Douglas Rayner Hartree | Encyclopedia.com

Complete Dictionary of Scientific Biography COPYRIGHT 2008 Charles Scribner's Sons
24-31 minutes

(*b*. Cambridge, England, 27 March 1897, *d*. 12 February 1958),

mathematics, theoretical physics, quantum chemistry, computing, numerical analysis.

Hartree played a fundamental role in the field of twentieth-century numerical analysis and its application to theoretical physics. He developed practical numerical methods for use with pen and paper, desk calculating machines, differential analyzers, and electronic computers, and he pioneered the application of calculating technologies to scientific problems. In mathematical physics Hartree's most well-known contribution was the invention of the method of the self-consistent field for calculating atomic wave functions, which became known as the Hartree-Fock approximation, following further work on the technique by Vladimir Fock. This and other contributions meant that during the 1920s and 1930s, Hartree played an important role in the development of atomic physics and quantum chemistry, work for which he was elected a Fellow of the Royal Society in 1932.

Hartree specialized in the numerical solution of ordinary and partial differential equations—equations that often described real world problems and therefore needed real world solutions. From his early work on ballistics through research on quantum chemistry, Hartree used the latest computing technology to find practical solutions to differential equations. He was responsible for bringing Vannevar Bush's differential analyzer technology to the United Kingdom and for developing a wide range of scientific and industrial applications for the machine. In the post–World War II period, Hartree was influential in gaining support for the development of electronic computers in England and devising numerical methods for their application to problems in theoretical physics. One of his final contributions was the book *Numerical Analysis*, first published in 1952 and regarded as a classic in the subject.

Origins and Early Career . Hartree was born in Cambridge, England, in 1897. His father, William Hartree, taught in the Engineering Laboratory at Cambridge University until his retirement in 1913 at the age of fortythree. William Hartree was very skilled in numerical computation and continued to undertake scientific work after his retirement from Cambridge, as an assistant to both A. V. Hill and, later, to his son. Hartree's mother, Eva Raynor, was very active in public affairs, working with the Red Cross, the suffragette movement, the League of Nations Union, and the British National Council of Women. She served on the Cambridge Borough Council for twenty years and was the first female mayor of Cambridge in 1925.

Hartree was educated first at a small school in Cambridge and then at Bedales School in Petersfield in Hampshire, from which he won a scholarship to study mathematics at the University of Cambridge in 1915. Hartree completed one year of his undergraduate degree before leaving Cambridge to undertake war work with the Ministry of Munitions. The main role of the Ministry of Munitions was to supply the British Forces with weapons and ammunition throughout World War I. Hartree was invited to join A. V. Hill's Anti-Aircraft Experimental Section of the Munitions Inventions Department of the Ministry of Munitions as a commissioned lieutenant in the Royal Naval Volunteer Reserve, as part of a team made up largely of Cambridge mathematicians and mathematical physicists, including Ralph Fowler, Edward Milne, and Hartree's father. William Hill, a Cambridge physiologist and later pioneer of operations research, had been charged by the Ministry of Munitions with undertaking ballistics research to assist in the development of new anti-aircraft weapons.

The workwas a mix of routine ballistics calculations and mathematical research on the ballistics of high-angled fire. Hartree became expert at both pencil and paper calculations and the use of hand-cranked calculating machines, such as the Brunsviga, but he also began to develop new numerical processes to calculate trajectories. His most lasting innovation was the use of time rather than angle of elevation as the independent variable in trajectory calculations, but it was his development and refinement of practical iterative methods for the numerical solution of differential equations that was to shape his future career. After the war Hartree wrote up his work on ballistics calculations for the journal *Nature*(1920) and coauthored a paper with Leonard Bairstow and Ralph Fowler on the pressure distribution on the head of a shell traveling at high velocities, published in the prestigious *Proceedings of the Royal Society*, thereby signaling the start of his career as a mathematical physicist.

Mathematical Physics Research . In 1919, Hartree returned to Cambridge; he completed his undergraduate studies in 1922. Fowler, who had also worked in Hill's group, had also returned to Cambridge as a lecturer, and he continued to influence Hartree. Hartree's experience of working with Fowler during the war made it an easy decision to stay on at Cambridge as a Cavendish Laboratory research student officially supervised by Ernest Rutherford but in practice mentored by Fowler. Inspired, according to his biographers Froese Fischer and Charles Galton Darwin, by the work of Niels Bohr, Hartree began studying the propagation of electromagnetic waves. Undertaken in collaboration with Edward Appleton, the work led to the magneto-ionic theory of the ionosphere and the development of the Appleton-Hartree equation for the refractive index.

The mid- to late 1920s was a time of great change and excitement in theoretical physics, and Hartree was becoming a well-known figure in the field. When news of Erwin Schrödinger's work on wave mechanics reached Cambridge, Hartree was ideally placed to make a contribution, and this is the area of study for which he achieved his PhD in 1926. His experience of numerical integration of differential equations, gained during his ballistics work in World War I, was invaluable. Hartree was able to develop and apply numerical techniques to the solution of increasingly complex atomic structures.

Integral to this work was Hartree's development of the method of the self-consistent field as a way of simplifying the numerical solution of the complex differential equations derived from the Schrödinger equation. Essentially the method enabled an approximation of the wave functions of the electrons of atoms to be described as ordinary differential equations that Hartree could then solve numerically by an iterative process. Hartree collaborated with John Slater, Ivar Waller, and others to continue to develop the method and its application. Later work by Vladimir Fock to further develop the technique resulted in the Hartree-Fock method of calculating molecular orbitals.

In 1929, at the relatively young age of thirty-two, Hartree was appointed Beyer Professor of Applied Mathematics at the University of Manchester. It was here that Hartree began to teach in seriousness and to supervise his own research students. Hartree was to become renowned for the help and support he gave to his students and others who sought his assistance. He continued his research and continued to develop numerical methods using calculating machines. In 1937, Hartree was appointed chairman of Theoretical Physics at the University of Manchester.

Differential Analyzers.

In 1931, Vannevar Bush published an article in the *Journal of the Franklin Institute* in which he described the construction at the Massachusetts Institute of Technology (MIT) of a large mechanical device designed to mechanically solve differential equations. The machine, the differential analyzer, consisted of six integrating units connected by means of bus shafts. Each integrating unit was made up of a horizontal disk with a vertical wheel resting on it. The output from the integrating unit was connected to the main bus system through a torque amplifier in order for it to generate sufficient force to drive other components of the machine. Additionally, the differential analyzer had input and output tables and multipliers attached to the bus system.

Hartree learned of Bush's differential analyzer through published accounts and from John Slater, a professor of physics at MIT with whom Hartree often collaborated. Hartree saw how the differential analyzer could be applied to his work on the electron fields of atoms, and he traveled to MIT in the summer of 1932 to see the machine. He again traveled to MIT in 1933, and this time he used the machine to work on the self-consistent field equations for Mercury. Hartree was very impressed by the power of the machine to not only solve differential equations in a fraction of the time it took using pen, paper, and a calculating machine, but also by the way in which solutions could be described by the operation of the differential analyzer. By watching the machine run, the operator obtained a better perspective of how the variables in an equation changed over time and therefore an improved understanding of the phenomena described by the equations.

Hartree's visits to MIT and his use of the differential analyzer on a real problem convinced him of the value of the device and of the potential value of constructing one in England. In order to raise the money to build a differential analyzer at Manchester University, Hartree decided to construct a model machine from the children's construction toy Meccano, and he recruited Arthur Porter, a final-year physics undergraduate at Manchester, to assist him. After graduating, Porter registered as a master's student under Hartree's supervision and built the model differential analyzer in 1934. Porter tested the machine by solving the already known self-consistent field equations for hydrogen before going on to solve the equations for chromium, for which he gained his master's degree.

The model differential analyzer was very much more successful than Hartree had dared hope it would be, and soon Porter was using it to solve a wide variety of problems. The value of a full-sized machine had been more than adequately demonstrated, and Hartree secured a gift of £6,000 from Sir Robert McDougall, the deputy treasurer of the University of Manchester, to build one. Bush supplied both plans and a list of possible improvements, and Hartree placed a contract with the Metropolitan-Vickers Electrical Company to build the machine. The Manchester differential analyzer was installed in the Physics Department at the University of Manchester in March 1935, initially as a four-integrator machine, but it was extended to eight integrators shortly afterward.

A succession of visitors to the both the Meccano model and the full-sized differential analyzer, coupled with Hartree's publications in the popular scientific press describing the machine, meant that the differential analyzer work at Manchester had a considerable influence on the computational landscape of the United Kingdom. In 1935, John Lennard-Jones, Plummer Professor of Theoretical Chemistry at Cambridge, approached Hartree and Porter about the possibility of building a model differential analyzer at Cambridge. Hartree and Porter provided advice and guidance, and the resulting Cambridge Meccano differential analyzer was a more accurate and reliable machine than that at Manchester. As in Manchester, the model machine was a precursor to a funding application to build a full-sized machine that would form the foundation of the Cambridge Mathematical Laboratory. In 1937, Maurice Wilkes joined the Cambridge Mathematical Laboratory to supervise the construction of the full-sized machine. The Cambridge Mathematical Laboratory led by Wilkes was at the forefront of electronic computer development in England in the post–World War II period. In additional to the model at Cambridge, several other model differential analyzers were built in the United Kingdom in the 1930s and 1940s in academic, industrial, and military settings and were found to be useful computing tools, especially in situations where an understanding of the problem was more important than highly accurate numerical solutions.

The original purpose of the Manchester differential analyzer had been to solve self-consistent field equations. However, by the time the machine was installed, Hartree and Fock had refined their methods in ways that no longer required the use of a differential analyzer but were more easily undertaken using desk calculating machines. Hartree therefore applied for and obtained a Department of Scientific and Industrial Research grant to investigate a wide range of problems applicable to the machine.

Using the grant to full effect, Hartree and his students explored many diverse applications for the differential analyzer, including several industrial problems such as the time lag in process control systems. What characterized much of the research was Hartree's ability to work with differential equations and devise practical solutions for them, alongside his ability to teach others how to do the same. While the differential analyzer was applicable only to specific types of problems, it demonstrated the growing need in Britain for large-scale computing resources—a need that was further demonstrated during World War II.

World War II . At the outbreak of World War II, Hartree, along with many other British scientists, immediately became involved in war-related work for the Ministry of Supply, which had a wide-ranging remit relating to the supply and research side of the British Armed Forces. Hartree had several roles throughout the war, some relating very closely to practical work on problems involving differential equations and some rather more on the advisory side. Initially Hartree was assigned to the Projectile Development Establishment to work on anti-aircraft rocket design, a project that had strong links to his work in World War I. This meant that he was no longer in dayto-day contact with the work of the Manchester differential analyzer. However, the differential analyzer was recognized as a valuable computational resource by the Ministry of Supply and was immediately applied to war-related problems, under Hartree's supervision when his other duties would permit. Over the course of the war, the differential analyzer group worked on a very wide range of problems, including ballistics work, control systems for radar and gun control, radio propagation, underwater explosions, motion and stability of aircraft, heat flow problems, and the solution of diffusion and shock wave equations for the British atomic bomb project.

Alongside his advisory role in the Ministry of Supply and his supervision of the differential analyzer group, Hartree was also responsible for the magnetron research group. This group was created with the specific purpose of understanding magnetron theory in order to better inform the design of magnetrons for use in radar. The work required investigating the motions of electrons in the electric field that the electrons themselves had produced—that is, a self-consistent field. Hartree was able to use methods similar to those he had developed in the 1920s for atomic structure calculations. Britain and the United States began to collaborate on aspects of the magnetron work from late 1940 onward, and Hartree and John Slater from MIT found themselves once again working on similar ideas and problems. Much of the work was not suitable for solutions using differential analyzers, so Hartree developed elegant numerical methods for his small team of human computers working with desk calculators.

In addition to his other wartime responsibilities, in 1942, Hartree set up and chaired the influential Interdepartmental Committee on Servomechanisms—usually known as the Servo Panel. The aim of the Servo Panel was to disseminate information about recent advances in servomechanisms and to promote the use of a common terminology. The panel consisted of representatives from the Admiralty, the Ministries of Supply and Aircraft Production, and industry. Under Hartree's leadership the Servo Panel set up a series of lectures and seminars on servomechanisms, which were attended by people from the armed forces, industry, and universities, largely from the United Kingdom but also from the United States and British Commonwealth countries. The Servo Panel addressed the concern that developments in servomechanisms in radar, gun control, aircraft stability, and other applications (such as in the control of power plants and chemical processes) should be shared in order to benefit both military and industrial applications. The influence of the Servo Panel was wide and led to the strong development of the field of control engineering in the postwar period.

Computers and Numerical Analysis . Hartree's wartime advisory experience, coupled with his understanding of practical computation, meant that he was ideally placed to play a significant role in the development and application of electronic computers in the United Kingdom. In addition, his position in the Ministry of Supply and his contacts at MIT allowed him access to and knowledge of electronic computing developments in the United States. In 1945, Hartree paid an official visit to the United States on behalf of the British government, during which he visited the Harvard MARK I and ENIAC projects—both large-scale calculating machine projects. The ENIAC was built at the Moore School of Engineering at the University of Pennsylvania; it led directly to the development of the stored program computer concept, influencing computer design around the world. In 1946, Hartree again visited the ENIAC at the express invitation of the U.S. War Department in order to explore the ENIAC's application to scientific problems, with particular reference to the laminar boundary flow problem. Hartree was thus well placed to understand the advances being made in the United States and to promote computer development in the United Kingdom. It is unclear whether Hartree knew of the top secret Colossus machines built at Bletchley Park for code-breaking purposes, but he certainly moved in social and scientific circles with those who did. Hartree sat on advisory committees and executive groups and gave very positive support to the development of computers. In the late 1940s and early 1950s, electronic computers were developed in three main locations in the United Kingdom—at the University of Manchester, Cambridge University, and the National Physical Laboratory at Teddington. Hartree influenced all three projects, usually acting behind the scenes to promote, enable, or support the work.

The first computer project that Hartree influenced turned out to be the last one to come to fruition. During the war, the need for large-scale, government-sponsored centralized computing facilities had been recognized, and in 1944, Hartree had been asked to join a committee to discuss the matter. The result was the creation of a Mathematical Division at the National Physical Laboratory (NPL) based in Teddington, England, which not only acted as a centralized computing resource for the United Kingdom but also developed the ACE computer designed by Alan Turing. Hartree supported the creation of the NPL Mathematics Division both at the committee stage and in putting plans in place.

On his release from war service, Hartree returned to Manchester University as professor of Engineering Physics. He stayed only a short time before his appointment to the Plummer Chair of Mathematical Physics at Cambridge in 1946, so he was not on site to support the computer developments taking place in the Electrical Engineering Department at Manchester by Frederic ("Freddie") Williams, professor of electrical engineering. However, through the Royal Society, Hartree influenced the financing of a computing laboratory at Manchester run by the mathematician Max Newman to explore the application of electronic computers in pure mathematics.

At Cambridge, Hartree had a more obvious and practical influence. Maurice Wilkes returned from war service to take up the post of director of the Cambridge Mathematical Laboratory, then based around the Cambridge differential analyzer. Hartree described to Wilkes the computer developments taking place in the United States and arranged for Wilkes to attend the now famous series of lectures given by the Moore School of Engineering at the University of Pennsylvania, which effectively disseminated the electronic stored program computer concept worldwide. Wilkes took this information, developed it, and went on to build the EDSAC computer at Cambridge. Hartree contributed to building a library of subroutines for EDSAC and played a role in advising potential EDSAC users.

In addition to helping to initiate computer projects at Cambridge, Manchester, and the NPL, Hartree played an important role in raising awareness of computers and promoting their application to real projects, both by working with machines and by publishing and speaking widely on the topic. On his appointment as Plummer Professor of Mathematical Physics, Hartree gave an inaugural lecture entitled "Calculating Machines: Recent and Prospective Developments and Their Impact on Mathematical Physics." This can be seen as the start of Hartree's work on bringing computers and their potential to the attention of the scientific community. In the summer of 1948, Hartree was invited to spend three months in Los Angeles as acting director of the Institute of Numerical Analysis, which had been set up by the National Bureau of Standards to start work on developing numerical methods applicable to electronic computers; Hartree contributed to the work by identifying numerical processes that needed to be developed in order for scientists to make the best use of the computers then under construction. While in the United States in 1948, Hartree also gave a series of lectures at the University of Illinois on calculating instruments and machines, later published as a book (*Calculating Instruments and Machines*, 1949), which was influential in shaping opinion during the 1950s.

The EDSAC computer in Cambridge went into operation in May 1949. Hartree was based in the Physics Department but regularly contributed to the work of the Mathematical Laboratory, influencing the programming and applications work of the machine. In particular he supervised an active program of research on atomic structure using EDSAC. More generally, however, he was on hand to give advice when it was needed. He also saw a growing need for those using, or proposing to use, EDSAC to have a good understanding of numerical methods; he developed lecture courses that he titled "Numerical Analysis" and in 1952 published a book of the same name that was regarded as a classic in the subject.

Hartree died suddenly in 1958, of heart failure, survived by his wife Elaine (née Charlton), along with a daughter and three sons. His career had spanned the computing problems of two world wars and saw the art of numerical computation develop from pencil and paper to electronics. While the solution of differential equations was a unifying factor in his work, Hartree had influenced the development of both calculating machines and methods by always focusing on developing numerical methods to further the solution of real life problems.

BIBLIOGRAPHY

A complete list of Hartree's publications can be found in Charlotte Froese Fischer, Douglas Rayner Hartree: His Life in Science and Computing *(River Edge, NJ: World Scientific Publishing, 2003), pp. 213–219. Correspondence and papers are held at Christ College, Cambridge; University of Manchester National Archive for the History of Computing; and the University of Cambridge Library. The American Institute of Physics Niels Bohr Library (College Park, Maryland) holds correspondence with Neils Bohr and interviews with Elaine Hartree, Neville Mott, and John C. Slater; additional correspondence with Bohr resides at the Neils Bohr Archive in Copenhagen.*

WORKS BY HARTREE

With Leonard Bairstow and Ralph Fowler. "The Pressure Distribution on the Head of a Shell Moving at High Velocities." *Proceedings of the Royal Society* Series A 97 (1920): 202–2218.

"Ballistic Calculations." *Nature* 106 (1920): 152–154.

"The Wave Mechanics of an Atom with a Non-coulomb Central Field: Part I, Theory and Methods." *Proceedings of the Cambridge Philosophical Society* 24 (1928): 89–110.

"The Wave Mechanics of an Atom with a Non-coulomb Central Field: Part II, Results and Discussion." *Proceedings of the Cambridge Philosophical Society* 24 (1928): 111–132.

"The Wave Mechanics of an Atom with a Non-coulomb Central Field: Part III, Term Values and Intensities in Series in Optical Spectra." *Proceedings of the Cambridge Philosophical Society* 24 (1928): 426–437.

"The Wave Mechanics of an Atom with a Non-coulomb Central Field: Part IV, Further Results Relating to Terms of the Optical Spectrum." *Proceedings of the Cambridge Philosophical Society* 25 (1929): 310–314.

With Arthur Porter. "The Construction and Operation of a Model Differential Analyzer." *Memoirs of the Manchester Literary and Philosophical Society* 79 (1934–1935): 51–72.

Calculating Instruments and Machines. Urbana: University of Illinois Press, 1949.

Numerical Analysis. Oxford, U.K.: Clarendon Press, 1952.

The Calculation of Atomic Structures. New York: Wiley, 1957.

OTHER SOURCES

Croarken, Mary. *Early Scientific Computing in Britain*. Oxford, U.K.: Clarendon Press, 1990.

Darwin, Charles Galton. "Douglas Rayner Hartree: 1897–1958." *Biographical Memoirs of Fellows of the Royal Society* 4 (1958): 103–116.

Froese Fischer, Charlotte. *Douglas Rayner Hartree: His Life in Science and Computing*. River Edge, NJ: World Scientific Publishing, 2003.

Porter, Arthur. *So Many Hills to Climb*. Silver Spring, MD: Beckham Publications, 2004.

Wilkes, Maurice V. "Introduction." In Douglas Rayner Hartree, *Calculating Machines: Recent and Prospective Developments and Their Impact on Mathematical Physics* and *Calculating Instruments and Machines*. Charles Babbage Institute reprint series in the History of Computing. Cambridge, MA: MIT Press, 1984.

Mary Croarken