NICHOLAS CHARLES HANDY

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Elected FRS 1990

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Nicholas Handy made significant contributions in the applications of quantum mechanics to molecules. In an academic career at Cambridge University he was involved with many advances in the computational methods that have turned quantum chemistry into a central tool for understanding modern molecular science.

EARLY LIFE AND CAREER

Nicholas Charles Handy was born in Swindon on 17 June 1941 and he spent his early childhood in Liddington, Wiltshire. His father and grandfather were corn merchants and his maternal grandparents were farmers. He was a pupil at Clayesmore Preparatory and Senior Schools in Dorset. In 1960 he started as an undergraduate student at St Catharine's College Cambridge to read for the Mathematical Tripos. He attended the course given by Paul Dirac (FRS, 1930), one of the founders of Quantum Mechanics. Apart from a period on a postdoctoral fellowship in the USA and sabbaticals, Handy spent his whole academic career at the University of Cambridge and at St Catharine's College.

At Cambridge he took Part III Mathematics and followed the lecture course "The Quantum Theory of Molecules" given by Frank Boys (FRS, 1972) who was then a University Lecturer in Theoretical Chemistry. Handy obtained a distinction in the examination and in 1964 started graduate research under the supervision of Boys in Lensfield Road where Theoretical Chemistry was based in the Department of Organic and Inorganic Chemistry. Boys himself did not publish many papers but his research contributions proved to be highly significant and

included his development of Gaussian basis functions for general use in electronic structure calculations. Handy's first calculations on the electronic structure of small atoms and molecules were carried out on the EDSAC II computer which was the successor to EDSAC built in the Mathematical Laboratory in Cambridge in 1948.

Nicholas Handy on receiving his BA in 1963 at Cambridge University

ELECTRON CORRELATION

Handy's PhD thesis was entitled "Correlated wavefunctions and energies of atoms and molecules" and was approved in 1967 (1). Five papers came out of his thesis research (2-5). He worked on the approximate solution of Schrödinger's equation for electrons using wavefunctions that depend explicitly on the interelectronic distance r_{12}. It was known for some time that a good wavefunction should have this form in order to satisfy the cusp condition that avoids an unphysical singularity at the point of coalescence of two electrons (Hylleraas 1929). However, the first calculations of wavefunctions with more than two electrons that included the correlation effect, pioneered earlier by Handy's supervisor Boys, were of the Configuration Interaction (CI) form in which the wavefunction was expanded as a linear combination of Slater Determinants. This type of wavefunction does not depend directly on r_{12} in order to avoid the computation of integrals over the coordinates of all of the electrons; only two-electron integrals are needed in CI. In his thesis research, Handy adopted

the transcorrelated method, in which Schrödinger's equation was projected against just those states for which most of the complicated many-electron integrals are eliminated. Applications were made to some small atoms and molecules.

Following completion of his PhD, Handy took up a Harkness Postdoctoral Fellowship in 1968 working with Robert Parr at the John Hopkins University, Baltimore, USA. Here he published a paper on the long-range behaviour of Hartree-Fock orbitals which has received several citations (6). In 1969 he returned to Cambridge where he was made an Official Fellow of St Catharine's. Then, in 1972, he was appointed to a University Demonstratorship in the Theoretical Chemistry section headed by David Buckingham (FRS, 1975) following the untimely death of Boys in that year.

Handy continued his research on improving the transcorrelated method in independent research in the early 1970s. One of the authors of this memoir, David Clary (FRS, 1997), joined Handy's group as a Ph.D. student in 1974. He performed variational calculations which included the r_{12} distance in the wavefunctions of atoms up to Ne (9) and diatomic molecules such as LiH (10) and calculated explicitly the required integrals over the coordinates of three and four electrons.

It was subsequently realised (Kutzelnigg 1985) that explicit r_{12} correlation could be included simply and effectively by reducing many-electron integrals to sums of two-electron integrals through approximate resolution in a basis of the identity operator. This approach was later adopted by many researchers (Klopper et al 2006) and Handy and co-workers did further research on the technique (37). The resulting "F12" approach, grounded in Boys' and Handy's original work, is a central feature in modern quantum chemistry, and is essential for very accurate treatment. A further legacy of Boys' and Handy's work was that it required them to develop numerical methods for quadrature suitable for molecular wavefunctions, and the insights gained in this period provided a platform for Handy's first contributions to the field of Density-Functional Theory (DFT) 25 years later.

A sabbatical visit to Berkeley in 1978-79 proved to be a major turning point in Handy's scientific direction through collaboration with the research groups of Fritz Schaefer and Bill Miller. Here he began to work with Schaefer on CI and on the analytic calculation of forces and higher energy derivatives. The collaboration flourished, and provided new inspiration for Handy, not least because of the new possibilities of a large and eager research group working

as a team, and also the availability of significant computing facilities at the Lawrence Berkeley Laboratory. Despite his earlier experience that explicitly-correlated electronic wavefunctions gave a much more compact and rapidly-convergent representation than that of CI, he realised that CI was the practical way forward at this time, and worked with Schaefer's group on the unitary group approach to spin-adapted CI (12, 17).

On his return to Cambridge, Handy realised that a much simpler, and potentially more powerful, way to do CI was by using individual Slater determinants, not spin-adapted combinations, as basis functions. His first paper on this (13) presented an extremely simple and general algorithm for both full CI (FCI) and multiconfigurational reference CI (MRCI) calculations. By use of data compression techniques, prescient of later developments by others of the exploitation of sparsity in quantum-mechanical wavefunctions and in many other fields, he was able to perform ambitious computations on the Cambridge IBM 370/165 computer which could provide at most a few hundred kilobytes of memory to a user's job. One key innovation in this code was the adoption of an outer-product representation of the wavefunction as a rectangular matrix, where alpha- and beta-spin parts of the wavefunction were explicitly separated, paving the way for algorithms that could support the vector-architecture computers (eg Cray-1S) that were emerging at the time; another innovation was the introduction of a canonical indexing scheme that allowed rapid addressing of the wavefunction from a compact look-up table. Later developments with Peter Knowles, one of the authors of this memoir, exploited the quantum-mechanical resolution of the identity (Siegbahn 1984) to generate an even simpler and more powerful FCI algorithm (21, 33, 34).

At the time of these CI developments, little was known about the accuracy of the various emerging approximate electronic structure methods. Schaefer and Handy together realised that FCI calculations opened the door to establishing error bounds, through 'benchmark' calculations that compared approximate methods with FCI in a small orbital basis set. Their first paper with Paul Saxe (16) on the water molecule (later extended to distorted geometries and other molecules by Robert Harrison (19, 20)) gave the first hard information on the performance of many-body perturbation theory (MBPT) and the coupled cluster and multireference CI methods that have become the widely-used standards of modern quantum chemistry. Further stimulation from the availability of new hardware (Cray-2 at NASA Ames) resulted in a more extensive series of larger benchmarks performed by Charlie Bauschlicher and Peter Taylor with Handy and others (28).

At about the same time, Handy realised that the ability to manipulate the Hamiltonian operator in a basis set offered more than the possibility to find the lowest eigenvalue of that Hamiltonian. Other quantum-chemical ansätze could be simulated; for example MBPT could be calculated up to arbitrary order, and the convergence, or otherwise, of the perturbation series – about which little was known analytically – could be investigated numerically (24,25). In collaboration with John Pople (FRS, 1961) it was realised that whilst MBPT is often rapidly convergent for closed-shell molecules, the same is not true for open-shell systems where the underlying breaking of spin symmetry in the reference wavefunction causes havoc in the perturbation series (30). This stimulated further work to avoid the spin contamination effects by projection (31, 32), or by adopting a spin-adapted reference wavefunction (38, 39).

Another fruit of Handy's interaction with Schaefer, together with his interests in molecular vibrational states, was his embarkation on a programme of the analytic computation of the derivatives of the energy with respect to nuclear displacements, and with respect to electromagnetic perturbations. Handy recognised that the way forward for theoretical spectroscopy of polyatomic molecules would need not only the gradient and curvature of the potential energy surface, but also 3rd and higher derivatives to address anharmonicity and absorption intensities, and that therefore analytical differentiation had to be used instead of finite differences. The methods addressed included Hartree-Fock (26), CI (14), Multi-Configurational Self-Consistent Field (18), MBPT (27), Coupled Cluster Single and Doubles (40) and, later, Density-Functional Theory (DFT). Crucial to the success of this endeavour was the assembly of a complete general program package, CADPAC (41), led by Roger Amos. An additional essential ingredient was "Nick's trick" (22), in which recognition of the hermiticity of the response kernel for molecular wavefunctions allowed one to avoid having to solve explicitly for parts of the perturbed wavefunction in each nuclear degree of freedom.

Handy recognised that there are other perturbations that one can usefully consider besides those associated with electromagnetic properties and nuclear motion. The dominant correction to the Born-Oppenheimer approximation, arising from the diagonal effect of the nuclear kinetic energy, can be formulated as an energy derivative and Handy and co-workers demonstrated its typical effect in hydrogen-containing molecules numerically (29). This work led to the realisation that in many cases, the dominant beyond-Born-Oppenheimer effects can be handled very simply, by using atomic (with electrons) rather than nuclear masses in the subsequent treatment of nuclear motion (45).

Handy's work on gradients speared other developments in electronic structure methods. Whilst thinking about the coupled-cluster method, and what would be necessary to obtain its analytic derivatives, he concluded that the formulation could be made much simpler if one did not have to deal with single orbital excitations. Together with Pople and others he translated the Brueckner orbital formalism from nuclear physics into an alternative to CCSD, which they named "Brueckner Doubles" theory, and formulated additionally the perturbation corrections to it (35, 36).

VIBRATIONAL STATES

When Boys died in 1972, Handy took over his small research group. As well as continuing work on the quantum mechanics of correlated wavefunctions described above this allowed him to take forward a project on the calculation of the vibrational states of molecules and this remained another research interest for his whole career. At that time it was becoming possible to develop functional forms for potential energy surfaces of small molecules and the accuracy of these functions needed testing by calculation of the vibrational energy levels. These calculations were straightforward using perturbation theory but Handy pioneered the development of more accurate variational methods using expansion of vibrational wavefunctions in suitable basis sets, applying appropriate numerical integration procedures and diagonalisation of the secular determinant to find the eigenstates and energies. The timely derivation of suitable Hamiltonians for ro-vibrational motion of small molecules in terms of normal coordinates by Jim Watson (FRS, 1987) made this project feasible (Watson 1968).

The variational calculations of Handy and Rosemary Whitehead (8) showed that more approximate perturbation methods for calculating vibrational energies for molecules such as H_2O could give vibrational frequencies with errors larger than 60 cm^{-1} which is not a suitable accuracy for high resolution spectroscopic analysis. This research was developed further through using valence internal coordinates in place of normal coordinates and molecules such as formaldehyde and acetylene were treated this way. Couplings of rotational, electronic and electron spin angular momenta in Renner-Teller and Jahn-Teller formulations were also included in calculations on molecules such as CH_2^+ (23). Potential surfaces directly derived from ab initio computations could also be included and calculations of radiative lifetimes and line intensities allowed for predictions of the full infrared spectra.

For some molecules Handy and collaborators were able to refine the force field to fit experimental spectroscopic data and give a definitive equilibrium structure for the molecule. They also derived the kinetic energy part of the Hamiltonian for use in calculations on different types of molecules including those with inversion modes such as NH_3 (50). A long-standing collaboration, started with Stuart Carter and subsequently continued with Carter and Joel Bowman, introduced a general computer program MULTIMODE which exploits normal modes and calculates the vibrational states and spectra from force fields for polyatomic molecules (48). This program was applied to predict the infrared spectrum for molecules as large as benzene (52). Another feature of this code is the option of treating wide amplitude motion using the Reaction Path Hamiltonian which is described below. Peter Schmidt from the US Office of Naval Research provided funding to support this research. The last paper which Handy published in the year of his death was a MULTIMODE calculation with Carter and Bowman on C_2H_4 and C_2D_4 (55).

Nicholas Handy, Fritz Schaefer, Stuart Carter, Peter Schmidt, Bill Miller and Joel Bowman at Emory University in 2003

In 1975 Bill Miller came to Cambridge from Berkeley, California for a sabbatical and through this developed a lifelong collaboration and friendship with Handy. Miller was an expert on using semiclassical theories to approximate quantum mechanics. Together with

research student Susan Colwell they used semiclassical theory to calculate the vibrational states of triatomic molecules (11), the accuracy of which could be checked by comparison with the benchmark variational calculations done by Handy and Whitehead.

Then, in his sabbatical visit to Berkeley in 1978-79, Handy derived the Reaction Path Hamiltonian for polyatomic systems with Miller and John Adams (15). This involved choosing an intrinsic reaction coordinate together with a set of orthogonal normal modes. The work complemented his collaboration with Schaefer in which second derivatives of electronic energies with respect to nuclear coordinates were being calculated *ab initio* and these were just the quantities needed in the Reaction Path Hamiltonian computations. In recent years this much cited paper has been particularly useful for use of its Hamiltonian in calculations on intramolecular hydrogen atom transfer and for calculating vibrational states of polyatomic molecules with a large amplitude motion.

When she was doing research in quantum chemistry, Angela Merkel performed calculations using the Reaction Path Hamiltonian (Zülicke and Merkel 1990) and in the late 1980s she invited Handy to speak at a symposium she organised in what was then East Germany. As Chancellor of Germany, Merkel was presented with the King Charles II Medal at the Royal Society in 2010 and Handy was present. She recognised him and was pleased to hear about the latest progress of research in their field.

DENSITY FUNCTIONAL THEORY

Walter Kohn (ForMemRS, 1998) and Pierre Hohenberg showed that the ground state of a many-electron system is uniquely determined by the electron density that depends on only three spatial coordinates (Hohenberg and Kohn 1964). This was then followed up with the derivation of self-consistent equations for implementing this theory (Kohn and Sham 1965). However, it then took nearly thirty years for the DFT method to be used by many chemists. The introduction of generalized gradient approximation (GGA) functionals in DFT in the late 1980s led to a notable improvement in accuracy for chemical systems. At the 1991 conference of the International Academy of Quantum Molecular Science, held in Menton, France, Axel Becke (FRS, 2006) presented impressive new DFT results obtained with the GGA that caught the eye of Handy and other prominent quantum chemists such as Pople. A few months later Pople visited Cambridge and encouraged Handy to work on DFT. Handy admitted to being discouraged at the time by the high computational cost and complexity of

wavefunction methods, and so he seized the opportunity to investigate this alternative approach.

John Pople and Nicholas Handy, Cambridge 2001

One of Handy's major contributions to DFT was a technical contribution described in one of his first DFT papers in 1993, co-authored with Chris Murray and Greg Laming (43). The key quantity in DFT is the exchange-correlation energy, which is written as an integral over some function of the electron density. Handy used a partitioning scheme (Becke 1988) to express the molecular integral as a sum of atomic integrals, although these integrals could not be evaluated analytically; numerical integration was required. Following his earlier work with Boys (7), Handy introduced a transformation of the radial coordinate to the range [0,1] such that the Euler-Maclaurin formula could be used to evaluate accurately the radial integral. By combining this with efficient angular integration, the exchange-correlation integrals of DFT could be evaluated to very high precision, meaning that DFT calculations performed by different groups using different computer programs could yield essentially identical results. Such reproducibility – which is a key feature of electronic structure methods – had been absent in many of the earlier DFT studies. The Euler-Maclaurin scheme is now the default radial integration scheme in many electronic structure programs.

With this efficient implementation of DFT in the CADPAC program, Handy and co-workers subsequently published a stream of papers in the early 1990s, demonstrating the quality and

computational efficiency of the method. This is exemplified by the study, with Murray, Laming, and Amos (42), on the bond lengths, harmonic vibrational frequencies, and dipole moments of small molecules calculated using fully self-consistent Kohn-Sham theory. Interestingly, this paper also highlighted the issue of non-separability of exchange and correlation within GGA DFT, which is a topic that Handy revisited on several occasions in later years, most notably his left-right correlation work with Aron Cohen (51).

Another longstanding interest of Handy was the issue of spin-contamination, whereby the expectation value of the spin-squared operator $<S^2>$ differs from the theoretical value of $S(S+1)$. In collaboration with Pople and Peter Gill, Handy published a key paper in 1995 on spin-contamination within DFT (44). The paper highlighted the fact that the value of $<S^2>$ computed in the usual manner from the Kohn-Sham determinant provides no information about the spin of the real system (since the determinant is the wavefunction of a fictitious non-interacting system, rather than the real system) and so a computed value different to $S(S+1)$ is not problematic. Indeed, the authors used the example of the CH_3 radical, for which the spin-density can be negative, to argue that a spin-unrestricted formalism must be used for describing open-shell systems in DFT and so reference-state spin-contamination is actually essential, rather than problematic.

One of the most important applications of modern DFT is the study of electronic excited states using Time-Dependent DFT (TDDFT), whereby vertical excitation energies are determined as the poles of the frequency-dependent polarisability. It was demonstrated (Casida *et al*. 1998) that for common exchange-correlation functionals, excitations to valence states were reasonably accurate (errors less than 0.5 eV), whereas excitations to Rydberg states were in very significant error (errors of several eV), and that this could be attributed to the incorrect asymptotic behaviour of the exchange-correlation potential. This led Handy and one of the authors of this memoir David Tozer to propose a simple correction to the exchange-correlation potential, whereby the correct $-1/r$ asymptotic behaviour was grafted on to a conventional GGA potential (46). A key feature of their approach was that the asymptotic potential approached a non-zero value asymptotically, a feature that was highly controversial at the time. This non-zero potential was a consequence of the fact that GGA functionals approximately average over the integer discontinuity in the exchange-correlation potential. At the time the implications of the integer discontinuity in DFT were not widely known, whereas nowadays they are widely accepted and the requirement of a non-zero potential is well-understood. This 'asymptotic correction' leads to a dramatic improvement in

the accuracy of calculations on Rydberg excitations, reducing errors by an order of magnitude.

Björn Roos had been following these TDDFT developments and in December 1998 he visited Cambridge and challenged Handy to determine excitation energies of a series of unsaturated organic molecules, for which he had already applied the state-of-the-art wavefunction method, Complete Active Space Perturbation Theory (CASPT2). Handy, Amos, and Tozer successfully applied the asymptotic correction to these molecules, at a fraction of the computational cost of CASPT2, illustrating the excellent accuracy to cost ratio that could be achieved using TDDFT. However, the study (49) also highlighted some important deficiencies of TDDFT. The first concerned double excitations, which are completely missing in linear-response TDDFT (although, perhaps surprisingly, the method can work well even when there is significant double excitation character). The second deficiency was that TDDFT using conventional functionals can break down completely for charge-transfer states, as exemplified by the n to π^* and π to π^* excitations in a model dipeptide, where there is minimal overlap between the orbitals involved in the excitation. This 'charge transfer problem' – which had not been highlighted prior to this study of Handy and co-workers – is now very widely known and has significant implications in a range of technologically important areas, such as organic electronics and photonics, molecular exciplexes, and photovoltaics.

The final aspect of Handy's DFT research – and where his scientific legacy will be particularly significant – concerns the exchange-correlation energy functional. This is the key quantity in DFT, the quality of which governs the accuracy of all DFT calculations. From the outset, Handy attempted to understand the deficiencies of existing approximations, provide insight into the failures, and develop improved approximations. Three of his contributions are particularly noteworthy and have been cited significantly. This first is the 1998 Hamprecht-Cohen-Tozer-Handy functional (47). A common approach in DFT functional development had been to choose a flexible functional form and determine the parameters through a fit to experimental thermochemistry (Becke 1993). Handy and co-workers realized that such an approach could not guarantee that the exchange-correlation potential – which is a key quantity in the calculation of molecular response properties – would be accurate. They therefore used a procedure to determine near-exact potentials from correlated *ab initio* electron densities (Zhao, Morrison and Parr 1994) and then explicitly included these

potentials (appropriately shifted to ensure a non-vanishing potential) in the fitting procedure, introducing important physics into the functional.

The second noteworthy functional is the 2001 OPTX exchange functional, commonly combined with Lee-Yang-Parr correlation to yield the OLYP exchange-correlation functional. Handy and Cohen (51) determined the parameters defining OPTX by fitting to atomic Hartree-Fock exchange energies, allowing the prefactor of Dirac exchange to be non-unity. The functional accurately reproduces atomic exchange energies by construction. However, when applied to molecules, the OPTX energy is notably lower than the Hartree-Fock exchange energy, emphasizing that such a local form includes both exchange and left-right correlation. The functional was therefore not only of practical use, but the work provided fundamental insight into the meaning of exchange and correlation within DFT.

Handy's most influential functional development work for DFT was the 2004 CAM-B3LYP functional, co-authored with Takeshi Yanai and David Tew (53). In the ten years since publication, it has already been cited more than 2,200 times, illustrating its impact. This contribution followed previous work (Savin 1996, Iikura *et al.* 2001) in partitioning the interelectron repulsion operator into short- and long-range components and then evaluating the short-range exchange using local DFT, but treating the long-range exchange exactly using Hartree-Fock theory. A key benefit of such an approach is that long-range properties – such as charge-transfer excitation energies, Rydberg excitations, polarisabilities, and bond-length alternation – are significantly improved at negligible additional computational cost. The novel feature of CAM-B3LYP is that the partitioning is highly flexible, allowing a fraction of exact exchange to be maintained at short interelectron distance, meaning long-range properties can be improved without degrading short-range properties.

In addition to the aforementioned DFT contributions – many of which were highlighted by Handy himself in the 2004 compilation of his selected papers (54) – it is pertinent to close by briefly mentioning the numerous other areas of DFT to which Handy contributed. These include electric response properties such as polarisabilities, hyperpolarisabilities, and frequency-dependent polarisabilities; magnetic response properties such as NMR shielding constants, magnetisabilities, and indirect nuclear spin-spin coupling constants; non-interacting kinetic energy functionals; correlation functionals; current-DFT; nuclear analytic derivatives; potential energy surfaces; vibrational frequencies; Slater basis sets and relativistic DFT.

AWARDS AND ACADEMIES

In 1988 Handy was elected a member of the International Academy of Quantum Molecular Sciences. A supporter in the foundation of this prestigious Academy was one of the pioneers of quantum mechanics Louis de Broglie (ForMemRS, 1953). In 1991 Handy became Secretary of the Academy and Pople was President for part of this period. The Academy meets each year usually in Menton, France and Handy took lessons in French to help him to communicate with the local mayor and other dignitaries.

The Nobel Prize for Chemistry was awarded in 1998 to Kohn for "his development of density functional theory" and to Pople for his "development of computational methods in quantum chemistry". Handy was delighted with these awards and his own significant contribution to these fields was cited in Pople's Nobel lecture.

Handy deservedly won several major awards for his contribution to quantum chemistry. This included election to the Royal Society in 1990, the Schrödinger Medal of the World Association of Theoretically Oriented Chemists in 1997, the Leverhulme Medal of the Royal Society in 2002 and, most appropriately, the Boys-Rahman Award of the Royal Society of Chemistry in 2003. Given his strong links with the USA, he was particularly pleased to go to Anaheim, California to receive the Theoretical Chemistry Award of the American Chemical Society in 2011. This was just one year before he died.

Upon his retirement in 2004 a conference was organised in Cambridge in his honour which was attended by more than 300 quantum chemists. The title of the conference was 'The No-Nonsense Path to Progress', which summarised accurately Handy's direct style for scientific interactions. In association with the conference, a book was published which featured his key papers and comments on them from himself and other experts (54).

CAREER AND PERSONAL LIFE

Despite the extensive time he spent on research Handy was dedicated to teaching both in his Cambridge College of St Catharine's and in his Department. He was also Steward of his College, which involved overseeing catering for students and Fellows, and eventually became President (equivalent to Deputy Master). He was a much valued supervisor in mathematics for undergraduates at St Catharine's for a period of over 30 years.
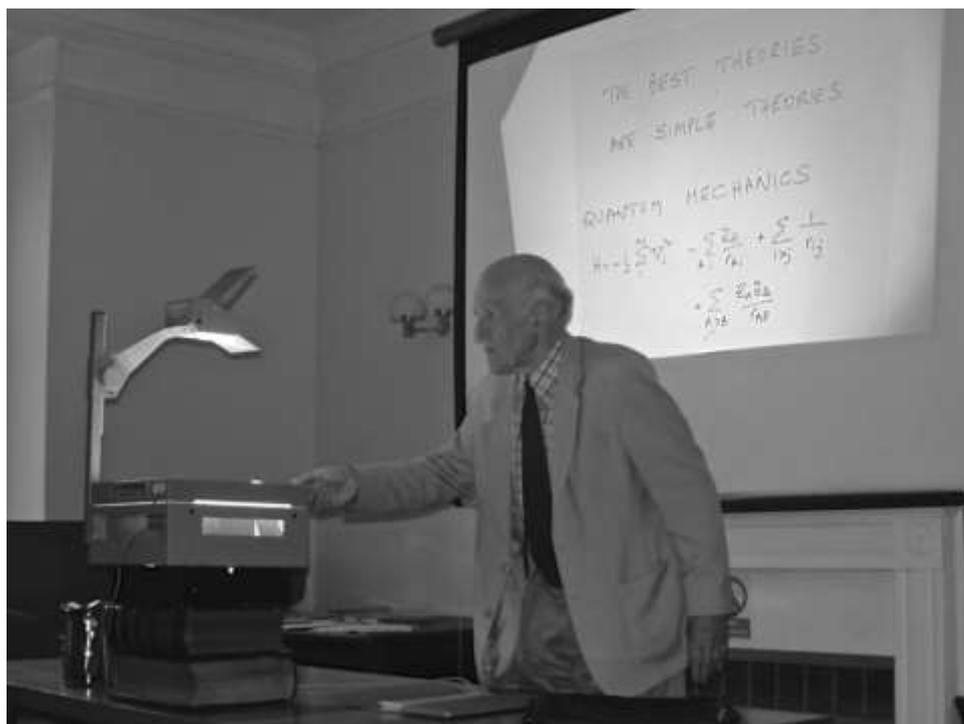
Nicholas Handy giving a typical lecture – "The best theories are simple theories".

Following on from his Demonstratorship, Handy was appointed Lecturer in Theoretical Chemistry at Cambridge in 1979. He was promoted to Reader in 1989 and then Professor of Quantum Chemistry in 1991 (such promotions being rare at that time in Cambridge).

During his PhD period he met Carole Gates at a college ball in Cambridge and they were married at her home village of Thornthwaite near Keswick in the Lake District. Carole joined him on his sabbaticals and regularly went with him to international conferences held all around the world. Through this she got to know well many of the members of the quantum chemistry community. They had two sons, Julian and Paul, and six grandchildren. Many former students and colleagues recall the warm receptions Carole and Nicholas provided in their home in Barton Road, Cambridge. After his retirement in 2004 they moved to Thornthwaite. With his family he helped to build a hydroelectric turbine there and he was delighted to tell how this enabled his house to be one of the few in the region to maintain electric power during a significant flood.

Handy's personality was honest and direct. He was an inspiring supervisor of students and postdocs. He managed most successfully to balance his family life with his research, teaching and college duties while at the same time making major contributions to his subject nationally and internationally.

SCIENTIFIC LEGACY

When Handy started out on his research career in the 1960s the influence of quantum mechanics on chemistry was largely pictorial and reliable quantitative calculations on molecules were rare. Handy played a central role in making the computational methods of rigorous quantum chemistry generally useful and applicable for chemists and other molecular scientists. Nowadays, some fifty years later, calculations are done routinely and reliably to confirm or predict the structures and properties of molecules containing many atoms.

As of October 2014 Handy's papers have received over 27,000 citations with an h-index of 83. His deep influence on quantum chemistry is arguably becoming even stronger after his death and in 2014 a major symposium in his memory was organised by the American Chemical Society in San Francisco.

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