MOLECULAR PHYSICS, 2000, VOL. 98, NO. 16, 1043–1050

Reminiscences at the end of the Century

CHARLOTTE FROESE FISCHER
Department of Computer Science, Vanderbilt University, Nashville, TN 37235, USA

I was born on 21 September 1929 in Nikolayevka, a little Mennonite village in the Ukraine some 60 kilometres north of Donetsk. When I was only 6 weeks old, my parents, along with my father's family, left for Moscow and managed to get to Germany on the last train allowed to leave before the Russian border was closed at the end of that year. My mother's family was to leave 2 weeks later but mother never saw any of them again. After several months in a refugee camp in Germany, our family got permission to immigrate to Canada during the height of the depression. The first few years were spent on a farm near Aberdeen, Saskatchewan, working mainly for food and housing. Then in 1935 the British Columbia Government wanted to develop the Lower Fraser Valley near Chilliwack for agriculture, offering a land grant of 10 acres to anyone willing to clear the undergrowth for farming. Several Mennonite families, including my parents, accepted the offer.

My father had a high-school education and, as his father before him, took up farming, working in a sawmill to supplement his income. He always was supportive of my search for education. Mother had only a grade-school education and never really understood my desire for learning. I was always expected to help at home, which meant that school for me was like a vacation. Homework was always done during study periods, except for English composition, which needed absolute peace and quiet.

At the end of the 12th Grade, I was placed highest in the junior matriculation examinations of 13 school districts around Chilliwack, qualifying me for a University Entrance Scholarship that covered tuition at the University of British Columbia (UBC). For financial reasons, I stayed on to take the 13th Grade at Chilliwack Senior High School, then the equivalent of first year at UBC. In the senior matriculation examinations the next year, I placed second in the province and got further scholarships, bursaries, and loans to support myself. On entering UBC, I had planned to specialize in bacteriology, but the microscope and I were not compatible. My aptitude tests also left no doubt: I should seek honours in mathematics, in which I was getting perfect grades. So I compromised by taking honours in mathematics and chemistry, an unusual combination at that time. Both the mathematics and chemistry programmes required that I take some physics. My first course was mechanics, from which I went to atomic physics and then quantum mechanics—the extent of my formal training in physics. In his 1995 memoirs (*Molecular Physics*, 1995, **86**, 551), Professor Douglas Henderson, well known for his work in statistical mechanics, provides a colourful description of the Physics Department at that time. Dr J. B. Warren, who taught atomic physics, had no problem with my taking his course without the specified prerequisites. I got a solid training in quantum mechanics in the course offered by Professor G. M. Volkoff, a long-time editor of the *Canadian Journal of Physics*. The Chemistry Department was quite different in that rules had to be followed rigidly. I was most interested in the more mathematical physical chemistry courses but was required to take analytical and organic chemistry, which required a lot of memorization. Maybe that is why, for my MA, I decided to get a degree in applied mathematics at which time I took a quantum chemistry course offered by Dr Chris Reid, a course which generated a lot of discussion among the students trying to understand the quantum mechanical description of the chemical bond.

While an undergraduate, I was fortunate in being introduced to research during the summer, first in geochemistry at UBC, analysing twigs from trees for trace minerals as part of Professor Harry Warren's research project in the Department of Geology, and then in the Canadian Forest Products Laboratory as a summer student in Ottawa, studying the properties of sawdust. With its extensive lumber industry, Canada produced a lot of sawdust which it was believed could be recycled into some useful product. However, in my last two years my research interests became more mathematical, and I spent two summers working with desk calculators. The last summer was in the Radio Physics Division of the National Research Council, under the direction of Dr James R. Wait. This work resulted in my first publication, 'Calculated diffraction patterns of dielectronic rods at centrimetric wavelengths,' in the *Canadian Journal of Physics*, of course.

At this point in my applied mathematics training I came to the conclusion that calculations were an integral part of problem solving and decided to learn all about

Molecular Physics ISSN 0026–8976 print/ISSN 1362–3028 online
http://www.tandf.co.uk/journals

computers and their application to science. Douglas R. Hartree at Cambridge University was recommended to me, and I was delighted that he accepted me as a student. Unfortunately, my National Research Council Scholarship was restricted to graduate study in Canada; thus, for financial reasons I was able to spend only two years at Cambridge, finishing my degree in another year at the University of Toronto, which had the largest computational facility in Canada at that time. The Computing Centre was under the direction of Calvin C. Gotlieb (Kelly), who later became known as the 'Father of Computing in Canada'. Also on the staff was Beatrice H. Worsley (Trixie) who had worked with Hartree and had obtained a PhD from Cambridge University in 1953.

During my first term at Cambridge, Hartree got me started on learning how to program the EDSAC. This was not so difficult. The booklet he had written, *Introduction to Programming for an Automatic Digital Calculating Machine and User's Guide to the EDSAC*, including exercises, consisted of only 69 pages, 6 by 9 inches in size. There was not a lot to learn! But users did not only program, they needed to maintain the hardware as well. The EDSAC was designed using vacuum tubes. These were not particularly reliable so engineers often spent the day trouble-shooting the computer and/or making modifications. Users could run short test programs during morning and afternoon teatimes. Serious computing was done in evenings and nights (figure 1). David Mayers (another of Hartree's students at the time) and I were usually assigned to Monday. Faculty with their Diploma students usually had first use of the machines when the engineers left. In our case, this often was Dr J. C. P. Miller, a number theorist, whose programs tended to use only the add operation. At about 8:00 PM he used to say 'My wife is expecting me', but it might still be an hour or so before he left. How frustrating it was to find, after he left, that the multiplier did not work! The memory of the EDSAC consisted of mercury delay lines in which information was stored as pulses that propagated through the tubes, were picked up at the other end electronically, regenerated, and recycled. But as any scientist knows, the velocity of a pulse in a liquid depends on temperature. The room in which the computer was housed had no environment control. As the night progressed, errors started to appear in that bits (pulses) were dropped, at which point it was necessary to run diagnostics and make adjustments to the hardware. Other failures could also appear. In such an environment, checking of results was extremely important. Typically, calculations were repeated until at least two runs would agree. Three were better! The extremely small memory of 1024 'short' 17-bit words also presented a challenge. From these early experiences with EDSAC, in my opinion, the improvement in accuracy of the hardware over the last 50 years is the most outstanding achievement, particularly in view of the tremendous gains in speed.

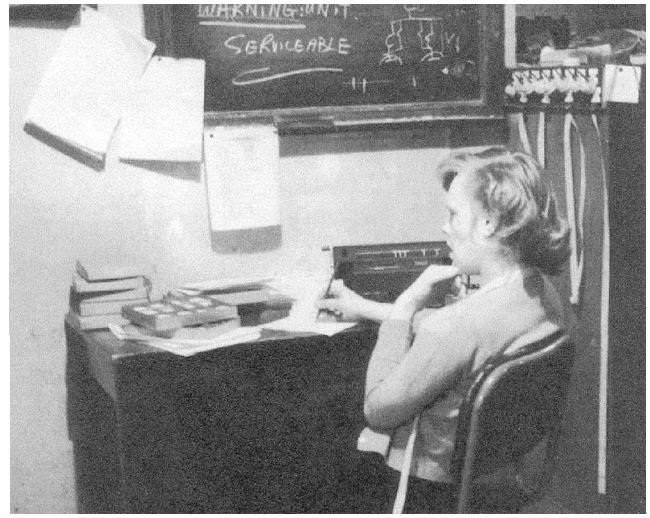
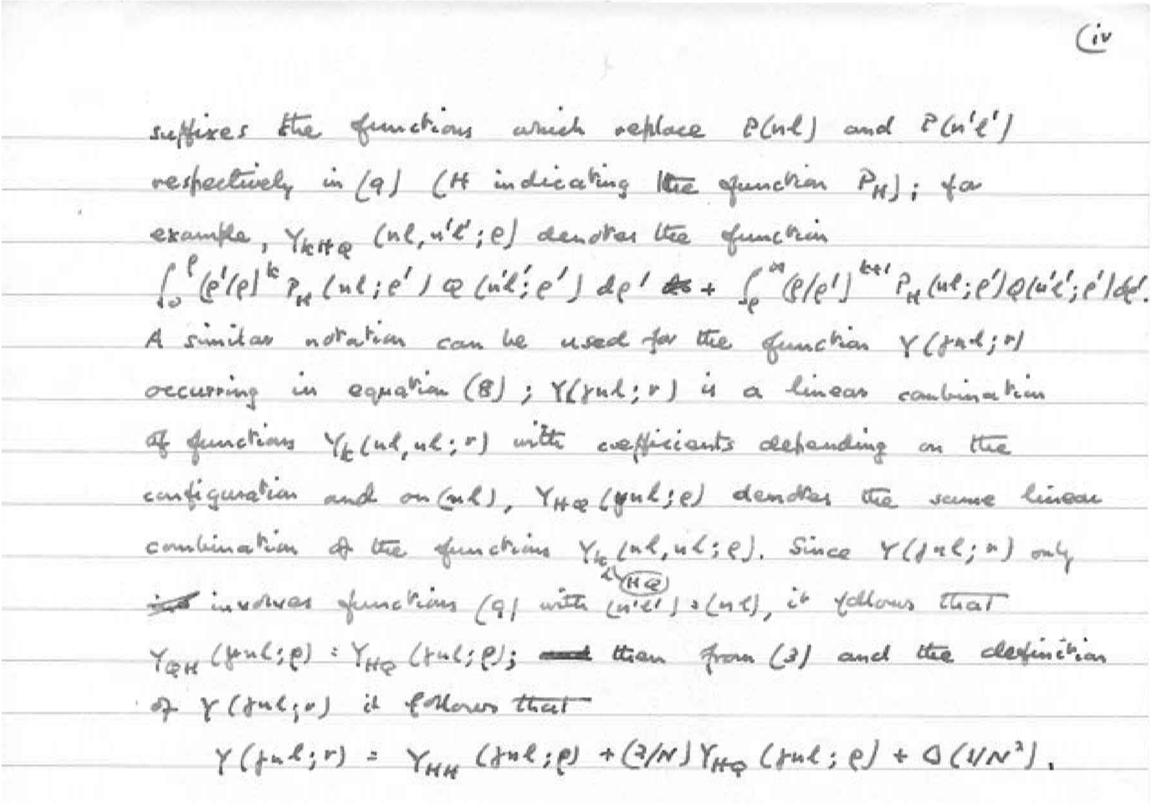


Figure 1. Late night computing on the EDSAC (note the paper tape for input/output and the mechanical calculator in the background).

As a research project, Hartree assigned to me the problem of solving 'equations with exchange' as he called them, whereas David Mayers, who started a few months before me, was assigned the relativistic problem without exchange. At the same time, Hartree was getting ready for a year at Haverford College in the USA. During his absence, my supervisor was Dr Maurice V. Wilkes, Director of the Mathematical Laboratory, who had designed and built the EDSAC and later obtained an A. M. Turing award from the Association for Computing Machinery for his work in computer architecture. In January 2000 in the Queen's New Year Honours List he was awarded a knighthood for services to computing, and now will be known as 'Sir Maurice'. As supervisor, his primary responsibility was to report on my research progress to the University at the end of every term. He would ask me to come in for a chat, inquiring how things were going. I always got the feeling he was relieved when I told him everything was going well because I am not sure he knew what to do otherwise. Although Cambridge did not require PhD students to take courses, I audited a course on the organization and design of the EDSAC computer and another on numerical analysis given by J. C. P. Miller (mentioned earlier) who spent much of the class time operating a mechanical Brunsviga to illustrate numerical concepts. I also had a chance to audit a course on quantum mechanics given by P. A. M. Dirac, whose lectures were always



(iv)

suffixes the functions which replace $P(nl)$ and $P(n'l')$ respectively in (9) (H indicating the function P_H); for example, $Y_{kHQ}(nl, n'l'; \rho)$ denotes the function

$\int_0^\rho (\rho'/\rho)^k P_H(nl;\rho') Q(n'l';\rho')\, d\rho' + \int_\rho^\infty (\rho/\rho')^{k+1} P_H(nl;\rho') Q(n'l';\rho')\, d\rho'$.

A similar notation can be used for the function $Y(\gamma nl; r)$ occurring in equation (8); $Y(\gamma nl; r)$ is a linear combination of functions $Y_k(nl, nl; r)$ with coefficients depending on the configuration and on (nl), $Y_{HQ}(\gamma nl; \rho)$ denotes the same linear combination of the functions $Y_{k(HQ)}(nl, nl; \rho)$. Since $Y(\gamma nl; r)$ only involves functions (9) with $(n'l') = (nl)$, it follows that $Y_{QH}(\gamma nl;\rho) = Y_{HQ}(\gamma nl; \rho)$; then from (3) and the definition of $Y(\gamma nl; r)$ it follows that

$$Y(\gamma nl; r) = Y_{HH}(\gamma nl; \rho) + (2/N) Y_{HQ}(\gamma nl; \rho) + O(1/N^2).$$

Figure 2. Sample of Hartree's handwritten notes.

presented in a very clear and logical fashion, but I must confess I had trouble seeing the big picture with my limited background in physics.

While at Haverford College, Hartree presented a series of lectures and completed his book, *The Calculation of Atomic Structures,* published by Wiley in 1957. To my recollection, he wrote to me twice. When he returned, he was extremely busy but quite interested in the results I had obtained during his absence. He helped me prepare several papers for publication, submitting them to the *Proceedings of the Cambridge Philosophical Society*, without being a coauthor. I have been told since, by Roy Garstang, that he believed the person who did the work should get the credit or take the blame! But I also remember going on a summer vacation and coming back to find he had written up some work for publication. In spite of having written the paper, he included his name as second author! This illustrates his helpfulness and extreme generosity of spirit. It also is my only joint publication with Hartree.

By that time, I was getting ready to return to Canada and I regret that, under these circumstances, I really did not get to know Hartree very well. However, during this last year when I was finishing my thesis, we corresponded extensively. In those days, papers to the Cambridge Philosophical Society or the Royal Society of London, needed to be submitted by Fellows. He read my drafts, gave suggestions for notation and pointed out errors. One piece of somewhat amusing advice in that it is no longer relevant is the following: 'The formulae need writing larger and more clearly, so that a printer who hasn't seen such formulae before can read them with certainty'. Hartree himself had no reluctance to fill pages with handwritten formulae which were always clear and had only few corrections, as the example in figure 2 shows.

I was extremely fortunate in the arrangements for my thesis defence. Normally, a student who had left Cambridge would have to take a written examination. It so happened that Professor John C. Slater invited Hartree to present a paper to a conference at MIT and to stay on as a consultant for several more weeks. My thesis defence was held during this time, with Hartree and Professor W. H. Watson, Chairman of the Physics Department at the University of Toronto, as my examining committee. For my defence, Hartree came to the University of Toronto and the three of us, two examiners and myself, had a friendly meeting. The most difficult question came from Professor Watson who asked if I believed in parity violation. I fumbled around a bit, but Hartree knew I had no idea what parity violation was. He turned around and asked Professor Watson, 'What is your opinion?', and the two of them had a little chat. On all occasions I found Hartree to be a very kind and helpful person. When he died suddenly in February 1958, about 6 months after my thesis defence, I lost a mentor who had provided me with a lot of guidance and support.

There were not many research opportunities for women in Canada when I obtained my PhD degree in 1957. I interviewed with IBM who offered me a position in their education division when I really wanted to be a systems engineer! But the University of British Columbia had just purchased their first computer, an ALWAC IIIE, so I accepted a position as Lecturer in the Mathematics Department. During my first year, I taught three courses, two of them back-to-back in time and some distance apart in space. In those days, teaching seemed easy. Much of calculus, for example, was taught by having students do problems at the board and very little preparation was needed. Summers were spent on computer work for the Pacific Oceanographic Group, Fisheries Research Board of Canada at Departure Bay, near Nanaimo, BC, under the direction of Dr N. Fofonoff. He taught me a very important lesson. He stated firmly that 'If you do not write up your work, there is no point in doing it'. To this day, I have bound copies of reports in the *Fisheries Research Board of Canada Manuscript Report Series*, in which every subroutine and program is described in detail, together with instructions on their use and even program listings. In those days the programs were short, though totally unreadable. Then in 1960, I was offered a summer position at the Boeing Airplane Company, Renton, Washington, where I was allowed to pursue my own research and use their advanced computing facilities. These included not only the latest IBM computer but also a FORTRAN compiler. For the first time, I saw there was a chance for portability of computer programs, and I began to develop numerical methods for atomic structure calculations. The following year, I was offered a summer position by David Layzer at the Harvard College Observatory, where the Smithsonian Institute also had excellent computing facilities that soon included an IBM 7090. This was an ideal environment. I spent several more summers, as well as a sabbatical, at the Harvard College Observatory and, in 1963, I was the first woman to be awarded an Alfred P. Sloan Foundation Research Fellowship. The objective of the Foundation was to select relatively young faculty members who have unusual potential for creative thinking in areas of the basic physical sciences, and then make unencumbered funds available for their research. It was a great honour for me to be selected. Thus, my research path had developed.

In 1967 I married Patrick C. Fischer, a computer scientist at Cornell University with an MIT degree in logic and computability theory, and we became a 'two-body problem'. Our first year was spent at the University of British Columbia, but UBC did not have a graduate programme in computer science. At that time, the University of Waterloo was rapidly expanding their computer science programme, so we both accepted positions there. Soon after, an extra dimension was added to our life with the birth of our daughter, Carolyn. Though she did not follow her parents into the hard sciences, we are proud of her success as an economist, interested in environmental issues. My husband soon became interested in administration, serving as Chairman first at the University of Waterloo, then Penn State University, and finally at Vanderbilt University. At each of these institutions, my primary appointment was in computer science, but my research interests were in numerical methods particularly as they related to atomic structure calculations, and to ideas of computational science.

In many respects, 1978 was a special year. Through the efforts of Brian Wybourne, I was offered a Visiting Erskine Fellowship to the University of Canterbury, at Christchurch in New Zealand. While there I had the opportunity of seeing the University's collection of medals and awards received by Lord Rutherford. My husband and I thoroughly enjoyed New Zealand. A week after my return, I left to give an invited talk at the Sixth International Conference on Atomic Physics in Riga, Latvia. The jetlag was horrendous. It also was the year I began to obtain funding from the US Department of Energy, which provided me with access first to what were called supercomputers and later to massively parallel systems. The funding also allowed me to collaborate with some excellent physics postdoctoral fellows: by combining their knowledge of physics with my computational experience, we were able to make significant contributions to atomic physics. Also, I learned a lot of physics in the process. In 1991, I was elected a Fellow of the American Physical Society: 'For developing the numerical approach to the Hartree–Fock method for atoms; for providing benchmark calculations of atomic energies and oscillator strengths; for the discovery of the calcium negative ion'.

Negative ions always held a special fascination for me. These atoms become bound because of the correlation in the motion of outer electrons. Chemical complexes often contain $O^{=}$: does it exist as an isolated atom? I spent many hours around 1970 trying to determine whether the system would bind if a sufficient amount of correlation were added. The answer is no.

Maybe this experience prepared me for showing very quickly in the Fall of 1986 that Ca^- existed and that the ground state was $4s^24p$. A year or so earlier, David Pegg of the University of Tennessee at Knoxville told me of an experiment in which he was convinced his group had created Ca^-. The problem was that they could not observe any decay. A possible answer was that the negative ion was in an exotic, high spin state with a long lifetime. I could find no such state. In the Fall of 1986, Jolanta Lagowski, a postdoc with S. H. Vosko working on density functional theory, asked many questions about the calculation of the electron affinity of Sc. Finally, I decided to do the calculations myself. Seeing how correlation yielded the $3d4s^24p\ ^1D$ ground state configuration for Sc^-, provided me with the insight that in Ca also the extra electron might be a 4p electron. Calculations very quickly showed a stable negative calcium ion. Of course, the electron affinity was very small and I did not expect my result to be quantitatively correct, but a ground state is stable and could explain the lack of any decay in experiment. A paper reporting these results was submitted to *Physical Review Letters* and was rejected twice. Then, when David Pegg and his group redesigned their experiment for photoelectron spectroscopy, and found a stable negative ion with almost identical electron affinity to my prediction, our two papers were accepted and published back-to-back. Later, both of our results were found to be in error quantitatively, but the negative ion was bound. This work demonstrated that the alkaline earths, at least from calcium on, could form negative ions, with the electron affinity increasing with increasing nuclear charge. The experience also taught me that experimental verification is extremely important for unexpected new theory to be accepted, though I suppose we could have tried another journal.

Also important to my research were collaborations with other scientists. My own interest was the radial problem, which leads to systems of coupled differential equations together with the eigenvalue problem. But for predicting atomic properties the angular problem, which has its basis in group theory, also needs to be solved. In early days, angular integrations were laboriously computed by hand using extensive tables. I was delighted when Paul Kelly (then at Lockheed) sent me a computer program for this task, but it had too many errors to be relied on. Then Alan Hibbert at Queen's University, Belfast, sent me a program. It too had errors but Alan always corrected them promptly. Thus a long collaboration started. These programs have now been replaced by faster, more efficient algorithms based on the theory developed by the A. Jucys' school at the Institute for Physics and Astronomy, at Vilnius, Lithuania, in particular by Z. Rudzikas and G. Gaigalas. The angular integration for transition probabilities was a special interest of Michel Godefroid at the Free University of Brussels, who was responsible for implementing powerful methods based on the biorthogonal transformations. Theorists also need to interact with experimentalists. In this regard, I have had a very rewarding collaboration with the Atomic Spectroscopy group at Lund University, where Indrek Martinson was extremely supportive, always finding ways to fund a visit, and getting me elected to the Royal Physiographical Society of Lund. Two postdoctoral fellows with whom I have had very productive collaborations are Tomas Brage and Per Jönsson. We even wrote a book together, entitled *Computational Atomic Structure: An MCHF Approach,* and participated in resolving a long-standing discrepancy between theory and experiment.

Both lithium and sodium, to an extent, are simple systems with one electron outside a closed shell core. For years, there was a discrepancy in the resonance transition between theory and careful experiment with extremely small error bars. In lithium, all theory was in essential agreement but outside error bars. This was a concern in that, if experiment was as accurate as it was claimed to be, the theory of transitions was inadequate. But in 1995, R. G. Hulet's group developed a new experimental method which deduced the radiative dipole moment from spectra of long-range, singly excited diatomic lithium atoms. In 1996, a slightly revised value was reported using more data points. With a small correction to the most accurate Hylleraas results for a relativistic correction, theory and experiment were now in excellent agreement. In Na, the situation was somewhat different. Some simple semi-empirical results were in perfect agreement with existing experiment taking into account only the polarization of the core. Tomas Brage showed that multiconfiguration Hartree–Fock (MCHF) calculations, taking into account only core polarization, also were in good agreement but that the oscillator strength changed when correlation within the core was included. There also was a small relativistic correction. At the 5th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas in Meudon, France, in 1995 new experimental data were reported for sodium, removing also this discrepancy between theory and experiment. For some systems it is now possible to predict oscillator strengths that are accurate to a fraction of 1%, but there are still many cases where such accuracy is difficult to obtain.

My research has revolved around the rapidly evolving computer technology. Unfortunately, this also meant that research results could soon become obsolete. I remember well that Douglas Hartree, in his last few years, had developed an elegant scheme for getting good initial estimates of wavefunctions so that the self-consistent field method used for solving the Hartree–Fock equations would converge in several fewer iterations. My thesis was related to this problem. But I never implemented any of these ideas into a computer program: by that time the computers were fast enough that a simple, but general, scheme was more convenient, even if the calculation required a few more iterations. From this experience, I learned that it was important to have a long-term view, that the human factor of 'ease of use' was extremely important. Early programs often were written to implement a single method, and all too often would terminate with 'method failed' when solving nonlinear problems. It was far more productive to have the program try a series of approaches before giving up. In other words, the program should encapsulate my knowledge about the solution of the problem and try a number of alternative methods if the first one failed. This was not always implemented in practice, but was my goal. In 1969, Professor Phil Burke at Queen's University Belfast was instrumental in establishing the journal *Computer Physics Communications,* in which programs were described in some detail. Along with the journal was the Computer Physics Library. I was invited to submit my multiconfiguration Hartree–Fock paper to this journal, which appeared in the first issue. Later on, in 1987, this paper was designated a 'Citation Classic' by *Current Contents,* for the numerous citations it generated. I was told by users that the program was easy to modify and adapt to specific problems because of its modular design. The dimension of the MCHF expansion was set to five (5): unlike chemistry, the physics community insisted they were interested in 'concepts', that any wave function with an expansion greater than five could not be visualized and was considered 'numerology'. Fortunately, that fashion has passed because, in the configuration model, expansions of up to 100 000 or more may be needed to get the required accuracy. So it is important to distinguish qualitative results that explain the physics from calculations that yield results to experimental accuracy, if not better.

In my reminiscences, I have referred frequently to Hartree. Those of us doing research in quantum mechanics may think of atomic structure as his primary interest, but this was not the case. A web search (using google.com) for 'Douglas Hartree' produces a list in which the first two entries are to the history of mathematics, followed by more than 10 in reference to the history of computing, whereas a similar search on 'Hartree' immediately produces many references to Hartree–Fock and Dirac–Fock, etc. Let me finish with some remarks about Hartree that illustrate some of his many facets, all based on extensive reading and interpretation† rather than personal knowledge.

Douglas R. Hartree started his university studies at Cambridge University in 1915, but at the end of the first year, his studies were interrupted. He went to join the team directed by A. V. Hill which was studying anti-aircraft gunnery and related matters. His father, W. Hartree, who had been on the teaching staff of the Engineering Laboratory at Cambridge, though retired, had joined the team a year earlier. Here, it seems, father and son started working together on numerical problems for the first time, and Hartree became interested in differential equations. He returned to university after the war, completing Part II of the Natural Sciences Tripos in 1921, after which he started his PhD studies under the guidance of R. H. Fowler, a leader in theoretical physics at Cambridge at that time. In 1921, Niels Bohr gave a lecture course in Cambridge which greatly influenced Hartree. Fowler believed that there was a great need, and opportunity, for a more quantitative application of Bohr's theory of spectra, and that Hartree was the ideal person for such an undertaking. In 1926 Hartree obtained his PhD for the validation of Bohr's theory for X-ray and optical terms of spectra. In the summer of 1925 Heisenberg visited Cambridge, and in the summer of 1926 Dirac gave his first course of lectures on 'Quantum Mechanics (Recent Developments)'. Hartree knew his work on Bohr's theory needed to be revised and on 21 November 1927 read a paper to the Cambridge Philosophical Society on 'The wave mechanics of an atom with a non-Coulomb central field', published in the 1927 *Proceedings*. In this paper he introduced atomic units, which simplify the equations tremendously, and also the term 'self-consistent-field method', which he described in a flowchart-like notation. Two years later, in 1929 he read a second paper, this time on 'The distribution of charge and current in an atom consisting of many electrons obeying Dirac's equations', in which he showed that a filled, spherical subshell, in non-relativistic theory becomes two spherical subshells in Dirac theory.

In 1929 Hartree accepted the Beyer Chair in Applied Mathematic at Manchester University. Here his interests seemed to have shifted. In the mid 1930's, he visited Vannevar Bush at MIT, who had built a differential analyser (first proposed by Lord Kelvin) that performed

† The most important of these are: C. G. Darwin, 1958, *Biographical Memoirs of Fellows of the Royal Society*, **4,** 103; M. V. Wilkes, 1958, *Computer Journal*, **1,** 48; M. Hartree Booth, 1986, personal memoirs, Christ's College, Cambridge, UK; B. Swirles Jeffreys, 1987, *Comments in Atomic and Molecular Physics*, **20,** 189; and J. Howlett, 1999, private communication.

integrations with a wheel rolling over a disk. This analogue device was particularly well suited to the solution of differential equations. Upon his return, he decided to build a similar device using 'Meccano' parts. His first PhD student was Arthur Porter, who helped with the design. A display of part of the model along with pictures of Hartree and Dr Porter can be seen at the Science Museum of London. Hartree also had a number of other students, such as Jack Howlett (1912–1999), who later was in charge of what was to become the Harwell Atomic Energy Establishment's computing section. During World War II, the Manchester differential analyser was probably Europe's most powerful calculating engine, and the group made valuable contributions to the atomic bomb project. In 1937 Hartree was promoted into the Chair of Theoretical Physics at Manchester, although in 1939–1945 during World War II he was working for the Ministry of Supply. Through his government contacts, Hartree was in touch with the development of electronic digital computers in the US. In 1945, just as the war in Europe was in its final stages, arrangements were made for him to see the Harvard Automatic Sequence Controller in action. The next year he was invited for a longer period to advise on the ENIAC computer being built at the University of Pennsylvania in the Moore School of Electrical Engineering. He was able to use the machine for a problem in laminar boundary fluid flow. In 1946 he returned to Cambridge as Plummer Professor of Mathematical Physics. His inaugural lecture 'Calculating machines: recent and prospective developments and their impact on mathematical physics' is included in an MIT Press reprint of his first book, *Calculating Machines,* published in 1947 by the Cambridge University Press. The address deals with computers and differential equations with no reference to quantum mechanics!

While at Manchester, Hartree had not completely lost interest in atomic structure calculations, as can be seen from the list of published papers included in the *Biographical Memoirs of Fellows of the Royal Society*. The publications show a wider range of topics, and though he published some papers by himself, far more are in collaboration with his father, W. Hartree, who performed the computations. In 1925, Bertha Swirles began her studies with R. H. Fowler at Cambridge, and Hartree passed on some problems from his thesis to her. In the Fall of 1928, she became an assistant lecturer in mathematics at Manchester University for a few years, returning in 1933 so she and Hartree were again at the same institution. At that time she again became involved with the self-consistent field method. She remembers Hartree suggesting the extension of the self-consistent field method to the Dirac equation at Euston (a railway station in London) when returning to Manchester from a conference in London. This led to one of the first papers on Dirac–Fock methods for atoms, applied to helium triplets. Bertha Swirles was more theoretical than Hartree, and not as interested in the computational process. So when the idea of 'superposition of configurations' for the calculations in oxygen was proposed, Hartree's father did the numerical work. This paper was published in 1939. When Bertha married Harold Jeffreys in 1940, Douglas Hartree attended the ceremony to give the bride away (see figure 3). Later on, when Harold Jeffreys was knighted, she became Lady Jeffreys, or 'Lady J.' as she says her friends call her.

Hartree had a number of other interests. His wife was an accomplished pianist and Hartree himself was a competent musician, playing not only clarinet and tympani, but also piano. So their house had to be large enough for two pianos. Sometimes he would conduct an orchestra, but apparently was happiest when he could be the timpanist. During the 1930s he founded the Faculty of Music at Manchester University and served as its first Dean. Another hobby was trains. During a strike in 1926, he had helped to man a signal box at a level crossing. Apparently he had enjoyed this a great deal, and this may have spurred his interests in railway signalling. He had an extensive train model at home which he made himself—track, rolling stock, signalling systems and all. It is likely that he was the first to point out that railway timetables could be constructed theoretically by solving differential equations, and had actually done this with the differential analyser. Apparently, there always were 'Meccano' sets around the house. His daughter, Margaret, in her personal memoirs of her father, writes that he introduced his children to the wonders of 'Meccano' in the mid 1930s, stimulating their interest in building more and more elaborate structures. However, parts kept disappearing; new boxes were given at birthdays and Christmas, yet more parts disappeared. They did not know they were being used to construct the differential analyser! Apparently another hobby was photography, and this came as a surprise to me. I myself had no picture of Hartree; and when I started contacting others who might have known him better, none had personal pictures that could be used with this article, except for two pictures from Lady Jeffreys that were group photographs taken in her mother's garden on the day of her wedding.

All sources of information refer to Hartree's kindness and his computational abilities. Apparently he performed calculations in all kinds of situations, including while travelling on a train. I remember being told that Hartree had deduced that the EDSAC was failing when multiplying by zero by calculations he performed on the train between Cambridge and

Figure 3. Douglas and Elaine Hartree at Bertha and Harold Jeffreys' wedding in 1940.

London. M. V. Wilkes reports that Hartree told him that he had something like 10 000 hours of personal computation to his credit.

In reviewing the history of Douglas R. Hartree, I was struck by the fact that he had collaborated with at least two women scientists (B. Swirles and B. Worsley) and, given the time in history, he had an unusual number of women PhD students, all in quantum mechanics. I was not able to research the situation at the University of Manchester, but believe he had at least one female PhD student, namely M. Black. Asearch of Cambridge University publications, shows that in his 11 years at Cambridge, he had two female PhD students (E. C. Ridley and I) and three male students (R. Garstang, A. S. Douglas, and D. F. Mayers) Thus, it seems appropriate to include, in this article, the picture of Douglas and Elaine Hartree at the wedding of Bertha Swirles to Harold Jeffreys. Lady J. was someone Hartree had collaborated with extensively, and the two of them laid the foundation for both multi-configuration Hartree–Fock and Dirac–Fock methods. Unlike Hartree, who died at the relatively early age of 60, Lady J. was 96 years of age when she died on 18 December 1999.

In my career, I have had a number of female graduate research students but only one female postdoctoral fellow, namely Lidia Smentek from Nicholas Copernicus University, Torun, Poland, an Editor of this issue. Though our research interests diverged since 1982 when she was at Vanderbilt University, we have remained friends. I am extremely grateful to her and her husband, Andy Hess, for organizing this tribute to my 70th birthday. My best wishes to both of them. I also want to take this opportunity to express my gratitude to all the authors who have contributed to this issue of *Molecular Physics*. It is a great honour to me and most unexpected. I look forward with great anticipation to reading this very special issue.

Also I wish to take the opportunity to thank Roy Garstang, Lady Jeffreys, and Joyce Wheeler for their invaluable assistance with my historical research, and to record my thanks to Christ's College for providing me with a copy of Margaret Hartree Booth's memoir of her father.