The Career and Scientific Legacy of Professor Ian Grant FRS (1930-2025)

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The University of Melbourne

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Image: Pembroke College Oxford

Origins

Albert Grant MP, by Carlo Pelligrini, published in Vanity Fair (1874)

Jewish on both sides of the family. Ian described himself as having a strong sense of his Jewish identity without being especially observant.

- Maternal side, Ornstien: Came to Britain in the 1690s, were involved in the early years of the Bank of England. One relative ran the Windmill Theatre in the 1940s, and was played by Bob Hoskins in *Mrs Henderson Presents*.
- Paternal side, Gottheimer. Family came to Britain around 1860 from Berlin, manufacturers of cloth caps and military headgear. Family changed name to Grant in 1915, following the precedent of Albert Grant, the flamboyant MP for Kidderminster who gifted Leicester Square to London.

The Grant Family

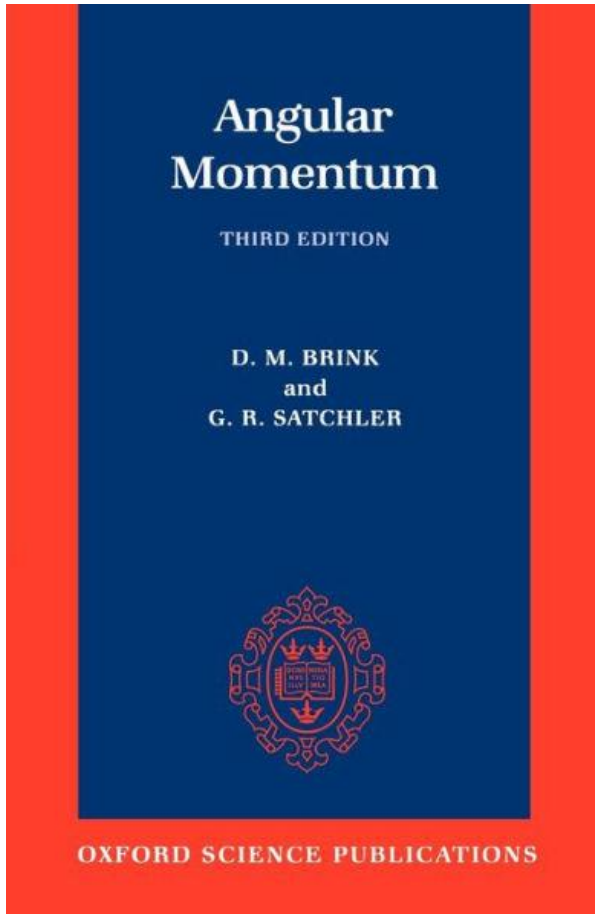
6 Woodlands Close, Headington, Oxford

Lived at 6 Woodlands Close, Headington, Oxford 1965-2005, later in Abbeyfield, Girton, Cambridge.

- Beryl Grant (Cohen, married 1958): Senior Lecturer in Law at Oxford Brooks University, wrote a text on employment law, 2002.
- Paul Grant (b 1960) Chartered Engineer
- David Grant (b. 1962) Health Economist

Ian's sons have forwarded biographical information to form the basis of his *Biographical Memoir* (with Steven Rose).

Education in Oxford (1948-1954)



- 1948-1951: Wadham College Oxford – BA First Class degree in Mathematics,
- 1951-1954: D. Phil. Clarendon Laboratory, on Coulomb effects in deuteron stripping reactions, initially with Professor Maurice Pryce FRS, after a year supervised by Professor Roger Blin-Stoyle. Examined by Sir Rudoph Peierls FRS and J. A. Spiers.

Ian said that a most significant aspect of his D.Phil. work was the time he shared an office and interacted with other students

- David Brink and Ray Satchler (angular momentum)
- Dick Steenberg (Racah algebra)
- Brian Judd (crystal field theory, tensor methods)
- Jean Yoccoz (numerical methods)

Cover of Brink and Satchler's *Angular Momentum (third edition, 1994)*

National Service (1955-1957)

Ministry of Defence, Whitehall, London (Image: MOD)

- Ian had to undertake National Service in the British Army at the conclusion of his D. Phil. This had been deferred for several years while at Oxford.
- Joined Royal Corps of Signals- January 1955.
- Mons Officer Cadet School, Aldershot May 1955, approached by R. A. Hulme, Chief of Nuclear Research, AWRE Aldermaston, invited to be “extracted” from the British Army.
- Indecision led to farce, and Ian was summoned to appear in full uniform at Whitehall…”Sit down Grant! You’re a sore trial to us!”
- He was given a choice: complete his regular Army Service as a subaltern in Germany or join AWRE Army Element as a sergeant working on scientific problems. After even more farce, he chose the latter, posted to AWRE.

AWRE Aldermaston (1956-1964)

AWRE (now AWE) Aldermaston, Berkshire, UK

He was initially assigned the task of studying interactions between matter and radiation, with a view to extending this to heavy element spectroscopy.

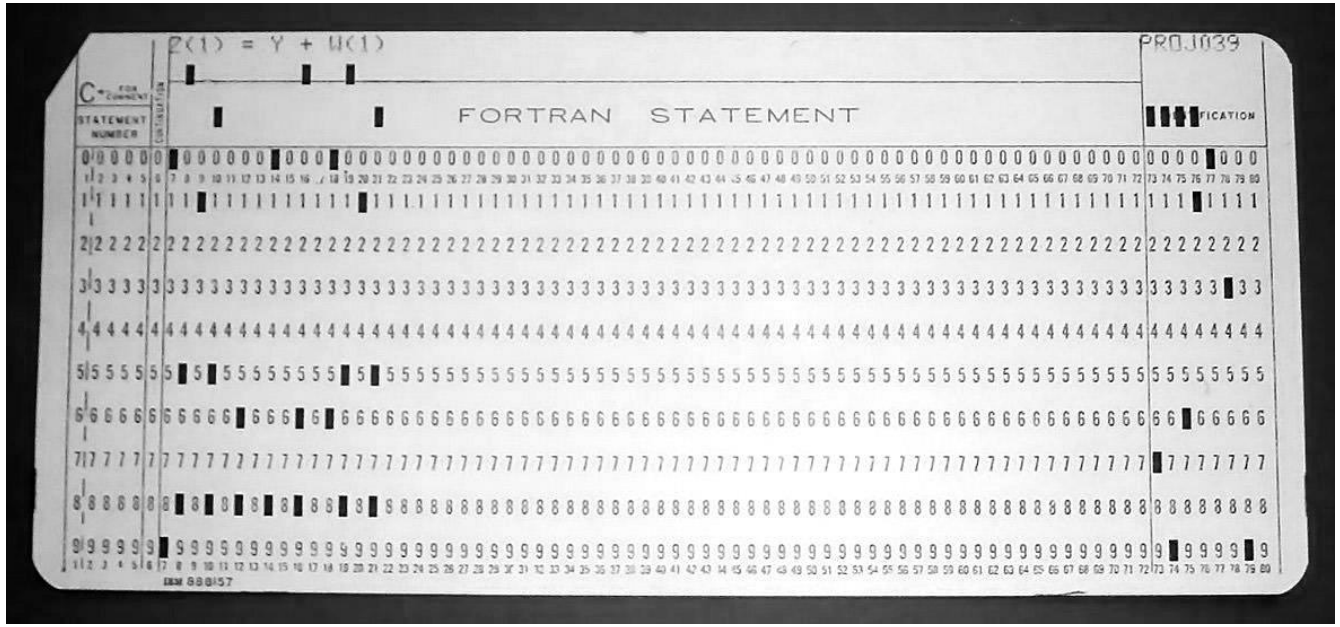
- Ian read Heitler's *Quantum Theory of Radiation* and realized a relativistic treatment was required for quantitative treatment of heavy elements.
- He then sat down with Condon and Shortley's *Theory of Atomic Structure* and saw the opportunity to formulate a relativistic theory of atomic structure.
- In December 1956, this led to an AWRE internal report that was published in 1961 as I. P. Grant, *Relativistic Self-Consistent Fields* Proc. Roy. Soc A **262**, 555-576 (1961).
- David Mayers (student of Douglas Hartree, contemporary of Charlotte Froese Fischer) completed Dirac-Hartree calculations on mercury on the IBM 704 at AWRE at around that time.

AWRE Aldermaston (1956-1964)

- Ian accepted a position in 1957 as Senior Scientific Officer at AWRE Mathematical Physics Division.
- Project was radiation-matter interactions at 10^7 K, completed around 1960.
- Used for modelling stellar interiors, radiative energy transfer processes
- Performed a detailed analysis of relativistic radiative transitions (Payne and Levinger 1957; Hulme, McDougall, Buckingham, Fowler 1935): found an error in the final step of Hulme *et al*. that resolved long-standing anomalies.

Some of Ian's work at Aldermaston remains "classified". My early readings at Oxford came from material stamped as "declassified" he was allowed to retain from AWRE.

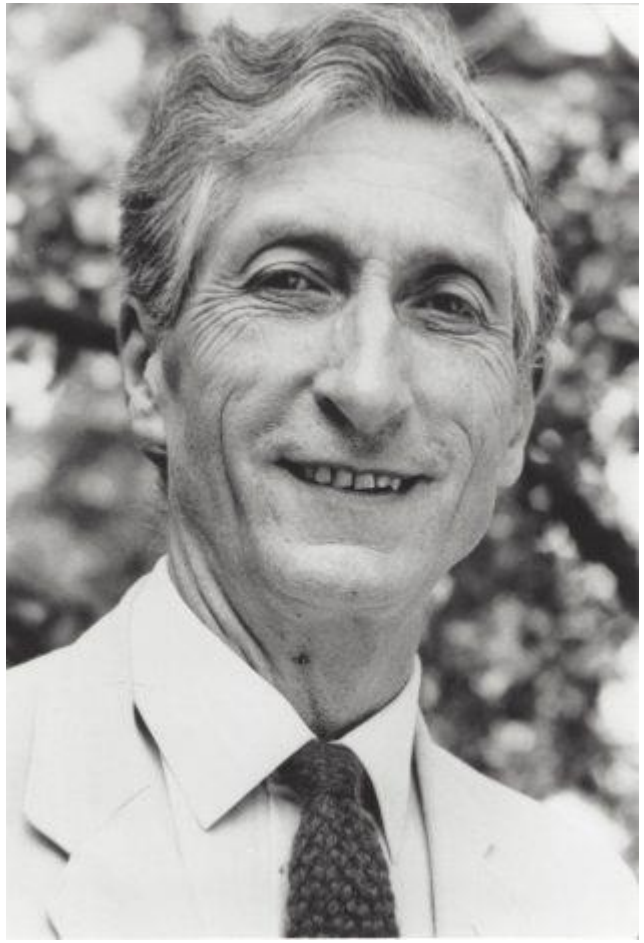
Atlas Fellow (1964-1969)



Fortran punch-card: Z(1)=Y+W(1)

- Appointed to a Research Fellowship at Atlas Computer Laboratory, Chiltern, Oxfordshire.
- Opportunity to use Britain's first supercomputer, the Ferranti Atlas 1
- Associated with a tutorial position in Mathematics at Pembroke College Oxford, six hours teaching per week, full dining rights.
- Kept formal position at AWRE for a couple of years and was allowed to retain declassified notes and reports.
- Mainly pursued research on radiative transfer in stellar atmospheres

Atlas Fellow (1964-1969)



Charles Coulson (1910-1974)

- Invited by Charles Coulson in 1965 to deliver a talk on relativistic quantum theory at the Mathematical Institute.
- Asked by Coulson at the end of the talk about whether it was possible to "visualize" effects of relativity on atomic structures.
- Led to publication with Valerie Burke "*The effect of relativity on atomic wavefunctions*", Proc. Phys. Soc. (Lond), **90**, 297-314 (1967).
- Wrote review of DHF methods, I. P. Grant, *Relativistic calculation of atomic structures,* Adv. Phys. **19**, 747-811 (1970).
- Ian identified this as the starting point of the GRASP project.

Pembroke College Oxford (1969-1998)

Pembroke College Oxford (Image, Andrew Shiva)

- Ian was appointed as a Tutorial Fellow at Pembroke College and University Lecturer in 1969
- Despite his research distinction, Ian was required to undertake an unusually heavy teaching and administrative load, including time as Vice-Regent of Pembroke College (1985-1987).
- Research was mainly a spare time activity.
- Promoted to *ad hominem* Reader (1990) and *ad hominem* Professor (1992), appointed Fellow of the Royal Society (1992).
- Statutory retirement in 1998.

Origins of the GRASP Project (1970)

Carl Moser, Director of CECAM (1969-1990)

Three-month workshop on relativistic atomic physics in Orsay (1970)

- Carl Moser (CECAM, Orsay)
- Ian Grant (Oxford)
- David Mayers (Oxford)
- Jim Waber (Northwestern)
- Jean-Paul Desclaux (CNRS)

A plan was developed to write two independent codes (based on work by Mayers and Desclaux), with Grant to construct the angular momentum modules, to be interfaced to both codes.

Theoretical Chemistry (1974-1990)

- Ian was given few resources in the Mathematical Institute, and quantum theory was in decline there when Roger Penrose was appointed Rouse Ball Professor in 1973.
- Charles Coulson started Theoretical Chemistry in 1 South Parks Road in 1972 but died in 1974.
- Ian was invited by Mark Child to use an office in Theoretical Chemistry, at the time to collaborate more closely Nick Pyper, Ian's SRC research fellow.
- This became a long-term arrangement, supported by the Coulson Chair, Norman March.
- Ian was very grateful for this generosity, because it allowed him the stability to develop a research group, albeit quite a small one.

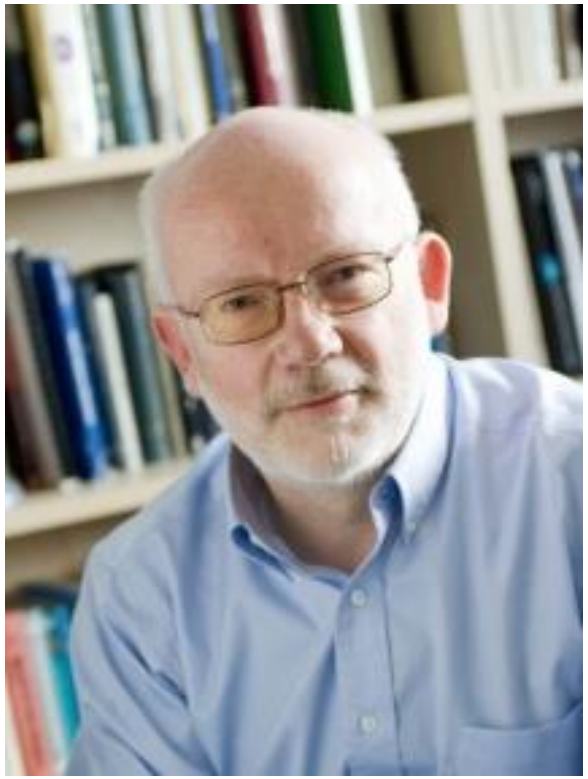
Department of Theoretical Chemistry, 1 South Parks Road, Oxford.

Mathematical Institute (1990-1998)

- Ian was promoted to Reader (1990) and Professor (1992).
- Fellow of the Royal Society (1992).
- He was finally given an office, research support and relief from his heavy teaching and administrative load.
- It was all welcome, but it was rather too late to pick up and develop his own active research program.
- Oxford required that academic staff retire at age 67: he was able to gain an extra year because he was born in December.
- He became Emeritus Professor in 1999 and later acquired visiting status at Imperial College and DAMPT in Cambridge.

Mathematical Institute, 24-29 St Giles, Oxford

Students



Emeritus Professor Steven Rose, Imperial College London

D. Phil. students
A Peraiah 1970–1972 (Professor of Astrophysics, Bangalore)
D Ellison 1971–1973 (emigrated to Canada)
D H Shun 1974–1977 (Lecturer, Hong Kong University)
S J Rose 1976–1979 (Head of Plasma Physics Group, Imperial College)
E P Plummer 1981–1984 (Senior Patent Examiner)
H M Quiney 1984–1987 (Head of Physics, Melbourne)
H Skaane 1996–1998 (finance sector, Norway)

Visitors and Collaborators

Post-Doctoral Fellows

Dr N C Pyper 1975–1977
Dr B J Mckenzie
Dr P H Norrington
Dr J Hata, 1981–1984
Dr C T Johnson 1985-1986.
Dr K G Dyall 1982–1984.
Dr W M Denny 1984
Dr L Laaksonen 1984–1985
Dr F A Parpia, 1987–1990
Dr W P Wijesundera 1989–1992
Dr M R Harston 1991–1992
Dr T C Scott 1992–1995
Dr S Ait-Tahar 1995–1996

Visitors

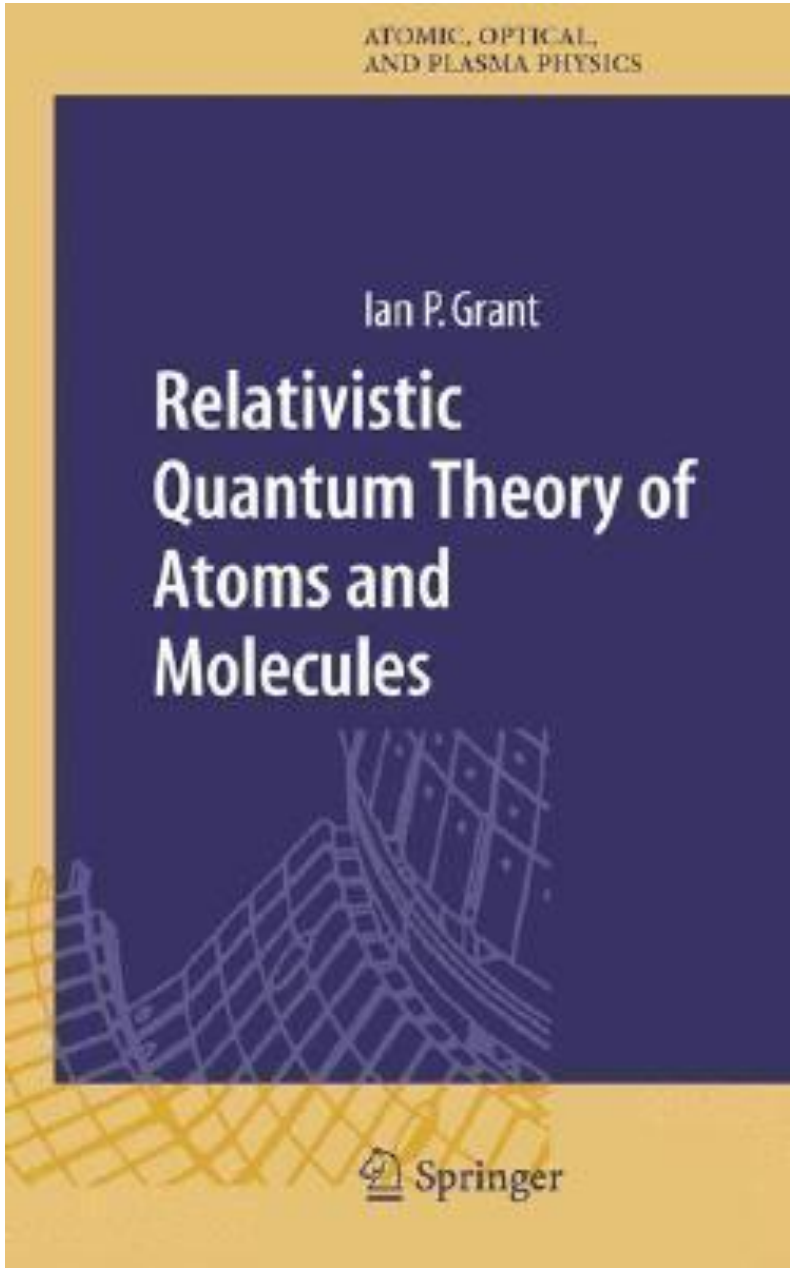
Prof D H Sampson 1992–1993 (Penn State)
Dr P Marketos 1991–1993 (Athens)
Dr S Fritzsche, Kassel 1992–1993 (Kassel).
Dr G Gaigalas, 1993 (Vilnius).
Prof J E Sienkiewicz, 1993, 1994, 1996, 1997 (Gdansk)
Asst. Professor V L Yakhontov 1994 (St. Petersburg)
Dr Elena P Ivanova, 1997, (Troitsk)
Dr J Bieron, 1996, 1997, 1999 (Krakow)

Community Service

- SRC Working Party on Computational Physics, Secretary 1969–1972 (CulhamLaboratory)
- Director, Oxford Synagogue and Jewish Centre Ltd 1974–2010(Chairman 1985–2005)
- Governor, Royal Grammar School, High Wycombe 1981–1999; Foundation Trustee 1999–2003.
- Governor St. Paul’s School, Barnes 1992–2000 (nominated by Oxford University)
- Board of Visitors, Blackett Laboratory, Imperial College 1992–1997.
- Steering Committee, Relativistic effects in heavy element chemistry and physics (REHE) 1991–1997.
- CCP2 (EPSRC Collaborative Computational Project) – member of Working Group for many years
- Occasional membership of SERC, EPSRC and Royal Society committees

Relativistic Quantum Theory of Atoms and Molecules

- First proposed in early 1970s as “Relativistic theory of atomic structures” for OUP.
- Existed in multiple versions as a set of notes, hand-written, typed, typeset in early word-processor formats and, finally, in Latex for thirty-five years.
- Was the subject of endless banter amongst family and colleagues
- It was always a work in progress, delayed first by the emerging field of basis set approximations, molecules, and scattering calculations, and then by the inclusion of QED and many –body effects.
- Second edition co-authored by Quiney, to be completed “soon”.



Achievements

With Bertha Swirles and Guilio Racah, Ian Grant is generally credited as having done the foundational work required for computational relativistic electronic structure theory.

Wrote many of the foundational papers on the theory of relativistic atomic structure.

Was an early adopter and enthusiastic developer of computational algorithms, including long service on editorial board of *Computer Physics Communications*.

Diagnosed many of the problems encountered by others, especially variational representations, and computational complexity.

Oversaw the development of the GRASP Project, from 1970, first published version in 1980, and into 21st Century.

Made significant contributions to relativistic models of the electron-electron interaction.

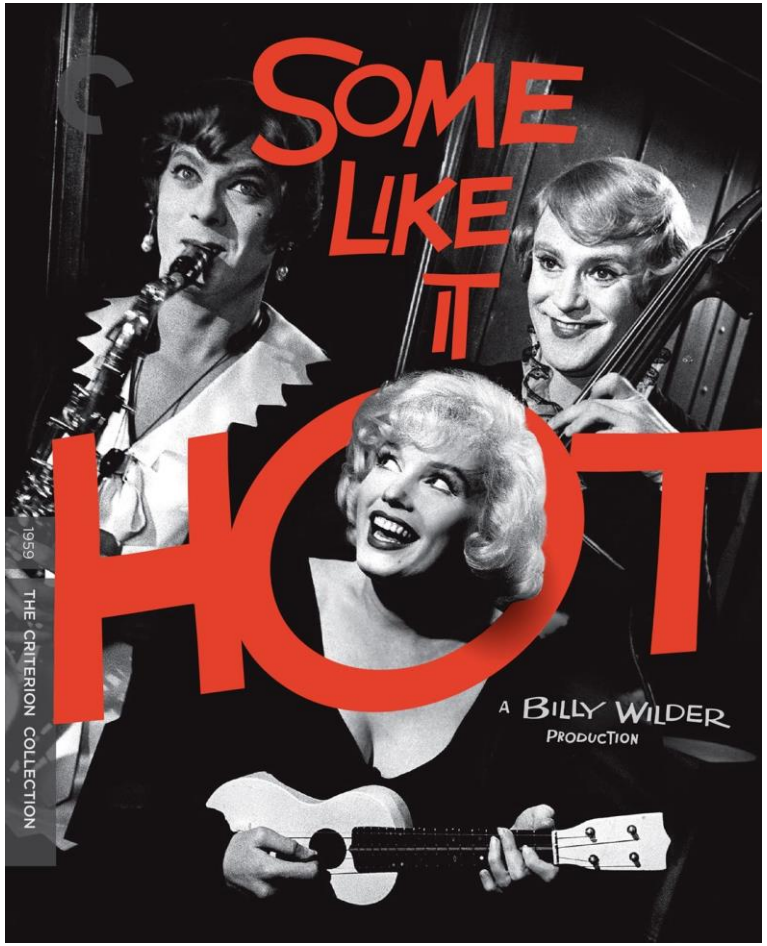
Led the development of basis set representations of Dirac operators, and facilitated the development of molecular methods, including BERTHA.

Extended GRASP to include continuum processes in the DARC code (Norrington).

Established many of the mathematical foundations of the discipline, and its pedagogical place within relativistic quantum field theories

Inspired this community that continues to contribute to the field seventy years later.

Favourite memory



On 25 December 1986, I went to 6 Woodlands Close in Headington for dinner.

I had to complete and submit by D.Phil. by 19 January 1987, and I took a draft of it with me. Ian had been unavailable for months, because he was acting Master of Pembroke.

We went through the draft in his study, and he identified a few things that still needed polishing. Beryl cooked something delicious.

I suggested that I should leave immediately to start work, but he said that would be “madness”, because one of his favourite movies was on television. I *had* to stay and watch it with him.

It was “Some like it Hot”, and we both laughed loudly throughout!

Poster for *Some Like It Hot*, United Artists (1959).

In memoriam: Professor Ian Grant FRS (1930-2025)

- Ian Grant was a formidable mathematician and numerical analyst, and equally precise in his use of language.

- He was unfailingly kind and generous, frequently humorous, but single-minded in his pursuit of excellence. He set high standards in everything he did.

- I am grateful that our professional relationship developed into a close friendship and count myself fortunate that I was able to visit him in Cambridge, still very much the Ian I always knew, just ten months ago.

- Let us all be grateful for the many opportunities that he has given to us.