PHILIP GEORGE BURKE
18 October 1932 — 4 June 2019
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Elected FRS 1978

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The development of theoretical and computational atomic and molecular physics in the second half of the twentieth century owes a great deal to Phil Burke. His knowledge and insight, his enthusiasm and encouragement, his vision and determination were essential characteristics for the success of his work and that of many others. He developed and used the R-matrix method in the study of the interaction between, on the one hand, atoms and molecules and their ions and, on the other, light or electrons. He published many original research papers and was author or editor of a number of books. Especially significant and far-reaching was his setting up of the journal Computer Physics Communications to enable an international field of scientists, initially to share computer codes, but subsequently also to discuss and develop methods in computational physics. While based at the Daresbury Laboratory, he established a number of Collaborative Computational Projects, thus providing a forum for scientists working in specific scientific disciplines to meet periodically to discuss current issues and in particular how the ever advancing cutting-edge of high-end computing could begin to address previously intractable problems. A consequence was his clarity of thinking about which new computer architectures were needed to make significant advances in each field of study, expertly guiding the UK’s provision of high-end computers to academia for over 20 years. He was a clear and methodical teacher, at both graduate and undergraduate level, and was generous with the time he gave to his students. In short, he demonstrated a balanced level of excellence in all aspects of his career. He was a consummate academic and a fine role model for his colleagues.

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Philip George Burke was born in London on 18 October 1932. His father, Henry Burke (born Hermann Burk), was a police constable born in London in 1882 of parents who had emigrated from Germany, while his mother, Frances Mary Burke (née Sprague), had been a nanny working in London. She was born in Forty Hill, Enfield, London, in 1888, where her father worked as a coachman.

Phil’s secondary education was in Wanstead County High School, London, during 1943 to 1950, although for a period of several months in 1944 his classes were held in a local secondary modern school after the high school was badly damaged in a bombing raid. He particularly excelled in mathematics and physics. So it was a natural next phase in his education, beginning in 1950, that he moved to the University College of the South West of England, in Exeter, and read for a BSc degree in physics. He achieved his degree with first class honours in 1953, awarded externally by the University of London because, at that stage, Exeter did not have its own degree-awarding rights. In due course, Exeter became a university in its own right, and in particular with the ability to award its own degrees. Phil was delighted when, in 1981, he was awarded by the University of Exeter the degree of DSc honoris causa in recognition of his outstanding achievements in physics, nationally and internationally. In 1992, Phil was accorded from the University of Exeter a first class BSc degree in physics ad eundem gradum, in parallel to his original BSc award from the University of London.

In 1953, Phil was awarded the Granville Scholarship by the University of London, which enabled him to go to University College (UCL) to undertake studies for a PhD. On arrival he was interviewed by Harrie (later Sir Harrie) Massey (FRS 1940), who suggested that Phil work on a problem in nuclear physics—the scattering of neutrons by deuterons. Massey also told Phil that the work would involve the application of electronic computers. The problem interested Phil, but he was rather wary about the use of computers, a new direction for him. The work was supervised jointly by Massey and R. A. Buckingham.

It soon became clear that Massey had been right and that substantial computing would be involved. Up to that time, most calculations had been done using Brunswega hand-operated machines, but Massey had arranged for a Booth computer to be acquired—designed by A. D. Booth and his wife; Booth was a lecturer at Birkbeck College, across the road from UCL. Initially, programs had to be entered in binary or had switches on the machine, while results were printed out on paper tape. This was slow and tedious, so Massey arranged for Phil to move his computing work to the pilot ACE computer at the National Physical Laboratory (NPL), Teddington. The ACE (later the DEUCE) computer was double the speed of the Booth machine. Programming was again in binary, but now on punched cards, as was the output.

The work was duly completed, and Phil’s PhD was awarded by the University of London. His thesis was entitled A theoretical investigation into the scattering of nucleons by light nuclei and the nature of nuclear forces. Several papers arising from this work were among the earliest of Phil’s publications. This work, both the methods used and the use of electronic computers in the solution of problems, proved to be a firm foundation for Phil’s subsequent research development.
On completion of his PhD, Phil accepted a post-doc position at UCL, funded by the Atomic Weapons Research Establishment (AWRE), to work on computational atomic physics problems of interest to AWRE. He spent the next year developing a computer program to solve the electron–atomic hydrogen collision problem, using the DEUCE computers at NPL and AWRE. In 1957, he visited Queen’s University Belfast (QUB) with Ian Percival (FRS 1985) to carry out further developments of the code and production runs on the DEUCE at Short Brothers and Harland, the aircraft building company in Belfast. This visit brought Phil into contact with the Department of Applied Mathematics (subsequently the Department of Applied Mathematics and Theoretical Physics—DAMTP) at QUB. The work enjoyed encouragement and support from the department head, David (later Sir David) Bates (FRS 1955), and from Alex Dalgarno (FRS 1972). Bates had been a student of Massey, in Belfast and later in UCL, and this work strengthened the link between the departments in UCL and QUB.

In the summer of 1957, the University of London set up its new Computer Institute, with Buckingham as its first head. Phil was appointed to the first lectureship position in computational science in the University of London. He spent two years in this position, but was also able to continue his research in atomic and nuclear collision theory, writing programs for the Ferranti Mercury computer that the Institute had acquired. It was during this time that he began a life-long collaboration with a new post-graduate student of Mike Seaton (FRS 1967)—Valerie Mona Martin—who had been assigned by Mike to develop further and to apply the electron–hydrogen atom program that Phil had written.

**United States 1959–1962**

This collaboration proved to extend beyond physics or computing. On 29 August 1959 Phil and Val were married, and shortly afterwards moved to the United States. Phil had been appointed to a post-doc position at the Lawrence Radiation Laboratory, Berkeley, CA, to work in the group of Luis Alvarez (later a Nobel laureate) on the analysis of the experiments involving the 72-inch Bubble Chamber. Phil worked on this problem for the first 18 months in the US, and began to program, using an early version of FORTRAN, an IBM 709 machine. He and Val also started to program the electron–hydrogen collision problem in FORTRAN, Val being employed part-time in Ken Watson’s theory group. For the last 18 months of his time in Berkeley, Phil also moved to the theory group, where he carried out theoretical and computational work on atomic physics and, with Harry Schey, in particle physics (the latter on Regge trajectories and on pion–pion scattering). In 1990, Phil received a letter from the Institute of Scientific Information to indicate that two of his papers published as a result of his work at Berkeley had emerged as two of the most cited papers in their field, as determined by the Science Citation Index. These papers, one written with Harry Schey (1)* and the other with Ken Smith (2), had had considerable influence on other authors working in atomic collisions over a substantial number of years (29). Specifically, the first paper reported the first accurate calculation of a doubly excited resonance in e-H scattering (1), and the second presented a

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* Numbers in this form refer to the bibliography at the end of the text.
Biographical Memoirs

comprehensive review of the field of electron–hydrogen and positron–hydrogen scattering at the time (2). This award was an encouraging accolade to Phil about his work, completed when he was still under the age of 30.

Phil and Val enjoyed the friendly hospitality of the other scientists throughout their stay in the US. Connie and Gerry Lynch were special friends, and were particularly helpful before and after the birth of Phil and Val’s first daughter, Helen. Less than a year after their arrival in the States, Phil and Val bought a Yamaha grand piano. This enabled Val, an accomplished pianist, to maintain her life-long enjoyment of making music.

Back to England 1962–1967

Phil, like many scientists of his generation, had decided that he wished to spend time in the United States after completing his PhD. It was becoming quite common for young UK scientists to work in the US for a few years, in order to gain a wider experience of their respective fields. Their motivation in travelling to the US was the availability of funding for science at a level that the UK could not at that time afford; so much of the cutting-edge science was being done in the United States.

Phil and Val chose to return to the UK after Phil’s three-year contract came to an end. The UK government had established a number of recruitment boards, chaired by Harry Hoff, with the aim of recruiting back British scientists from North America. Sir Harrie Massey alerted Phil to the role of the Hoff Committee. Walter Marshall (later Lord Marshall of Goring, FRS 1971) was a member of the committee and was interested in bringing Phil to the UK Atomic Energy Research Establishment at Harwell. As a result, Phil was offered a position at Harwell, which he accepted. A few years later, Phil himself was invited by Marshall to serve on the committee, and so Phil was responsible for a number of British scientists returning to positions in the UK.

In the autumn of 1962, Phil and Val and their young daughter moved from Berkeley to Harwell. The following year Susan, their second daughter, was born, followed a year or so later by Pamela.

Almost immediately after the family’s return to the UK, Phil started work in the Theory Division at AERE Harwell, whose head was Walter Marshall. Phil began to collaborate with other members of the Division, particularly John Tait and Joanna Taylor. Their work followed on from the research described in the papers by him with Schey (1) and by him with Smith (2). This was based on the close-coupling approximation in the study of electron–hydrogen and electron–He$^+$ scattering. The target has a single electron, so there are two electrons in the system under consideration. The Hamiltonian of this system can be expressed in atomic units (for which $\hbar = e = m = 1$) as

$$H = -\frac{1}{2} \nabla_1^2 - \frac{1}{2} \nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}$$ \[1\]

where the subscripts 1 and 2 refer to the bound electron and the scattered electron respectively, so that $r_1$ and $r_2$ are the radial distances of the two electrons from the nucleus, while $r_{12} = |r_1 - r_2|$. The first two terms in [1] are the kinetic energy operators for the two electrons; the next two terms are the potentials due to the interaction between the nucleus and each
electron; the final term is the potential due to the Coulomb interaction between the electrons, and $Z$ is the nuclear charge.

In the close-coupling method, the two-electron wave function is written, assuming $LS$ coupling of the angular momenta of the electrons, as

$$\psi^{LS}(1, 2) = A \left\{ \sum_{\nu} \frac{1}{r_1 r_2} P_{nl_1}(r_1) \mathcal{Y}^{M_L}_{L_1 l_1}(1, 2) F^{LS}_{\nu}(r_2) \right\} + \sum_{\ell} \alpha^{LS}_{\ell} \phi^{L,M_L}_{\ell}(r_1, r_2) \quad [2]$$

where $\nu = n l_1 l_2$, with $l_1$ and $l_2$ being the orbital angular momenta of the two electrons, and the summation over $\nu$ can involve several target states, to allow for both elastic and inelastic collisions. $P_{nl_1}$ is an (exact) reduced radial hydrogenic function, $F^{LS}_{\nu}(r_2)$ describes the scattered electron, $\mathcal{Y}$ is a Clebsch–Gordan combination of products of the spherical harmonics of the two electrons, and the functions $\phi$ represent antisymmetrized two-electron bound configurations of the scattering system needed for completeness and also to provide some electron–electron correlation. $A$ is the antisymmetrization operator that ensures the total wave function is antisymmetric with respect to an interchange of the coordinates (space and spin) of the electrons. Substitution of [2] into the time-independent Schrödinger equation with Hamiltonian given by [1] leads to a set of coupled integro-differential equations (the Close-Coupling equations) for the functions $F_{\nu}$.

The effect of scattering is seen in the asymptotic behaviour of the scattered electron, and particularly in the form of $F_{\nu}(r)$ as $r \to \infty$. This leads to the determination of the reactance matrix (K-matrix) from which quantities such as the cross section of the scattering can be obtained, and then compared with experimental results.

Phil and his colleagues undertook specific calculations of the scattering of electrons by hydrogen and $\text{He}^+$ (5–8). For elastic scattering, they found that the correlation terms $\phi$ in equation [2] had only a small effect on the cross sections, but for inelastic collisions, they were crucial in obtaining results in good agreement with experiment. Further significant developments, motivated by the potential for astrophysical applications, were made in the theory of the scattering of electrons by more complex atoms with open p-shells (3), which led to calculations that accorded well with experimental results (4).

Phil’s colleagues at Harwell and other neighbouring laboratories formed the core of a group of friends for Phil and Val on their return to the UK. Joanna Taylor was an excellent singer, so Phil and Val, together with Joanna and her husband Bob (who worked at the Rutherford Laboratory), were able to organize informal weekly musical evenings. At these, Val accompanied Joanna’s singing, while John Tait’s wife, Hilary, also played the piano.

In 1965 Phil was invited to spend three months working with Ugo Fano at the National Bureau of Standards in Washington, DC, and so the whole family departed for the United States. On their return at the end of the three months, Val applied for a post at the Atlas Computer Laboratory, and she was appointed as a part-time Senior Scientific Officer to work assisting Ian Grant (FRS 1992).

In 1967 Phil was promoted from Principal Scientific Officer to Senior Principal Scientific Officer. His interview board was chaired by Dr (later Sir) Arthur Vick, who was head of AERE Harwell at that time. A few months later, Alex Dalgarno resigned his chair in the Department of Applied Mathematics at QUB to take up an appointment at the Harvard Department of Astronomy, and Phil was encouraged to apply for the vacant chair. Phil was surprised to find that the chair of the appointment panel at Queen’s was none other than Dr Vick, who had very
recently been appointed as Vice-Chancellor of Queen’s. Phil was duly appointed to the chair. In the following few years, before he retired, Vick’s careful management of the university was instrumental in keeping it out of the worst of the difficulties that dogged the Province during the early part of the ‘Troubles’.

**QUB 1967–1977**

Phil, Val and the girls moved to Belfast towards the end of October 1967. Two years later, Phil’s father died and so his mother came to join the family in Belfast. The Troubles affected every-day life in Belfast in a variety of ways. The daily news was grim, especially in the first half of the 1970s when each day we heard of bombs, shootings or knee-cappings. Sometimes bombs were detonated without warning; at other times warnings of bombs could be hoaxes. People in Belfast, as in other towns in the Province, were very wary of venturing into the centres of those towns. Though the Burke family remained safe through this time, the Troubles did impinge on them. One incident to affect them occurred in 1972 on what came to be known as Bloody Friday, when during the afternoon of 21 July bombs were let off in many parts of Belfast, in the suburbs as well as in the centre. Val and the girls were in the university when a bomb exploded nearby, blowing in the window of the room where Val was working.

The following year, Val gave birth to their fourth daughter, Alice. Earlier that year, Phil and Val purchased a former labourer’s cottage on a half-acre site in the townland of Rossglass, across Dundrum Bay from the Mourne Mountains. It was a country location, within a few minutes’ walk to the beach, and allowed the family to spend weekends and longer holidays away from Belfast.

Phil began to gather a small group of enthusiastic researchers around him who, under his leadership and overall direction, set about developing what came to be known as the R-matrix theory of atomic collisions and the associated computer packages. The aim was to extend from target atoms or ions having a single electron, as modelled by equation [2], to ones with any number of electrons. For an \( N \)-electron target, the Hamiltonian of the complete system is

\[
H_{N+1} = \sum_{i=1}^{N+1} \left( -\frac{1}{2} \nabla_i^2 - \frac{Z}{r_i} \right) + \sum_{i<j}^{N+1} \frac{1}{r_{ij}} \quad [3]
\]

A fundamental feature of the R-matrix method is the division of space into an internal region, in which short-range correlation has to be included among all \( (N+1) \) electrons, and an external region in which short-range correlation between the free electron and the electrons of the target atom or ion can be ignored. The boundary between these two regions, \( r = a \) (where \( r \) denotes the distance from the target nucleus), is usually defined as the distance beyond which the included wave functions of the target are essentially zero.

Hence in the internal region, the wave function for state \( k \) of the \( (N+1) \)-electron system is usually written as

\[
\psi_k (X_{N+1}) = A \sum_{ij} \Phi_i (X_N; \{ \hat{r}_{N+1} \sigma_{N+1} \} r_{N+1}^{-1} u_{ij}^0 (r_{N+1}) a_{ij} + \sum_j \chi_j (X_{N+1}) b_{jk} \quad [4]
\]
where $X_N$ denotes all the space and spin coordinates for electrons labelled $1, \ldots, N$, with a similar definition for $X_{N+1}$. Comparing with [2], $\Phi_i$ represents the wave function of the target, combined with the angular and spin coordinates of the scattered electron (paralleling $P_{nl}$ in [2]), $u_{ij}^0$ represents the scattered electron and $\chi_j$ represents the short-range correlation among all $(N+1)$ electrons. In [2] the functions $P_{nl}$ are known exactly. For a multi-electron target, the corresponding functions $\Phi_i$ are not known exactly; customarily they are expressed as configuration interaction functions.

Equation [4] applies only to the internal region $(r \leq a)$, so on that interval the Hamiltonian $H_{N+1}$ is not hermitian. This defect is corrected by adding the Bloch operator (Bloch 1957)

$$L_{N+1} = \sum_{i=1}^{N+1} \frac{1}{2} \delta(r_i - a) \left( \frac{d}{dr_i} + \frac{b - 1}{r_i} \right)$$  \[5\]

where $b$ is an arbitrary constant. Eigenvalues $E_k$ as well as the coefficients $a_{ijk}$ and $b_{jk}$ of equation [4] are determined by diagonalizing $H_{N+1} + L_{N+1}$ over only the internal region. The $R$-matrix at $r = a$ is determined from the $E_k$, $a_{ijk}$ and the $u_{ij}^0(r = a)$. The form of the wave function in the external region reduces to a close-coupling expansion without exchange:

$$\Psi(X_{N+1}) = \sum_i \Phi_i(X_N; \hat{r}_{N+1} \sigma_{N+1}) r_{N+1}^{-1} F_i(r_{N+1}) a_{ijk}$$  \[6\]

The link between the internal and external regions (and therefore with the $R$-matrix) is provided by the requirement that the wave function and its derivative with respect to $r$ must both be continuous at $r = a$.

There are three features of the $R$-matrix method that have made it the method of choice for many researchers in electron–atom/molecule collisions. First, it can be applied to any atomic or molecular system; second, the diagonalization relating to the internal region needs to be undertaken only once—in other words, it is independent of the energy of the incident electron; third, the division of space into suitably chosen internal and external regions means that, in the latter, exchange between the scattered electron and those of the target can be ignored, simplifying the associated equations and so reducing the computational effort required. The theory was laid out in two papers (10, 19). A further fundamentally important aspect of the method is that, besides having effective connection on the boundary between regions of space where the physics differs drastically, it permits advantageous use in each such region of the theory and numerical methods appropriate to the physics there. For example, this philosophy allowed the first successful calculations on Ba and Sr atoms in strong magnetic fields (O’Mahoney & Taylor 1986).

The initial thrust of the group’s work was to obtain expressions for the elements of the Hamiltonian matrix between single configuration functions, and an algorithm for this, based on Racah algebra, had been given by Ugo Fano (1967). The key constituents were angular momentum recoupling coefficients, a code for which was already being developed by Phil (9), fractional parentage coefficients, the coding of which was undertaken by Donald Allison (1969), while Alan Hibbert (1970) put together these components to give the Hamiltonian matrix elements. Computer codes developed for these stages benefited from the assistance of Alfie Chivers. Following this, Phil developed codes for the scattering part of the project.

Shortly after Phil moved to Belfast, he was approached to be the founding editor of a new journal, Computer Physics Communications (CPC), which would publish articles about
computing and also the computer programs themselves. The programs would be stored and
distributed to researchers via a program library, and it was suggested that Val would be the
program librarian. Subscribers to the journal and library were encouraged to interact with
the authors of the programs, and in some cases this established the possibility for ongoing
research collaboration. Further details of the development of CPC can be found in the fiftieth-
anniversary issue of the journal (Scott et al. 2020).

The development of this new journal proved to be ideal for Phil’s research group at Queen’s
because it provided an outlet for their programming work. The research group began to grow;
potential research students were attracted to work on the overall R-matrix project. In particular,
Derek Robb came to work on the development of the scattering codes, and especially on the
matrix elements of the dipole operator (Robb 1973). A little later, Ken Taylor developed (under
Phil’s overall direction) the application of the R-matrix method to the study of photoionization
(18). The group was further strengthened by the arrival of Keith Berrington from Durham, who
worked on developing the codes for a number of applications. The success of the R-matrix
method encouraged others in the department, who were separately working on electron–atom
collision problems, to begin to apply the R-matrix process in their work. Of these, Ken Bell
and Arthur Kingston were to sustain their activity for many years.

Calculations were commenced using the R-matrix method in a range of related
applications: oscillator strengths (11); electron–atom collisions, including the use of
pseudostates that proved to be important for neutral atom targets in order to represent the
polarizability of the target atoms (12); atomic polarizabilities (13); and van der Waals forces
(15). When the group was confident that the codes were working well, the first published
versions of the R-matrix codes were published in CPC (17, 22), along with the associated
atomic structure code CIV3 (Hibbert 1975). These codes, which could be applied to any
atomic system, represented a significant scientific advance in theoretical and computational
atomic physics, and fulfilled the stated aim of CPC to offer to the atomic physics community
the means by which much further work could be achieved.

As Phil’s reputation grew, the department hosted an increasing number of overseas visitors,
which allowed for the application of the R-matrix method in new avenues. Long-term
research collaborations were begun with Verne Jacobs (14) on photoionization, with Naresh
Chandra and Franco Gianturco (16) on electron-molecule scattering, and with Vo Ky Lan
and Maryvonne Le Dourneuf (20) on the use of polarized pseudo-states for neutral atomic
targets. These visits provided encouragement to the group during a difficult time in Northern
Ireland society. Additionally, a few conferences and other meetings were able to be organized,
but it wasn’t wise to entertain visitors in restaurants in the city. Instead, hospitality was
provided by members of the department, and particularly by the professors: Bates, Burke
and Moiseiwitsch.

In 1972, the department was rehoused in a new building, overlooking the Botanic Gardens.
This had been the brainchild of David Bates and was renamed the David Bates Building
following David’s retirement in 1982. The new building also housed the CPC office as well
as the CPC secretary, Marie Murray, and the senior programmer, Shirley Jackson.

Shortly after this, David Bates suffered a serious heart attack, and he was advised to
limit his administrative activities. He gave up the role of head of applied mathematics,
while continuing with his teaching and research. The headship mantle fell to Phil, which he
commenced in 1974. It was a role not entirely unfamiliar to him. For a number of years, Phil
had been responsible for the research activities of the department, while Benno Moiseiwitsch
Philip George Burke

had taken on a similar role for the teaching, with David in overall charge. The three of them had worked closely together. Also, in 1968, an informal ‘School’ had been created, comprising the Departments of Applied Mathematics and of Physics. This arrangement facilitated common interests in both research and teaching. Later, the School was expanded to include computer science and then also pure mathematics, again to enhance interactions in areas of common interest. Years later, the School was to form the model for the development of schools right across the university.

During this period in Belfast, Phil had a wider exposure to the UK physics environment, particularly with the Science Research Council (SRC). He was a member of the SRC Physics Committee from 1967 to 1971, while from 1969 to 1971 he was chair both of Sub-Committee X of the Physics Committee and of the Synchrotron Radiation Panel. Then from 1971 to 1975 he was a member of the Synchrotron Radiation Research Committee, and was therefore involved in the decision to site the new Synchrotron Radiation Source at the Daresbury Laboratory (DL) in Cheshire. This prospect was stimulating new projects in, for example, atomic and molecular processes, surface science, X-ray diffraction, crystallography and electronic structure of solids.

In light of his growing expertise and reputation, in 1974 Phil was elected member of the Royal Irish Academy. The Academy covers the whole of the island of Ireland (its founding in 1785 coming long before political divisions were formulated) and is Ireland’s premier learned society, embracing both the sciences and the humanities.

Phil’s expertise in high performance computing led to his appointment to SRC’s Atlas Computer Committee in 1973. Following the retirement of Jack Howlett as director of the Atlas Computer Laboratory (ACL) in 1975, ACL became a division of the Rutherford Laboratory. This stimulated discussion about the future of high performance computing in the UK, and Phil was appointed chair of the Panel on Future Computing Needs in Science in 1975. In 1976, he was appointed chair of the Science Board’s computing sub-committee, and this gave the impetus to bring together key people in the development of a future strategy for high performance computing in the UK. As a result, a small group met at DL. The group comprised Alick Ashmore, the director of DL, Sir Sam Edwards (FRS 1966), chair of SRC, John (later Sir John) Pendry (FRS 1984), head of the Theory Group at DL, and Phil. The group proposed the establishment of a new Theory and Computational Science (TCS) Division at DL, which would incorporate the existing Theory Group. This proposal was accepted by SRC, and in 1977 Phil became head of the new TCS Division at DL, as a joint appointment, initially for five years, involving DL and QUB.

QUB and the Daresbury Laboratory 1977–1982

The detail of Phil’s joint appointment arrangement included an agreement that he would work in QUB on Thursday and Friday of each week in term-time and at DL for the remaining time, though with a little flexibility to accommodate circumstances. As a result, and because of the continuing civil unrest in Belfast, Phil and Val decided that their home base should be in Cheshire. They bought Brook House, a large Victorian house built around 1850 in the village of Crowton, a short distance from DL and ideal as a family home, including suitable accommodation for Phil’s mother. Moreover, the house gave Phil the opportunity to indulge his passion for tree-planting. As Brook House became a long-term home for the family, Phil
was able to watch and nurture his trees, which grew to be very tall and which he was very proud to show to visitors.

So, on Wednesday nights in term-time, Phil would take the overnight ferry from Liverpool to Belfast, arriving very early on Thursday mornings, and then leave on the return boat on Friday evenings. This gave Phil two full days in Belfast, when he was able to undertake his teaching, meet research students and colleagues and attend any meetings, which the university would hold while he was there. His students, both graduate and undergraduate, much appreciated the time he devoted to them and the way he gave them his full attention.

An important aspect of the new TCS Division in DL was the support for and extension of the Collaborative Computational Projects (CCPs). The first CCP, on ‘Correlation in molecular wave functions’, had been set up at the ACL in 1974 by a working group chaired by John Murrell (Sussex). This pilot project provided a template for the development of more CCPs when the work was transferred to the TCS Division. The researchers associated with each CCP were able to coordinate their work and to meet regularly to discuss progress. The rapid growth of the CCPs at DL required a major increase in computer power. A prototype Cray was installed at DL in the summer of 1979, with SRC purchasing 40 hours per week from Cray Research. This yielded a major increase in computer power, with many researchers in the UK belonging to one or sometimes more than one CCP, and it opened up a new era of high performance computations. The pressure of working in two venues was a factor in Phil relinquishing his work as principal editor of CPC at the end of 1979. That role was taken up by Keith Roberts, who had been a strong supporter right from the beginning of the journal, and whose approach to programming Phil had long admired. However, Phil continued his links with the journal through his appointment as honorary editor and he continued as director of the program library through until 2000.

Phil’s work on applications of the R-matrix method continued apace, with numerous publications in conjunction with colleagues both in Belfast and in DL; for example, earlier work on electron-molecule scattering was extended by Phil and Brian Buckley (23). It became apparent that the limit to LS angular momentum coupling would be insufficient to meet the need for data to be used in astrophysical modelling, which required the study of transitions between specific J-dependent levels. This led to the incorporation of relativistic effects into the R-matrix codes. For such applications, and for medium-sized elements generally, the R-matrix theory was extended through the inclusion into the Hamiltonian of operators arising from the Breit–Pauli approximation, by Phil with Stan Scott (24) and with the modified R-matrix codes described by Stan Scott and Ken Taylor (1982). A fully relativistic version was needed for the treatment of heavier systems. Based on the Dirac equation, the theory was set out by Jwei-Jun Chang (1975) while working with Phil in Belfast. This was subsequently developed in Oxford by Ian Grant and Patrick Norrington (Norrington & Grant 1981) into what is now the Dirac Atomic R-matrix code (DARC).

In recognition of Phil’s growing standing as a national and international scientist, he was elected as Fellow of the Royal Society in 1978. Living now in England, he was more easily able to get to meetings of the Society (and other scientific meetings), held usually in London.

By 1980, Phil’s mother had become much more frail and in the September, at the age of almost 92, she passed away. Her loss was hard for the family, of which she had been an integral part, living with them since Phil’s father had died and playing an active role as the children grew up.
The following year there was a significant impact on Phil’s health. In August 1981 he returned home after attending a conference in the United States and collapsed with a slipped disc in his back. He was forced to take bed rest for several months and was still in a lot of pain, which precluded the renewal of his DL/QUB contract when it was completed in the summer of 1982. It was clear it was time to return to QUB full-time.

**QUB 1982–1998**

For their return to Belfast, and as Phil was still having problems with back pain, Phil and Val bought a house within easy walking distance to the department. The medical advice had been for Phil to undergo surgery to relieve his pain, but as there were significant risks in that, he asked for alternatives and was recommended to try exercise and particularly swimming. The university’s PE Centre, with swimming pool, was also close by, so Phil went there several times a week, a regime he continued for many years. Slowly, his mobility increased and pain diminished, although for the rest of his life he would suffer bouts of pain and had to take rest to overcome it. Within a year, he was able to drive and so the family moved to a house in the hills on the outskirts of Belfast, but still within an easy drive to the university.

Phil’s return to a full-time role in QUB coincided with the retirement of David Bates. Benno Moiseiwitsch had taken on the role of head of department in 1977, and he continued with this, leaving Phil time to lead the research effort and to engage more fully in scientific policy-making, both within the university and at national and international level. Within the university, he chaired the QUB Computer Committee (1982–1986), the IT Planning Committee (1987–1989) and the Research Advisory Group (1991–1993). His work on the development of national policy on high performance computing, begun during his time at DL, was recognized through invitations to join a number of national policy-making committees, often as chair. He was chair of the Computer Board’s Computer Consultative Council (1983–1985), of the Science and Engineering Research Council (SERC) Science Board Computer Committee (1984–1986), the SERC Atlas Centre Supercomputer Committee, the SERC Computing Advisory Panel, the SERC Supercomputing Management Committee (1991–1994), the Inter-Council HPC Management Committee (1996–1998) and the Joint Policy Committee on National Facilities for Advanced Research Computing Allocations and Resources Panel (1989–1990). Recalling that the Royal Irish Academy covers the whole of the island of Ireland, he was a member of the RIA’s National Committee for Physics (1984–1990). Additionally, he was a member of the Joint Policy Committee for National Facilities for Advanced Research Computing (1989–1990), the Council of SERC (1989–1994) and the Council of the Royal Society (1990–1992). He remained the Royal Society representative on the Court of the University of Ulster (1984–2003). He was also a member of the Scientific Steering Committee of the Isaac Newton Institute for Mathematical Sciences at Cambridge (1990–1994) and of the Advisory Board of the Edinburgh Parallel Computing Centre (1990–1996).

In recognition of his national and international achievement in science, and of his leadership and expertise in the field of high performance computing, he was awarded the CBE in 1993, an accolade of which he was very proud. His colleagues in QUB benefited greatly as a result of his work in this area, for they were kept abreast of the most up-to-date advances in computing, and for many years had access to the best available national computing facilities.
This access enabled the research group in Belfast to participate fully in the Opacity Project, a research project proposed and led by Mike Seaton at UCL to try to explain what in the 1980s was the poor agreement between theoretical determinations of stellar opacity and observational results (Seaton 1987). It required a systematic calculation of atomic data for all stages of ionization of most elements up to iron. Phil encouraged the group to get involved with this work, alongside colleagues at UCL and Royal Holloway College and with scientists from many other countries too. The calculations involved the determination of oscillator strengths of ionic transitions and of photoionization cross sections of the ions being studied. For the former, the combined team made use of different codes that individual groups had developed, mainly the CIV3 code of the QUB group (Hibbert 1975) and the SUPERSTRUCTURE code (Eissner et al. 1974) of the UCL group. These codes provided target state wave functions for the photoionization calculations. The two main groups also had individual codes for this process: IMPACT (Crees et al. 1978) from UCL, and the R-matrix codes from QUB (22). Mike Seaton quickly realized that Phil’s R-matrix package was the more efficient and later calculations were undertaken almost exclusively by this method. After several years’ work and the publication by different team members of a long series of atomic data papers, the use of these data in the opacity calculations did indeed result in much closer agreement between theory and observation (Seaton et al. 1994).

The range of applications of the R-matrix approach grew. Barry Schneider (1975) and then Phil with Ian Mackey and Isao Shimamura (21) had developed the R-matrix theory applied to electron-molecule scattering. Further developments were undertaken by Gillan et al. (25), while a new code applying R-matrix methods to electron-molecule scattering was developed by Charles Gillan, Lesley Morgan and Jonathan Tennyson (FRS 2009) (Morgan et al. 1997, 1998); an overview was presented later (36).

The original R-matrix theory was based on the assumption of low-energy incident electrons. A modification to include intermediate-energy electrons was developed by Phil in collaboration with Tim Scholtz and Penny Scott (26), and this method was used by Katrina Higgins and James Walters (27) to consider positron scattering.

A time-independent R-matrix-Floquet theory was initiated by Phil to study multiphoton processes (28), and early applications were later described (30, 31). The theory was developed further by Hugo van der Hart (1996, 2000), and extensions to multiphoton processes for molecules were added in collaboration with James Colgan, David Glass and Katrina Higgins (33, 34). Phil and Val (32) developed a new time-dependent R-matrix theory for multiphoton processes for arbitrary many-electron atoms in intense laser fields.

**Retirement**

To mark Phil’s retirement from QUB in 1998, a conference was held to honour his many contributions to theoretical atomic physics. Many of Phil’s collaborators were present (see figure 1) and the programme included presentations in all of the areas to which the R-matrix method had by that date been applied. A book incorporating the talks was published shortly afterwards (Bell et al. 1999). Following this, Phil and Val settled permanently in Brook House, but came to Belfast regularly, initially for one week each month. Phil and Val were then able to advise on the progress of the QUB group’s research projects. Equally, Phil was able to offer to the university his unique expertise in the context of the university’s physics entry in the periodic Research Assessment Exercise.
Figure 1. The participants at Phil’s retirement conference. Phil and Val are standing in the front row, fifth and sixth from the left, respectively, between Mike Seaton (left) and Alex Dalgarno (right).

For Phil, retirement was always going to be something of a misnomer. He did of course give up his undergraduate teaching, but his research continued. A number of new developments were initiated. These included the implementation of the R-matrix method on massively parallel computers, which permitted much larger calculations to be undertaken without taking inordinately long to complete (35).

A major effort during Phil’s ‘retirement’ was the writing and publication of his *magnum opus*: his book on the R-matrix theory of atomic collisions (37). This large volume discussed both the theory and its applications in the many branches of atomic, molecular and optical (AMO) physics that had been developed by Phil and others from the ideas and computer codes Phil had initiated. It was published in 2011, just in time for the International Conference on Photonic, Electronic and Atomic Collisions conference, which was held that year in Belfast, under the local chairmanship of Derrick Crothers.

Having his main base in England, Phil was able to continue with his scientific advisory role. He was a member of peer review and advisory panels for the Ministry of Defence (1997–2008) and of the AWE reviews of physics methodologies (2001, 2004) and of high performance computing (2001, 2005).

In August 2009, Phil and Val celebrated their golden wedding anniversary. The whole family, which now included seven grandchildren, gathered at Brook House for the weekend to mark this special occasion (see figure 2).
Figure 2. Phil and Val outside Brook House on the occasion of their golden wedding celebration.

In 2012, Phil was awarded the Will Allis Prize by the American Physical Society for his pioneering and sustained theoretical development of R-matrix computational methods. He had been nominated by the Division of Atomic, Molecular and Optical Physics (DAMOP) and it was customary for the presentation to be made at the DAMOP annual conference, accompanied by a lecture from the recipient. The DAMOP conference in 2012 was held in California, and Phil rightly considered it unwise to undertake such a long flight. Arrangements were made at QUB for a video to be made of his lecture and this was shown, to acclaim, at the conference.

Over time, the frequency of visits by Phil and Val to Belfast started to diminish. By 2015, Phil’s back problems made further visits too difficult. He continued to take an interest in the department and particularly the theoretical AMO physics research group, and they were always pleased to welcome at Brook House his old friends and colleagues. In the following years, he became frail and passed away in June 2019, just a few weeks short of their sixtieth wedding anniversary.

But his legacy lives on, in the methods he developed, in the continuing work of many other scientists world-wide who are now using those methods and in the ongoing work of the journal CPC and the CCPs. A very recent and detailed account of Phil’s contribution to AMO physics has been given by Bartschat et al. (2020). Ken Taylor, who worked with Phil for nearly 50 years, has written the following appreciation:
Working with Phil was always both a pleasure and an inspiration. The period involved ran from his supervision of my Honours project in 1973; through the years as one of his PhD students right up to and beyond my eventual return as a Professor to Queen’s in 1993 and his subsequent retirement. Phil was kind from the start but gave out difficult, though nevertheless attackable, research challenges to his students. Supervision sessions were quick and concentrated. He rapidly introduced me to many members of the international community and made me feel part of it.

In 1979 I became part of Phil’s group at Daresbury Laboratory. Phil encouraged Charles Clark and myself to exploit the newly-installed Cray-1 computer to explore the then new field of quantum chaos.

Later, a timely Lectureship at Royal Holloway enabled me to spend most Wednesdays working with Mike Seaton at UCL extending the R-matrix methods and codes appropriately, initially for use in the Opacity Project.

On my return to Queen’s in 1993 Phil and I found we had then a common desire to provide an accurate description of the response of few- and many-electron atoms to laser fields. While Phil used his recently developed R-matrix Floquet theory for handling fairly long laser pulses of moderate intensity, I, along with Jonathan Parker (who came to Belfast as a Cray Research Inc post-doc), concentrated on implementing a method for solving the full time-dependent Schrödinger equation for a two-electron atom in short, intense, fields that would harness efficiently the massively-parallel computers then emerging. Once again Phil had secured the then best instance of this new architecture, namely a Cray T3D, for UK science. This work with Jonathan Parker and others gave rise to the HELIUM code. Lambros Nikolopoulos (as holder of an EU Individual Marie Curie Fellowship in the group) worked with Jonathan Parker and myself bringing together R-matrix and HELIUM concepts to develop an R-Matrix approach incorporating Time (RMT) for multi-electron atoms that would be especially efficient on the massively parallel computers required (Nikolopoulos et al. 2008).

Phil thus was an unrivalled positive influence right through my career. He nurtured not only my scientific curiosity but also the wish to develop new theory and carry it through appropriate numerical methods and algorithms to exploit effectively the latest and most powerful computer architectures. Looking back over the years I fully realize my great good fortune.

**Publishing activities**

Over a period of almost 60 years, Phil authored or co-authored over 380 research papers, which were published in international research journals, as well as over 50 refereed conference reports. Additionally, he wrote eight books, two as sole author and six jointly with others. He was also founding editor of CPC (1969–1979), honorary editor of CPC (1979–2019), principal editor of the Plenum Series on Physics of Atoms and Molecules and series editor of the Springer Series on Atomic, Optical and Plasma Physics (2005–2019).

**Honours and awards**

1970  Fellow of the American Physical Society
1974  Member of the Royal Irish Academy
1978  Fellow of the Royal Society
1981  DSc *honoris causa*, University of Exeter
1986  Fellow of University College London
1993  Commander of the Order of the British Empire
1994 Guthrie Medal and Prize, Institute of Physics
1999 DSc honoris causa, The Queen’s University of Belfast
2000 Sir David Bates Prize, Institute of Physics
2012 Will Allis Prize, American Physical Society
Fellow of the Institute of Physics
Member of the European Physical Society
Fellow of the Royal Astronomical Society

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The frontispiece photograph was taken by Dr Gleb Gribakin, School of Mathematics and Physics QUB, and is reproduced with his permission. The photographs in figures 1 and 2 are from the Burke family collection.

AUTHOR PROFILE

Alan Hibbert MBE MRIA is emeritus professor of applied mathematics at Queen’s University Belfast. After completing his doctorate in Oxford under the supervision of Charles Coulson (FRS 1950), he moved to Belfast in 1967 as a post-doc, and started to work on the development of the R-matrix code as part of Phil’s small team. His interest lay primarily in atomic structure, but much of the initial coding was for routines that were common to structure and collisional calculations. This work led to the structure code CIV3, developed alongside the R-matrix code. After a year in Belfast, Alan became a member of the teaching staff in applied mathematics in QUB, eventually becoming head of the department; prior to retirement in 2009, he was director of education in the School of Mathematics and Physics. He also represented QUB on the Board of Governors of Armagh Observatory (2005–2009), remaining on its management committee (deputy chair 2012–2017) after his retirement from Queen’s. He was elected Member of the Royal Irish Academy in 2000, and appointed MBE in 2014. In 2017, he returned for family reasons to his native Lancashire, and continues research facilitated by his honorary professorship at Queen’s.

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