in this broad-based program were contributed by energetic dedicated research associates and graduate students. Prominent among the former were Reinhart Ahlrichs, Paul Cade, Enrico Clementi, Serafin Fraga, Juergen Hinze, Sigeru Huzinaga, Wlodzimierz Kolos, Sigrid Peyerimhoff, Bernie Ransil, Robert Sack and Lutek Wolniewicz; and among the latter, Paul Bagus, Howard Cohen, John Detrich, Winnifred Huo, Yong-ki Kim, Gulzari Malli, Doug McLean, Charles Scherr, Chris Wahl, Andy Weiss, Bill Worley and Megumu Yoshimine.

While the first LCAO-SCF model could deal satisfactorily with closed-shell systems, an analogous satisfactory treatment of open-shell systems remained elusive for quite a while. In fact, this problem was endemic in virtually all SCF formulations, and had been side-stepped by Hartree for atoms by introducing somewhat artificial approximations in implementing the N -electron variation principle [1].

The solution to this puzzle, which I discovered in 1958, was another instance where one had to ask the right question: the variation principle had to be modified so that all degenerate N -electron wavefunctions, which jointly represent the open

shell, participate equally in the variational process [10]. While this extension of LCAO-SCF theory did not lead to a simple scheme for all conceivable cases, nevertheless a large class of open-shell problems now became easily accessible.

In 1962 I became director of the University of Chicago Computation Center; I held that position until 1968. Since then I have spent considerable time and effort on the design and development of computer hardware and software for large-scale scientific calculations. However, I never lost interest in physics and quantum chemistry. During the mid-1970s I worked intensively, in collaboration with my former student John Detrich, on relativistic effects in atoms and molecules [11,12], and from about 1980, again with John Detrich, on the MCSCF (multi-configuration self-consistent field) model of electronic structure [13,14]. I expect to continue alternating between physics, quantum chemistry, and computer development for the foreseeable future.

In conclusion, I want to thank Professor Orville-Thomas for his kindness and patience, and for inviting me to write this account. I also thank all my friends and colleagues who have contributed to this issue of "Theochem".

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