NEWSLETTER

No. 1

March 1987

DISCORSI B DIMOSTRAZIONI

MATEMATICHE, intorno à due nuoue fcienz,e

Attenenti alla

MECANICA & I MOVIMENTI LOCALI;

del Signor GALILEO GALILEI LINCEO, Filofofo e Matematico primario del Serenifimo Grand Duca di Tofcana.

Con una Appendice del centro di granità d'alcuni Solidi,



IN LEIDA, Appresso gli Elsevirii. M. D. C. XXXVIII.

The title page of Galileo's <u>Mathematical Discourses and</u> <u>Demonstrations concerning Two New Sciences</u> (Leiden 1638).

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Facsimile cover illustration of the first newsletter 1987

Contents

| Fea | atures | | |
|-----|---|--------------------|----|
| | Volta, Ampère & Ohm: brief biographies | by Vincent Smith | 3 |
| | A note on Guillaume Amontons and the laws | of friction | |
| | | by Ian M Hutchings | 11 |
| | A personal history of the pseudopotential | by Volker Heine | 24 |
| | From bombs to bubbles: the extraordinary career of Cyril Stanley Smi | th | |
| | | by Denis Weaire | 33 |
| | The Birth, Life and Death of the Bohr Atom | | |
| | | by A Whittaker | 36 |
| | Rutherford's transmutation experiment: At the time what did he think had occurred? | by E A Davis | 54 |

Book Review

Editorial

| Paul Langevin, My Father, The Man & His Work | 60 |
|--|----|
|--|----|

Committee and contacts

Editorial

Dear readers,

This will be the last Newsletter/Bulletin under my editorship. I've edited 22 normal issues and 7 special issues - roughly 750,000 words - over the last 20 years and in all that time I have had to reject only one submission. I think that speaks for itself regarding the quality of scripts and I should like to express my sincere thanks to all the contributors who have made the publication such a great success. The circulation in 2004 was around 300 and it now stands at over 2000 worldwide and I like to think that the newsletter has contributed in some small way to that success.

I have just read one of the articles in that 2004 issue '60 YEARS OF MEDICAL PHYSICS seen through the eyes of one who went through it' by Dr. Sidney B Osborn. I remember this article, which had been submitted to (I think) the Journal of the Institute of Radiology, and was rejected on the grounds that it was insufficiently 'academic'. Well, maybe it was but it remains a fascinating account of working in the field of the diagnostic and therapeutic uses of radiation in the post war period. It had been published in the IOP Medical Physics Group Newsletter and received further attention by the readers of the History of Physics Group Newsletter. This was possible because our newsletter (and I presume that of the Medical Physics Group) is not peer reviewed and acceptance is up to the editor - I regard this as one of its great strengths. Had this not been the case this account would have never seen the light of day!

You will see that the newsletter has been renamed the 'bulletin', and yet another change is that the bulletin is proposed to be an online publication. For those who are at ease with the medium will be content to read it on your laptops but I'm sure the Institute will be happy to continue providing a print copy for those who prefer more versatile reading conditions - (soaking in the bath with a glass of wine in one hand and the bulletin in the other perhaps!).

Finally I send my best wishes to your new editor and I'm sure the bulletin will continue to provide a great service to our members.

Malcolm J Cooper

Volta, Ampère & Ohm: brief biographies

Vincent Smith, University of Bristol

Introductory remarks

I originally prepared this as a presentation for a joint meeting of the IOP History of Physics and Physics Communicators Groups on the subject of 'SI Units', held at IOP HQ on 25 April 2022. I was interested to find out more about the founders of the elements of the equation V=IR. However, I was very struck by the various vicissitudes all three scientists had in their personal lives, problems related to (a) death and disease and (b) social attitudes of their times. Medicine and morals have progressed a lot since then!

Alessandro Guiseppe Antonio Anastasio Volta

Born 18 February 1745 in Como, Duchy of Milan.

Died 5 March 1827 in Como, Lombardy, Austrian Empire. (From 1805 to 1814, Como was in the Napoleonic 'Kingdom of Italy')

His parents were Filippo Volta and Maria Maddalena Inzaghi.

Alessandro was 6th of 7 children. "An impoverished noble family" ⁽¹⁾.



"Filippo Volta was reckless with money. He died when Alessandro was only seven, leaving his wife and seven surviving children in debt. Alessandro, together with his mother and two sisters, lived with an uncle, also named Alessandro Volta, who was archdeacon of the Como Cathedral. Alessandro's siblings all went into service of the church" ⁽¹⁾.

Education and employment

A late developer, he did not speak until age 4. But before he left school, had learned Latin, French, English and German. Taught by Uncle Alessandro from 7 to 12, then sent to a Jesuit boarding school, who expected him to become a priest. His family wanted him to become a lawyer, so he moved to another school until age 18. (But he wanted to be a scientist.)

After leaving school, he worked in the laboratory of a wealthy friend, Giulio Cesare Gattoni. In 1769 he proposed that electricity was only attractive (repulsion was just attraction from infinity.) He abandoned this idea later, but it gained him enough fame that he got a job at a local school in Como in 1775.

In 1778, he was appointed to the Chair of Experimental Physics at the University of Pavia, which he held for nearly 40 years.

Scientific achievements

- 1. Improvement of the Electrophorus
- 2. Perfection of the Eudiometer
- 3. Discoverer of Methane
- 4. Measured thermal expansion coefficient of air (Charles' Law / Loi de Gay-Lussac)
- 5. Study of condenser (capacitor)
- 6. Dispute with Galvani
- 7. Inventor of Voltaic pile
- 8. Measured electrochemical potentials of many metals

The Electrophorus



Used for carrying charge from one place to another. It was Invented in 1762 by Johan Wilcke but improved, popularised and named by Volta in 1772 (Letter to Joseph Priestley.) '*Elettroforo perpetuo*', because charge can be obtained indefinitely. In 1780 he reported on the ratio of charge to electric tension in different Leyden jars and invented the 'condenser'. He used this to increase the sensitivity of the electroscope.

The Eudiometer and the Discovery of Methane

Thomas Paine, Benjamin Franklin and others (even Pliny the Elder) had observed 'inflammable air' or marsh gas, bubbling up in ponds. In 1776-1777 Volta succeeded in collecting samples of the gas and studied its reaction with air in a device called a Eudiometer (a sealed, graduated tube) in which he ignited the mixture with an electric spark. He developed the 'electric pistol', using the explosion to fire a bullet. (Forerunner of the internal combustion engine) He also suggested this could be done remotely, the forerunner of the telegraph.

Dispute with Galvani and invention of the electric pile (battery.)

In 1786, Luigi Galvani had observed the twitching of the legs of dead frogs when connected to an electrostatic spark, and also when placed with copper hooks on iron railings. (Actually, it could well have been his wife, Lucia, who first noticed it and mentioned it to her husband!) Galvani believed the electricity came from within the frog. Volta at first accepted this and conducted his own experiments, which led him to conclude that the electricity came from the junction of the two dissimilar metals. To prove this he immersed copper and zinc plates in brine, later using discs of these metals separated by cloth soaked in brine. As part of the development of the pile, Volta measured what we now know as the Electrochemical potentials of many metals.



Personal Life



Alessandro Volta and his friend, the soprano Marianna Paris (See: 'an intense love affair'...) ⁽²⁾ Alessandro saw her for the first time in a performance of "The Barber of Seville" in 1789 and it seems it was love at first sight! It also seems that Marianna felt the same way, and they were lovers for many years.

However, society would not approve of their marriage.



Alessandro with his wife (they married in 1794): Maria Teresa Peregrini. This too did not go smoothly: his wife was the youngest of six sisters and they had to wait until the older sisters were all married! They honeymooned in Gravedona,

together with his brother, the Archdeacon.

Children: Zanino, Flaminio, and Luigi. (Flaminio, the "most promising" died of encephalitis at age 18)

Volta was elected FRS in 1791 and received the Copley Medal in 1794. He was created Count by Napoleon in 1810.

Below is his image on an Italian banknote (1984.) NB 10,000 lire = $\pounds 4.50$ today.



André-Marie Ampère

Born 20 Jan 1775, Lyon, Kingdom of France (King Louis XVI, Bourbon)

Died 10 June 1836, Marseille, Kingdom of France (King Louis Philippe, Orleans)

The French Revolution and then Empire under Napoleon Bonaparte, created some turmoil in between...!

Ampère's name is one of the 72 names inscribed on the Eiffel Tower



Early Life

Parents: Jean-Jacques Ampère, Jeanne Antoinette Desutières-Sarcey. André-Marie had two sisters, Antoinette and Josephine. When André-Marie was five, the family moved to their country estate in Poleymieux, near Lyon. He was educated to a high standard by his father in Latin and Mathematics.

Sadly Antoinette died in 1792. After the Revolution, his father became Justice of the Peace, but he was guillotined by the Jacobians in 1793.

Personal life and Career

In 1796, he met Catherine-Antoinette (Julie) Carron, whom he married in 1799. In 1800, they had their first child, Jean-Jacques, who was later to become a professor of linguistics. Sadly, Julie died in 1803. Ampère got married again in 1806, to Jeanne-Françoise Potot. The couple quickly realized their marriage had been a mistake. Their daughter Albine was born in 1807, and the couple legally separated in 1808. Albine came to live with her father and his younger sister Josephine.

In 1797, aged 22, Ampère began work as a successful private tutor in Mathematics in Lyon, and proceeded to a job in a school in Bourg-en-Bresse in 1802. Here, he published an important paper on probability (the theory of games.) Later, in 1804, he moved to Paris and became a tutor in Mathematics at the Ecole Polytechnique. He was promoted to full professor in 1809, in spite of having no formal qualifications.

He also held prestigious posts at the University of Paris and the College de France. He died at Marseille in 1836. He is buried in the Montmartre cemetery in Paris. He chose his own epitaph: 'Tandem felix': 'Happy at Last'.

Scientific achievements

Theory of Games Force between currents Ampère's circuital law Discovery of Fluorine Precursor of Periodic Table

Ampère's Force Law & Ampère's circuital law

Both these are best expressed in terms of vector calculus. The first gives the element of force between two current elements in different circuits. The second relates the closed line integral of the magnetic vector to the current enclosed. Ampere, of course, never saw these expressions in modern notation.

He showed experimentally that the force between two wires carrying parallel currents is attractive, while the force is repulsive if the currents are anti-parallel.

James Clerk Maxwell said of Ampère: "The experimental investigation by which Ampère established the laws of the mechanical action between electric currents is one of the most brilliant achievements in science. The whole, theory and experiment, seems as if it had leaped, full grown and full armed, from the brain of the 'Newton of electricity.' It is perfect in form, and unassailable in accuracy, and it is summed up in a formula from which all the phenomena may be deduced, and which must always remain the cardinal formula of electro-dynamics."³⁾

Ampère's work is covered very fully in the book by Assis and Chaib: Ampère's Electrodynamics⁴⁾

Discovery of Fluorine

Ampère noted in 1801 that Hydrogen fluoride (produced by the action of sulphuric acid on calcium fluoride) had properties similar to hydrogen chloride. He proposed a new element, Fluorine, and suggested it could be produced from fluorides by electrolysis. He corresponded with Sir Humphrey Davy, who attempted this, but without success. In fact Fluorine was not isolated until 1886, by Henri Moissan, for which he received the Nobel Prize for Chemistry in 1906.

Similarities between Elements

Ampère noticed many similarities in groups of the known elements at that time. In this sense, he had a precursor of Mendeleev's periodic table, although Ampère did not use atomic weights to order them.

An anecdote about Ampère:

"One day, as he was going to his course of lectures, he noticed a little pebble on the road; he picked it up, and examined with admiration the mottled veins. All at once the lecture which he ought to be attending to returned to his mind; he drew out his watch; perceiving that the hour approached, he hastily doubled his pace, carefully placed the pebble in his pocket, and threw his watch over the parapet of the Pont des Arts."⁵

Georg Simon Ohm

Born 16 March 1789, Erlangen, Bavaria.

Died 6 July 1854, Munich, Bavaria. (Erlangen is also the birthplace of Emmy Noether (1884)

His father, Johann Wolfgang Ohm, was a locksmith while his mother, Maria Elizabeth Beck, was the daughter of a tailor.

He was one of seven children, but only three survived to adulthood.



Although his parents had not been formally educated, Ohm's father was a rather remarkable man who had educated himself to a high level and was able to give his sons an excellent education through his own teachings. His younger brother Martin later became a well-known mathematician. Their mother died when Georg was ten.[Georg] was a student at the University of Erlangen for three terms, but rather than concentrate on his studies he spent much time dancing, ice skating and playing billiards.

In 1806, Georg obtained a position as a teacher in a school in the canton of Bern, Switzerland. In 1809, he became a private tutor in Neuchatel. He continued to study mathematics, and received a doctorate from the University of Erlangen, then joined the faculty there in 1811. But with little prospects, he then became a teacher of mathematics in two schools in Bamberg, Bavaria.

Ohm wrote a textbook on geometry, and sent it to King Wilhelm III of Prussia. The King was impressed and gave Ohm a job teaching in the Jesuit Gymnasium in Cologne (1817.) He was given a sabbatical year in Berlin at half pay in 1826, to concentrate on his research. He later moved to Nuremberg, and in 1849 to Munich as curator of the Bavarian Academy's Physics cabinet.

Ohm never married, as he felt he had insufficient means to support a family in the appropriate style. Finally, he was given the Chair of Experimental Physics at Munich University (1852), just two years before his death.

Ohm was awarded the Royal Society's Copley Medal in 1842, and became a Foreign Member in 1842. (Full member of the Bavarian Academy in 1845.)

Ohm's Law

"His first paper in 1825 examined the decrease in the electromagnetic force produced by a wire as the length of the wire increased." I was sure this was a mistake, since it sounds directly opposed to Ampere's research (above), until I realised Ohm was talking about constant tension (voltage) from presumably, his Voltaic pile. So he found that increasing the length of the wire decreased the current. He published his Law: the current is proportional to the potential difference, in 1827. (In fact, Henry Cavendish had already discovered this some 50 years before, but did not publish it.)

References

Much use has been made of relevant articles in Wikipedia. In addition the following are of interest:

(1) Alessandro Volta | 10 Facts On The Inventor of Battery | Learnodo Newtonic (learnodo-newtonic.com)

(2) <u>Alessandro Volta and Marianna Paris: an electric love (evolvere.com)</u> (in Italian: use Google Translate for an English version.)

(3) Maxwell, J. C. (1954). A Treatise on Electricity and Magnetism. Dover, New York. [vol. 2, article 528, p. 175].

(4) Ampère's Electrodynamics, A. K. T. Assis and J. P. M. C. Chaib 2015 Amperes-Electrodynamics.pdf (unicamp.br)

(5) Camille Flammarion in Popular Astronomy: a General Description of the Heavens (1884)

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Introduction

Duncan Dowson's important book on the history of tribology (1) is the natural starting point for any physicist wishing to learn about the origins of this subject, and together with David Tabor's chapter published 15 years earlier (2) was responsible for sparking my own interest. The purpose of this note is to extend the discussion presented by Dowson and shed a little more light on the contribution of a key figure in the development of our understanding of friction: Guillaume Amontons (1663-1705).

Amontons' papers of 1699

The so-called 'laws of friction', which state that the friction force is proportional to the normal load and independent of the apparent area of contact, are usually ascribed to Amontons although they were in fact clearly enunciated by Leonardo da Vinci more than two hundred years earlier (3). The source that is widely cited for Amontons' first statement of these laws is a paper presented at a meeting of the Académie Royale des Sciences in Paris on 19 December 1699 and published in the Mémoires de l'Académie, entitled 'De la resistance causée dans les machines, tant par les frottemens des parties qui les composent, que par la roideur des cordes qu'on y employe, et la manière de calculer l'un et l'autre' (On the resistance caused in machines, by the friction of their components as well as by the stiffness of the ropes they use, and the method of calculating these; author's translation) (4). Numerous writers on the history of tribology over the past eighty years have cited this paper (e.g. 1,2,5–14). However, the key importance of a previous contribution by Amontons is nearly always overlooked¹.

¹ The paper in Japanese by Yoshitake written for the tercentenary of Amontons' paper (10) is perhaps the most accurate, but has been cited by no subsequent authors.

Six months before the December meeting, in June 1699, Amontons presented to the Académie a lengthy paper entitled 'Moyen de substituer commodement l'action du feu à la force des hommes et des chevaux. (Method of conveniently substituting the action of fire for the force of men and of horses) (15). The main topic of that paper was the design of a novel heat engine, a 'moulin à feu', based on the thermal expansion and contraction of air. Sheet metal cells arranged around the rim of a giant wheel were alternately heated by a furnace and cooled by immersion in water as the wheel rotated (16). Expansion of the air in these cells pushed water through tubes into another ring of cells, and the unbalanced distribution of the weight of water around the wheel led to a gravitational torque and could thus generate mechanical work. Amontons' ingenious design of what we would nowadays regard as a Stirling engine was based on a series of detailed experiments in which he investigated the expansion of air by heating, its contraction on cooling, and rates of heat transfer through metal sheet. In order to estimate the power of the engine, he also compared the effort produced by men with that of horses, carrying out experiments which showed that a man could work at about one sixth of the power of a horse. As a result, he calculated that a heat engine with a wheel 30 feet (9 m) in diameter rotating once every 9 seconds would be equivalent in power to 39 horses or 234 men.

In order to estimate the rate of mechanical working by a human worker, Amontons measured the forces and displacements involved in the manual polishing of plate glass, and in doing so made a significant contribution to the concept of mechanical work (17). It is from these observations that Amontons first drew his important conclusions about friction.





Figure 1. Eighteenth century illustrations of the manual polishing of glass (18). A glass sheet (E in the lower image) is polished with progressively finer abrasives by the action of a polishing block (F) that is dragged backwards and forwards by the operative. The downward force on the block is supplied by a springy wooden strut or *flèche* (H) bent between an upper board (K) and the block.

Diderot's *Encylopédie* of 1765 provides details of the polishing process that Amontons observed, as illustrated in Figure 1 (18). The polishing block was moved repeatedly backwards and forwards over the surface of the glass sheet in the presence of abrasives such as sand and emery. As explained in the *Encylopédie* (19), the task of the operative was made easier by the fact that the block was pressed down on to the glass by a long springy wooden rod or *flèche* bent between an upper board and the block. The worker thus did not need to press down on the block, nor continually to accelerate and decelerate a heavy mass, and all his effort could be employed in sliding the block horizontally.

Amontons explains that he measured the downward force on the block with a spring balance arranged to pull the end of the *flèche* upwards, as well as the horizontal force required to cause sliding by the same method. He measured the sliding forces for three different sizes of polishing blocks, with areas of 6, 11 and 24 pouces (literally, inches, but implicitly, square inches; the pre-Revolutionary French inch was 27.07 mm). He reported values for two slightly different downward forces: 28 and 30 livres (pounds force, one livre being 489.5 g). Amontons' results, given as values of the sliding force within the text of the original paper, are plotted in Figure 2 in terms of the ratio between the sliding (frictional) force F and the normal load N. In most cases he gave two values for the sliding force: a maximum value that applied when the *flèche* was vertically above the centre of the polisher (and presumably applying the maximum normal force) and a minimum value when the *flèche* was most obliquely inclined. These are plotted in Figure 2 as solid and open points respectively. In Figure 3 the mean values of sliding force are plotted against the normal load.



Figure 2. Ratio between sliding force, *F*, and normal load, *N*, plotted against nominal area of contact, as reported by Amontons for the polishing of glass. The filled points relate to maximum values of *F*, and the open points to minimum values



Figure 3. Sliding force, *F*, plotted against normal load, as reported by Amontons for the polishing of glass. Values of *F* are the means of the maximum and minimum values reported.

In his paper of June 1699 (15) Amontons wrote:

'From these observations one can note, in passing, that it is an error to believe that friction in machines increases or decreases in proportion to the size of the sliding surfaces, and, for example, that the wheel of a mill turns more easily if its bearings are shorter, which is in any case poor practice because they wear the bushes in which they turn unacceptably. But friction increases or decreases in proportion to the loads which are moved, and in the ratio of the length of the levers which move them along (the bodies) on which they are pressed.'

Apart from the formal papers published in the *Mémoires*, other sources of information about the proceedings of the *Académie* include the original handwritten minute books, maintained by Bernard Le Bovier de Fontenelle, *secrétaire perpétuel* for 42 years, which record not only the texts of the papers read at meetings but also the names of members present on each occasion. The minutes for 1699 (20) reveal that Amontons started to read his lengthy paper on the *moulin à feu* on Saturday 20 June 1699, and completed its presentation at the following meeting on Wednesday 24 June (erroneously referred to in the minutes as 23 June). The minute book provides the full text for his paper almost exactly as it was later printed in the *Mémoires*, but includes one further data point not present in the published version: that point has been included in Figs. 2 and 3.

Summaries of the most important material presented at the meetings of the *Académie*, intended for the non-specialist reader, were also prepared by Fontenelle and published in the *Histoire* (21). The *Histoire* and the *Mémoires* for each year were published together in a single volume, but with the pages of each part separately numbered. The first edition of the volume for 1699 was published in Paris in 1702, with subsequent editions in 1718 and 1732; although these later editions contained some corrections and revisions, Amontons' papers remained unaltered and their pagination was the same in all the Paris editions. A further version of the first edition was published in Amsterdam in 1706 with different pagination. English translations of some of the content of both the *Histoire* and the *Mémoires*, in abridged form, were also published in 1742 in London (22).

The extract from Amontons' paper on the *moulin* à *feu* quoted above is followed by a significant passage in both the published *Mémoires* and the minute book, but which is omitted from the abridged English version:

'I greatly wish to have had the opportunity to carry out the same experiments with samples of iron, copper and wood, on surfaces of the same materials, because from those one could deduce some very important rules to calculate friction in machines.'

It is thus clear that in June 1699, based on his experiments on polishing, Amontons was making definite claims that the friction force was independent of the area of contact, and also that it varied in proportion to the normal load. Having carried out his initial experiments only in the context of glass polishing, it is not surprising that Amontons expressed the wish to extend his work to other materials more relevant to machinery construction, presumably in the absence of polishing abrasives.



Figure 4. Apparatus used by Amontons and described in his paper of December 1699 (original drawing from the minutes of the *Académie*) (20)

The widely-cited paper of December 1699 in which Amontons restated his laws of friction more forcefully and explicitly (4) describes his further experiments on the sliding of copper, iron, lead and wood against samples of the same materials, all lubricated with aged pork fat. While the minute book entry for 19 December 1699 (20) describes these experiments in the same way as the paper later published in the *Mémoires*, and contains much of the text of that paper, the paper had been substantially edited and additional material added by the time the published version was printed in 1702. For example, Amontons' thoughts on the problem of friction in a stack of interleaved plates, contained in the paper on friction' at its meeting of 27 February 1700 (23). But as far as the experimental work is concerned, the 1702 paper and the minutes of the meeting on 19 December 1699 are consistent.

Amontons' apparatus is shown in Figure 4: he used a bent elastic strut to provide the (effectively constant) downward force on the slider, and a spring balance to measure the (variable) horizontal force. This arrangement appears unusual and unnecessarily complex to the modern eye, and immediately raises the question as to why, more simply, he did not apply the normal load with a weight on the slider. The reason is, however, clear: Amontons was using exactly the same methods that he had employed in his experiments on glass polishing. Apart from the statements that the samples were of various (unspecified) sizes, and that he tested a wide range of combinations of the different materials, other information about the experimental conditions is completely absent from the record. Only a single value of normal load, 30 livres, is mentioned, although that was in a theoretical discussion on the effect of moment on friction in a rotating system (which develops a point he had already raised in the June paper). This is the same load as that used in his polishing experiments. It seems probable that Amontons used exactly the same type of *flèche* as in his glasspolishing studies, and may well have performed his new experiments in the same workshop.

According to the minutes of the meeting, Amontons made it clear to his audience on 19 December that in stating his laws of friction he was repeating a claim he had already made in June, based on his work on glass polishing:

'the resistance caused by friction only increases or decreases, as I have already said in the experiments reported to the meetings on 20 and 23 June, in proportion as the load is larger or smaller, and not according to whether the bodies that slide are more or less extended.'

The italicized reference to the June meetings, present in the minutes, is absent from the version published in the *Mémoires*.

An important difference between the published version of Amontons' paper (4) and the minutes of the meetings of 19 December 1699 and 27 February 1700 is the absence in the minutes of any comments on the physical basis of friction. In the printed paper, Amontons provides a diagram showing elastic asperities as springs attached to the surface; he ascribes frictional resistance to the effect of surface roughness, and discusses the origins of friction in terms of the force needed to lift asperities, whether flexible or rigid, over each other. All these ideas are missing from the contemporary accounts of his talks in the minutes of the *Académie*, the only occasions on which Amontons presented his work on friction. The paper he actually presented at the December meeting was more strongly focused on the question of quantitatively predicting the effects of friction and rope stiffness in machinery than was the subsequently published paper, and omitted any discussion of the presence or role of asperities.

La Hire's study of friction

Amontons' paper was the second to be presented to the *Académie* on 19 December 1699. It was preceded by a paper by Philippe de la Hire, entitled '*Expériences et observations sur les corps qui frottent l'un contre l'autre*' (Experiments and observations on bodies that slide against each other). Although its main substance was included by Fontenelle in the *Histoire* (24) no quantitative data are provided in that summary, and this paper, the text of which is recorded in the minute book, was never published in the *Mémoires*. Nor was Fontenelle's piece on friction in the *Histoire* included in the English translation of 1742 (22).

Philippe de la Hire (1640 -1718) was considerably older than Amontons (59 years old compared with Amontons' 36) and a senior figure within the *Académie*, his membership being as a *pensionnaire* while Amontons had only recently been admitted as an *élève* (25). Although initially trained in the visual arts, by this time La Hire had had very wide practical experience in geometry, cartography and observational astronomy, and lived in the Paris Observatory. He made several contributions in mechanics (26) and in 1695 had published a comprehensive textbook on the subject (27). La Hire

has been described as 'an empirical and eclectic scientist who made a modest contribution to a broad range of subjects rather than to a narrow field of research' (25) and his interests were extremely diverse. His contributions to the *Académie* were certainly prolific: the *Mémoires* for 1699 alone include no fewer than seven papers, including reports of eclipses, notes on the optical properties of mirrors and experimental techniques relevant to telescopes, as well as a paper on the forces that could be exerted by humans in various ways.

On 19 December La Hire reported the results of the experiments on friction that he had initiated following Amontons' paper in June, which Fontanelle had recorded as having caused some astonishment to the members of the Académie (24). Details of his experiments are provided in the minute book (20,26). La Hire used several blocks of wood, well finished but not polished, and with surface areas in the proportions 1, 2, 3, 4, 5, 6, 7 and 8. He placed them on a well finished but unpolished wooden table, and loaded them all to provide the same normal load of 2¹/₄ livres. By using a weight attached to a string over a well-turned pulley with a small axle, he found that the load needed to cause the blocks to slide was in all cases 1³/₄ livres. He commented, perhaps unnecessarily, that the part of the string that was horizontal was parallel to the table. La Hire was a careful experimenter; indeed, he has been said to 'have been noted for meticulousness bordering on pedantry in his scientific research.' (25). La Hire's journal of astronomical observations for 1699, preserved in the Observatory (28), shows no record of any tribological experiments, but is testimony to his detailed observation and careful recording of measurements.

La Hire repeated these experiments with two flat but unpolished blocks of marble, with areas of 6 and 20 (square) *pouces* on a table of the same material, and both loaded to 4½ livres. He found that both started sliding at a force of 1 *livre* 5 *onces* (i.e. 1.31 *livres*). Adding water to the contact region made little difference to the friction force. La Hire then stated (20):

'These experiments are contrary to the common beliefs about the sliding of bodies against each other, since one had always believed that friction was in proportion to the areas touching, the load on the areas being equal, and that is how I reasoned in my treatise on mechanics. But M. Amontons having found in his experiment on the polishing of mirror glass that the friction increases in the ratio of the loads and not of the areas, as soon as I was notified of this I became convinced by physical reasoning, clarified by the experiments that I then made.'

La Hire went on to provide an explanation for these observations. He suggested that if the bodies in contact had soft, flexible regions (as in wood) one could consider them as tiny springs that would deform under the load, and that the deformation of each of these springs would be proportional to the load it carried, and independent of the total area of the bodies. Similar arguments would apply if the regions were hard and inelastic (as in marble): then the regions that engaged with each other would either rub against each other and become worn, or rise over each other as sliding occurred. In all these cases, he argued that the friction force would be independent of the apparent area of contact, and depend solely on the normal load.

Discussion

Many previous accounts have either failed to mention La Hire's contribution, or understated its importance in confirming Amontons' proposed laws and influencing Amontons' thinking. In some cases, even when La Hire's role has been mentioned the sequence of events has been described unclearly or in a misleading way. One reason for the confusion is that Fontanelle's account in the *Histoire* (24) provides meagre chronological information.

As discussed in the previous sections, the minute book of the Académie shows that both Amontons and La Hire regarded the former's paper on the moulin à feu, presented in June 1699, as including a definitive statement of the laws of friction: both referred to it in their papers read in December. Fontanelle's account (24) states that on hearing Amontons' paper in June, La Hire immediately carried out his own experiments, but this has been wrongly interpreted by some authors as occurring after the December paper. In fact, it is clear not only that La Hire's investigation took place between June and December 1699, but that at the December meeting he presented his own results to the Académie before Amontons' presented his paper. However, Amontons' priority in the discovery of the laws was in no doubt: the minutes describe him as 'M. Amontons who had first had occasion to examine this matter in detail', and in his own remarks La Hire explicitly acknowledged Amontons' role. La Hire freely admitted that his previous understanding of friction had been wrong; in his textbook on mechanics, for example, he had erroneously suggested that the friction of the axle of a pulley wheel could be reduced by reducing the area of contact with its housing (27).

As Figure 2 shows, the evidence on which Amontons based his statement in June 1699 that friction is independent of contact area was strong, but the evidence in Figure 3 of its proportionality with load was much less

convincing: his exploration of the effect of load involved the use of only two, marginally different loads of 28 and 30 *livres*. It is completely unclear how many values of load he investigated before presenting his December paper: only a single value is mentioned in his reports, and in any case his apparatus which used a bent spring to provide the load was probably not well suited to changing this variable. La Hire was helped by using weights to apply the normal load, and as far as can be judged, his experiments, while restricted to only two materials (wood and marble) under unlubricated conditions, seem to have been more systematic and certainly in the case of area to have explored a wider range of values.

Many writers have assumed that because in his December paper Amontons stated that he had found the force of friction in all cases to be close to one third of the normal load, he believed that to be true for all sliding conditions. That is emphatically not the case: the ratio F/N that he had himself measured for the polishing of glass was around 0.8 to 0.9, and he also stated clearly in the published version of the December paper (although this part is not found in the minutes) that the friction between a wooden beam and the ground was 'around $\frac{3}{4}$ of the weight' (4). He was also aware of La Hire's results, which gave ratios of 0.8 for his experiments with wood and 0.3 for marble. Amontons' value of about one third, as Dowson has also stressed (1), applied to the particular conditions of boundary lubrication with pork fat that he had investigated.

It is striking that there is no record in the minute book of any discussion by Amontons of the physical origins of friction at either of the meetings in December 1699 or February 1700. Nor is the topic mentioned in Fontenelle's summary of Amontons' work on friction in the *Histoire* (24): Fontenelle presents it solely as the work of La Hire. Amontons must have been aware of La Hire's ideas about the behaviour of what we would now call asperities from the December meeting, and then included very similar concepts in his published paper. It is therefore clear that La Hire should be credited with the first statement of these important ideas in the development of theories of friction, and not Amontons as has been suggested by many previous writers.

Conclusions

Guillaume Amontons' first statement of the laws of friction was made in his paper on a novel heat engine, presented at a meeting of the *Académie Royale des Sciences* in June 1699, rather than in the paper on friction of December 1699 that is usually cited. Amontons based his original statement

on measurements of the forces involved in the polishing of glass, which demonstrated convincingly that the friction force was independent of apparent contact area, but less persuasively that it was proportional to the normal load.

In his paper on friction Amontons re-stated his laws more explicitly, and described the use of the same unusual apparatus in which the normal load was applied with a spring, to study the grease-lubricated sliding of several combinations of materials more relevant to machine construction. Both Amontons and Philippe de la Hire, who had carried out his own independent measurements and reported them at the same meeting of the *Académie*, acknowledged the priority of Amontons' earlier work.

However, priority for the idea that the physical basis of the laws originated in the behaviour of small protuberances or asperities in contact should belong to Philippe de la Hire, who enunciated it before Amontons, and of whose work Amontons must have been aware.

References

- 1. Dowson D. History of Tribology. London: Longman; 1979.
- 2. Bowden FP, Tabor D. The Friction and Lubrication of Solids, Part 2. Oxford: Oxford University Press; 1964.
- Hutchings IM. Leonardo da Vinci's studies of friction. Wear. 2016 Aug;360– 361:51–66.
- Amontons G. De la resistance causée dans les machines, tant par les frottemens des parties qui les composent, que par la roideur des cordes qu'on y employe, et la manière de calculer l'un et l'autre. Hist Académie R Sci. 1699;mem. 206-227.
- 5. Schnurmann R. Amontons' Law, ``Traces'' of Frictional Contact, and Experiments on Adhesion. J Appl Phys. 1942;13(4):235–45.
- Kragelsky IV, Shchedrov VS. Razvitie nauki o trenii (Development of the science of friction). Moscow: Soviet Academy of Sciences; 1956.
- 7. Dowson D. Men of Tribology: 2 Guillaume Amontons; 3 John Theophilus Desaguliers. Trans ASME J Lubr Technol. 1978 Jan;100:2–5.
- Deresiewicz H. Amontons and Coulomb, friction's founding fathers. In: Approaches to modeling of friction and wear, eds FF Ling, CHT Pan. Columbia University, December 17–19, 1986: Springer-Verlag, New York; 1988. p. 56–60.
- Singer IL. Amontons' Rules of Friction Formulated 300 Years Ago. MRS Bull. 1999 Dec;24(12):52–52.
- Yoshitake T. Amontons' first experiment on friction looking back on 300 years of tribology. J Jpn Soc Tribol. 1999;44(2):111–4.

- 11. Zhuravlev VPh. On the history of the dry friction law. Mech Solids. 2013 Jul;48(4):364–9.
- Popova E, Popov VL. The research works of Coulomb and Amontons and generalized laws of friction. Friction. 2015;3(2):183–90.
- Desplanques Y. Amontons-Coulomb Friction Laws, A Review of the Original Manuscript. SAE Int J Mater Manuf. 2014;8(1):98–103.
- Blau PJ. Amontons' Laws of Friction. In: Wang QJ, Chung YW, editors. Encyclopedia of Tribology [Internet]. Springer International Publishing; 2013. Available from: https://doi.org/10.1007/978-0-387-92897-5_166
- Amontons G. Moyen de substituer commodement l'action du feu à la force des hommes et des chevaux. Hist Académie R Sci. 1699;mem. 112-126.
- Talbot GR, Pacey AJ. Antecedents of Thermodynamics in the Work of Guillaume Amontons. Centaurus. 1972 Mar;16(1):20–40.
- Fonteneau Y. Les antécédents du concept de travail mécanique chez Amontons, Parent et Daniel Bernoulli : de la qualité à la quantité (1699-1738). Dix-Huit Siècle. 2009;41(1):339–68.
- Diderot D. Glaces, Planche 42. In: Encyclopédie, ou Dictionnaire raisonné des sciences, des arts et des métiers: Planches. 1765.
- Diderot D. Verrerie. In: Encyclopédie, ou Dictionnaire raisonné des sciences, des arts et des métiers vol 17. 1765. p. 153.
- 20. Académie royale des sciences. Procès-verbaux T18 (12 novembre 1698 23 décembre 1699). Bibliothèque nationale de France; 1699.
- 21. Seguin MS. Fontenelle et l'Histoire de l'Académie royale des sciences. Dix-Huit Siècle. 2012;44(1):365–79.
- 22. Martyn J, Chambers E. The philosophical history and memoirs of the Royal Academy of Sciences at Paris. Vol. 1. 1742.
- 23. Académie royale des sciences. Procès-verbaux T19 (1700). Bibliothèque nationale de France; 1700.
- 24. Anon. (B. de Fontenelle). Sur les frottemens des machines. Hist Académie R Sci. 1699;hist. 104-109.
- Sturdy DJ. Science and social status. The members of the Académie des Sciences, 1666-1750. Woodbridge: Boydell Press; 1995.
- Schmit C. Philippe de La Hire, physicien : philosophie mécanique, mécanique rationnelle, mécanique appliquée. Arch Int Hist Sci. 2019 Jan;69(182–183):272– 351.
- 27. La Hire P. Traité de mécanique. Paris: Imprimerie Royale; 1695.
- La Hire P. Journal des observations faites à l'Observatoire de Paris, 4 janvier 1697 au 20 juillet 1704 [Internet]. Paris; Available from: https://bibnum.obspm.fr/ark:/11287/23FNc

A personal history of the pseudopotential

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This is a very personal history of development of the pseudopotential in the theory of the electronic structure of materials, from its inception up to the development and implementation of the CASTEP, CETEP and ONETEP computer codes.

Foreword

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In the second half of the twentieth century the world was transformed by the inventions of solid state physicists. The relentless march of semiconductor technology continues to this day. Up to about 1950 the subject had presented a hodgepodge of miscellaneous effects, with fragmentary understanding here and there. It must have discouraged many from choosing such an unpromising line of research; Hans Bethe was one who profited little by his early venture into it [1]. At the heart of many of its puzzles lay the key question: how are we to describe the quantum-mechanical energy levels of electrons in a solid? Since they generally consist of continuous bands rather than sharp levels, this became known as the problem of *band structure*. How are we to calculate it, describe it, interrogate it? For many it must have seemed a hopeless task: the quantum-mechanical description of a sea of interacting electrons moving in in a dense forest of ions. But there were important clues that pointed towards simplicity. In a few instances the limited success of a familiar but paradoxical description of the electrons as *free* particles gave hope.

A small number of optimists took this as their cue, and conceived theories of *nearly free* electrons, whose wave functions were to be manageable mixtures of plane waves outside the ion cores. Their "OPW Method" was to be transformed into the more transparent pseudopotential theory that is the subject of Volker Heine's personal account.

While the astonishing success of solid state physics was (at least in my opinion) mainly an experimental and technological triumph, it needed a sound and transparent theoretical underpinning, which pseudopotential theory provided for many purposes. Its story is an essential thread of that of modern physics, yet it has rarely been recounted. Its earliest history is briefly sketched (up to about 1950) in the compendious history of solid state physics, *Out of the Crystal Maze* [2]. What happened after that?

Heine was involved from the very beginning of the modern developments, mainly in association with Cohen, Phillips and other members of the Institute for the Study of Metals at the University of Chicago. The Institute was founded by Cyril Stanley Smith after WW2: it amply fulfilled his ambition as an exciting and informal research environment with an ever-widening perspective and a new title, the James Franck Institute.



Morrel H Cohen

James C Phillips

Marvin L Cohen

The Chicago Gang. Three academic generations (successive advisors) who contributed to the inception and application of pseudopotential theory in the late 1950s.

Back in Cambridge Heine found plenty of inspiration and challenge from experimentalists who were measuring, for example, the Fermi Surfaces of metals. Sabbaticals (surely one of the greatest inventions of academics) played a large role at the outset, in connecting with his American counterparts.

His involvement in the theory and applications of the pseudopotential continued for several decades, evolving from a creative and supervisory role to a more avuncular presence. In the article which follows he has recorded his view of the development of the pseudopotential, still ongoing as the twenty-first century advances.

It has been an honour and a pleasure for me to assist him in this, and to help to pay tribute to his collaborators.

1. Introduction

In the 1930s the new quantum theory was being applied to atoms and molecules for the first time, for example in explaining the bonding of the hydrogen molecule and the tetrahedral arrangement of the bonds of a carbon atom. The formalism of electronic band structure and Bloch wave functions was developed for crystalline solids, explaining for example how the electrons in a metal could behave rather freely as evidenced by conductivity and Hall effect, while not contributing very much to the specific heat.

But the details of energy band structure remained obscure. There were two extreme approaches to its description: the nearly-free-electron model and the tight binding model. In the book of Mott and Jones [3] the band structures of several metals were sketched from the point of view of the nearly-free-electron model. Even carbon (as diamond) seemed to conform to this picture. I remember asking Nevill Mott how people could have the temerity to use it for such a case. He replied: "We knew something from the soft x-ray spectra, already measured by Skinner". Indeed these showed that the band widths and band shapes were rather close to that of the free electron gas. *Why* that should be so remained a mystery.

2. Realistic calculations

Perhaps the first realistic band calculation is that of Herring and Hill from 1940 [4]. They invented the OPW (orthogonalised plane wave) method, in which the wave functions of electrons were built out of plane waves (the wave functions of free electrons), orthogonalised to the wave functions of the electrons in the core of each atom. Then Herman, around 1950, performed heroic pioneering calculations of the band structure of silicon and germanium with the same method [5]. His results were roughly consistent with the emerging experimental evidence.

In these OPW calculations, contributions to electron energies were found to largely cancel, so that the results were describable in terms of nearly-free-electron theory.

Such was the situation in 1954 when I arrived in Cambridge: I too adopted the OPW method, applying it to calculate the band structure of aluminium in connection with some experiments on the shape of the Fermi surface conducted in the Mond Laboratory, within the Cavendish Laboratory. My formulation and results improved upon previous work. An alternative "cellular" method was being tried in the group of Harry Jones in London: it seemed to have insurmountable problems.

The success of OPW calculations set the scene for the advent of the pseudopotential. It had antecedents in the work of Fermi and others, relating to scattering theory [6]. Its rapid development and application up to 1970 are contained in Volume 24 of Solid State Physics [7]. which will serve to fill in much of the technical detail that is absent below.

3. The idea of the pseudopotential

A little later, in Chicago JC Phillips and Len Kleinman [8] also undertook OPW calculations. For the first time, in talking about their work, they lumped the two energies (potential and kinetic) in the atomic core together into one quantity which they called the *pseudopotential*. Their pseudopotential was a *non-local* operator, but for many purposes this complication can be swept under the carpet, and a simple picture emerges from this change of perspective.

Morrel Cohen was quick to see the promise of this new perspective. He showed that the pseudopotential idea could be generalised. Travelling on the train from the General Electric Company research labs in Schenectady to Chicago, he and I quickly wrote a paper on this [9]. We rather grandiosely called it *The general theory of pseudopotentials*.

It was not very long before it was realised that yet more general forms could be adduced. One was particularly simple: it was formulated by a graduate student, Brian Austin, in our Cambridge group.

This work also gave us the Cancellation Theorem, helping us to understand the weakness of the pseudopotential, which implies that (pseudo)wavefunctions of energy eigenstates may be well represented as combinations of just a few plane waves.

4. Perturbation theory and screening

The pseudopotential is weak enough to enable perturbation theory to be used for a variety of purposes, including the inclusion of electron-electron interactions which "screen" the potential. It may also be used to compute the total energy of sp-bonded metals and compare these, as well as the frequencies of lattice vibrations. Morrel Cohen had already pointed out at an early stage that with a weak pseudopotential one should be able to describe many properties simply by using perturbation theory. Walter Harrison pioneered much of this development in the first handbook of pseudopotential applications [10]. covering a remarkable range of topics. His preface offers a snapshot of how things stood in 1966.

In the fullness of time, as we shall recount later, less approximate methods could be used, as computer power increased dramatically.

5. Better pseudopotentials

Another fresh idea opened the door to an even wider concept of the pseudopotential. It was realised that *any* potential may be considered to be a valid pseudopotential if it "gives the right answer"; that is, if it yields essentially the same results as a full calculation. This notion was already current in the St Petersburg (Leningrad) School, in relation to the theory of colour centres in ionic crystals. It was Igor Abarenkov that brought those ideas from Russia to the West as a post-doctoral visitor to Cambridge in the early Sixties. He used simple square well potentials (different for each angular momentum component) inside the core: the depth of the square well was adjusted to give the correct energy levels for a single atom, which could be looked up in tables derived from optical spectra. This was called a Model Potential. We used it to calculate Fermi Surfaces of metals

A graduate student from Nigeria, Alex Animalu, set up model potentials for 25 elements. They served in their original form for many useful calculations and were still occasionally employed in the 1980s.

Calculations with model potentials were found by Marvin Cohen (who came out of the Chicago school) to be in good agreement with experimentally measured optical spectra of silicon and a range of other semiconductors. There was even good agreement for the pseudopotential of indium metal as fitted to the spectra of the semiconductors such as InSb and to the Fermi surface of indium metal. All this was reassuring.

However it became clear by 1970 that the model potential was still in need of refinement. Bob Shaw showed how to remove energy dependence, leading to the inception of "norm-concerning" potentials, as developed by Don Hamann and others. This refinement became standard practice.

In the same period John Pendry, another Cambridge graduate student, developed a new perspective on the pseudopotential. It ran counter to the trend towards transparent simplicity that had produced the model potential.

6. Total energy

The pseudopotential concept has relevance to all types of atom, including transition and rare-earth elements as well as the sp-bonded elements, but it is for the latter that the idea made its greatest initial impact. Perturbation theory could be used to compare energies of different crystal structures. With the advent of the model potential, such calculations became even easier. Another early and transparent application was to the electrical resistivity of a molten metal. John Ziman showed that this gives good results for the molten alkali metals with the new model potential.

It also worked for polyvalent elements including aluminium. Denis Weaire and myself pursued the structures of simple metals (especially strange ones, as in Ga and Hg). Those early perturbative methods have since been superseded by less approximate ones, with ever-widening applications in materials science.

7. Density functional theory

Although electron-interactions could be incorporated in a very simple approximation by perturbation theory, there still remained serious questions concerning additional many-body effects, cheerfully swept under the carpet, or crudely modelled by pseudopotential practitioners.

The favourite formalism to deal with this was Density Functional Theory. Initially I was not an enthusiastic supporter of it. It seemed a rather crude approximation based on the theory of a free electron gas. However, the strength of DFT progressively emerged with experience, and it is now widely used.

Walter Kohn received the Nobel Prize in 1998 for the development of Density Functional Theory. Important contributions were made by Lou Sham, who began his career in Cambridge.

8. Towards computer experiments

At the end of the 1970s, the norm-conserving pseudopotentials, with the incorporation of Density Functional Theory, seemed to be yielding many correct results. Other ingredients were contributed by Richard Martin, another who was inspired by the "Chicago Gang" as a graduate student in the sixties. Eventually he was to write an excellent book on band theory and practical methods [11], another useful source of information omitted in the present sketch.

The stage was then set for what we may call computer experiments (large simulations), exploring the energy of crystal structures and other properties. For example, one can follow the path of a chemical reaction, such as that which occurs when the surface of a metal is corroded.

9. A spectacular breakthrough by Car and Parrinello

So far so good, though the calculations were quite laborious. Then in 1985 a short Physical Review Letter [12] from Roberto Car and Michaele Parrinello burst on the scene. Usually such a Letter introduces a single new idea, but this one offered three or four - no wonder we had difficulty understanding it! No new pseudopotentials were introduced, but rather ideas that made the computations much simpler and quicker.

Mike Payne in Cambridge was quick to code up the new method, developing his own code, later called CASTEP. This, and the Vienna code VASP, developed by Gerhard Kresse, became the leading workhorses of simulations across the world that used pseudopotentials and plane wave expansions.

After a few years, the UK Research Council(EPSRC) declined to fund its further development, in spite of its huge potential. The commercial scientific software company MSI developed the code further with Payne. Marketed commercially, it has been a great success. The downside of this arrangement is that the source code has not been freely available to academic researchers around the world.

10. Parallisation and achieving order N

Around 1992 the UK Research Council had bought the first massively parallel computer. Its use for high-energy particle physics was envisaged, but others were brought on board, to the extent of 25%. The development of the Car-Parrinello method was seen as a suitable large project for a concentrated effort, and duly approved. However its practical implementation on such a machine remained a challenge.

Some of us had tentatively discussed in general terms how one might parallelise electronic structure calculation, and it was not obvious. Now we were challenged. Payne solved the problem: one parallelises the problem by breaking up the wave function into its many separate Fourier components. The result was the CETEP code (Cambridge Electronic Total Energy Package). A dedicated CP consortium of physicists, chemists and materials scientists was created to carry the whole project forward as rapidly as possible.

There remained one serious challenge: the required computational time grew as the *cube* of the number of atoms in the simulation. This would inhibit applications to many real problems of scientific interest, including those related to biology.

Chemical bonding is a local affair, depending local configurations of atoms. How could one use this insight to invent a method for which the required computation time of a given task increases *linearly* with the number of atoms, that is, it is "of order N". This was achieved in the ONETEP code (Order N Electronic Total Energy Package), developed by Peter Haynes, Chris Skylaris, Arash Mostofi and Mike Payne in 2005. Using it, computer simulations involving a few thousand atoms are now carried out, extending even to biological systems.

11. Cooperation and the Psi-k European Network

When we had started advanced total energy calculations and computer simulations in Cambridge around 1982, they made great demands upon us. We now had our own inhouse computer to manage and maintain. The greatest demand was that of the expert manpower needed for the research. We had just one junior staff member, Richard Needs. In all of Europe, there were about five other young people who had brought this new field of research across the Atlantic from USA. We had a meeting together at the end of a conference, during which I said to them "You don't have a hope in hell of matching successfully the work of two or three established groups in USA, as individual young researchers with little support." As Nevill Mott once said, "In basic research, second-class work is almost not worth doing."

So I called for collaboration, and it soon began to take shape. For example, beginning in 1983 we held a workshop each winter to discuss the latest ideas and developments and experience from around the world. We shared computer codes, developed collaborations, and exchanged students and postdocs.

Around 1978 the Research Council had bought a Cray 1S supercomputer. It was the first such machine available to academic users anywhere in Europe. In order to make good use of this expensive piece of new equipment, the Research Council set up a series of Collaborative Computational Projects (CCP's). Ours was CCP-9. It linked theoreticians and experimentalists with each other, spreading the use of computing and computer simulation through the scientific community. It trained new young graduate students, developed new codes, and generally stimulated collaboration through workshops and tutorials.

CCP-9 was extremely successful, and had a European outlook from the beginning, perhaps due in part to its instigators, with such names as Temmerman, Szotek, Gyorffy and Heine! In 1992 the European Union began funding research networks.. Together with our collaborators we used one to spread and expand our ideas throughout Europe.

The mission of our network, Psi-k, was threefold. First came excellence in science through cooperation and sharing, rather than the pursuit of national prestige or money or competitiveness. The second commitment was to try to serve the needs of all researchers in our field, across all of Europe, not just the big players. Our calculations are often done by one researcher at one computer, so that individual practitioners can spring up in small universities or research institutes anywhere. Many of us could remember that when we started out in the research field of electronic structure of solids, we were rather isolated. Thirdly, we wanted to help graduate students and young researchers enter the field. We drew them in from countries and universities where opportunities for our kind of research did not exist.

As well as workshops to share ideas and codes, there were Working Groups for collaboration on simulations in different areas of science. An expanded number of Summer Schools covered everything from introduction to electronic structure of solids to training in the use of specific codes. CCP-9 had already started a Newsletter, eventually issued monthly.

Every five years we gather together for a meeting: in 2010 in Berlin about twelve hundred of us were there. And, after more than half a century, this story continues....

REFERENCES

[1] H Bethe, "Energy on Earth and in the Stars" *in* "From a Life in Physics", World Scientific, 1-18 (1989).

[2] L Hoddeson, E Braun, J Teichmann, W S Weart, "Out of the Crystal Maze", Oxford University Press (1992).

[3] N F Mott and H Jones, "The Theory of the Properties of Metals and Alloys". Oxford University Press, ACS publications (1937).

[4] W C Herring, "A new method for calculating wave functions in crystals", *Phys Rev* 57, 1169-1177 (1940).

[5] F Herman, "Theoretical investigation of the energy band structure of solids", *Rev Mod Phys*, **30**, 102-122 (1958).

[6] E Fermi, "Displacement by pressure of the high lines of the spectral series". *Nuovo Cimento* **11**, 157 (1934).

[7] "Solid State Physics", eds F. Seitz, D Turnbull and H Ehrenreich 24, (1970).

[8] J C Phillips and L Kleinman, "New Method for calculating wave functions in crystals and molecules", *Phys Rev* **116**, 287-294 (1959).

[9] M H Cohen and V Heine, "Cancelation of kinetic and potential energy in atoms, molecules and solids", *Phys Rev*, **122**, 1821-1826, (1961).

[10] W Harrison, "Pseudopotentials in the theory of metals", Benjamin (1966).

[11] R M Martin, "Electronic Structure: Basic theory and Practical Methods", Cambridge University Press (2020).

[12] R Car, M Parrinello, "Unified Approach for Molecular Dynamics and Density-Functional Theory", Physical Review Letters 55, 2471-2474 (1985).

From bombs to bubbles: the extraordinary career of Cyril Stanley Smith

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Smith meets Oppenheimer

The excellent movie "Oppenheimer", recently released, understandably places nuclear physicists front-and-centre in its story. But at one stage Oppie explains to his colleagues that the Manhattan Project depends on much more than their theories. Engineering, metallurgy and chemistry were to play essential roles. Of these the last was particularly challenging. A primary task was to determine the properties of Plutonium, of which practically nothing was known. Furthermore, adequate samples for lab work would be some time in coming...

The man entrusted with leadership of the crucial metallurgy programme was Cyril Stanley Smith. In time of war, talent trumps all else, so that his non-American origins (in Birmingham) did not matter. (One is reminded of Klaus Fuchs, recommended to the Americans by Nevill Mott, a less fortunate recruitment!). Smith had established a fine record as a research metallurgist in industry, before joining the war effort in administration. Sitting with Oppie on a park bench he was persuaded to go to Los Alamos.

Plutonium is radioactive and highly reactive chemically: it required extraordinary dedication for Smith's team to succeed in good time. It seems they had no qualms about the eventual purpose of their work, being carried along by magnitude of the challenge to their abilities.

The rest is history, but not very well recorded. Despite its substantial length "The Making of the Atomic Bomb" [1] barely mentions Smith and his team, yet he was the very last person to lay hands on the Plutonium bomb (making an improvised last-minute repair.)

Chicago

After the war, his career his career took another turn, as he became an academic, founding and directing the Institute for the Study of Metals at the University of Chicago. It looked out on Moore's impressive piece, commemorating Fermi's achievement of a chain reaction in the tennis courts. He saw his new institute as a counterweight to the neglect of his subject by the universities, and the "aloofness of physicists".

I had the privilege and pleasure of being at the Institute for a year in the mid-Sixties, when it comprised many leading solid state physicists. I enjoyed its inclusive

collegiate atmosphere: Smith had drawn inspiration from the mutual support and teamwork that characterised the work of his Los Alamos metallurgists.

Personally I regret that the Institute was listed as such only until 1967, when it was renamed as the James Franck Institute - not dissimilar in spirit but with a much wider remit. Did the aloofness of physicists win out?

A final move

By then Smith had undergone his last migration/transformation, to MIT. His interests steadily grew wider, taking in history, philosophy and art, all drawing inspiration from his metallurgical insights. Eventually he summed all this up in his book "A Search for Structure" [2], consisting of his relevant published papers, with detailed notes. A recurrent theme was the disordered nature of many materials, and their history-dependence. He chided the solid state physicists for their obsession with very pure and perfect materials. No doubt this fell on deaf ears, as crystalline silicon played its central role in the emergence of semiconductor technology, as it does today.

Most materials, he insisted, are funeous, a word that he introduced. A character called Funes in a Borges short story sadly lost the ability to forget! Material objects are the products of their individual history, not just of their composition, and do not forget the past.

Perhaps some of his grander ideas were tenuous or tentative, but one elementary paper was transparent and intriguing, at least to me.

The 2D soap froth



Fig 1 Cyril Stanley Smith and his 2D soap froth.

In the book's first paper, Smith gives pride of place to a very simple system that could be used to illustrate some of his principles. His 2d soap froth is not the bubble raft of Bragg - rather it is a bubble sandwich between two glass plates. It was taken up by E N da C Andrade, of the Royal Institution.

In a somewhat tangled tale of misleading error, I was drawn into study of foam coarsening (the growth of average bubble size with time, involving sudden local topological changes). Paul Kermode and I developed a computer simulation for this phenomenon, closely analogous to grain growth in metals. Smith did have a weak spot: like many of his generation. He could not see the coming impact of large computers in simulating the kind of systems that interested him. He urged me to concentrate more on experiments, which turned out to be good advice, anyway. For me this was the inception of several decades of research in a field that has expanded to the present day, in a group now led by Stefan Hutzler.



Smith died at the age of 88. Eventually his grandson, Stuart Denman, has become interested in his work, and he is busy exploring odd corners of it. Being a software expert, he developed a computer game based on the 2d soap froth, which was successfully commercialised (Fig 2).

Smith's soap froth.

Fig 2 Denman's computer game based around

Perhaps the title that Smith would have most appreciated was philomorph (lover of form) – he was indeed a member of the Society of Philomorphs in Cambridge, Mass. No doubt he is well remembered there: Birmingham should be proud of him too.

References

- 1 Richard Rhodes, The making of the Atomic Bomb, Simon and Schuster, New York, 1986
- 2 C S Smith, A Search for Structure, MIT Press, 1983

The Birth, Life and Death of the Bohr Atom

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The Bohr atom¹ deservedly plays a major part in the history of quantum theory. The physics community considered it an enormous achievement and it was developed during the next few years to explain many features of atomic physics. Even those who found the ideas difficult to grasp had to admit to its exceptional empirical success. Einstein described it as 'a miracle' and 'one of the greatest discoveries', and Bohr was justifiably awarded the Nobel Prize for Physics in 1922.

Yet the Bohr atom was very much a shooting star. Conceived in 1913, ten years later it was very clearly on its last legs, its many successes being more and more overshadowed by a range of problems which appeared to be terminal. The question asked here is why its lifetime was so short and what lasting gains the Bohr atom left us.

Background

Niels Bohr was born in 1885 in a strongly academic background, his father, Christian Bohr, being Professor of Physiology at the University of Copenhagen. This was helpful for Niels as he understood how the academic system worked, and it also gave him good contacts. He studied physics, and rather remarkably, while he was still a student, based on a student project he published two papers on surface tension in Royal Society journals, one experimental in the *Philosophical Transactions* and the other theoretical in the *Proceedings*.

For his doctorate, his thesis was a critical examination of the current state of the electron theory of metals. It dealt extremely thoroughly with what was understood at the time, also making clear what aspects of the theory were totally unsatisfactory and would only be explained later when quantum theory emerged. Bohr made great efforts over several years for an English translation of this to be published, sending around 250 copies to every known physicist but without success. The problem may have been that the translator was much better at English than at physics.

Cambridge, Manchester and the Crucial Elements of Bohr's Theory

In 1911, on a grant from the Carlsberg Foundation, Bohr travelled to Cambridge, where he hoped to convince J.J. Thomson of some of the problems in Thomson's theory of electronic conduction, but unsurprisingly without much success.

Fortunately he obtained an introduction to Ernest Rutherford, then in Manchester. Rutherford was, of course, recognised as an exceptionally important scientist, having been awarded the Nobel Prize for Chemistry in 1908 for his discoveries in on radioactivity. Nevertheless his demonstration of the nuclear atom had not been generally acknowledged very positively until Bohr's work, and it might be said that he gained as much from Bohr as Bohr gained from him in the creation of the Rutherford-Bohr atom (as it was often called at the time).

During this time, Bohr became certain that a model of the atom must be based on Rutherford's idea of the nucleus, but he added one or more rings of electrons surrounding the nucleus, and he argued that as electrons were added to a particular ring, the addition of a further electron might make the ring mechanically (not electromagnetically) unstable, and so this electron would have to commence a new ring. Bohr suggested that thus the properties of the atom would largely depend on number of electrons in the outermost ring, and so this was a primitive explanation of the Periodic Table, properties of the atoms changing systematically as the number of electrons in the outermost ring increased. Rutherford's nucleus was the first crucial element that led to Bohr's great theory.

A second equally important element was the importance of the quantum theory, at least in a general form using a simple equation broadly analogous to Planck's fundamental law. Bohr's ideas would become much firmer in the crucial trilogy of papers published in 1913.

While in Manchester he had extremely useful discussions with Rutherford, who gave him great support. In these early days of his career Bohr prepared a document for him with many interesting suggestions concerning the nuclear atom but nothing very concrete. Throughout his career, Rutherford was always extremely and positive towards Bohr, though sometimes dubious about some of the ideas.

Back in Copenhagen, the last crucial element in Bohr's seminal work emerged in February 1913. This was his discovering (or remembering) Balmer's formula for the wavelengths of the lines in the visible of the hydrogen spectrum. Writing this in terms of frequency we obtain

$$v = cR\left(\frac{1}{2^2} - \frac{1}{n^2}\right), \ n = 3, 4...$$

where c is the speed of light and R is the Rydberg constant.

We may generalise this result, using the ideas of Ritz and Rydberg, by including lines in the infra-red and the ultra-violet, and also by allowing the nucleus to have a charge of Z rather than 1 for hydrogen. There must still be only one electron so, for example, Z = 2 corresponds to He⁺ and Z = 3 to Li⁺⁺. We then obtain:

$$v_{n} = Z^{2} cR \left(\frac{1}{m^{2}} - \frac{1}{n^{2}}\right) m = 1, 2, 3 ...; n = m + 1, m + 2 ...$$

(Some lines in the Paschen, with m = 3 had been discovered earlier, for which see later.)

According to Bohr's memory a good deal later, he immediately recognised that this formula could be regarded as the difference between two energies. The resulting paper, the first of his trilogy, was dispatched in April.

John Nicholson

Meanwhile he had been somewhat concerned by noticing a series of papers by John W. Nicholson published in the *Monthly Notices of the Royal Astronomical Society*. The first was written in 1910 and they were to continue until 1914. They contained some ideas and techniques quite similar to those Bohr was planning to use.

Nicholson was four years older than Bohr. He had been a Lecturer at the Cavendish and later at Queen's University Belfast, and in 1912 he had been appointed Professor of Mathematics at King's College London. He was extremely well regarded, having published several excellent papers and being awarded the Adams Prize in 1912. He was to receive it again in 1918, and he became a Fellow of the Royal Society in 1917.

Quote differently from those of Bohr, Nicholson's atoms were based on astronomical ideas. Like Bohr's they were nuclear in nature, though they were not connected directly with the ideas of Rutherford. His model, rather like Bohr's, involved electrons descending to the nucleus. Like Bohr he took quantum ideas on board and made use of Planck's constant, *h*. Also, and this was to become interesting later, he showed that the angular momentum of an atom could only change by integral multiples of $h/2\pi$.

Nicholson's theory contained four 'proto-elements', the smallest having a nuclear charge of 2*e*, and he compared the ratios between frequencies of the various spectral lines to those of the vibration of his models, with a good deal of success. He was able to explain the positions of some lines and predict others.

Naturally Bohr was concerned that there might be overlap with his own work, though he concluded that it could be that the two theories were complementary; while his work dealt with emission of radiation, Nicholson's dealt with its scattering.

The Famous Trilogy

Now, with the use of the crucial elements mentioned above, Bohr wrote his great trilogy, *On the Constitution of Atoms and Molecules*, the papers being sent by Bohr to Rutherford to forward to the *Philosophical Magazine*. The first paper of the trilogy was sent to Rutherford in March 1913, He replied to Bohr suggesting that the paper was a little verbose and that he was sure Bohr would not mind him cutting it down a little. However Bohr did mind very much and he travelled to Manchester to make sure that the paper was published just as Bohr had written it. It was finally published in July. (The second and third papers contained mainly applications of the ideas in the first.)

Bohr included the crucial proof in the first paper of his trilogy, and rather unusually he presented three methods of obtaining his main result, the first admittedly being remarkably unconvincing.

Method 1

In this proof he considers an electron rotating round a nucleus. He ignores, for the moment, radiation, and he expresses the frequency of revolution and the radius of the orbit in terms of W, the energy required to take the electron an infinite distance from the nucleus, and also the mass and charge of the electron. He then points out that the kinetic energy of the electron in its orbit is also equal to W. (The potential energy is - 2W so the total energy is equal to -W.) We obtain:

$$\omega = \frac{2^{1/2}}{\pi} \frac{W^{3/2}}{e^2 m^{1/2}} \qquad a = \frac{e^2}{2W}$$

Including radiation, one would expect the electron to spiral into the nucleus gaining in energy emitting a steadily increasing frequency of radiation. Clearly this does not happen. Instead, following Planck, Bohr suggests that, as the electron moves from its orbit to infinity, radiation is emitted at frequency v, the energy being *nhv*.

Obviously the value of v is now crucial, and Bohr assumes that v is equal to $\omega/2$, where ω is the frequency of revolution of the electron in its final state. Bohr does not make the reason for this choice at all clear, though it may be that there is an averaging between initial and final states of the movement of the electron. Thus Bohr assumes that the amount of energy emitted in the process is equal to $nh\omega/2$. (Initially Bohr assumed that this corresponds to *n* individual emissions of energy $h\omega/2$, and only subsequently he realised that he needs a single emission at frequency $nh\omega/2$.)

We then obtain:

$$W = \frac{2\pi^2 m e^4}{n^2 h^2}; \quad a = \frac{n^2 h^2}{4\pi^2 m e^2}$$

So n = 1, gives the lowest energy and smallest radius:

Ground state energy = -13.6 eV

Bohr radius = $5.3 \times 10^{-9} \text{ eV}$

both in good agreement with experiment. This is a remarkable success.

The difference in energy then leads to the frequencies of the lines of the spectrum, in agreement with experiment and Bohr obtains a value for the Rydberg constant:

$$R = \frac{2\pi^2 m e^4}{h^3 c} = 1.09 \text{ x } 10^5 \text{ cm}^{-1}$$

also in good agreement with experiment.

Thus the choice $v = \omega/2$, whatever its merits, has the great virtue of leading to the right answers!

At this point in the paper, Bohr gives a fair account of Nicholson's ideas. He makes a number of criticisms, pointing out that a system in which the energy is decaying cannot, as Nicholson suggests give off homogeneous radiation, remarking also that Nicholson's model cannot produce the Rydberg expression, and that, according to Nicholson's own rules, his systems must be unstable for some of his modes of vibration.

However, as already mentioned, he did say that these problems might occur because Nicholson is dealing with scattering rather than emission, and it may be mentioned that in the whole paper, Nicholson's name is mentioned twelve times.

Method 2

This first proof was fragile at best, the main positive, as we said, being that it gave the right answer. Kragh called it 'ad hoc' and even Bohr must have been unhappy, since he added second proof, which uses what we would now call the correspondence principle. This is highly significant because this principle was absolutely central for all his work on quantum theory right up till 1925 and even beyond.

Here, instead of $nh\omega/2$, he takes W to be $f(n)h\omega$ and from the form of the Balmer series it is clear that f(n) must be proportional to n and so writes it as kn, with k a constant. (Thus for the first proof k is equal to $\frac{1}{2}$.)

He now considers a transition between two values of n, N and N-1, where N is extremely large.

The frequencies of the radiation for a transition between states with quantum numbers N and N - 1 will be

$$\nu = \frac{\pi^2 m e^4}{2h^3 k^2} \left\{ \frac{1}{N-1^2} - \frac{1}{N^2} \right\} = \frac{\pi^2 m e^4}{2h^2 k^2} \left\{ \frac{N^2 - (N-1)^2}{N^2 (N-1)^2} \right\} = \frac{\pi^2 m e^4}{k^2 h^3 N^3}$$

Meanwhile the frequency of revolution of the electron its orbit (N or N - 1) is

$$\omega = \frac{\pi^2 m e^4}{2k^3 h^3 N^3}$$

Since, according to the correspondence principle, these should be the same for large N we see (from denominators) $k^2 = 2k^3$ so $k = \frac{1}{2}$ which agrees with the 'ad hoc' result.

The Correspondence Principle

We will now say a few general remarks about the correspondence principle, centred around two remarks. The first is by Arnold Sommerfeld, who played a massive role building up the Bohr model, so he was a fellow-worker with Bohr, but also, in some sense, a competitor. He said that the principle was a 'magic wand that did not act outside Copenhagen'. Clearly he was somewhat frustrated that the same results he was able to produce by good hard genuine physics could, it seemed, be pulled more or less out of thin air by Bohr via the correspondence principle.

We may ask - what, in fact is the principle? Léon Rosenfeld, who was Bohr's closest supporter, almost an acolyte, suggested to Bohr that the principle recognises that the results of classical and quantum mechanics should converge as h or hv tend to zero. This is indeed how the principle is very often described and used today. But Bohr denied that this was the principle. Rather, he said, it was an obvious requirement of the theory. (Rosenfeld actually was not totally convinced.)

Bohr often used the principle in the way we have already seen, relating frequencies of radiation between arbitrarily close states to the classical frequency. However it does not seem that there was a general definition of the principle, either by Bohr or by anybody else.

A more useful approach to the principle may be found in Bartel Van der Waerden's introduction to his *Sources of Quantum Mechanics*². He describes the research work between 1919 and 1925 that led to the discovery of quantum mechanics as 'systematic guessing, guided by the principle of correspondence'. This remark perhaps gives a useful idea of the principle in practice, providing hints and suggestions to help the creative work forward.

Max Jammer³ goes a little further: 'There was rarely in the history a comprehensive theory which owed so much to one principle as quantum mechanics owed to Bohr's correspondence principle.'

One further point about the principle, stressed by Bohr in particular, is that it definitely does not state that the difference between the *quantum description* of the phenomena in the appropriate limit and those of the classical case tend to zero, only *the statistical results*.

Method 3

We now return to Bohr's description of his third method of obtaining his result. This is broadly the method that is used in textbooks today, starting with the angular momentum being a multiple of $h/2\pi$. This method is well-known, and we will not discuss it here, but it should not be forgotten that Nicholson had previously used this expression for angular momentum – Nicholson certainly didn't forget it!

Bohr stressed as the central point of the theory was that it was a strange mixture (perhaps unholy mixture) of classical ideas and quantum ideas. The whole idea of quantum jumps was so much opposed to classical ideas that it could only conceivably be justified by its empirical success.

Initial Reactions

Slowly but steadily Bohr and his theory attracted attention. It certainly helped that his appearance and personality were attractive – somewhat later Sommerfeld was to write 'Bohr is just like Einstein only better washed and much neater.'

The novelty of his idea meant that there could have been a risk that he might have been dismissed as a crank, but his general bearing and obvious clear understanding of physics made this impossible. Max Born said that 'All this is queer and incredible but the Danish physicist looks so like an original genius that I cannot deny that there must be something in it.'

On the actual theory, one extremely positive point was the agreement with experiment, though Carlo Runge, for example, suggested that Bohr's achievement might be just a set of rules with no reference to actual atoms. He was among a number of physicists who dismissed the ideas as nonsense. For some, particularly those of the older generation, the novelty of the new ideas was just too much to take. Rayleigh, for example, said they were no use to him. He did not deny that they could be useful to others, but just not for him.

A good number of physicists, though, were prepared to follow Bohr, partially or totally, strange as the theory appeared. However many naturally brought up concerns. For many, the main defect of the Bohr model was exactly the point he stressed as its central feature, the combination of classical and quantum ideas. Although Rutherford was generally very much in favour of Bohr's ideas, of course, this was an aspect of him that perturbed him. Wilhelm Wien, winner of the Nobel Prize for Physics in 1911, for example, and many others, criticised the theory merely for its disobedience of classical electromagnetism.

There were also many more specific criticisms of the theory. J.J. Thomson, among others, complained that the frequency of the radiated emission was not that of any frequency, rotation or vibration, of the atom. This went so much against longstanding successful physical theory that it was unsurprising it was a stumbling block to the acceptance of the theory. Interestingly, in contrast Einstein regarded this as one of the most positive points of the theory, perhaps because he realised that major breaks with the past would be required,

Rutherford, again with others, also perceived another difficulty in the theory. Suppose, it might be said, the electron 'intends' to pass from state A to state B. It must commence to vibrate at the appropriate frequency $\frac{E_A - E_B}{h}$. Suppose, though, it 'decides' to bypass state B and move to state C. Clearly it would be vibrating at the wrong frequency. To put it another way, as Rutherford did, one must assume that the electron 'knows' beforehand where it is going to stop. (Many of these objectors did, as implied above, broadly assume teleology, with the electron deciding what path it may take.)

Bohr did not argue with these arguments. His general response to such objections was to agree that there was a problem, but suggest that it would be solved in future workings of the theory; ideas were "preliminary and hypothetical". If asked to explain his ideas, he replied that there was no "explanation".' Within a very few years, it would become clear that, sensible as these objections were, in fact they would be seen as inappropriate or irrelevant.

Nicholson Again

Bohr could not ignore the ideas of Nicholson. In fact, for a few years the two theories, those of Bohr and of Nicholson appeared to be of roughly equal standing. Nicholson criticised Bohr's model, a major complaint being its undeniable failure with helium. Bohr largely ignored that of Nicholson, though he occasionally picked up on a particular point with which he disagreed, in particular the problems he raised in his great paper.

It appeared that some physicists favoured one theory, some the other. For example, in 1915 John Stanley Plaskett felt that 'The question between Nicholson and Bohr cannot be regarded as settled, although Nicholson appears to have the last word.' Many of those who supported Nicholson did so *because* it used solely classical mechanics and simple quantum theory, in contrast to Bohr's quantum jumps. In retrospect, of course, it could be said that this was precisely the reason to favour Bohr.

Yet within a few years of the birth of the Bohr model, it became clear that very little support for Nicholson remained. Bohr's model was achieving success after success while, even when Nicholson attempted to improve his own model, it actually became less convincing. This was obviously extremely discouraging for him, but he still thought that, even though his own model had proved unsuccessful, he should have received more recognition for his contribution to that of Bohr.

He became a Fellow of Balliol College Oxford in 1919, and the summary report on mathematics fellows of Balliol over the years⁴, <u>Mathematics at Balliol: modern</u> (ox.ac.uk), presents his view that Bohr coupled the ideas of Rutherford and Nicholson. However this account was not generally accepted, and Nicholson became extremely depressed. The summary reports an over indulgence in the college wine-cellar, and, from 1930, an inability to perform his tutorial duties. He spent the last twenty-five years of his life in a mental institution.

Initial Progress

Over the next few years, progress was made on the basic structure of the Bohr theory. With

$$v = Z^2 cR\left(\frac{1}{m^2} - \frac{1}{n^2}\right), n = m + 1, m + 2 \dots$$

Series were found with

$$Z = 1$$

| Lyman | (Theodore), | 1914 | m = 1 | UV |
|----------|---------------|------|--------------|----|
| Paschen | (Friedrich }. | 1908 | <i>m</i> = 3 | IR |
| Brackett | (Frederick), | 1922 | m = 4 | IR |
| Pfund | (August,), | 1924 | m = 5 | IR |

| Z = 2 | Pickering (Edward)-Fowler (Alfred) | 1896, 1912 | $\mathrm{He^{+}}$ |
|-------|---------------------------------------|------------|-------------------|
| Z = 3 | (theoretical ideas - Nicholson, Bohr) | 1913 | Li ⁺⁺ |

For the Z = 3 series, Nicholson had speculated that Z was equal to 1, and quantum numbers were 'thirds' e.g 5/3. It was Bohr who pointed out that Z must be equal to 3, and quantum numbers were integers.

Criticism had been made that, especially as Z increased, it became clear that there were systematic discrepancies between the theoretical values and those found experimentally. Bohr showed that one should take into account the finite mass of the nucleus, Then with m and M the mass of electron and nucleus respectively, one should use the reduced mass μ where

$$\mu = \frac{mM}{m+M} = m \left(\frac{1}{1+\frac{m}{M}}\right)$$

When this is done, theory and experiment agree within experimental error.

Experimental Support

Soon after Bohr's theory there were two experimental discoveries strongly supporting his work

(Henry) Moseley and characteristic X-rays, 1913

Moseley (Figure 2) studied frequencies of X-rays emitted from targets made of the great majority of elements; a graph of $\sqrt{E_x}$ against atomic number showed K, L, M series. (Fig. 1).

For the K series, an electron dropped from a higher level to a hole in the n = 1 state, so the energy produced an X-ray

For $n = 2 \rightarrow n = 1$ K_{α} $n = 3 \rightarrow n = 1$ K_{β}

For the L series, the initial hole is in the n = 2 level.

For the M series it is in the n = 3 level

Moseley' work led to clarification of the idea of atomic number and showed gaps in the Periodic Table and places where re-ordering was required.

Most important here is that it agreed with Bohr's theory



Figure 1



It was expected that Moseley would be awarded for the Nobel Prize for Chemistry for 1915, but apparently the decision was to delay the prize because the work was so recent. Sadly he died at Gallipoli in 1915. It has even been suggested that in the very special circumstances the rule night be broken and the prize be awarded posthumously, but this idea was not accepted.

Figure 2 Photograph of Moseley in uniform, 1915.

Franck-Hertz experiment



Figure 3

The second important experiment supporting Bohr was performed by James Franck and Gustav Hertz in 1914. In this experiment mercury was bombarded with electrons of increasing energy. We explain Figure 3 by realising that 4.86 volts corresponds to transition from the ground state to excited state thus removing electrons from the current. The experiment is clearly in agreement with the Bohr theory. Franck and Hertz were awarded the Nobel Prize for Physics in 1925.

Bohr-Sommerfeld Theory

The first important development of the Bohr theory came from Arnold Sommerfeld and led to the famous Bohr-Sommerfeld theory

As Sommerfeld pointed out, the limitation of the Bohr theory was that it had only one coordinate: r.

He introduced a general momentum $\int p_i dq_i = n_i h$ Then for radial momentum: $\int p_r dq_r = n'h$ For ngular momentum $\oint p_{\varphi} dq_{\varphi} = kh$ Then we use n = n' + k; n = 1, 2, 3...; k = 1, 2..., nFor our usual l, l = k - 1

The energy is independent of the value of k The orbit is an ellipse with $\frac{b}{a} = \frac{k}{n}$

With n = 4



Figure 4

It has been suggested that there might be 'pendulum orbit' with k = 0, but this disagrees with the calculations and also goes straight through the nucleus.

Sommerfeld also introduced a third quantum number which implied that only certain orientations of the orbit were allowed with respect to an applied magnetic field.

$$\oint p_{\psi} \, d\psi = mh$$

where *m* may take on one of 2k + 1 values between -k and *k*

m denotes the orientation of the orbit relative to the direction of the field

The energy is independent of the value of k (as it must be as these are different orientations of the same system)

For a given Bohr transition there will be several possibilities for values of k at each level.

For example for the transition n = 3 to n = 2 there will be $3 \ge 2 = 6$ components

Sommerfeld realised that there would be selection rules. Discussion of these is where some of the disagreement between him and Bohr on methods arose. As well as allowed frequencies, one needs to know the polarisation and intensities of the various permitted lines and this development produced the famous Bohr-Sommerfeld atom

Hydrogen fine structure

In 1887, Michaelson and Morley, showed that the hydrogen lines were doublets

Sommerfeld used special relativity to create a picture of a precessing ellipse, with the electron rotating either with the precession or against it thus producing a doublet.

Sommerfeld's formula was $W(n,k) = E_{Bohr} \{1 + \frac{\alpha^2 Z^2}{n^2} (\frac{n}{k} - \frac{3}{4})\}$ where $\alpha = \frac{2\pi e^2}{hc} = \frac{1}{137}$ is the fine-structure constant

For a period, the Bohr-Sommerfeld atom was looked on as the most perfect of theories

But in 1925, a transition discovered by Gerhard Hansen that disobeyed Sommerfeld selection rule, and there were a few other problems. It seemed that, rather strangely, the Bohr-Sommerfeld theory was extremely near to being absolutely correct but not quite.

Stark effect

The effect was discovered by Johannes Stark in November 1913. (He won the Nobel Prize for Physics for 1919). It said that lines of hydrogen Balmer series and helium lines were split by electric field into several components with the splitting proportional to the magnitude of field.

An explanation of the effect using Bohr theory was provided by Karl Schwarzschild and by Paul Epstein in 1916.

Bohr's work supported Stark and Stark's work supported Bohr, and yet they intensely disliked each other, at least in part because Stark had his own model of the atom, very different from that of Bohr and totally unsuccessful. This dislike became much stronger when Stark become Hitler's most important supporter on physics matters.

Normal Zeeman effect

The normal Zeeman effect was discovered by Pieter Zeeman in 1896. (He won the Nobel Prize for Physics in 1902) In this effect, under a magnetic field, lines split into triplets, the splitting being proportional to the size of the field. An explanation using

classical physics was given by Hendrik Lorentz who shared the 1902 Nobel Prize with Zeeman. An explanation using Bohr theory was given by Sommerfeld and Epstein in 1916

Anomalous Zeeman effect

This effect was discovered by Thomas Preston in 1897. Here the pattern is not a triplet. [Really the words 'normal' and 'anomalous' should not be used. There is just one effect and for some cases the pattern is the 'normal' triplet.]

Preston is not very well-known. He lived from 1860-1900 and was Professor of Physics at University College Dublin (UCD). The UCD website suggests that if he had lived, he might have shared the 1902 Nobel Prize with Lorents and Zeeman.

The anomalous Zeeman effect could not be explained by Bohr theory, and this was a massive blow to the its prestige.

Paschen- Back effect, 1912

Paschen and Ernst Back showed that at high fields, all cases change to the triplet pattern.

This again could not be explained for hydrogen by Bohr theory

Trouble shooting

It cannot be exaggerated how much effort was made between roughly 1914 and 1924 to clear up the remaining difficulties of the theory by the most powerful physicists in the world including Bohr, Kramers, and the young Pauli and Heisenberg between roughly 1914 and 1924 using many old and new weapons. Many different versions of the correspondence principle were used. There were major differences of opinion on the whether use of half-integral quantum numbers was permissible, Bohr being very slow to accept these, Heisenberg and Pauli much faster. Heisenberg promoted a core model in which the core of the atom and the valence electron shared a quantum half each. Expressions such as $\sqrt{j(j+1)}$ were also used. Success was extremely limited.

There is a story that when a friend met Pauli at this time, he commented that Pauli did not look happy and Pauli replied– 'How can one be happy when he is thinking about the anomalous Zeeman effect?'

Gradually among these leaders, belief in the physical model itself decayed. As late as mid-1923 Pauli semi-apologised that his latest theory was largely model-independent and phenomenological. But Pauli and Heisenberg soon abandoned determinist trajectories, leaving ideas that were symbolic, formal, heuristic.... Alfred Landé produced useful rules for the anomalous Zeeman effect (the famous Landé interval rules) but they were empirical and numerological, and Landé himself admitted that he found them incomprehensible.

In retrospect at least it was clear that the life of the Bohr model at least in the initial relatively unsophisticated form was drawing to an end.

The helium atom

From the time of origin of the Bohr model, it was clearly crucial to apply the ideas to the helium atom in order to show that the effect was not restricted to problems with one electron. and it seems that Bohr thought that it might not be too difficult. His first model was of two electrons rotating in the same orbit round the nucleus. Unfortunately there was no agreement with experiment, particularly for the ionisation energy.

In 1919, Landé worked with a model with inner and outer orbits for the two electrons. The two orbits could be coplanar, which he interpreted as orthohelium, or at right angles (parahelium). Again unfortunately there was no agreement with experiment. Over the next few years many other models were suggested, by, for example, John van Vleck and Kramers, but again without success. Finally in 1924, Born and Heisenberg provided a completely general approach to excited helium atom but this was still a total failure.

By now it was clear that the Bohr atom could not explain the relatively simple problem of the helium atom

Periodic Table

This was a topic where the Bohr atom had a greater, though not complete, success. In his trilogy of 1913, Bohr had suggested what seem now to be naïve shell-type models. At the time chemists suggested static models while physicists suggested dynamic models.

With the greater understanding of quantum numbers, in 1921 Bohr suggested a comprehensive approach to a full Periodic Table. He claimed it was based on the correspondence principle, though in practice it used chemistry and physics as well as the principle itself. Indeed Pauli complained that Bohr used aspects of the Periodic Table to produce the table itself. It should be mentioned that, though Bohr's work attracted the most attention, others contributed or competed, including Charles Bury, John Main Smith and Edmund Stoner. In the end, Stoner's work was the most complete.

A basic point for Bohr was the aufbau principle: Adding the cth electron to an atom does not affect the initial c - 1 electrons. Without this principle, analysis would obviously be massively more difficult.

One of the interesting points in his work was that initially n went down in outer 'shells'. For example, writing the number of electrons in a shell or sub-shell, with n as a subscript, we have $2_1 8_2 18_3 32_4 18_3 8_2$. Only later did he decide that n in outer shell increases systematically as the atom builds up, so n is a shell number, which of course we now take for granted

Bohr recognised the occurrence of intermediate shells. At points in building up the atom, the outer shell remains unchanged while an interior shell builds up for example:

[with (n, k)] The structure of calcium is (1, 1), (2, 1), (2, 2), (3, 1), (3,2) but then (4, 1) forms before (3, 3) followed by (3, 3)

Atoms formed while (3, 3) is added are transition metals. Another example are the rare earths.

Bohr explained intermediate shells by the use of penetrating orbits (remembering that Bohr though of orbits totally physically).

An orbit with (n, k) = (5, 5) will be wholly outside the orbit with (4, 4) as both are circular and the first has a larger radius than the second. However an orbit with (5, k) with k < 5 will be elliptical and will penetrate into the (4, 4) orbit. Bohr said that this would couple together the various orbits. The electron in e.g. the (5, 2) orbit will experience a reduced nuclear charge, a lower effective value of n and an increased energy.

We now come to a difference between Bohr and Stoner. For Bohr and for given n, the electrons in the group were divided equally between the various values of k:

 $(2_1)^4 (2_2)^4 (3_1)^6 (3_2)^6 (3_3)^6$

He was presumably basing this on the correspondence principle but Stoner, by more specific analysis of spectra, obtained the situation we accept today:

 $(2_1)^2(2_2)^6$ $(3_1)^2(3_2)^6(3_3)^{10}$

X-ray spectroscopy and the Periodic Table

Extension of Moseley's work showed the opening of sub-shells by noting at what atomic number particular lines first appeared. This work was carried out by groups in Sweden (led by Manne Siegbahn and cloely associated with Bohr) and in France. The two groups were very much in competition.

Element with Z = 72

Bohr's Periodic Table claimed that the element with Z = 72 was *not* a rare earth while George Urbain in France said that it was.

In the rare earth group, the atoms have 0 or 1 5d electrons and the number of 4f electrons gradually builds up. Bohr said that for the element with Z = 72, the 72nd electron was a second 5d electron i.e. the 4f sub-shell was full. Thus the element was analagous to zirconium which has the structure $(1s)^2(2s)^2(2p)^6(3s)^2(3p)^6(4s)^2(3d)^{10}(4p)^6(5s)^2(4d)^2$ In particlar zirconium has two 4d electrons while Bohr said the atom with Z = 72 has two 5d electrons.

Then in 1922 Urbain and Alexandre Dauviller claimed detection of lines of the atom with Z = 72, announced that it was a rare earth and named it *celtium*.

At fist Bohr was inclined to accept this, but his colleagues George von Hevesy and Dirk Coster pesuaded him to dispute it. They searched for the element in zirconium minerals and found it comparatively easily. X-ray spectra showed that it was not a rare earth. Together with Bohr they named it *hafnium*. (*Hafnia* is Latin for Copenhagen.) Quite fairly this was loked on as a triumph for Bohr.

The way ahead

Overall though by 1924-5 it was clear that the Bohr model was failing. There had been many successes but, while in the early days of the model, one could glory in these successes and regard dificulties as problems to be solved, by now the many successes were taken for granted and the many failures seemed permanent.

It is interesting to have a glance at the path from the Bohr atom to the new quantum theory. For this purpose the most useful guide is the book by Van der Waerden², *Sources of Quantum Mechanics.* The list of the authors of papers included from 1921 on is interesting as it takes us right through to Heisenberg's work of 1925:

Ladenburg 1921

[Slater 1924] (not actually included by Van der Waerden though he discusses it)

Bohr Kramers and Slater 1924 Kramers 1924 Born 1924 Kramers 1924 Van Vleck 1924 Kramers and Heisenberg 1925 Kuhn 1925 Heisenberg 1925

We first briefly look at Rudolf Ladenberg's paper of 1921. For its interaction with a radiation field, Ladenburg replaced the atom by a set of virtual harmonic oscillators with frequencies equal to the absorption frequencies of the atom.

Next we discuss the 1924 paper of John C Slater, an American PhD student. Following Ladenberg quite closely, he suggested that each atom is the source of a 'virtual field of radiation' emitted by virtual oscillators. This field oscillates with the frequencies of the various quantum transitions, and interacts with all the other atoms by guiding photons and specifying the paths they take between particular atoms.

We may remember the common complaint that Bohr's theory contained nothing oscillating at the frequency of the radiation. We see that this 'defect' is remedied here.

[We now present a potted history of the photon. The idea of the photon came from Einstein in 1905. His theory of the photolectric effect using the photon was confrmed by the experiments of Robert Millikan 1914-16, but few physicists accepted the photon. Millikan certainly didn't. For example in 1914 most influential Prussian physicists whole-heartedly recommended Einstein for Membership of the Prussian Academy but excused his idea of photons because 'it is not possible to introduce really new ideas without taking risks.'

Then in 1923 came the Compton Effect which studied the collision between an X-ray photon and an electron in metal foil. This was generally accepted as proof of the photon concept. BUT NOT BY BOHR!!]

Slater now travelled to Copenhagen.

Bohr and Kramers persuaded Slater to remove the photons with the result that in the Bohr Kramers Slater (BKS) paper:

- (1) Energy and momentum were conserved only statistically
- (2) There was only statistical independence of processes of emission and absorption in distant atoms

Experiments by Walther Bothe, Hans Geiger, Compton, Alfred Simon soon showed that neither (1) nor (2) were true and Bohr had to give BKS an 'honourable funeral'.

Slater was furious! He felt that Bohr and Kramers had ruined his theory. He already had a bad impression of Bohr because before he came to Copenhagen he had asumed, though Bohr published only results, they must be on the basis of substantial calculations. Only when he arrived in Copenhagen did he realise that there were no calculations.

BKS

Was this a chronic failure

OR

A last attempt to show that semiclassical physics (matter and radiation completely separate conceptually) would not work?.

It led Heisenberg to realise that there would be no easy solutions.

Indeed Kramers and later Heisenberg based their work on BKS

Jammer³: 'It is hard to find in the history of physics a theory which was so soon disproved after its proposal and yet was so important for the future development of physical thought.'

A Final Question

How much did Bohr and the Bohr model contribute to final (Heisenberg) quantum mechanics?

¹ Helge Kragh, *Niels Bohr and the Quantum Atom: The Bohr Model of Atomic Structure 1913-1925* (Oxford University Press, Oxford, 2012). Kragh and this book in particular are the central authority for this topic.

² B. L. Van der Waerden, *Sources of Quantum Mechanics* (North-Holland, Amsterdam, 1967).

³Max Jammer, *The Conceptual Development of Quantum Mechanics* (McGraw-Hill, New York, 1966).

⁴ <u>Mathematics at Balliol: modern (ox.ac.uk)</u>

Rutherford's transmutation experiment: At the time what did he think had occurred?

Edward A Davis, University of Cambridge

1. Introduction

In 1919 Ernest Rutherford undertook a significant experimental investigation in which nitrogen gas in a cylindrical container was bombarded with alpha particles from a radium source. Viewing the products of the collision by the scintillations they produced on a cadmium sulphide screen situated at the opposite end of the container to the radium source, he deduced that atoms of nitrogen struck by the alpha particle had disintegrated, ejecting a hydrogen atom in the process.

Accounts of the experiment, its historical background, and reports in the newspapers at the time were covered comprehensively during a one-day meeting at Manchester University in June 2019. The presentations at that meeting were written up for a special issue of an IOP History of Physics Newsletter in October 2021. Here I elaborate a little on the story, with apologies in advance for any overlap with the articles in that publication.

2. What did Rutherford suggest had occurred?

There is no doubt that Rutherford not only achieved – but also realised he had achieved – artificial transmutation in the experiments reported in the Philosophical Magazine of 1919 [1] and deserves credit for this. What he did not claim, or even contemplate at the time, was that the residual atom left behind after the alpha particle had struck a nitrogen atom and ejected a hydrogen atom from it, was in fact oxygen. Indeed, he called the residuals 'swift *nitrogen* atoms' [2].

Why did Rutherford suggest the residual atoms could still be nitrogen, knowing that a proton had been ejected? The answer can be found in his Bakerian lecture '*Nuclear constitution of atoms*' delivered to The Royal Society in 1920 [3], one year after publication of the paper in which he reported the experimental results. In this lecture, Rutherford suggested that the residuals could be either carbon or nitrogen. In his own words:

'It is natural to inquire as to the nature of the residual atoms after the disintegration of ... nitrogen, supposing that they survive the collision and sink into a new stage of temporary or permanent equilibrium. The expulsion of an H atom carrying one charge from nitrogen should lower the mass by 1 and the nuclear charge by 1. The residual nucleus should thus have a nuclear charge 6 and mass 13, and should be an isotope of carbon. If a negative electron is released at the same time, the residual atom becomes an isotope of nitrogen.' It is clear from the above statement that Rutherford knew the atomic mass of nitrogen was 14 and that its nucleus carried a charge of 7. So, his first suggestion that loss of a proton would lead to the residual atom being carbon is the obvious one, although he did not suggest this in his 1919 paper.

The above extract from the Bakerian lecture gives equal weight to the suggestion that the residual atoms could also be nitrogen. In the lecture he described a possible model for the nitrogen nucleus containing electrons that are quite independent of the orbiting outer electrons. He pictured (in the absence of knowledge of the existence of neutrons) the nucleus as being composed of four atoms of mass 3, two hydrogen atoms of mass 1, plus a binding electron between the hydrogens, as he illustrated below.

NITROGEN Mass 14 CHARGE 7

Rutherford postulated that when a proton was knocked out, an electron from this nucleus might be released at the same time. In today's terms we would say an electron emitted from a nucleus would convert a neutron to a proton, compensating for the proton that was ejected and leaving the atomic number unchanged. The nitrogen left behind would of course be a different isotope with mass 13.

3. The satellite model

There is no suggestion in any of Rutherford's papers prior to 1924 that he considered the possibility that the alpha particle was absorbed by, or integrated with, the nitrogen nucleus, a fact later shown to be the case via the cloud-chamber experiments of Blackett [7]. In several papers written with Chadwick between his move from Manchester to Cambridge and Blackett's experiments, he attempted to explain why protons were knocked out of some nuclei more easily than from others. His model [4] shows that he considered the ejected proton (marked H for hydrogen) to sit as an outrider to the main nucleus (marked N). Depending on how the alpha particle struck

this hydrogen satellite determined the direction (forward or backward) of ejection, as illustrated.



There is no indication in these diagrams of the alpha particle entering the nucleus. Indeed, Rutherford and Crawford specifically refer to *three* particles after the collision, namely the proton, the residual atom and the alpha particle. Furthermore, using the conservation of momentum, they calculated the energy with which the alpha particle escapes relative to its initial energy.

4. First light

The first suggestion that the alpha particle might be captured by the nucleus was made by J.B. Perrin at the third Solvay Conference held in Brussels in October 1921 while commenting on Rutherford's experimental results. The same suggestion was also made later by Pettersson and Kirsch in correspondence to Rutherford in June 1924. Both communications were referred to by Rutherford in 1925 (see below), after the experiments by Blackett had convinced him that this was indeed what had occurred.

In a paper co-authored with Chadwick in 1924 [6], Rutherford acknowledged the possibility that the alpha particle might have attached itself to the nitrogen.

'The fate of the alpha particle is a matter about which we have no information. It is unlikely that the field of force remains central at very close distances. It is possible that the alpha particle is in some way attached to the residual nucleus. Certainly it cannot be re-emitted with any considerable energy, or we should be able to observe it.' In a letter dated Sept 1924 to Rutherford (while he was in Canada) from Chadwick (who was in Scotland) wrote:

'I think I ought to tell you of the results of the last experiments but I don't know when you will get this letter as I very seldom see a post office. I corrected the number of disintegration particles from aluminium under as definite conditions as were feasible. As near as the experiments allow, the number agrees with that calculated on the assumption of an attractive inverse fourth and repulsive inverse square taking (1) zero force at 4 x 10⁻¹³ and (2) that the H particle appears when the alpha disappears. Of course the agreement cannot be very good on account of the counting errors and even in estimating the solid angles of the alphas used. Blackett has got two more photographs which are somewhat clearer than the others. They show the track of the H particles and the track of the recoil atom, but no track for the alpha (unless it is a very short one or what he calls the recoil track is the alpha track). If this is true it is a very fine addition to the evidence for the attractive field, and fits in very well with our expectations.'

5. Confirmation

In 1925 Blackett reported the results of a more extensive study, confirming these initial observations, namely that the alpha particle is absorbed on collision with the nitrogen atom [7]. Quoting from this paper:

It was to be expected that a photograph of such an event would show an alpha-ray track branching into three. The ejected proton, the /residual nucleus from which it has been ejected, and the alpha-particle itself, might each have been expected to produce a track. The forks however branch only into two. The path of the first of the three bodies, the rejected proton, is obvious in each photograph. It consists of a fine straight track, along which the ionisation is clearly less than along an alpha-ray track, in must therefore be due to a particle of small charge and great velocity, the second of the two arms of the fork is a short track similar in appearance to the track of the nitrogen nucleus in a normal fork. Of a third arm to correspond to the track of the alphaparticle itself after the collision there is no sign. On the generally accepted view, due to the work of Rutherford, the nucleus of an atom is so small, and thus the potential at its surface so large, that a positively charged particle that has once penetrated its structure (and almost certainly an alpha-particle that ejects a proton must do so) cannot escape without acquiring kinetic energy amply sufficient to produce a visible track. As no such track exists the alpha-particle cannot escape. In ejecting a proton from a nitrogen nucleus the alpha-particle is therefore itself bound to the nitrogen nucleus. The resulting new nucleus must have a mass 17, and, provided no electrons are gained or lost in the process, an atomic number of 8. The possibility of such a capture has already been suggested by Rutherford and Chadwick in a recent paper.

Commenting on Blackett's experiments and referring to the Perrin and the Pettersson & Kirsch earlier proposals, Rutherford wrote in 1925 [8].

The fine track of the proton was clearly visible, also that of the recoiling nucleus, but there was no sign of a third track to be expected if the alpha particle escaped after the collision. He concluded that the alpha particle is captured by the nitrogen nucleus under these conditions, and that in consequence the mass of the recoiling nucleus should be 17 and its charge 8 – namely an isotope of oxygen.

In view of the evidence obtained by Blackett of the capture of an alpha particle, I have thought it of interest to bring to the attention of readers of Nature two clear statements of the likelihood of such a capture in a collision which leads to the expulsion of a proton. In a discussion of a paper on the structure of the atom, read by me before the Solvay International Institute of Physics in 1921, ... a reference to this question was made by Prof. J. Perrin. A selection of the remarks made by him will be given in full, as the above publication may not be generally accessible to readers of Nature:

'Mr Rutherford's own experiments seem to prove that this idea of a simple collision must be given up. The alpha projectile, despite its high speed, and due to a very strong electrical repulsion, can arrive, very slowly, in the immediate vicinity of the nucleus. At this moment, a 'transmutation' occurs, probably consisting of an intranuclear rearrangement, with possible capture of the incident alpha nucleus (because we do not know what becomes of it), emission of the hydrogen nucleus forming the H-ray observed, and perhaps even with other less important projections.'

A suggestion of a similar kind has also been made by Pettersson and Kirsch. They forwarded to me, in June 1924, a short paper intended for publication....A paper including a statement of their views on this question was published in the Physikalische Zeitschrift 25 (1924) p 588.

In a lecture of 1925 to the Royal Institution, Rutherford (1925, p. 588) stated: "He [Blackett] concluded that the α particle was captured in a collision which led to the ejection of a proton. ... It thus appears that the nucleus may increase rather than diminish its mass as the result of collisions in which a proton is expelled."

6. Summary

In summary, Rutherford undoubtedly achieved transmutation in his 1919 experiments. However, he did not suggest or realise that he had transmuted nitrogen into oxygen. Rutherford guessed at carbon or nitrogen as the end product. The latter might seem strange – transmutation of nitrogen into nitrogen! However, in his Bakerian lecture he

explains why he thought that could be a possibility. Rutherford did not contemplate at the time that the alpha particle had been absorbed into the nitrogen nucleus. Suggestions of this possibility made by Perrin and later by Pettersson & Kirsch were acknowledged by Rutherford after Blackett's experiments confirmed that this was indeed what had occurred.

7. Acknowledgements

The author was inspired to write this article following his reading of Jeffrey Alan Hughes's PhD thesis: *The Radioactivists, Community, Controversy and the Rise of Nuclear Physics*, University of Cambridge 1993. He is grateful for discussions on the topic with Dr Michael Jewess.

Addendum: To this writer, the measured tone of Rutherford's Phil. Mag. paper is surprising. Is it possible that he was not as excited about his experimental findings as much as others were later? After all, he had observed and was completely familiar with natural transmutation in radioactive decay when he was at McGill University. To execute it artificially (albeit using a naturally occurring alpha emitter) in the way he did at Manchester was possibly not that great a surprise to him.

1. E. Rutherford *Collision of alpha particles with light atoms. IV. An anomalous effect in nitrogen*, Philosophical Magazine 1919, 37, pp. 581-587.

2. Tantalisingly, Rutherford did mention that the residuals were observed to have a range lower than that expected of nitrogen and more like that of oxygen. However, he explained this away in terms of the expelled hydrogen taking away some of the residual atom's energy.

3. E. Rutherford *Nuclear Constitution of Atoms* (Bakerian Lecture), Proceedings of the Royal Society A 1920, 97, pp. 374-400.

4. E. Rutherford and J. Chadwick *The Artificial Disintegration of Light Elements*, Philosophical Magazine 1921, 42, **pp.**809-825

5. E. Rutherford and J. Chadwick (1922) *The disintegration of elements by α particles*, Philosophical Magazine Vol. 44, pp.417-432.

6. E. Rutherford and J. Chadwick *Further experiments on the artificial disintegration of elements* Proc. Phys. Soc. 1924, 36, pp 417-422.

7. P.M.S. Blackett, *The Ejection of Protons from Nitrogen Nuclei, Photographed by the Wilson Method*, Proceedings of the Royal Society A 1925, 107, pp. 349-360.

8. E. Rutherford, Disintegration of Atomic Nuclei Nature 1925, 115, pp 493-494.

BOOK REVIEW



Paul Langevin, My Father, The Man & His Work

Andre Langevin

English edition by Francis Duck

Published by EDP Sciences, 2022

Reviewed by Alexander R. May

In this book, faithfully translated by Francis Duck, we take a journey into the world of a physicist who, at least outside of French society, is little known by the public. Paul Langevin lived in a time of seismic shifts in physics and society. He was that rare phenomenon of a talented physicist and humanist who appreciated the arts and history. He also refused to accept the then-popular logical positivist view that meaningful solutions and knowledge could only emerge following logical analysis. Through his experiences during World War One and Two, we learn that principles meant a lot to him, even when it meant putting himself at risk professionally and of bodily harm.

Paul Langevin began studies at the Ecole de Physique et Chimie Industrielles (ESPCI) (1889 -1891), where he would later return as Director of Studies. Although he wished to continue his studies, he was initially reluctant to apply to the Ecole Normale as he felt it was beyond his ambitions. However, he was motivated to do so by Dommer, a professor of industrial physics, and upon examination by Marcel Brillouin and Jules Tannery, passed all the tests with flying colours. Before long, he was at the University of Cambridge working in the laboratory of J. J. Thomson on the topic of ionised gases, and he defended his PhD in 1902. Shortly after, when the eminent Eleuthère Mascart requested he act as his substitute lecturing physics at the Collège de France, it placed

him among the most prominent members of Paris's scientific community. Returning to ESPCI as a Professor of Physics in 1905, he climbed to the upper echelons of Physics. He was appointed in 1909 to the prestigious position of titular Professor at the College de France and participated in and later led the Solvay Physics conferences.

While his scientific career was rocketing skyward, he continued to take a great interest in human rights, having joined the Ligue des droits de l'homme earlier in 1899. He was an active pacifist who supported worker's strikes and fought against nationalism in all its forms. However, he renounced what he felt was blind pacifism in the face of Hitler. This contrasted with other members of the Committee of Vigilance of Antifascists Intellectuals (CVIA) and led to his resignation. Shortly afterwards, he solidified his leanings towards active resistance through interactions with Communist militants as the Second World War broke out. It wasn't long before he was arrested, imprisoned, and interrogated. Luminaries such as Einstein, then in the United States, and Kapitza in the USSR requested their respective leaders to intervene on Langevin's behalf, and he was released to house arrest. As the war progressed and the situation in Germany became critical, he was forced to flee to Switzerland before returning to Paris upon its liberation. There he continued his support of causes until he died in 1946.

Langevin's scientific work is rich and varied, spanning Magnetism, Relativity, Brownian Motion, and Ultrasonics. He pioneered the study of magnetic properties, which he related to the interaction of atomic or molecular magnetic moments and the competition between the action of the magnetic field and random thermal motion. It has been said that Langevin grasped the main points of special relativity while Einstein was racing to publish it elsewhere. His equation relating the molecular fluctuations in several systems, including non-equilibrium thermodynamics, is still used by biophysicists today to study the movements of particles in biological fluid suspensions.

Most of all, during World War 1, he pioneered the development of sonar using piezoelectricity to detect submarines through their reflection of ultrasonic waves. The first transducer he developed, the Florisson-Langevin probe, consisting of a mosaic of quartz plates glued between two steel foils, can still be seen working in the ESPCI in Paris.

However, the most intriguing aspect of this book is the snapshots of relationships and the social circles within which Langevin moved. This book contains details of which this review has only covered a fraction. It is also beautifully presented with relevant photographs and footnotes and fits perfectly into its place within the EDP Sciences and History series.



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