DOUGLAS RAYNER HARTREE*

C. G. DARWIN.

Douglas Rayner Hartree was born in Cambridge on 27 March, 1897, and he died also in Cambridge on 12 February, 1958.

His genealogy furnishes an admirable illustration of the principle of heredity in ability, for he could claim to inherit many of his gifts and his scientific tastes from one or other of his parents.

His father, who was a grandson of the famous Samuel Smiles, was for many years on the teaching staff of the Engineering Laboratory at Cambridge. He had retired from these duties in 1913, but on the advent of war in 1914 he took up work in the team led by Prof. A. V. Hill which was studying anti-aircraft gunnery and cognate matters. This brought his son Douglas into the same team, and started him on the lines of doing numerical computation. After the war William Hartree cooperated with A. V. Hill in physiological experiments for a time, and then joined his son in numerical work. This he continued almost until his death in 1943, but the relationship was an exceptional one, because the son was the leader and the father ranked as the junior in this work.

His mother, originally Eva Rayner, was daughter of a prominent physician in Stockport, and sister of E. H. Rayner who for many years was Superintendent of the Electricity Division of the National Physical Laboratory. She herself was active in public service and in various women's organizations. She was at one time Mayor of Cambridge and she also served for a time as President of the National Council of Women.

These remarkable parents had three sons, of whom Douglas was the eldest. The other two unhappily have not survived. He was educated, first in Cambridge and later at Bedales School, Petersfield, from 1910-15. He attributed to the excellent teaching of this school, in particular in mathematics, the actual trend of all his tastes in later life. He entered St. John's College, Cambridge, as a Major Scholar in 1915, but at the end of his first year his course was interrupted by the war and he went into the team of A. V. Hill which has been referred to above. He returned to Cambridge after the war and graduated in 1921, having obtained First Class Honours in Part I of the Mathematical Tripos, but, no doubt on account of the disturbance of his career by the war, only Second Class

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Honours in Part II of the Natural Sciences Tripos. The details of his professional career were as follows. He was awarded the Ph.D. degree in 1926. He was a fellow of St. John's College 1924-27, of Christ's College 1928-29. From 1929-37 he held the chair of Applied Mathematics in the University of Manchester, and in 1937 there was a substantive promotion there into the chair of Theoretical Physics, though during the period of the war he was mainly on leave of absence while serving the Ministry of Supply. In 1946 he returned to Cambridge as Plummer Professor of Mathematical Physics in succession to R. H. Fowler, and he held this chair until his untimely death in 1958. He was elected Fellow of the Royal Society in 1932.

In 1923 he married Elaine, the daughter of Eustace and Beatrice Charlton, of Keswick, who had herself been a pupil at Bedales School. They were not there together but it was the school link that first brought them into contact. She survives him. There are three children of the marriage, a daughter and two sons. They are all now married and have children. They have followed the tradition of the family in their scientific tastes and employments.

In his personal character, apart from his high intelligence, I think modesty and unselfishness would be recognized as Hartree's leading traits. In general company he would be apt to be silent, unless the subject of discussion should chance to be one in which he was an expert, and then he could speak up clearly and lucidly but not in the least aggressively. He was an admirable lecturer, and when he wanted to explain a problem to someone who was to work on it, he had a quick perception of the degree to which the listener was able to follow his talk, so that he could always make the subject easy to understand.

In the work he undertook his unselfishness was outstanding in the sense that he was always ready to help people with their problems, even at the expense of his own work. Actually this was perhaps a good thing, because there were a number of other people attacking the same kinds of problem in atomic physics as he was, so that the work would have been done anyhow, whereas there was no one in the world with the same gift for putting into shape *any* problem that was susceptible to numerical analysis. The unselfishness sometimes went to extreme lengths. Thus during 1939-45, when he was working with the Ministry of Supply, he had frequent occasion to travel between Manchester and London, and he always took with him some piece of calculation he had promised to do for somebody so as to employ the time in the train. It is related that after one such occasion he apologized to the man he had been working for on account of the small amount he had managed to get done, explaining that the train had been so crowded that he could not get a seat, and that in the corridor his elbow had been jogged so often.

His main interest was certainly in his work, but he also had strong outside tastes. One was for music which was a bond between him and the whole of his family. He played the piano, but his main activity in this was in an orchestra where he played the drums, and sometimes acted as conductor. Another strong interest was in railways, and in particular in railway signalling, and he records the fact that at the age when other small boys wanted to be engine-drivers his ambition was to be a signalman. This interest had its reward in much later life when he was consulted by the railway traffic staff on the question of the optimum running times for trains between Rugby and Euston, and was able to use both his general experience and his computing methods and instruments to give the answer. Still later he served on a Committee of the British Transport Commission and showed them how to use the new digital high-speed computing machines to solve the very complicated problems of traffic control, which previously had required months of work by the specialists in the subject.

In the many fields in which he worked, much that he did was necessarily in collaboration with others. It would hardly be possible to refer to all these in the detail of what is written below, but among his collaborators a few may be cited. The list includes the late J. R. Womersley, B. Swirles (now Lady Jeffreys), A. Porter, H. G. Booker, the late P. J. Daniel. I cannot attempt to apportion credit among these workers, and indeed I think that in some cases Hartree would have given most of the credit to his collaborators.

It is undoubtedly for his quite outstanding ability in the use of numerical analysis that Hartree's name will be best remembered. This began with the work he did on the technically new science of anti-aircraft gunnery in 1916-18. The science of ballistics has, of course, a very old history, but high-angle fire presented many new problems. His main activity was in the integration of the differential equations for trajectories, and in this at the age of 20 he introduced a reform which may not now seem very revolutionary, but which must have been rather disturbing for the older practitioners of the science. By tradition the angle of elevation of the trajectory had always been used as the independent variable, and the coordinates and the time were expressed in terms of it. He showed that there would be great advantages in using the time itself as the independent variable, and expressing all the other quantities in terms of that. He introduced this practice and it is now generally accepted.

After the war he returned to Cambridge for two further years as an undergraduate, taking the Natural Sciences Tripos and he then continued there doing research under the stimulating influence of R. H. Fowler. He considered later that the most important event in his scientific career was a visit to Cambridge paid by Niels Bohr, in 1921, who gave a course of lectures on the Quantum Theory. This was of course the " Old Quantum Theory ", and it is difficult for anyone who grew up later under the Wave Mechanics to realize what a curious period that was. It was both exciting and thwarting, for one had to believe in two fields of knowledge, each of which surely must be right, and yet they seemed mutually contradictory. It was under this stimulus that one of Hartree's earliest papers was done, in which, with a view to getting closer to understanding the light-quantum, he studied the propagation of an electromagnetic wave that was not uniform over the wave front. There were many other attempts going on at that time on similar lines, which were aimed at reconciling quantum and classical theories, but, as might be expected from our present knowledge, none of them had any success.

However, Hartree soon turned to a more profitable part of this field. The formula for the reflexion of X-rays from crystals can be made to give information about the distribution of electric density in the atoms of the crystal by means of Fourier analysis, and this type of problem was exactly suited to his skill. He also did work on various details of the Bohr atom model in the course of which he estimated the corrections that might be expected for various atomic energy levels on account of the inner shells of electrons. All this work was the germ that later flowered into one of his major contributions to physics, that of the Self-consistent Field.

With the advent of the Wave Mechanics, which was started in 1925, it became possible to feel confidence in much of the detail of atomic structure, and whereas previously the work had been mainly guided by the principles of general dynamics, now it came into the wave-theory. Second order linear differential equations replaced the earlier non-linear first order equations. The new work exactly suited Hartree's gifts, for it was in the numerical integration of differential equations that he had served his apprenticeship. In the new field the only problem that could be accurately solved was that of the hydrogen atom, but of course many efforts were being made to go beyond that, at first to such problems as the helium atom and the hydrogen molecule, and then to more complicated structures. He soon contributed to this subject by the introduction of the Self-consistent Field.

To see the importance of this, reference may be made to one of his much later writings, a Report for the Physical Society of 1948, where the subject is described, together with various extensions of it. The actual wave equations for the electrons in one of the heavier atoms are certainly not expressible in terms of ordinary mathematical functions. Some form of approximation is essential, and this would mean the construction of tables. " It has been said that the tabulation of a function of one variable requires a page, of two variables a volume, and of three variables a library; but the full specification of a single wave function of neutral *Fe* is a function of 78 variables. It would be rather crude to restrict to 10 the number of values of each variable at which to tabulate this function, but even so, full tabulation of it would require 10^{78} entries, and even if this number could be reduced somewhat from considerations of symmetry, there would still not be enough atoms in the whole solar system to provide the material for printing such a table."

The principle of the Self-consistent Field evades these quite insuperable difficulties by imagining that each electron is moving in a sort of smudged field due to all the others, and furthermore it takes advantage of the fact that in a heavy atom the inner electrons have filled up many of the lower-level groups completely, and the influence of their field on the rest is therefore comparatively easy to estimate.

As a start these fields are guessed and it becomes possible by the numerical solution of ordinary differential equations to find the wave function belonging to each of the electrons in these fields, which is a very much simpler problem than that of considering the simultaneous equations which would be required to represent the atoms' behaviour accurately. The computed wave functions for the electrons then yield an electric density which is likely to be rather different from its first guessed estimate, and from this density new values of the field are calculated. The calculation is done over again with the new field, and it must be repeated until the two processes of finding the wave-functions and of their electric fields are mutually consistent. It will readily be believed that there are many opportunities for ingenuity in simplifying this work, by recognizing how large it is admissible to take the steps of the integrations and in other ways, so as to make the series of operations converge most rapidly to the final self-consistent results. Hartree had such a deep understanding of the subject that he saw quicker than anyone else how to take advantage of any short cuts that might offer themselves.

Working in this manner he attacked problems very much more advanced than others had attempted. For example, sometimes working in conjunction with his father, he solved the problem for such elements as copper and even mercury. All this work was being done with pencil and paper, but the situation was changed about this time, when Vannevar Bush developed his differential analyser in America. This immediately excited Hartree's interest.

The differential analyser is a machine which can do integrations by making a wheel roll on a rotating disc, while its distance from the centre of the disc is varying all the time. The principle of it was originally proposed by Kelvin, but in those days it could not work because the loads on the various shafts became so heavy that wheels would slip. With modern electric techniques, however, a torque-amplifier can multiply up any mechanical force many times, and so it overcomes this difficulty, and the integrations can be done with considerable accuracy. The machine could obviously be adapted for the solution of differential equations, though in order to do this they have to be written in a form rather different from those usually given in the older text-books.

Hartree saw that this machine would much lighten the very heavy numerical work of his computations on self-consistent fields. He therefore made a journey to Boston to see the machine work, and on returning home he set up one for himself, the first model being made in 1934 of Meccano parts*. Starting from this, with the help of A. Porter, he obtained a number of results and later, again with his help and aided by a generous gift of £6,000 from Sir Robert McDougall, in 1935 he had a much larger machine made. This was later copied in other places, but for long it was much the largest, best and certainly most used differential analyser outside America.

It was a general purpose machine, and with his invariable generosity Hartree gave service with it to a very great many enquirers, and the service included giving them his intimate experiences of the general way that numerical problems should be solved. Indeed, in some cases he could show them how with a little ingenuity it might be quite unnecessary to use the machine. One example of this arose out of the first German magnetic mine that was recovered. There were questions posed about its fusing and firing, and a team from the Admiralty went all the way to Manchester to ask Hartree for the help of his machine in solving them. After two hours' study he could given them the answers without using the machine at all!

His main purpose in making the machine had been to use it for the Self-consistent Field problem, but not long afterwards the problem itself was very considerably changed by Fock, who showed that what are known as the " exchange forces " would play an important part in the matter. These forces arise because electrons cannot be treated as recognizable individuals, but are mutually interchangeable. They made very notable changes in the fields of the atom, and it turned out that they did not lend themselves so readily to solution by the differential analyser. There was something of a reversion to pencil and paper, to which Hartree himself contributed again.

It thus came about that the most valuable work that Hartree did with the machine was the solution of a great number of general problems with a great variety of applications, rather than the purpose for which it was originally intended. I do not think there is any reason at all to regret this, because though Hartree made a contribution of first rate importance to quantum theory by his work on the Self-consistent Field, he could only

* Meccano is a well-known toy with which schoolboys can put together quite elaborate structures.

claim to be one among quite a number of workers who were making equally important contributions to the general subject, whereas in his particular gift for numerical calculation he was unique.

With the use of the differential analyser, but of course very much more by his skill in seeing how it could best be used, he made important contributions during the next decade to a very great variety of subjects. Thus during the war he applied it to the study of anomalous radar pulses in the troposphere, to the behaviour of the magnetron, in particular to the effect of its "straps", and to the steering of tanks. In the subject of anti-aircraft gunnery the matter of automatic following of the hostile aeroplane by radar devices gave difficult problems which were exactly suited to his gifts. One example that may be cited is a result on this subject which he obtained in collaboration with the late Prof. P. J. Daniel, of Sheffield, whom he had brought into the subject, which was forgotten when the war ended, and in fact was rediscovered in America 10 years later.

Apart from the solution of special military problems perhaps the most important contribution that he made in this field was to the subject which has now become dignified by the title of automation. This, of course, is not a new subject, for Watt had invented the centrifugal governor in the 18th century, and the theory of this device was worked out by Clerk Maxwell, but the new developments have been so great as to constitute a real revolution, and in this revolution Hartree played a conspicuous part. It began as early as the days of his original model differential analyser. With the help of this he was the first to study fully the "three-term controller", which has become the basic instrument for the control of chemical plants of all kinds, so that now millions of pounds of manufacturing production depend on it.

The "three-term controller" is essentially an instrument which controls the next stage in the production of something by measuring the past stages of its production, for example it might be the control of the temperature of some chemical process. This might be determined either by the quantity that has been just produced, by its differential coefficient, or by some integral of its past production. For some manufactures one of these will be best, for others another, and often best of all will be a suitable combination of all three. In working out these things he made use of the invaluable Heaviside Operational Calculus, which was for long regarded with suspicion by many orthodox mathematicians, though more recently it has been recognized as identical with the method of the Laplace transform, so that it has become respectable. In particular it seems to have been he who, by the use of the operator $e^{-p\tau}$, first saw how to attack a practical difficulty that plays a great part in many manufactures, that of finite time-lag. This occurs when it is a considerably later stage in a long process which is to be used in giving the instructions that concern some much earlier stage. It would hardly be an exaggeration to say that very possibly, but for Hartree's work, a great deal of present day manufacture would be different from what it in fact is.

The Differential Analyser had scarcely become a well established instrument when signs began to appear that it would be replaced by an even more powerful instrument, the Electronic Digital Computer, and in the development of this Hartree again played an important part. The first such instrument, the ENIAC, was set up in America for the special purpose of calculating the trajectories of projectiles. Its potentialities had not been much developed by the end of the war, and one of the first acts of the designers was to send for Hartree so as to get him to advise them in its use.

I do not think it would be an exaggeration to say that it was he who taught them the way in which advantage could be taken of its extreme rapidity of action. The problem is formidable, as are all the problems which depend on two constants one at each end of a range of integrations. Here the two constants are respectively the initial elevation and the position of the target. With the older methods several trajectories had to be laboriously calculated from the start, some of which would go above the target and some below, and there then had to be a final interpolation to find the true trajectory. He showed them how to make ENIAC do one of these trajectories and at its end automatically make a correction for a new trial. It then repeated this process with new corrections again until it finally found the right path. All this was done without making any records, but as soon as the machine had the solution, it automatically received a new order, which was to go through the whole of this trajectory again, but this time printing out the answer. I believe the calculation of each trial trajectory took less than a second to do; the final printing was much the slowest part of the proceedings, but even so the whole calculation was done in about half-a-minute.

The speed of working of electronic computers is very much greater than that of the differential analyser and their accuracy is very much higher and the consequence has been that they have entirely superseded the differential analysers in most of the work for which these had proved themselves so useful. The analysers are still used for purposes of automation in manufacture, but even there they are being superseded in some cases and in the research institutions most of the analysers, so laboriously installed a few years ago, are now lying idle because their work can be so much better done by the new instruments.

In this change Hartree played a leading part, largely by the advice he could give to those who were supporting the installation of the new machines. These included the EDSAC at Cambridge, which had been set up through the initiative of M. V. Wilkes, the Ferranti one at Manchester, and also many others including ones in America and Australia, both of which countries he visited as a consultant. Though he continued to the end to give advice in the use of these machines, and indeed often to help in the planning of the programmes for them in a great variety of subjects, he would not have claimed to do anything in the way of directing their use, and for this he would certainly have given all credit to their actual directors. When he returned to Cambridge in 1946 he was largely concerned with directing the researches of a number of junior men. These researches were in a great variety of fields, some of them concerned with atomic structures, and others with hydrodynamics, including questions both of diffusion and of the boundary layer; all these subjects demanded skill in the manipulations of arithmetic or in seeing how to adapt the machines to do this work for them.

In these later years I think it may be said that the central interest in Hartree's thinking was the adaptation of the electronic machines for dealing with partial differential equations. This subject had come up even in the earlier days of the differential analyser, but there it had been a matter of deciding which of the two independent variables should have its differentials replaced by finite differences, while the other remained as a continuous variable. He had done some work for a steel-works on this matter in connection with the cooling of steel ingots, and this work brought out the important differences according to whether it was time or position that was expressed in finite differences. Now with the electronic machine both had to be replaced by finite differences, and the centre of difficulty was the decision how big the steps might be taken for each of these variables. This is a technical matter to be studied for any problem before the machine can be used, and it is hardly possible to exaggerate its importance. Not long ago a case was cited of an equation which could be handled in two different ways according as to whether it was time or position that was considered first. Both methods looked equivalent at first sight, but it turned out that without any loss of accuracy the steps of the finite differences taken one way could be no less than 8,000 times as great as if they had been taken the other way about. It will be readily appreciated from this example what an important part of the task is the arrangement of the lay-out of the work before it should be placed on the machine.

Partial differential equations constitute the central feature of many branches of mathematical physics, and the adaptation of such problems to the machines, much of it started by Hartree, holds the promise of leading to great advances in many subjects. In one respect fruit has already been borne, for in the old days the mathematician could in effect only solve linear equations and this meant a great limitation to the problems he could discuss, whereas non-linear equations continually present themselves, and the differential analyser or the electronic machine can handle them just as well as the linear type. It may well prove that this freedom from the limitation to linear equations, a freedom which he was among the very first to gain, will grow into a transformation of the whole shape of the applied mathematics of the future. In his inaugural address as Plummer Professor in Cambridge in 1946 he said: " It may well be that the high-speed digital computor will have as great an influence on civilization as the advent of nuclear power."

One of the most important contributions made to mathematics by Hartree has been his books, and in particular the book entitled *Numerical Analysis* which first came out in 1952; the second edition, emended in a few ways, only actually appeared after his death. Numerical analysis may be an austere subject, but he succeeded in producing a real work of art on it. This is partly because it calls not merely for deep understanding, but also for craftsmanship, and a craft is always interesting to contemplate for its own sake. Thus the reader, accustomed to mathematical works where the author is only concerned with the rigorous proofs of his theorems, and never thinks of looking beyond that, will find it most refreshing to read that everyone can always be sure of only one thing—that he will himself make mistakes sometimes. " Anyone intending to undertake a serious piece of calculation should realize that adequate checking against *mistakes* is an essential part of any satisfactory numerical process. No one, and no machine, is infallible, and it may fairly be said that the ideal to aim at is not to avoid mistakes entirely, but to find all mistakes that *are* made, and so free the work from any *unidentified* mistakes." All through the book attention is given to the best ways of detecting the mistakes that have been made. " One kind of ' check ' is so inadequate as to be almost worthless, namely, repetition of a calculation by the same individual that did it originally. It is much too easy to make the same mistake twice. . . ."

There are also a number of other examples where his practical experience contradicts the results given in most books. Thus he indicates that even the common formula for the solution of an ordinary quadratic equation with one unknown, as given in elementary books on algebra, is often nearly useless, in particular when the two roots are far apart. And again in dealing with the solution of linear simultaneous equations with many unknowns he says that there are many different ways appropriate in various cases, but " though there may be no one best way of evaluating the solution, it can be said with some certainty that the direct evaluation of the determinants and of the expression for the solution in terms of them is *never* the best way . . ." although in fact this is given as the complete answer in many books on algebra.

An interesting general point in the book is that it almost unconsciously shows how much methods of computation have been changed by the use of machines, whether the desk-machine type or the newer digital machines.

The older mathematicians who had to do numerical work would certainly regard logarithms as the key to such work, but logarithms have now gone so much out of use that, apart from occasional references to the slide-rule, they are never mentioned in the text, and in the index of this work there is not to be found an entry under the word " logarithm ".

In writing an account of Hartree's life work it has not been possible to describe in detail a great many of the things to which he applied his gifts. They have been in so many different fields that to have explained them all would have taken any reader far beyond anything that would be likely to be among his own special interests.