Having graduated in Mathematics in 1951, I began research in Theoretical Physics in the Clarendon Laboratory, and was awarded the D. Phil. in 1954. I was still liable for National Service; conscription into the Royal Corps of Signals in January 1955 eventually led to a posting to the AWRE Army Element in December 1955. Although still a Sergeant in the Signals, my job was that of a Scientific Officer in the Mathematical Physics Divisions at AWRE Aldermaston (now AWE). This introduced me to problems involving the interaction of intense electromagnetic radiation with matter, in particular matter containing heavy element constituents, which required the development of new methods of relativistic quantum theory [1] which have since dominated my research. I also became acquainted with other areas of mathematical physics, in particular particle and radiative transport theory, radiation hydrodynamics and the use of numerical methods for solving integral and differential equations in these fields.

On demobilization in January 1957, the UKAEA appointed me a Senior Scientific Officer in the Mathematical Physics Divisions at Aldermaston and I was promoted to Principal Scientific Officer in January 1962. The potential applications of relativistic quantum theory in atomic, molecular and solid state physics were not fully understood in 1961, and I was soon obliged to move on to new problems involving radiative transfer theory. In May 1964, I was elected to a 5 year Research Fellowship at the Science Research Council's newly formed Atlas Computer Laboratory, Chilton (now part of the Rutherford Laboratory) associated with a Research Fellowship at Pembroke College, Oxford. As well as developing an astrophysically oriented project to exploit the new Atlas computer, I was also expected to organize Pembroke's mathematics teaching to undergraduates, and give up to 6 hours a week of tutorials.

Although not formally attached to the Mathematical Institute, I was invited to meetings of Prof. Charles Coulson's Quantum Theory Group. At the time, this was one of the major groups studying applications of quantum theory to the structure and properties of atoms and molecules. It was his question at one of these seminars that encouraged Valerie Burke and me to investigate how relativity affects the shapes of hydrogenic wavefunctions [2], the first step in visualizing how relativity alters the electronic structure of atoms [3] and molecules and the way they interact with the environment.

At the time, radiative transfer theory was still dominated by simple models with plane parallel stratification, modelled by integral and differential equations solved analytically. The most sophisticated numerical techniques available were mainly devised for neutron transport, where the particle mean free paths were typically of similar order to the dimensions of the system. I was interested in a range of problems in stellar and planetary atmospheres in which the medium may be neither uniform nor stratified in planes and mean free paths can change by orders of magnitude for radiation of different colours and from one place to another. To meet this challenge, I came up with the idea of combining imbedding methods, which exploit the semigroup structure of the equations relating reflection and transmission operators at the interface of adjacent regions, with finite difference approximations to these operators. The article, written jointly with Garry Hunt, describing the mathematical structure [4], continues to be

cited occasionally, mainly in studies of the flow of radiation in planetary atmospheres and remote sensing from space.

Pembroke elected me to a Tutorial Fellowship and I became a CUF lecturer in 1969. I soon found I had little time to continue active collaboration on planetary radiation problems with Garry Hunt [5] at the Atlas Lab. Some further work on radiative transfer in the atmospheres of giant stars was done with a student, Annamaneni Peraiah (now Emeritus Professor in Bangalore) [6], but rising activity in the applications of my 1961 article *Relativistic self-consistent fields* [1] impelled me to devote most of the limited time available for research to this growing field. There had already been extensive studies of the ground states of atoms from Helium to Fermium (and even to hypothetical "superheavy" elements), and the opportunity to write a review of the field [7] in 1969 suggested a strategy for further development. This was refined during a 3 month Workshop at CECAM, Paris, in 1970, attended by David Mayers (Oxford Comlab), Jim Waber (Los Alamos/Northwestern Univ), Jean-Paul Desclaux (Centre d'Etudes de Limeil, France) and me. Two major program packages for the relativistic calculation of atomic structure and properties, now used world-wide, were conceived at this meeting: GRASP (see below) and MCDFGME [10], mainly due to Paul Indelicato and Jean-Paul Desclaux, maintained by the Laboratoire Kastler-Brossel in Paris.

Professor Coulson left the Mathematical Institute to found the Oxford Department of Theoretical Chemistry in 1970, and I was encouraged by his offer of an office in the department to my first postdoc, Nick Pyper, who was a theoretical chemist. After Coulson's death in December 1974, the Acting Head of Department, Mark Child, invited me to join the department, enabling me to build a small research group with a few research students and a succession of postdocs, supported by SRC/SERC research grants. This group, which included Nick Pyper, Jiro Hata, Dick Shun. Bruce McKenzie, Steven Rose, Ed Plummer, Patrick Norrington, Ken Dyall, Leif Laaksonen, Harry Quiney, Farid Parpia, Wasantha Wijesundera and Slimane Ait-Tahar at various times, continued to develop what later became GRASP (General-purpose Relativistic Atomic Structure Package) [8] and to expand its range of applications along with studies of electron-atom/ion scattering using a relativistic version of the R-matrix method (the DARC code) [11].

Promotion to *ad hominem* Reader in Mathematical Physics in 1990 and then *ad hominem* Professor in 1992 brought the group back to the Mathematical Institute. Farid Parpia left Oxford to work with Charlotte Froese Fischer (Vanderbilt Univ/ NIST), producing a new version, GRASP92, for multi-processor systems. With further development, renamed `grasp2K`, this package continues to be developed and maintained by the CompAS group [9] coordinated from Malmö University in Sweden. Overseas visitors to Oxford, Josef Sienkiewicz (Gdansk), Jacek Bieroń (Krakow), Gediminas Gaigalas (Vilnius) and Stephan Fritzsche (Jena) further contributed to the project; Bieroń, Gaigalas and Fritzsche are members of the CompAS group.

Interest in relativistic modelling of molecular electronic structure became a hot topic in the 1980s. Molecular electronic structure is usually modelled

nonrelativistically using Galerkin methods introduced by Roothaan in 1951 to approximate the electronic Schrödinger equation. Early attempts to use similar methods to calculate molecular electronic structures relativistically by replacing Schrödinger's operator with Dirac's relativistic operator failed miserably, and it was even claimed that the relativistic self-consistent field equations for atoms or molecules had no valid bound state solutions. Investigation of the reasons for failure were studied by Ken Dyall, Stephen Wilson (Atlas Centre, Rutherford Laboratory) and me [12, 13], leading to a practical demonstration, by Harry Quiney in his 1987 D. Phil thesis, of a well-posed stable method for atomic electronic structure [14], opening the way for extension to molecules. Here, the bottleneck was an efficient algorithm for calculating multi-centre interaction integrals over four-component Dirac spinors. The algorithm we developed, described in Haakon Skaane's D. Phil. thesis in 1998, is central to the BERTHA code [15] for relativistic molecular electronic structure (named, with her permission, after the late Bertha Swirles (Lady Jeffreys) who wrote the first paper on relativistic self-consistent fields at Cambridge in 1935). Quiney, now A/Professor at the University of Melbourne, has recently collaborated with Professor Francesco Tarantelli's group at the Chemistry Department, University of Perugia, to develop a Dirac-Kohn-Sham version of BERTHA to study the electronic structure of chemical systems with many heavy atoms [16]. They suggest the method is now sufficiently powerful to permit the time-dependent modelling of the behaviour of molecules in strong electromagnetic fields, accurately accounting for relativistic kinematic effects and spin-orbit coupling.

High precision calculations of atomic and molecular structure, especially if atoms with high nuclear charge are present, require inclusion of radiative corrections predicted by quantum electrodynamics, of which a major contributor is the lowest order self-energy of an orbital electron. Self-energy is dominated by the strong fields near the atomic nucleus, and is usually approximated in many-electron atoms today by scaling tabulated self-energies for hydrogen-like ions using the ratio of the actual electron density near the nucleus to the electron density in the appropriate hydrogen-like ion. Harry Quiney and I investigated direct *ab initio* calculation of the self-energy in a many-electron atom using a novel renormalization scheme that avoids the subtraction of formally infinite quantities of standard treatments [17, 18, 19]. This approach merits further work. A visitor from St. Petersburg, Victor Yakhontov (now in Basel) studied an alternative approach [20].

My book [21] reviews the field of relativistic atomic and molecular structure to the mid-noughties.

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