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Obituary

Werner Eissner (1930–2022): A Pioneer in Computational Atomic Physics

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Werner Eissner (Figure 1), a pioneer in computational atomic physics, was born on 16 October 1930 in the city of Görlitz, Germany, to Bernhard and Frieda (née Eckert) Eissner. He lost both parents early in life, his father in the War and later his mother at the age of 15. He attended elementary school in his hometown (1937–1941) and high school in both Görlitz (1941–1945) and Lüdenscheid (1946–1951). His higher education was at Göttingen University (Preliminary Diploma in physics, 1954) and Tübingen University (Diploma under Professor Dr. Hubert Krüger, 1959, and doctorate degree under Professor Dr. Gerhard Elwert, 1967). His doctoral thesis dissertation was entitled “Rechnungen zur Elektronenstoßanregung der M-Schale von Wasserstoff und zur Polarisation des Stoßleuchtens der Hα-Linie” (Calculations for the electron collision excitation of the M-shell of hydrogen and for the polarisation of the collisionally excited Hα line), which he presented in preliminary form at the Third International Conference on the Physics of Electronic and Atomic Collisions (ICPEAC, 22–26 July 1963) held at University College London (UCL) [1]. For most of Werner’s career, he was a member of two major research groups in atomic physics led by Professor Michael J. Seaton FRS at UCL and by Professor Philip G. Burke FRS at Queen’s University Belfast (QUB) and Daresbury Laboratory (DL).

After graduating at the University of Tübingen, Werner joined Mike Seaton at UCL on a Culham stipend and later as Associate Research Fellow of the Royal Society through an exchange arrangement with the Deutsche Forschungsgemeinschaft. One of us (HN) recalls those early days in some detail:

> Professor Mike J. Seaton was planning a grand project in atomic physics. Space research was expected to soon provide astrophysics with a plethora of UV-spectra coming from the most varied objects such as the solar corona, AGNs, and planetary nebulae, originating from medium and highly ionised atoms. To identify and interpret these spectra, the atomic data were mostly missing. A computer should construct the atomic structure along the lines of Condon and Shortley, and no longer be performed by hand with Clebsch–Gordan coefficients adding stepwise one-electron functions to arrive at the desired n-electron atom. I remember that,

on a visit late in 1966, Mike Seaton told me about his plans and offered me a position on the project. The European Space Research Organisation (ESRO) provided the required grant. Mike also told me that a grant had already been found for Werner Eissner. Early in 1967, the group was formed with four members: John Belling, Werner Eissner, John Tully, and me. In a long session, Seaton explained the task. We should organise the way we felt best. He would always be available for advice but did not want to be involved in details. However, as Belling and Tully were also involved in other tasks, the atomic structure group was soon reduced to Eissner and me.

Once it was clear what the computer program should and might be able to do, we split the work. Werner developed the algebraic structure and I the radial functions. I was also supposed to look at the astrophysically required data. The programming was not a straightforward thing. We soon hit storage problems, and a lot of work went into the organisation of the overlay structure. To economise computer time, Werner's flair for finding clever solutions for the algebraic problems was exceedingly helpful. As our first aim was highly ionised systems, we initially thought that a $1/r$ potential might serve for constructing the radial functions. However, after a few trials and in the view of the long-term aim of having a truly general program, we chose a modified Thomas–Fermi potential. There were plenty of occasions when we consulted Mike: his advice was invaluable.

Werner was a very gentle, lively, and interesting person. We had many discussions over and after coffee, particularly on history. What initially complicated our collaboration was his quest for perfection. Looking for a solution was always fun, but agreeing when the solution was good enough was another matter. However, we soon developed a mutual feeling for the right moment of mutual consent.

We finished STRUCTURE and published it in 1969. Werner and I wanted Mike Seaton to be a co-author, but he very generously refused. We acknowledged his contribution with: "The advice of Professor M.J. Seaton at every stage of this work was of great help". Werner then went full speed to develop his collision program. Werner was a godsend for Mike Seaton's atomic data project. For Werner, the project was a godsend as well, he loved it and dedicated all his energies to it.

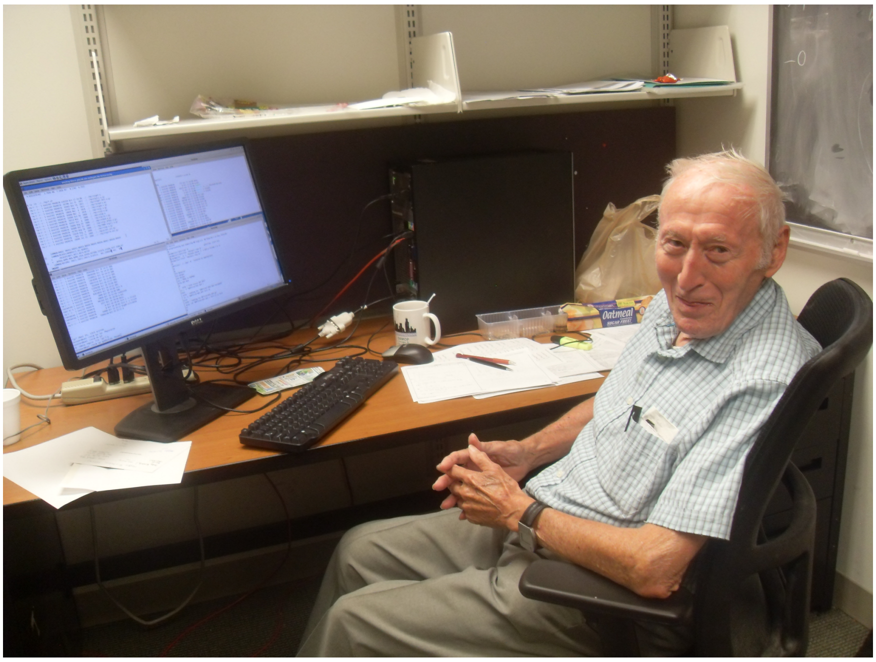

Figure 1. Werner Eissner at his desk as a Visiting Fellow (2014) of the Department of Astronomy, Ohio State University, Columbus, OH, USA.

As mentioned above, Werner first teamed up at UCL with Harry Nussbaumer to write the non-relativistic version of the major atomic structure code known as SUPERSTRUCTURE (SST) [2,3]. Later, the two co-authors were joined by Michael Jones for the inclusion of the Breit–Pauli relativistic corrections in the code. Werner also co-wrote with Claude Zeippen the subroutine that allows for the inclusion of relativistic corrections in the magnetic-dipole operator [4]. SST can be and has been widely used on its own for accurate atomic structure and radiative calculations. Such structure codes can also be used as a starting point in coupled-channel scattering calculations to provide accurate "target" descriptions. Users have cited the two papers by Werner and Harry more than a thousand times! In addition, Werner developed the UCL Distorted Wave code [5], which has not only been used for many calculations but also inspired different versions including SST variants [6].

After being a Postdoctoral Resident at the Center for Theoretical Studies of the University of Miami in Coral Gables, Florida, during 1972–1973—where he co-edited, under Arnold Perlmutter, the Proceedings of the Coral Gables Conference on Fundamental Interactions in Physics (22–26 January 1973) [7], which was attended by renowned scientists such as Paul Dirac, Abdus Salam, Robert Wilson, Robert Hofstadter, Gregory Breit, Harrie Massey, Larry Spruch, and Arvid Herzenberg—he returned to UCL in 1974 to be hired as a Science Research Council Fellow and Senior Lecturer during 1975–1978 and thereafter as an Honorary Research Associate until February 1980.

Together with Mike Seaton, Phil Burke, and their collaborators, Werner played a major role in laying the theoretical and computational foundations of the electron scattering close-coupling method [8–13]. This formalism forms the basis of high-precision, state-of-the-art computations of electron–atom collisions, most notably the *R*-matrix suite of codes [14,15] employed by many researchers worldwide, especially from the Opacity Project [16,17] and Iron Project [18–20] teams. While at UCL, he was instrumental in the development of the IMPACT suite of close-coupling codes [14], and later adapted SST to interface with the *R*-matrix package also leading to a relativistic version of those codes.

By 1973, it had become obvious that the scientific community needed to document, maintain, and provide state-of-the-art computer programs for general use. The Atlas Laboratory, which became part of the United Kingdom (UK) Rutherford and Appleton Laboratory in 1975, accordingly proposed the formation of Collaborative Computational Projects (CCPs). Funding was approved by the then UK Science Research Council, and, in 1978, Werner was appointed the Research Assistant for the second CCP (known a CCP2) on "The Continuum States of Atoms and Molecules" for which Phil Burke had overall responsibility as Chairman of the CCP2 Working Party.

As the CCP2 Research Assistant, Werner documented and maintained a library of atomic physics codes, many of which he had written, and ensured these were readily available to anyone in the world with a genuine interest in computing atomic data. In addition, Werner edited the CCP2 newsletter, organised CCP2 workshops, and attended and minuted meetings of the CCP2 Working Party. The success of CCP2 was very much to Werner's credit: it allowed and installed a collaborative spirit among atomic physicists and astrophysicists, which the more famous Opacity and Iron Projects were subsequently able to adopt and exploit.

In 1978, Professor Burke held appointments at the DL and QUB, spending most of his time at the former. Werner therefore relocated to DL in March 1980 and, then, in 1985, to the QUB Department of Applied Mathematics and Theoretical Physics, as Professor Burke's appointment there became full-time in 1982 and, by 1985, he had negotiated Werner's transfer. Werner remained at QUB until his formal retirement in 1993, after which one of us (GW) offered him a position as a project scientist at the Ruhr University Bochum. While at Bochum, he supervised two master's theses and a PhD thesis related to the applications of the *R*-matrix code. In Bochum, he also completed his review article on the UCL Distorted Wave code [5]. In 2000, he followed GW to the University of Stuttgart, where he continued his calculations based on contract work. An example of these activities was his work with Vo Ky Lan on the photoionization of Ti^{3+} presented at ICPEAC 2009 [21].

Werner was always keen on improving codes wherever possible. In particular, he strived to provide foolproof versions of SST. Together with Keith Berrington and Patrick Norrington, he was instrumental in optimising the Breit–Pauli version of the RMATRX code, thus rendering it more reliable and user-friendly [15]. When the Opacity Project was launched in 1983 and the Iron Project in 1993 for the calculation of astrophysical opacities and a vast array of collisional and radiative parameters using the *R*-matrix codes, Werner played a key role in their adaptation and applications. He was a founding member of both international endeavours and remained an active contributor to the end of his life.

He spent much of his time at UCL, QUB, and DL as already mentioned and was also a welcome visitor at the Observatoire de Paris (Meudon), the Observatoire de la Côte d'Azur (Nice), Ohio State University (Columbus), NASA Goddard Space Flight Center (GSFC, Washington), and the Joint Institute for Laboratory Astrophysics (Boulder). One of us (AKB) reminisces about Werner's collaboration at GSFC [22,23]:

> In 1974, I met Werner while spending a few days at University College London learning how to use the SUPERSTRUCTURE and Distorted Wave codes. Having performed most of the coding, he was an expert in both of them. I acquired these programs, but I did not learn enough. I needed a lot of help not only in the beginning but for many years into the future. With the help of a systems engineer, we sometimes had three-way discussions on the telephone about adapting these codes. Werner visited me at the Goddard Space Flight Center many times and helped me a lot. Without his help, I would not have progressed much. He stayed at my house, and he was so familiar with my place that while entering the house he would say, "I know where I am going to sleep". He was always very active. If he was not helping with the codes, he would try to find something to do around the house. Once I was in Belfast having a gathering on a very cold evening; while returning home, Werner found that his bicycle lamp had been stolen, but he managed to travel home on that cold and dark night. He was always determined to do whatever was needed. I will always miss his sage advice.

The present summary provides a general idea of Werner's known and acknowledged scientific contributions. He was a brilliant scientist and programmer; a great, loyal, and sincere human, a true "family friend". Many researchers owe him gratitude for the efficient tools he ensured were available to the community, thus directly and indirectly adding to the wealth of atomic data required for the advancement of many fields such as astrophysics, plasma physics, and, of course, atomic physics. For many of his colleagues, he was a generous provider of sound advice, even acting as a mentor for some of them. Werner is mourned by them and many other colleagues for his selfless devotion to solving their problems without seeking benefit for himself. That quality alone highly distinguished him from most people.

Although it was difficult to not bother him with queries about the scientific problems many of us faced (which, owing to his immensely good nature, he never minded), he was also delightful company otherwise. He could hold forth on several topics with remarkable and in-depth knowledge of history, photography, and architecture, and was fond of food and outdoor activities such as cycling and alpine skiing. He also appreciated music and literature, not least the writing of his contemporary Günter Grass. He could exercise very precise focus as a photographer showing the finer details of the architecture and sculptures in churches and other buildings he frequently visited. His almost annual skiing trip to the Austrian Alps—often Kaprun at the base of the Kitzsteinhorn Glacier, where he delighted in daring off-piste challenges even in his early 70s—always left us in complete amazement. The parcels of *Elisenlebkuchen* (famous German ginger bread) his friends received from his ritual New Year's visit to Nuremberg showed attentive care and generosity.

Werner Eissner passed away on 6 April 2022 leaving no descendants, having been a bachelor all his life. His memory is profoundly cherished by all those who knew him. In particular, the authors extend their deepest sympathy and condolences to surviving relatives and friends on the passing of this most remarkable man.

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Abbreviations

The following abbreviations are used in this manuscript:

AGN	Active galactic nucleus
CCP	Collaborative Computational Project
DL	Daresbury Laboratory
ESRO	European Space Research Organization
FRS	Fellow of the Royal Society
GSFC	Goddard Space Flight Center
ICPEAC	International Conference on the Physics of Electronic and Atomic Collisions
NASA	National Aeronautics and Space Administration
PhD	Doctor of Philosophy
SST	SUPERSTRUCTURE
QUB	Queen's University Belfast
UCL	University College London

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