LIVES IN MATHEMATICS

John Scales Avery

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INTRODUCTION[1]

I hope that this book will be of interest to students of mathematics and other disciplines related to mathematics, such as theoretical physics and theoretical chemistry.

An apology

I must apologize for the fact that the level of the book is uneven. Chapters 1-8, as well as Appendices A and B, are suitable for students who would like to learn calculus and differential equations. However, the remainder of the book is more demanding, and is suitable for more advanced students.

Human history as cultural history

We need to reform our teaching of history so that the emphasis will be placed on the gradual growth of human culture and knowledge, a growth to which all nations and ethnic groups have contributed.

This book is part of a series on cultural history. Here is a list of the other books in the series that have, until now, been completed:

- Lives in Education
- Lives in Poetry
- Lives in Painting
- Lives in Engineering
- Lives in Astronomy
- Lives in Chemistry
- Lives in Medicine
- Lives in Ecology
- Lives in Physics
- Lives in Economics
- Lives in the Peace Movement

[1]This book makes use of chapters and appendices that I have previously written, but most of the material in the book's 19 chapters is new. My son, Associate Professor James Emil Avery of the Niels Bohr Institute, University of Copenhagen, is the co-author of Appendices D, E, F and G.

The pdf files of these books may be freely downloaded and circulated from the following web addresses:

https://www.johnavery.info/

http://eacpe.org/about-john-scales-avery/

https://wsimag.com/authors/716-john-scales-avery

Contents

Chapter 1

PYTHAGORAS

1.1 The Pythagorean brotherhood

Pythagoras, a student of Anaximander, first became famous as a leader and reformer of the Orphic religion. He was born on the island of Samos, near the Asian mainland, and like other early Ionian philosophers, he is said to have travelled extensively in Egypt and Mesopotamia. In 529 B.C., he left Samos for Croton, a large Greek colony in southern Italy. When he arrived in Croton, his reputation had preceded him, and a great crowd of people came out of the city to meet him. After Pythagoras had spoken to this crowd, six hundred of them left their homes to join the Pythagorean brotherhood without even saying goodbye to their families.

For a period of about twenty years, the Pythagoreans gained political power in Croton, and they also had political influence in the other Greek colonies of the western Mediterranean. However, when Pythagoras was an old man, the brotherhood which he founded fell from power, their temples at Croton were burned, and Pythagoras himself moved to Metapontion, another Greek city in southern Italy. Although it was never again politically influential, the Pythagorean brotherhood survived for more than a hundred years.

The Pythagorean brotherhood admitted women on equal terms, and all its members held their property in common. Even the scientific discoveries of the brotherhood were considered to have been made in common by all its members.

1.2 Pythagorean harmony

The Pythagoreans practiced medicine, and also a form of psychotherapy. According to Aristoxenius, a philosopher who studied under the Pythagoreans, "They used medicine to purge the body, and music to purge the soul". Music was of great importance to the Pythagoreans, as it was also to the original followers of Dionysus and Orpheus.

Both in music and in medicine, the concept of harmony was very important. Here Pythagoras made a remarkable discovery which united music and mathematics. He discovered that the harmonics which are pleasing to the human ear can be produced by dividing a lyre string into lengths which are expressible as simple ratios of whole numbers. For example, if we divide the string in half by clamping it at the center, (keeping the tension constant), the pitch of its note rises by an octave. If the length is reduced to 2/3 of the basic length, then the note is raised from the fundamental tone by the musical interval which we call a major fifth, and so on. The discovery that harmonious musical tones could be related by rational numbers[1] made the Pythagoreans think that rational numbers are the key to understanding nature, and this belief became a part of their religion.

Having discovered that musical harmonics are governed by mathematics, Pythagoras fitted this discovery into the framework of Orphism. According to the Orphic religion, the soul may be reincarnated in a succession of bodies. In a similar way (according to Pythagoras), the "soul" of the music is the mathematical structure of its harmony, and the "body" through which it is expressed is the gross physical instrument. Just as the soul can be reincarnated in many bodies, the mathematical idea of the music can be expressed through many particular instruments; and just as the soul is immortal, the idea of the music exists eternally, although the instruments through which it is expressed may decay.

In distinguishing very clearly between mathematical ideas and their physical expression, Pythagoras was building on the earlier work of Thales, who thought of geometry as dealing with dimensionless points and lines of perfect straightness, rather than with real physical objects. The teachings of Pythagoras and his followers served in turn as an inspiration for Plato's idealistic philosophy.

Having found mathematical harmony in the world of sound, and having searched for it in astronomy, Pythagoras tried to find mathematical relationships in the visual world. Among other things, he discovered the five possible regular polyhedra. However, his greatest contribution to geometry is the famous Pythagorean theorem, which is considered to be the most important single theorem in the whole of mathematics.

The Mesopotamians and the Egyptians knew that for many special right triangles, the sum of the squares formed on the two shorter sides is equal to the square formed on the long side. For example, Egyptian surveyors used a triangle with sides of lengths 3, 4 and 5 units. They knew that between the two shorter sides, a right angle is formed, and that for this particular right triangle, the sum of the squares of the two shorter sides is equal to the square of the longer side. Pythagoras proved that this relationship holds for every right triangle.

In exploring the consequences of his great theorem, Pythagoras and his followers discovered that the square root of 2 is an irrational number. (In other words, it cannot be expressed as the ratio of two integers.) The discovery of irrationals upset them so much that they abandoned algebra. They concentrated entirely on geometry, and for the next two thousand years geometrical ideas dominated science and philosophy.

[1] i-e-. numbers that can be expressed as a ratio of two integers

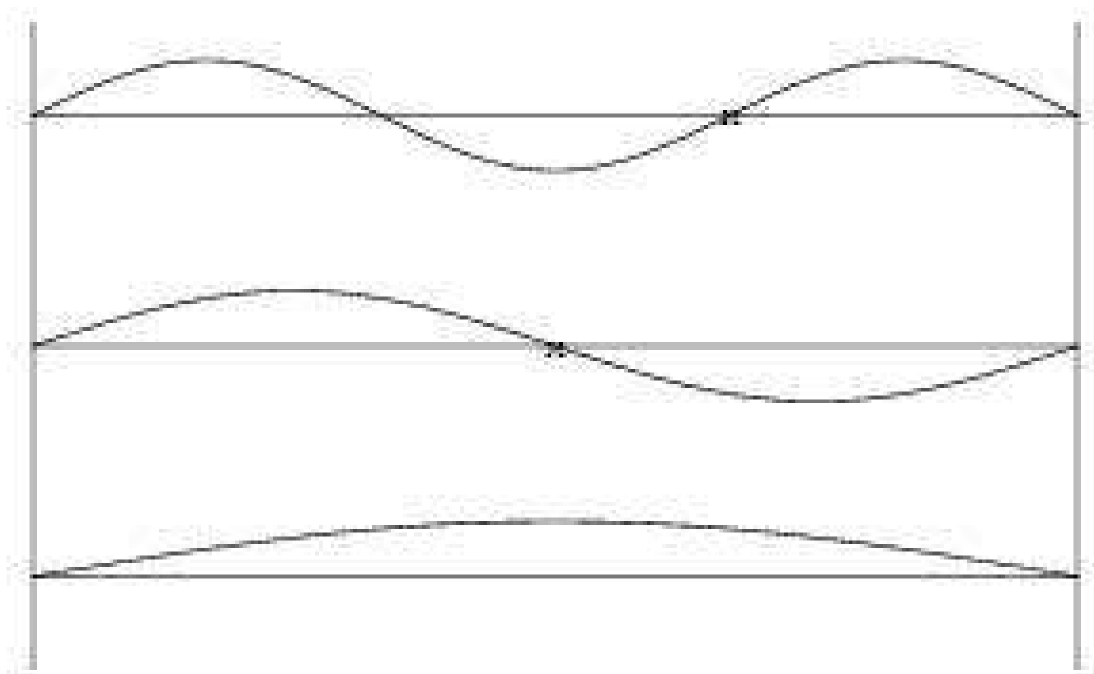

Figure 1.1: **Pythagoras (569 B.C. - 475 B.C.) discovered that the musical harmonics that are pleasing to the human ear can be produced by clamping a lyre string of constant tension at points that are related by rational numbers. In the figure the octave and the major fifth above the octave correspond to the ratios 1/2 and 1/3.**

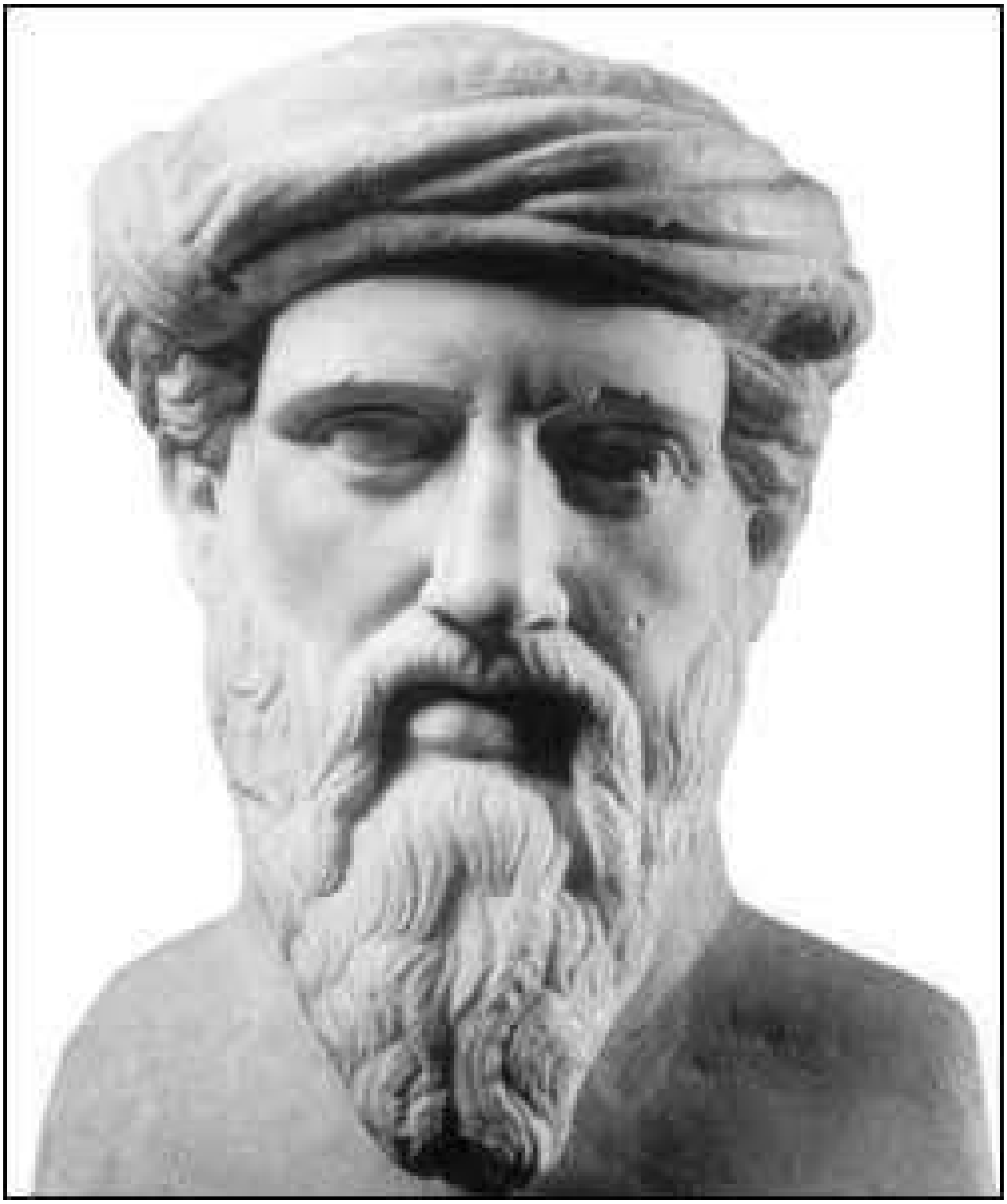

Figure 1.2: **Pythagoras founded a brotherhood that lasted about a hundred years and greatly influenced the development of mathematics and science. The Pythagorean theorem, which he discovered, is considered to be the most important single theorem in mathematics.**

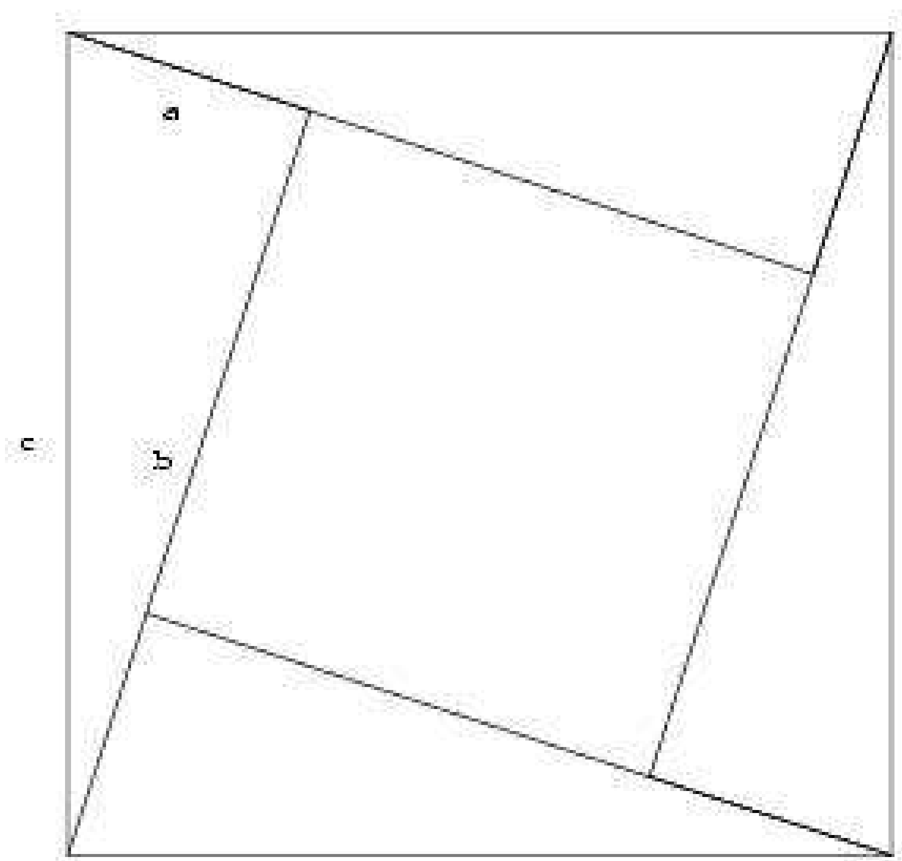

Figure 1.3: **This figure can be used to prove the famous theorem of Pythagoras concerning squares constructed on the sides of a right triangle (i.e. a triangle where two of the sides are perpendicular to each other). It shows a right triangle whose sides, in order of increasing length, are a, b and c. Four identical copies of this triangle, with total area 2ab, are inscribed inside a square constructed on the long side.**

1.3 Geometry as a part of religion

The classical Greek geometers, most of whom were Pythagoreans, discovered many geometrical theorems. They believed that the contemplation of eternal geometrical truths was a way of finding release from the suffering of human existence, and geometry was a part of their religion. There were certain rules that had to be followed in geometrical constructions: only a compass and a straight ruler could be used. The theorems of the geometers of classical Greece were collected and put into a logical order by Euclid, who lived in Alexandria, the capital city of Egypt founded by Alexander of Macedon.

Suggestions for further reading

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25. L Ya Zhmud', *Pythagoras as a mathematician (Russian)*, Istor.-Mat. Issled. 32-33 (1990), 300-325.

Chapter 2

EUCLID

2.1 Alexandria

Alexander of Macedon's brief conquest of the entire known world had the effect of blending the ancient cultures of Greece, Persia, India and Egypt, and producing a world culture. The era associated with this culture is usually called the Hellenistic Era (323 B.C. - 146 B.C.). Although the Hellenistic culture was a mixture of all the great cultures of the ancient world, it had a decidedly Greek flavor, and during this period the language of educated people throughout the known world was Greek.

Nowhere was the cosmopolitan character of the Hellenistic Era more apparent than at Alexandria in Egypt. No city in history has ever boasted a greater variety of people. Ideally located at the crossroads of world trading routes, Alexandria became the capital of the world - not the political capital, but the cultural and intellectual capital.

Miletus in its prime had a population of 25,000; Athens in the age of Pericles had about 100,000 people; but Alexandria was the first city in history to reach a population of over a million!

Strangers arriving in Alexandria were impressed by the marvels of the city - machines which sprinkled holy water automatically when a five-drachma coin was inserted, water-driven organs, guns powered by compressed air, and even moving statues, powered by water or steam!

2.2 The Museum and the Great Library of Alexandria

For scholars, the chief marvels of Alexandria were the great library and the Museum established by Ptolemy I. Credit for making Alexandria the intellectual capital of the world must go to Ptolemy I and his successors (all of whom were named Ptolemy except the last of the line, the famous queen, Cleopatra). Realizing the importance of the schools which had been founded by Pythagoras, Plato and Aristotle, Ptolemy I established a school at Alexandria. This school was called the Museum, because it was dedicated to the muses.

Near to the Museum, Ptolemy built a great library for the preservation of important manuscripts. The collection of manuscripts which Aristotle had built up at the Lyceum in Athens became the nucleus of this great library. The library at Alexandria was open to the general public, and at its height it was said to contain 750,000 volumes. Besides preserving important manuscripts, the library became a center for copying and distributing books.

The material which the Alexandrian scribes used for making books was papyrus, which was relatively inexpensive. The Ptolemys were anxious that Egypt should keep its near-monopoly on book production, and they refused to permit the export of papyrus. Pergamum, a rival Hellenistic city in Asia Minor, also boasted a library, second in size only to the great library at Alexandria. The scribes at Pergamum, unable to obtain papyrus from Egypt, tried to improve the preparation of the skins traditionally used for writing in Asia. The resulting material was called *membranum pergamentum*, and in English, this name has become "parchment".

2.3 Euclid is called to the Museum

One of the first scholars to be called to the newly-established Museum was Euclid. He was born in 325 B.C. and was probably educated at Plato's Academy in Athens. While in Alexandria, Euclid wrote the most successful text-book of all time, the *Elements of Geometry*. The theorems in this splendid book were not, for the most part, originated by Euclid. They were the work of many generations of classical Greek geometers. Euclid's contribution was to take the theorems of the classical period and to arrange them in an order which is so logical and elegant that it almost defies improvement. One of Euclid's great merits is that he reduces the number of axioms to a minimum, and he does not conceal the dubiousness of certain axioms.

Euclid's axiom concerning parallel lines has an interesting history: This axiom states that "Through a given point not on a given line, one and only one line can be drawn parallel to a given line". At first, mathematicians doubted that it was necessary to have such an axiom. They suspected that it could be proved by means of Euclid's other more simple axioms. After much thought, however, they decided that the axiom is indeed one of the necessary foundations of classical geometry. They then began to wonder whether there could be another kind of geometry where the postulate concerning parallels is discarded. These ideas were developed in the 18th and 19th centuries by Lobachevsky, Bolyai, Gauss and Riemann, and in the 20th century by Levi-Civita. In 1915, the mathematical theory of non-Euclidean geometry finally became the basis for Einstein's general theory of relativity.

Besides classical geometry, Euclid's book also contains some topics in number theory. For example, he discusses irrational numbers, and he proves that the number of primes is infinite. He also discusses geometrical optics.

Euclid's *Elements* has gone through more than 1,000 editions since the invention of printing - more than any other book, with the exception of the Bible. Its influence has been immense. For more than two thousand years, Euclid's *Elements of Geometry* has served as a model for rational thought.

Figure 2.1: **Euclid, detail from "The School of Athens", a painting by Raphael. It is not proven that this is Euclid. Some references point this person out as Archimedes.**

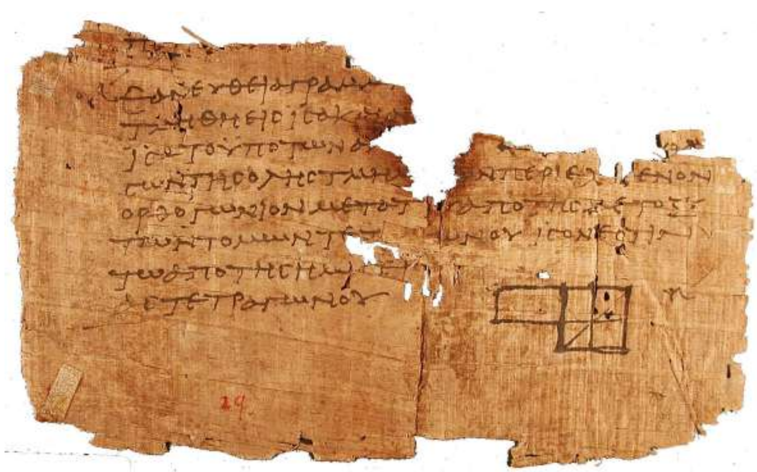

Figure 2.2: **One of the oldest surviving fragments of Euclid's Elements, found at Oxyrhynchus and dated to circa AD 100 (P. Oxy. 29). The diagram accompanies Book II, Proposition 5.**

2.4 The eight books of Euclid's *Elements*

Here are the titles of the eight books of Euclid's *Elements of Geometry*:[1]

1. **Book I, On basic plane geometry**
2. **Book II, On geometric algebra**
3. **Book III, On circles and angles**
4. **Book IV, On construction of regular polygons**
5. **Book V, On Eudoxes' of abstract theory of ratio proportions, abstract algebra**
6. **Book VI, On similar figures and geometric proportions**
7. **Book VII, On basic number theory**
8. **Book VIII, On continurs proportions (geometric progressions) in number theory**

2.5 Euclid's Book I, *On basic plane geometry*

Definitions

1. **A point is that which has no part.**
2. **A line is breadthless length.**
3. **The ends of a line are points.**
4. **A straight line is a line which lies evenly with the points on itself.**
5. **A surface is that which has length and breadth only.**
6. **The edges of a surface are lines.**
7. **A plane surface is a surface which lies evenly with the straight lines on itself.**
8. **A plane angle is the inclination to one another of two lines in a plane which meet one another and do not lie in a straight line.**
9. **And when the lines containing the angle are straight, the angle is called rectilinear.**

[1] https://mathcs.clarku.edu/ djoyce/elements/trip.html

10. When a straight line standing on a straight line makes the adjacent angles equal to one another, each of the equal angles is right, and the straight line standing on the other is called a perpendicular to that on which it stands.

11. An obtuse angle is an angle greater than a right angle.

12. An acute angle is an angle less than a right angle.

13. A boundary is that which is an extremity of anything.

14. A figure is that which is contained by any boundary or boundaries.

15. A circle is a plane figure contained by one line such that all the straight lines falling upon it from one point among those lying within the figure equal one another.

16. And the point is called the center of the circle.

17. A diameter of the circle is any straight line drawn through the center and terminated in both directions by the circumference of the circle, and such a straight line also bisects the circle.

18. A semicircle is the figure contained by the diameter and the circumference cut off by it. And the center of the semicircle is the same as that of the circle.

19. Rectilinear figures are those which are contained by straight lines, trilateral figures being those contained by three, quadrilateral those contained by four, and multilateral those contained by more than four straight lines.

20. Of trilateral figures, an equilateral triangle is that which has its three sides equal, an isosceles triangle that which has two of its sides alone equal, and a scalene triangle that which has its three sides unequal.

21. Further, of trilateral figures, a right-angled triangle is that which has a right angle, an obtuse-angled triangle that which has an obtuse angle, and an acute-angled triangle that which has its three angles acute.

22. Of quadrilateral figures, a square is that which is both equilateral and right-angled; an oblong that which is right-angled but not equilateral; a rhombus that which is equilateral but not right-angled; and a rhomboid that which has its opposite sides and angles equal to one another but is neither equilateral nor right-angled. And let quadrilaterals other than these be called trapezia.

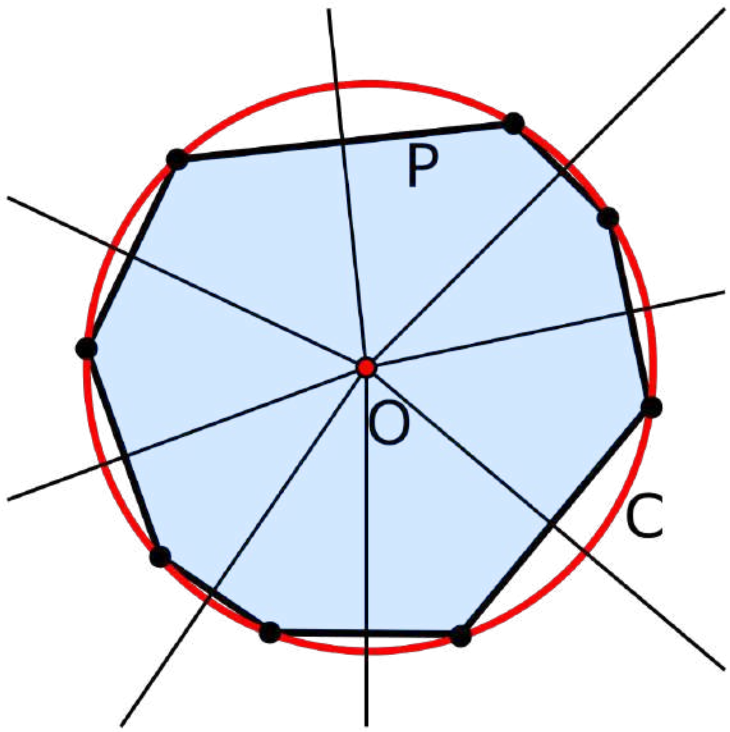

Figure 2.3: **Circumscribed circle, C, and circumcenter, O, of a cyclic polygon, P.**

23. Parallel straight lines are straight lines which, being in the same plane and being produced indefinitely in both directions, do not meet one another in either direction.

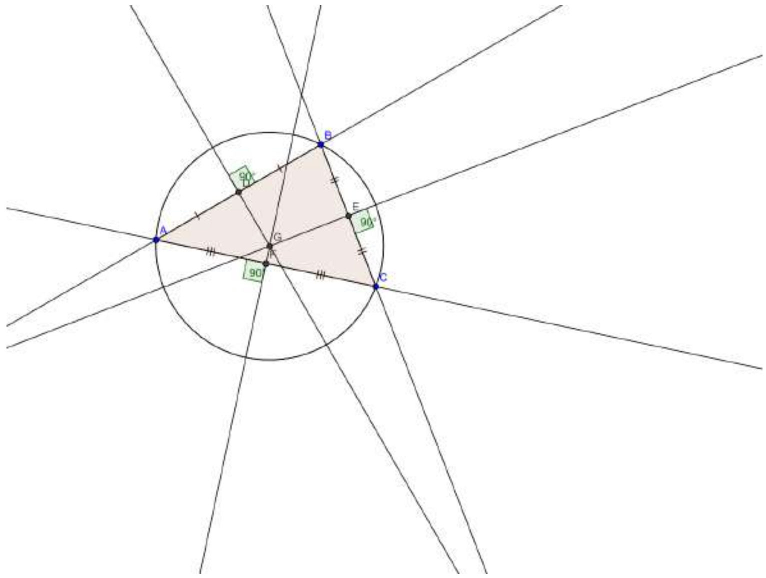

Figure 2.4: **Construction of the circumcircle and the circumcenter.**

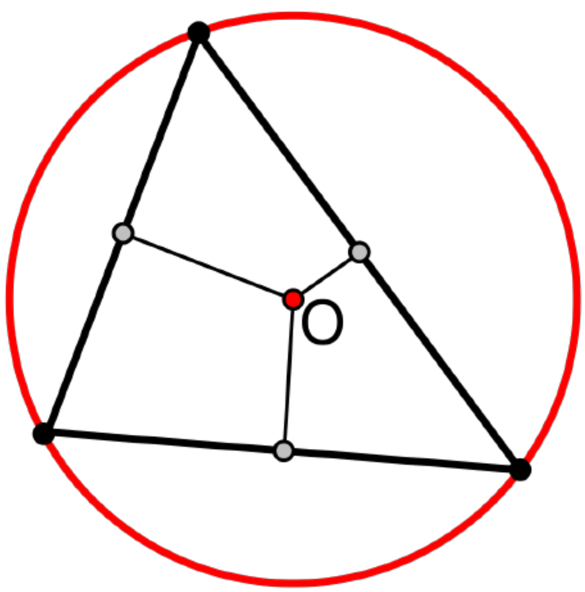

Figure 2.5: **The circumcenter of an acute triangle is inside the triangle.**

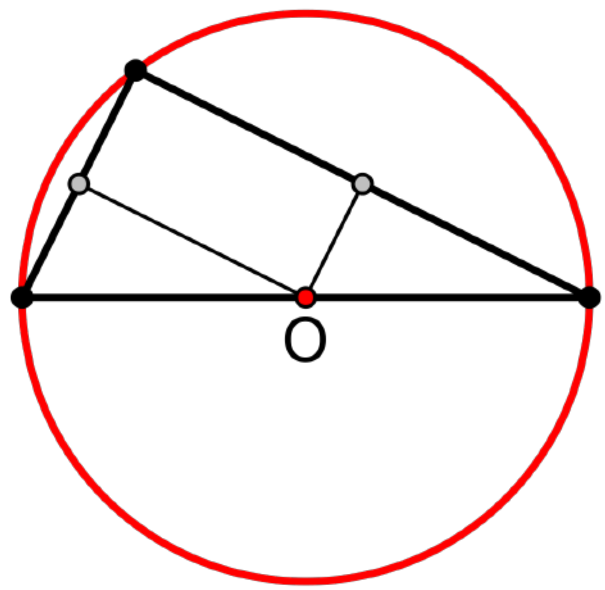

Figure 2.6: **The circumcenter of a right triangle is at the midpoint of the hypotenuse.**

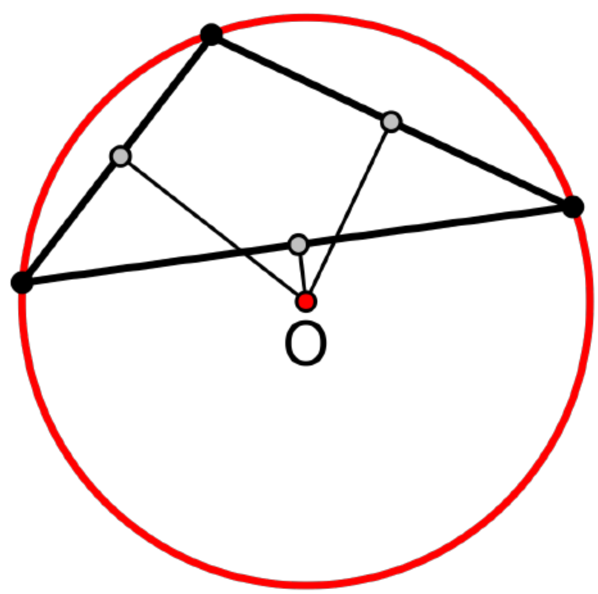

Figure 2.7: **The circumcenter of an obtuse triangle is outside the triangle.**

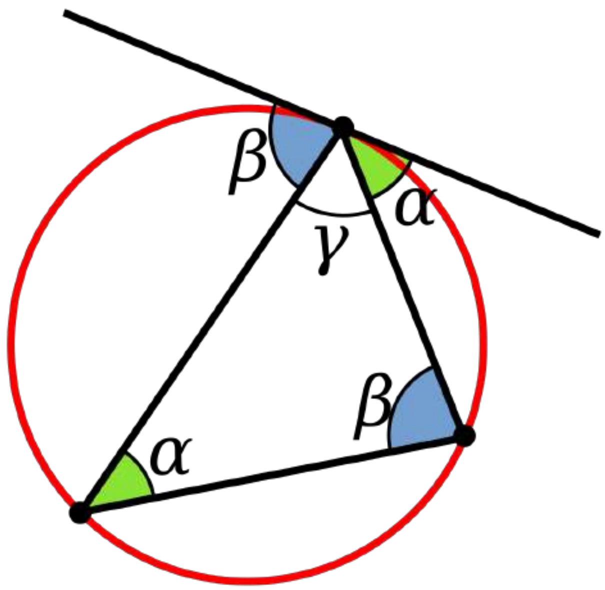

Figure 2.8: **A diagram of the angles in a cirumcircle of a triangle, showing the alternate angle theorem.**

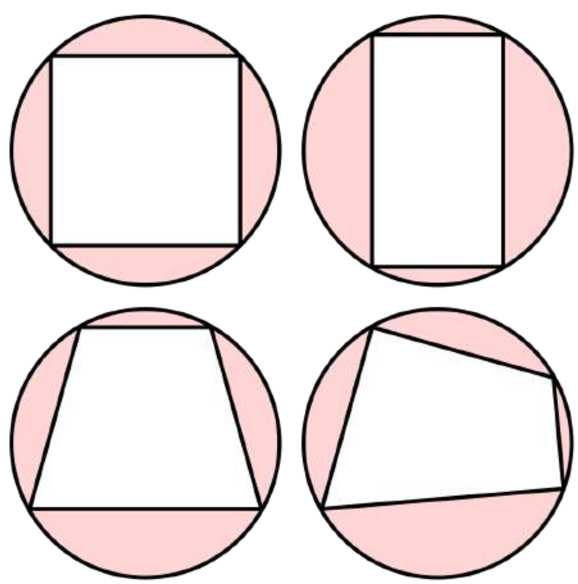

Figure 2.9: **Cyclic quadrilaterals.**

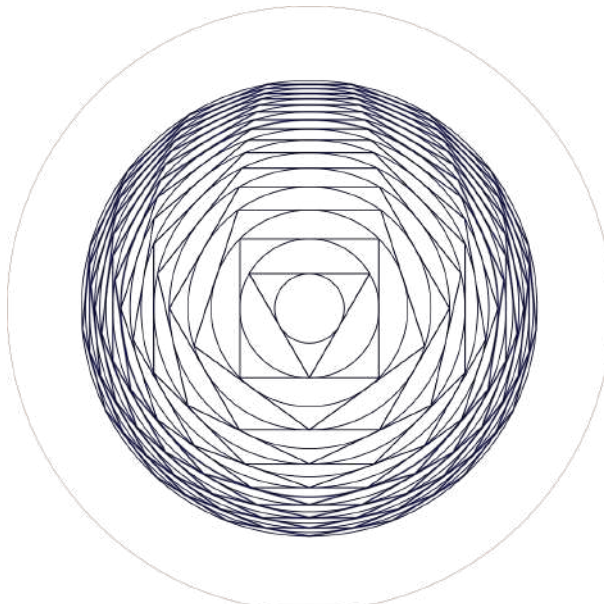

Figure 2.10: **A sequence of circumscribed polygons and circles.**

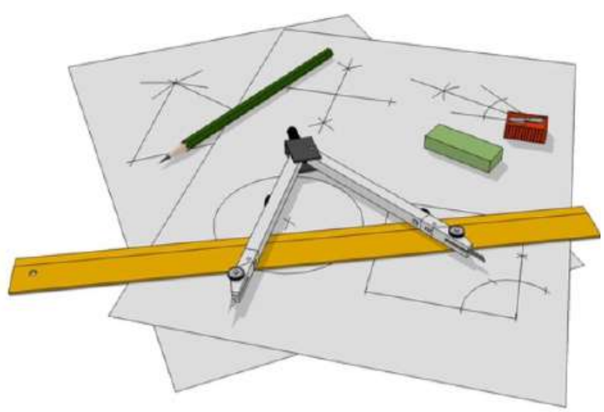

Figure 2.11: **Straightedge and compass, the only tools that classical geometers were allowed to use.**

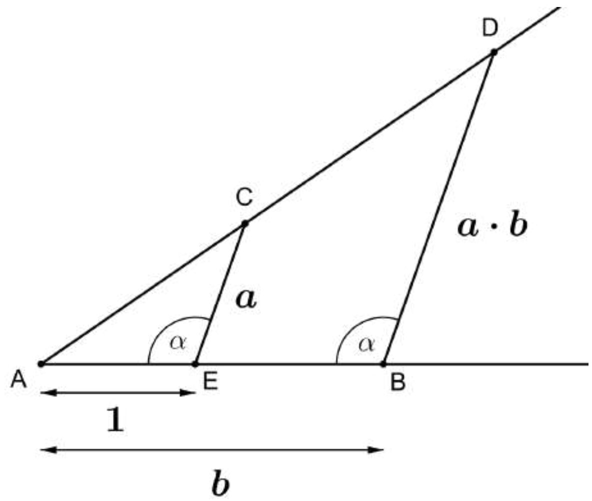

Figure 2.12: **The intercept theorem.**

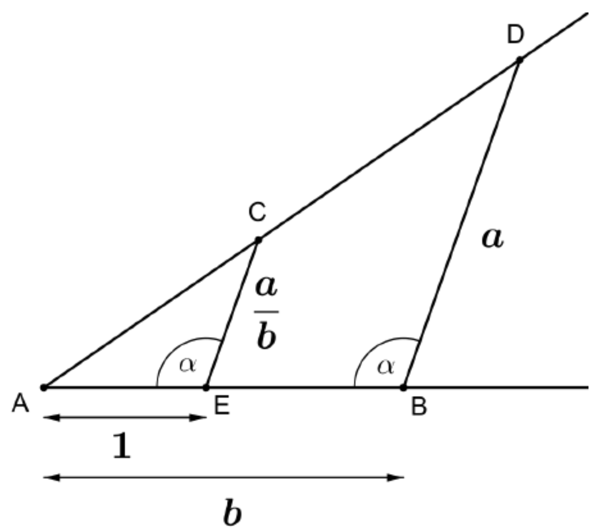

Figure 2.13: **Another form of the intercept theorem.**

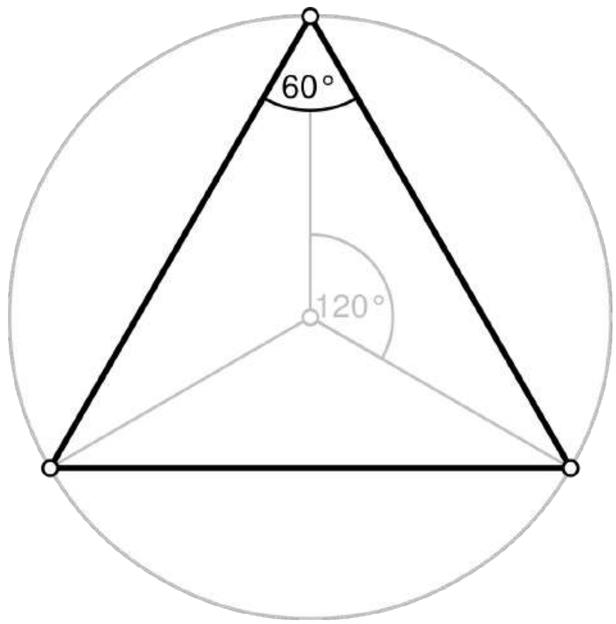

Figure 2.14: **Equilateral triangle with angles.**

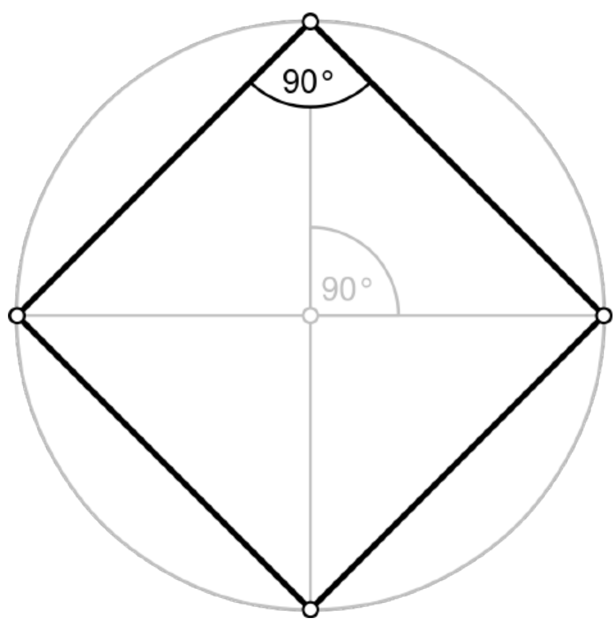

Figure 2.15: **Square with angles.**

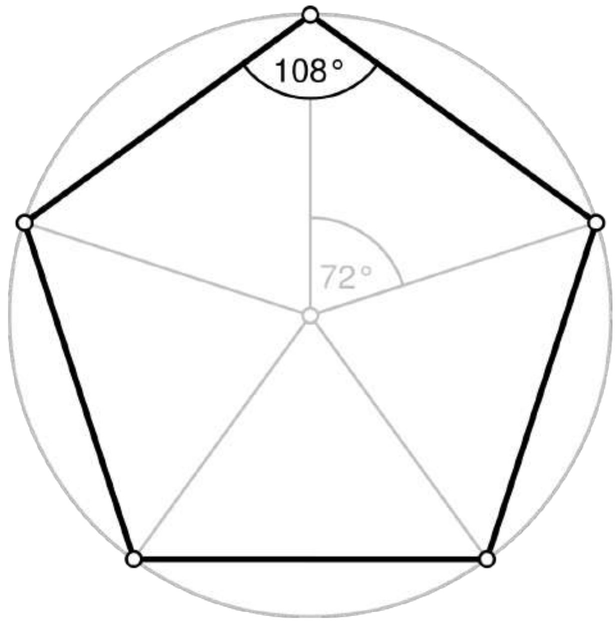

Figure 2.16: **Regular pentagon with angles.**

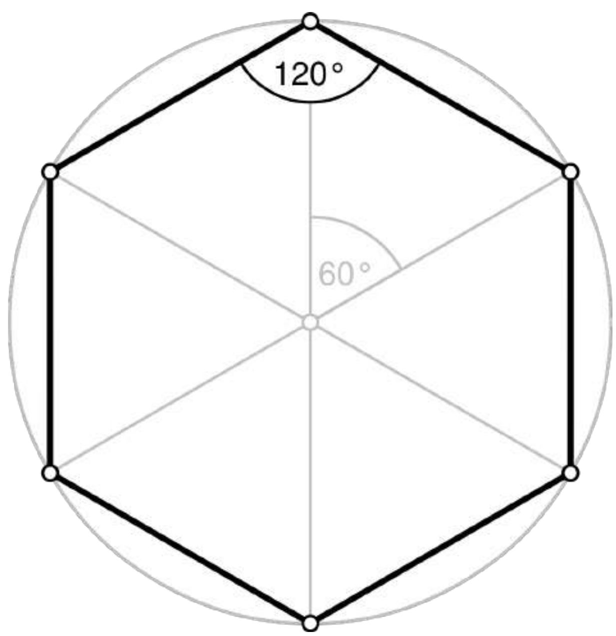

Figure 2.17: **Regular hexagon with angles.**

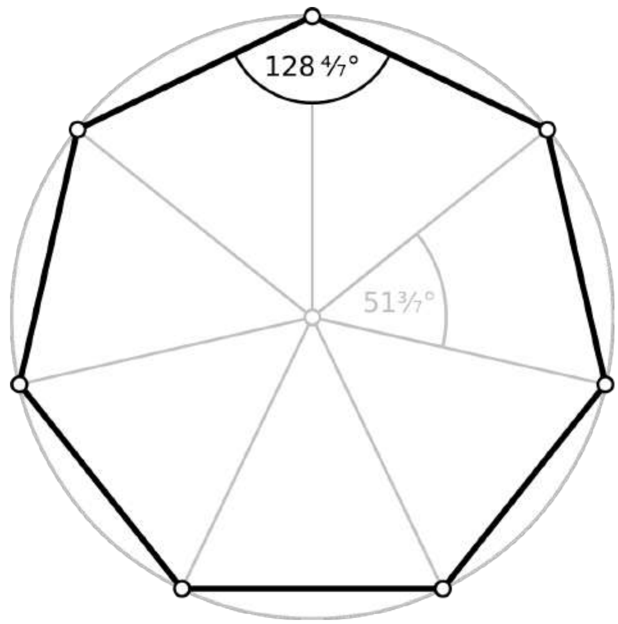

Figure 2.18: **Regular heptagon with angles.**

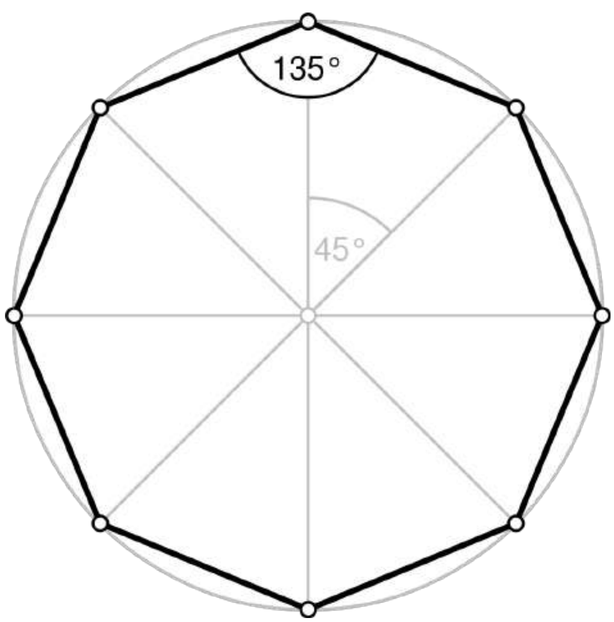

Figure 2.19: **Regular octagon with angles.**

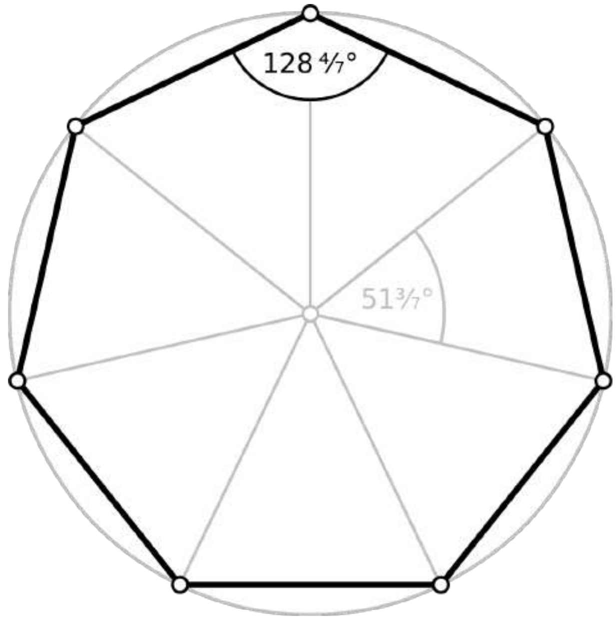

Figure 2.20: **Regular nonagon with angles.**

Suggestions for further reading

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Chapter 3

ARCHIMEDES

3.1 Heiron's crown

Archimedes was the greatest mathematician of the Hellenistic Era. In fact, together with Newton and Gauss, he is considered to be one of the greatest mathematicians of all time.

Archimedes was born in Syracuse in Sicily in 287 B.C.. He was the son of an astronomer, and he was also a close relative of Hieron II, the king of Syracuse. Like most scientists of his time, Archimedes was educated at the Museum in Alexandria, but unlike most, he did not stay in Alexandria. He returned to Syracuse, probably because of his kinship with Hieron II. Being a wealthy aristocrat, Archimedes had no need for the patronage of the Ptolemys.

Many stories are told about Archimedes: For example, he is supposed to have been so absent-minded that he often could not remember whether he had eaten. Another (perhaps apocryphal) story has to do with the discovery of "Archimedes Principle" in hydrostatics. According to the story, Hieron had purchased a golden crown of complex shape, and he had begun to suspect that the goldsmith had cheated him by mixing silver with gold. Since Hieron knew that his bright relative, Archimedes, was an expert in calculating the volumes of complex shapes, he took the crown to Archimedes and asked him to determine whether it was made of pure gold (by calculating its specific gravity). However, the crown was too irregularly shaped, and even Archimedes could not calculate its volume.

While he was sitting in his bath worrying about this problem, Archimedes reflected on the fact that his body seemed less heavy when it was in the water. Suddenly, in a flash of intuition, he saw that the amount by which his weight was reduced was equal to the weight of the displaced water. He leaped out of his bath shouting *"Eureka! Eureka!"* ("I've found it!") and ran stark naked through the streets of Syracuse to the palace of Hieron to tell him of the discovery.

The story of Hieron's crown illustrates the difference between the Hellenistic period and the classical period. In the classical period, geometry was a branch of religion and philosophy. For aesthetic reasons, the tools which a classical geometer was allowed too use were restricted to a compass and a straight-edge. Within these restrictions, many problems

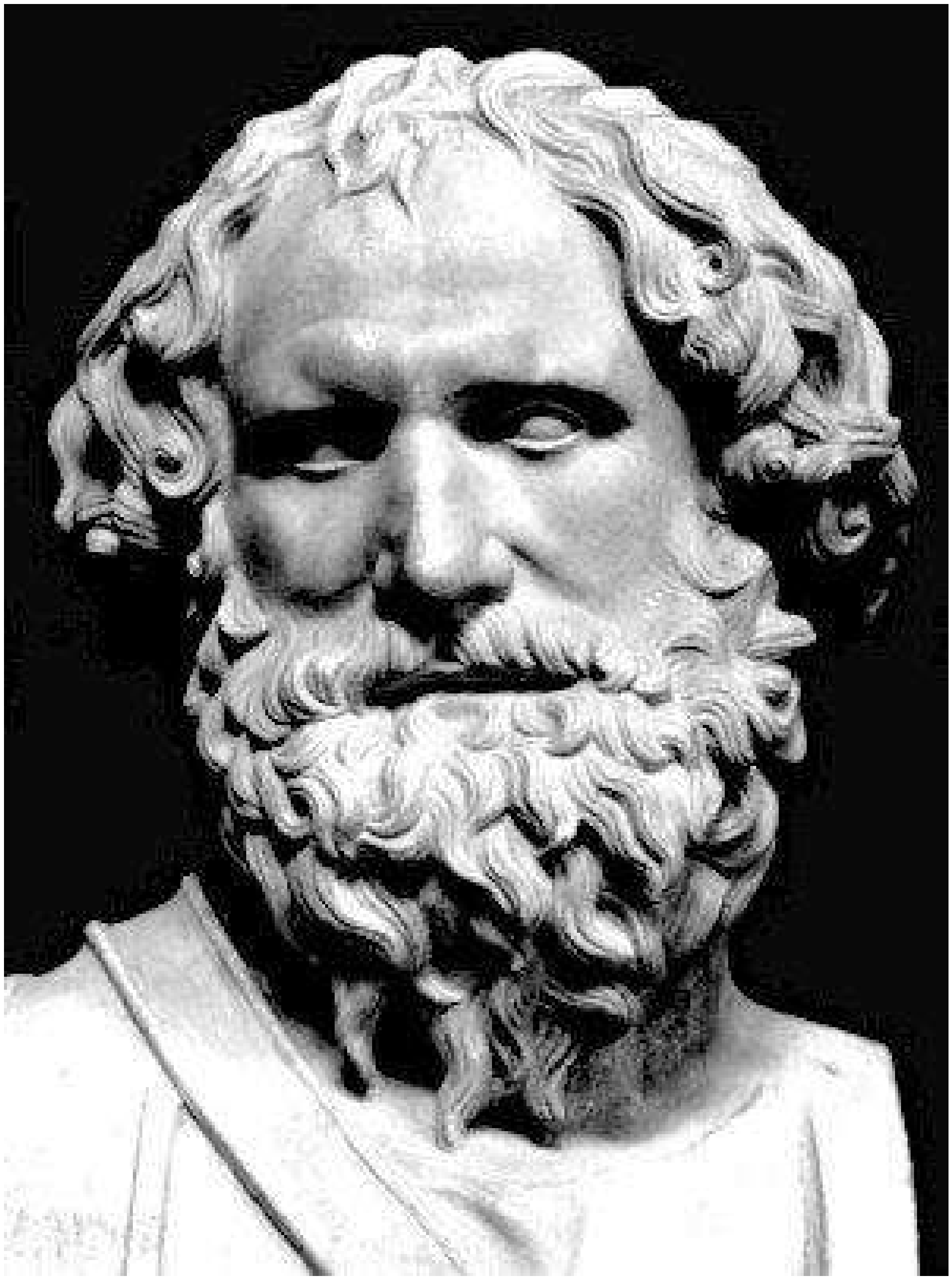

Figure 3.1: **A statue of Archimedes (287 BC - 212 BC**. He invented both differential and integral calculus almost two millennia before Newton, but he was unable to teach his methods to his contemporaries.

are insoluble. For example, within the restrictions of classical geometry, it is impossible to solve the problem of trisecting an angle. In the story of Hieron's crown, Archimedes breaks free from the classical restrictions and shows himself willing to use every conceivable means to achieve his purpose.

One is reminded of Alexander of Macedon who, when confronted with the Gordian Knot, is supposed to have drawn his sword and cut the knot in two! In a book *On Method*, which he sent to his friend Eratosthenes, Archimedes even confesses to cutting out figures from paper and weighing them as a means of obtaining intuition about areas and centers of gravity. Of course, having done this, he then derived the areas and centers of gravity by more rigorous methods.

3.2 Invention of differential and integral calculus

One of Archimedes' great contributions to mathematics was his development of methods for finding the areas of plane figures bounded by curves, as well as methods for finding the areas and volumes of solid figures bounded by curved surfaces. To do this, he employed the "doctrine of limits". For example, to find the area of a circle, he began by inscribing a square inside the circle. The area of the square was a first approximation to the area of the circle. Next, he inscribed a regular octagon and calculated its area, which was a closer approximation to the area of the circle. This was followed by a figure with 16 sides, and then 32 sides, and so on. Each increase in the number of sides brought him closer to the true area of the circle.

Archimedes also circumscribed polygons about the circle, and thus he obtained an upper limit for the area, as well as a lower limit. The true area was trapped between the two limits. In this way, Archimedes showed that the value of pi lies between 223/71 and 220/70.

Sometimes Archimedes' use of the doctrine of limits led to exact results. For example, he was able to show that the ratio between the volume of a sphere inscribed in a cylinder to the volume of the cylinder is 2/3, and that the area of the sphere is 2/3 the area of the cylinder. He was so pleased with this result that he asked that a sphere and a cylinder be engraved on his tomb, together with the ratio, 2/3.

Another problem which Archimedes was able to solve exactly was the problem of calculating the area of a plane figure bounded by a parabola. In his book *On method*, Archimedes says that it was his habit to begin working on a problem by thinking of a plane figure as being composed of a very large number of narrow strips, or, in the case of a solid, he thought of it as being built up from a very large number of slices. This is exactly the approach which is used in integral calculus .

Archimedes must really be credited with the invention of both differential and integral calculus. He used what amounts to integral calculus to find the volumes and areas not only of spheres, cylinders and cones, but also of spherical segments, spheroids, hyperboloids and paraboloids of revolution; and his method for constructing tangents anticipates differential calculus.

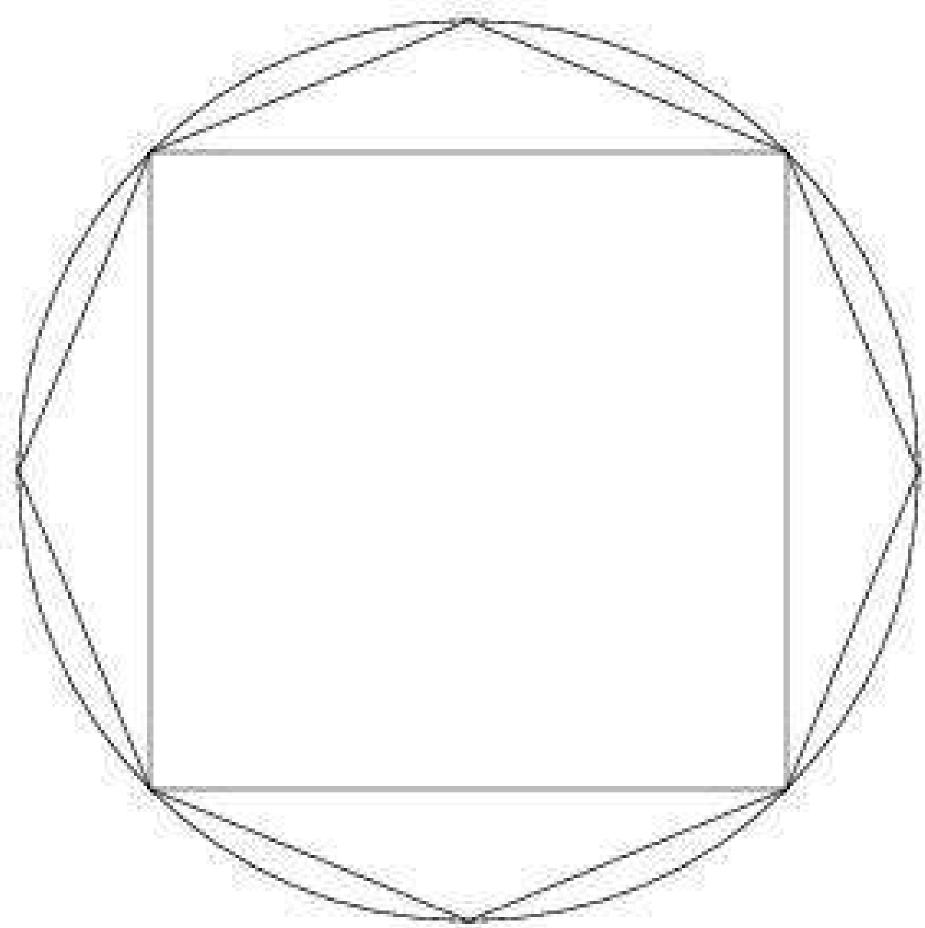

Figure 3.2: **This figure illustrates one of the ways in which Archimedes used his doctrine of limits to calculate the area of a circle. He first inscribed a square within the circle, then an octagon, then a figure with 16 sides, and so on. As the number of sides became very large, the area of these figures (which he could calculate) approached the true area of the circle.**

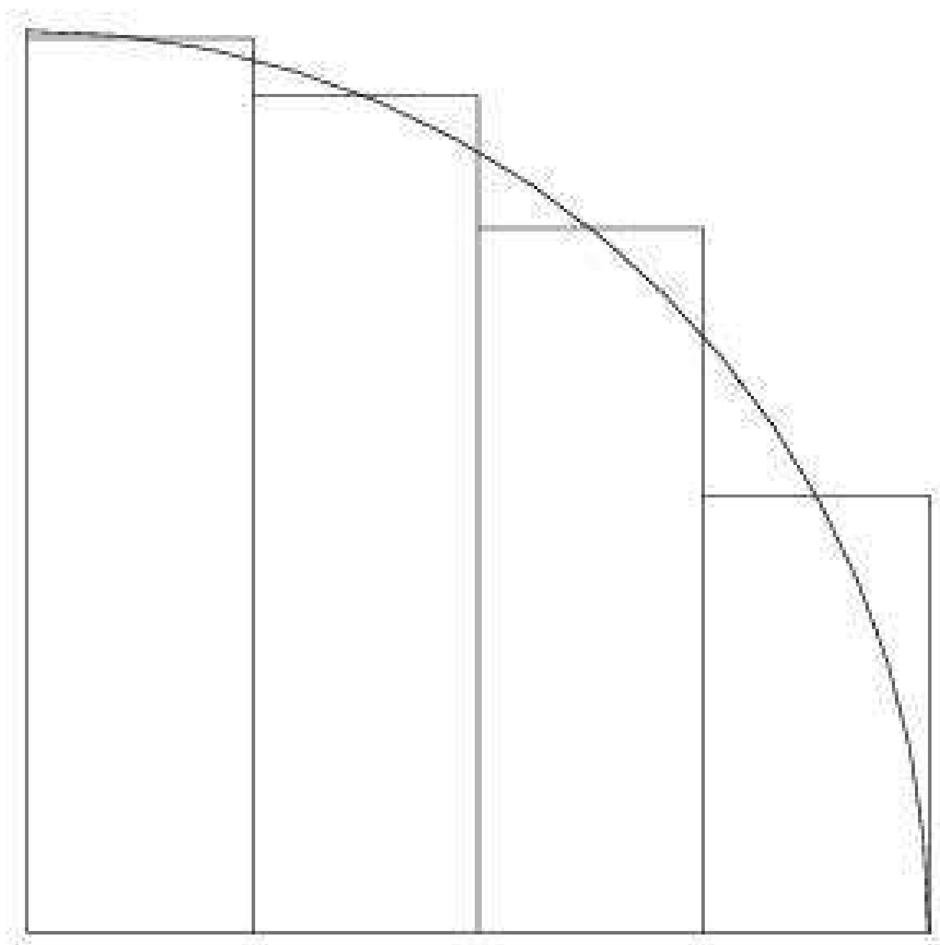

Figure 3.3: **Here we see another way in which Archimedes used his doctrine of limits. He could calculate the areas of figures bounded by curves by dividing up these areas into a large number of narrow strips. As the number of strips became very large, their total area approached the true area of the figure.**

Unfortunately, Archimedes was unable to transmit his invention of the calculus to the other mathematicians of his time. The difficulty was that there was not yet any such thing as algebraic geometry. The Pythagoreans had never recovered from the shock of discovering irrational numbers, and they had therefore abandoned algebra in favor of geometry. The union of algebra and geometry, and the development of a calculus which even non-geniuses could use, had to wait for Descartes, Fermat, Newton and Leibniz.

3.3 Statics and hydrostatics

Archimedes was the father of statics (as well as of hydrostatics). He calculated the centers of gravity of many kinds of figures, and he made a systematic, quantitative study of the properties of levers. He is supposed to have said: "Give me a place to stand on, and I can move the world!" This brings us to another of the stories about Archimedes: According to the story, Hieron was a bit sceptical, and he challenged Archimedes to prove his statement by moving something rather enormous, although not necessarily as large as the world. Archimedes good-humoredly accepted the challenge, hooked up a system of pulleys to a fully-loaded ship in the harbor, seated himself comfortably, and without excessive effort he singlehandedly pulled the ship out of the water and onto the shore.

Archimedes had a very compact notation for expressing large numbers. Essentially his system was the same as our own exponential notation, and it allowed him to handle very large numbers with great ease. In a curious little book called *The Sand Reckoner*, he used this notation to calculate the number of grains of sand which would be needed to fill the universe. (Of course, he had to make a crude guess about the size of the universe.) Archimedes wrote this little book to clarify the distinction between things which are very large but finite and things which are infinite. He wanted to show that nothing finite - not even the number of grains of sand needed to fill the universe - is too large to be measured and expressed in numbers. *The Sand Reckoner* is important as an historical document, because in it Archimedes incidentally mentions the revolutionary heliocentric model of Aristarchus, which does not occur in the one surviving book by Aristarchus himself.

In addition to his mathematical genius, Archimedes showed a superb mechanical intuition, similar to that of Leonardo da Vinci. Among his inventions are a planetarium and an elegant pump in the form of a helical tube. This type of pump is called the "screw of Archimedes", and it is still in use in Egypt. The helix is held at an angle to the surface of the water, with its lower end half-immersed. When the helical tube is rotated about its long axis, the water is forced to flow uphill!

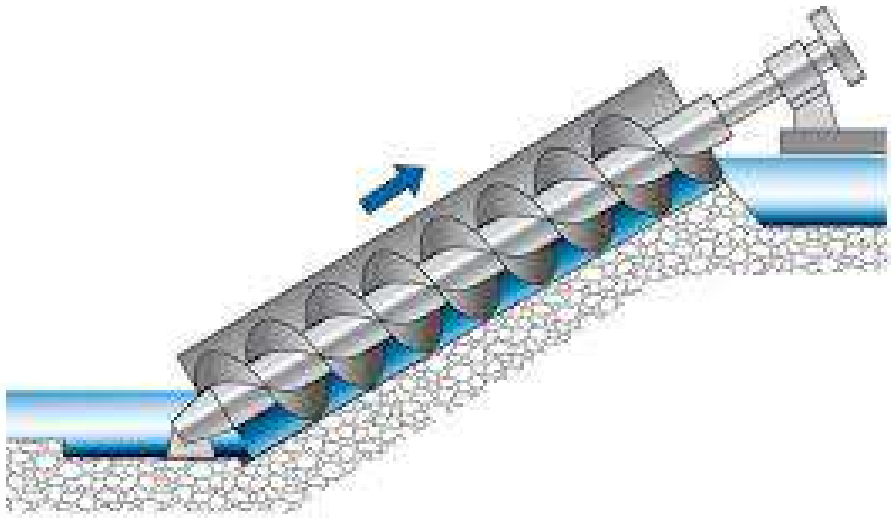

Figure 3.4: **Archimedes' screw, the helical pump which he invented, is still in use today.**

3.4 Don't disturb my circles!

His humanity and his towering intellect brought Archimedes universal respect, both during his own lifetime and ever since. However, he was not allowed to live out his life in peace; and the story of his death is both dramatic and symbolic:

In c. 212 B.C., Syracuse was attacked by a Roman fleet. The city would have fallen quickly if Archimedes had not put his mind to work to think of ways to defend his countrymen. He devised systems of mirrors which focused the sun's rays on the attacking ships and set them on fire, and cranes which plucked the ships from the water and overturned them.

In the end, the Romans hardly dared to approach the walls of Syracuse. However, after several years of siege, the city fell to a surprise attack. Roman soldiers rushed through the streets, looting, burning and killing. One of them found Archimedes seated calmly in front of diagrams sketched in the sand, working on a mathematical problem. When the soldier ordered him to come along, the great mathematician is supposed to have looked up from his work and replied: "Don't disturb my circles." The soldier immediately killed him.

The death of Archimedes and the destruction of the Hellenistic civilization illustrate the fragility of civilization. It was only a short step from Archimedes to Galileo and Newton; only a short step from Eratosthenes to Columbus, from Aristarchus to Copernicus, from Aristotle to Darwin or from Hippocrates to Pasteur. These steps in the cultural evolution of mankind had to wait nearly two thousand years, because the brilliant Hellenistic civilization was destroyed, and Europe was plunged back into the dark ages.

Figure 3.5: **Machines used by Archimedes to defend Syracuse against the Roman attack.**

Figure 3.6: **"The death of Archimedes", a painting by Thomas Degeorge.**

Figure 3.7: **The Great Library of Alexandria was partially burned during an attack by Julius Caesar in 48 BC. Much of the library survived, but during the Roman period which followed, it declined through neglect. With the destruction of the advanced Hellenistic civilization, much knowledge was lost. Had it survived, the history of human culture and science would have been very different.**

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Chapter 4

AL-KHWARIZMI

Wikipedia says of him:

“Muhammad ibn Musa al-Khwarizmi (c.780-c.850), Arabized as al-Khwarizmi and formerly Latinized as Algorithmi, was a Persian polymath who produced vastly influential works in mathematics, astronomy, and geography. Around 820 CE he was appointed as the astronomer and head of the library of the House of Wisdom in Baghdad.

“Al-Khwarizmi’s popularizing treatise on algebra (The Compendious Book on Calculation by Completion and Balancing, c. 813-833 CE) presented the first systematic solution of linear and quadratic equations. One of his principal achievements in algebra was his demonstration of how to solve quadratic equations by completing the square, for which he provided geometric justifications. Because he was the first to treat algebra as an independent discipline and introduced the methods of ‘reduction’ and ‘balancing’ (the transposition of subtracted terms to the other side of an equation, that is, the cancellation of like terms on opposite sides of the equation), he has been described as the father or founder of algebra. The term algebra itself comes from the title of his book (the word al-jabr meaning ‘completion’ or ‘rejoining’). His name gave rise to the terms algorism and algorithm, as well as Spanish and Portuguese terms algoritmo, and Spanish guarismo and Portuguese algarismo meaning ‘digit’.

“In the 12th century, Latin translations of his textbook on arithmetic (*Algorithmo de Numero Indorum*) which codified the various Indian numerals, introduced the decimal positional number system to the Western world. The *Compendious Book on Calculation by Completion and Balancing*, translated into Latin by Robert of Chester in 1145, was used until the sixteenth century as the principal mathematical text-book of European universities.

“In addition to his best-known works, he revised Ptolemy’s *Geography*, listing the longitudes and latitudes of various cities and localities. He further produced a set of astronomical tables and wrote about calendaric works, as well as the astrolabe and the sundial. He also made important contributions to trigonometry, producing accurate sine and cosine tables...”

Figure 4.1: **Statue of al-Khwarizmi in front of the Faculty of Mathematics of Amirkabir University of Technology in Tehran. Iran.**

Figure 4.2: **A stamp issued September 6, 1983 in the Soviet Union, commemorating al-Khwarizmi's (approximate) 1200th birthday.**

Figure 4.3: **Statue of Al-Khwarizmi in Uzbekistan.**

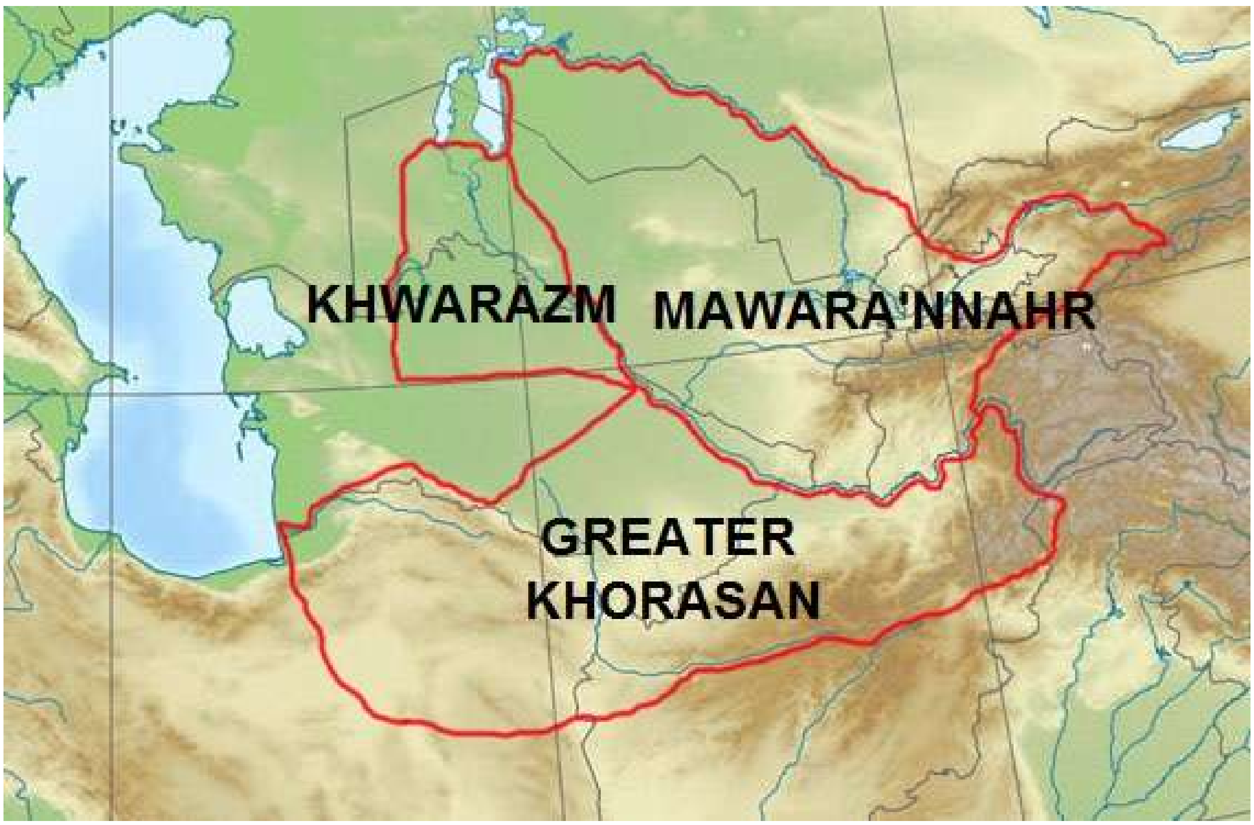

Figure 4.4: **This map shows Khwarazm, the place of Al-Khwarizmi's birth. It lies to the east of the Caspian Sea.**

Figure 4.5: **Scholars at the library of the House of Wisdom in Baghdad. Illustration by Yahyá al-Wasiti, 1237.**

4.1 Al-Khwarizmi's life

Muhammad ibn Musa al-Khwarizmi (c.780-c.850) was born in the Persian province of Khwarazm, shown on the map in Figure 4.4. During his lifetime, Muslim conquests made Baghdad the most important intellectual center, and scholars from as far away as China were attracted to the Arab capitol. Al-Khwarizmi also traveled to Baghdad, where he worked at the "House of Wisdom", which had been established by Caliph al-Ma'mun. Here he was able to study both Greek and Sanskrit manuscripts on science and mathematics, and to carry out his highly influential original work.

4.2 The father of algebra

Al-Khwarizmi has been called "the father of algebra". J. J. O'Connor and E. F. Robertson wrote in the MacTutor History of Mathematics archive:

"Perhaps one of the most significant advances made by Arabic mathematics began at this time with the work of al-Khwarizmi, namely the beginnings of algebra. It is important to understand just how significant this new idea was. It was a revolutionary move away from the Greek concept of mathematics which was essentially geometry. Algebra was a unifying theory which allowed rational numbers, irrational numbers, geometrical magnitudes, etc., to all be treated as 'algebraic objects'. It gave mathematics a whole new development path so much broader in concept to that which had existed before, and provided a vehicle for future development of the subject. Another important aspect of the introduction of algebraic ideas was that it allowed mathematics to be applied to itself in a way which had not happened before."

In modern terms, one of the methods introduced by al-Khwarizmi corresponds to moving terms in an equation freely to the right or left of the equal sign in an equation, with a change of sign. He also introduced a systematic method for solving quadratic equations. However, modern notation had not been invented at the time, and al-Khwarizmi described all of the operations for solving a problem in words, even using words rather than symbols for numbers. He introduced the decimal positional number system to the west. When we speak of "Arabic numerals", it is because of his work. However, positional number systems had long been in use, both in Mesopotamia and in India.

Wikipedia states that:

"Al-Khwarizmi's work on arithmetic was responsible for introducing the Arabic numerals, based on the Hindu-Arabic numeral system developed in Indian mathematics, to the Western world. The term 'algorithm' is derived from the algorism, the technique of performing arithmetic with Hindu-Arabic numerals developed by al-Khwarizmi. Both 'algorithm' and 'algorism' are derived from the Latinized forms of al-Khwarizmi's name, Algoritmi and Algorismi, respectively."

In 1145. Al-Khwarizmi's book *Compendious Book on Calculation by Completion and Balancing,* was translated into Latin by Robert of Chester, and for many centuries it was the principle book on mathematics used at European universities.

4.3 Contributions to astronomy

Al-Khwarizmi's book on astronomy, *Zij al-Sindhind*, consisted of approximately 37 chapters on calendars and calculations. and 116 tables. The tables give the values of trigonometric functions and calculated locations of the sun, moon and the five planets that were known at the time. The fact that al-Khwarizmi performed original calculations of these positions marked a turning point in Islamic astronomy. The original manuscript has been lost, but copies of a Latin translation, thought to be by Adalard of Bath, exist in four European libraries, in Chartres, Paris, Madrid and Oxford.

4.4 Contributions to geography

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Chapter 5

OMAR KHAYYAM

5.1 Omar's family and education

Omar Khayyam (1048-1131) was born in the city of Nishapur, which is located in the northern part of Persia, or present-day Iran. His father was a wealthy physician, who paid a tutor to give his son Omar an excellent education. The tutor, Bahmanyar bin Marzban, was a Zoroastrian, and had been a student of the great physician, scientist, and philosopher Avicenna. Thus Omar Khayyam received an unusually good education in science, philosophy and mathematics.

In 1066, Omar's father died, and his tutor also died soon afterwards. Two years later, in 1068, Omar joined a caravan for a three-month journey to Samarkand, then a great center of learning in Uzbekistan. He arrived there at the age of 20, and introduced himself to the governor of the city, Abe Tapir, an old friend of his father. Tahir soon recognized Omar's extraordinary mathematical ability and have him a job in his office. Soon afterwards, Omar was promoted to a job in the king's treasury.

Two years later, in 1070, Omar Khayyam published one of his greatest mathematical works, *Treatise on Demonstration of Problems of Algebra and Balancing*. This book contains a discussion of cubic equations, and it shows that they may have more than one root. Like other Islamic mathematicians, Omar did not consider negative roots. The book established Omar's reputation as a mathematician, and his fame spread throughout Persia,

5.2 Invited to Isfahan

In 1073, the young but already famous Omar received an invitation to come to Persia's capitol city, Isfahan. The invitation came from the two most powerful men of the Seljuk Empire, Malik Shah, Sultan of the empire, and Nizam al-Mulk, his vizier. Omar's job was to produce a calendar that would be valid over a long period, without the need for adjustment. He was given an enormous salary, and the means to hire many assistants. With these ample means, he recruited many talented scientists and founded an astronomical observatory.

Omar measured the length of the tropical year with extraordinary accuracy. His value, 365.2422 days. is extremely close to the currently-accepted value.

5.3 Linking algebra and geometry

The Pythagoreans had abandoned algebra when they discovered irrational numbers, such as $\sqrt{2}$, since their religion was based on the idea rationality both in mathematics and in the social sphere. Ancient Greek mathematics concentrated on geometry.

The union of geometry and algebra was pioneered in the western world by Pierre de Fermat and René Descartes. However, both Fermat and Descartes were preceded in the Islamic world by Omar Khayyam, whose mathematical work united algebra and geometry.

5.4 Omar Khayyam anticipates non-Euclidean geometry

Throughout history, many authors have doubted that Euclid's fifth postulate concerning parallel lines was necessary. Many, including Khayyam, have tried to prove the fifth postulate from the first four. Omar's attempt is particularly interesting because in it we can see the first glimmerings on non-Euclidean geometry, later developed in Europe by Gauss and Riemann. One of Omar's diagrams is shown in Figure 5.6.

5.5 The Rubáiyát

translated by Edward Fitzgerald. Only the first few verses are shown here

Awake! for Morning in the Bowl of Night
Has flung the Stone that puts the Stars to Flight:
And Lo! the Hunter of the East has caught
The Sultan's Turret in a Noose of Light.

Dreaming when Dawn's Left Hand was in the Sky
I heard a voice within the Tavern cry,
"Awake, my Little ones, and fill the Cup
Before Life's Liquor in its Cup be dry."

And, as the Cock crew, those who stood before
The Tavern shouted – "Open then the Door!
You know how little while we have to stay,

And, once departed, may return no more."

Now the New Year reviving old Desires,
The thoughtful Soul to Solitude retires,
Where the White Hand of Moses on the Bough
Puts out, and Jesus from the Ground suspires.

Iram indeed is gone with all its Rose,
And Jamshyd's Sev'n-ring'd Cup where no one Knows;
But still the Vine her ancient ruby yields,
And still a Garden by the Water blows.

And David's Lips are lock't; but in divine
High piping Pehlevi, with "Wine! Wine! Wine!
Red Wine!" – the Nightingale cries to the Rose
That yellow Cheek of hers to incarnadine.

Come, fill the Cup, and in the Fire of Spring
The Winter Garment of Repentance fling:
The Bird of Time has but a little way
To fly – and Lo! the Bird is on the Wing.

Whether at Naishapur or Babylon,
Whether the Cup with sweet or bitter run,
The Wine of Life keeps oozing drop by drop,
The Leaves of Life kep falling one by one.

Morning a thousand Roses brings, you say;
Yes, but where leaves the Rose of Yesterday?
And this first Summer month that brings the Rose
Shall take Jamshyd and Kaikobad away.

But come with old Khayyam, and leave the Lot
Of Kaikobad and Kaikhosru forgot:
Let Rustum lay about him as he will,
Or Hatim Tai cry Supper – heed them not.

With me along the strip of Herbage strown
That just divides the desert from the sown,
Where name of Slave and Sultan is forgot –
And Peace is Mahmud on his Golden Throne!

A Book of Verses underneath the Bough,

A Jug of Wine, a Loaf of Bread, – and Thou
Beside me singing in the Wilderness –
Oh, Wilderness were Paradise enow!

Some for the Glories of This World; and some
Sigh for the Prophet's Paradise to come;
Ah, take the Cash, and let the Promise go,
Nor heed the rumble of a distant Drum!

Were it not Folly, Spider-like to spin
The Thread of present Life away to win –
What? for ourselves, who know not if we shall
Breathe out the very Breath we now breathe in!

Look to the Rose that blows about us – "Lo,
Laughing," she says, "into the World I blow:
At once the silken Tassel of my Purse
Tear, and its Treasure on the Garden throw."

The Worldly Hope men set their Hearts upon
Turns Ashes – or it prospers; and anon,
Like Snow upon the Desert's dusty Face
Lighting a little Hour or two – is gone.

And those who husbanded the Golden Grain,
And those who flung it to the Winds like Rain,
Alike to no such aureate Earth are turn'd
As, buried once, Men want dug up again.

Think, in this batter'd Caravanserai
Whose Doorways are alternate Night and Day,
How Sultan after Sultan with his Pomp
Abode his Hour or two and went his way.

They say the Lion and the Lizard keep
The Courts where Jamshyd gloried and drank deep:
And Bahram, that great Hunter – the Wild Ass
Stamps o'er his Head, but cannot break his Sleep.

I sometimes think that never blows so red
The Rose as where some buried Caesar bled;
That every Hyacinth the Garden wears
Dropt in its Lap from some once lovely Head.

And this delightful Herb whose tender Green
Fledges the River's Lip on which we lean –
Ah, lean upon it lightly! for who knows
From what once lovely Lip it springs unseen!

Ah, my Beloved, fill the Cup that clears
To-day of past Regrets and future Fears –
To-morrow? – Why, To-morrow I may be
Myself with Yesterday's Sev'n Thousand Years.

Lo! some we loved, the loveliest and best
That Time and Fate of all their Vintage prest,
Have drunk their Cup a Round or two before,
And one by one crept silently to Rest.

And we, that now make merry in the Room
They left, and Summer dresses in new Bloom,
Ourselves must we beneath the Couch of Earth
Descend, ourselves to make a Couch – for whom?

Ah, make the most of what we may yet spend,
Before we too into the Dust descend;
Dust into Dust, and under Dust, to lie;
Sans Wine, sans Song, sans Singer, and – sans End!

Alike for those who for To-day prepare,
And those that after some To-morrow stare,
A Muezzin from the Tower of Darkness cries
"Fools! Your Reward is neither Here nor There!"

Why, all the Saints and Sages who discuss'd
Of the Two Worlds so learnedly, are thrust
Like foolish Prophets forth; their Works to Scorn
Are scatter'd, and their Mouths are stopt with Dust.

Oh, come with old Khayyam, and leave the Wise
To talk; one thing is certain, that Life flies;
One thing is certain, and the Rest is Lies;
The Flower that once has blown forever dies.

Myself when young did eagerly frequent
Doctor and Saint, and heard great Argument

About it and about; but evermore
Came out by the same Door as in I went.

With them the Seed of Wisdom did I sow,
And with my own hand labour'd it to grow:
And this was all the Harvest that I reap'd –
"I came like Water and like Wind I go."

Into this Universe, and Why not knowing,
Nor Whence, like Water willy-nilly flowing:
And out of it, as Wind along the Waste,
I know not Whither, willy-nilly blowing.

Up from Earth's Centre through the Seventh Gate
I rose, and on the Throne of Saturn sate,
And many Knots unravel'd by the Road;
But not the Master-Knot of Human Fate.

There was the Door to which I found no Key:
There was the Veil through which I could not see:
Some little talk awhile of Me and Thee
There was – and then no more of Thee and Me.

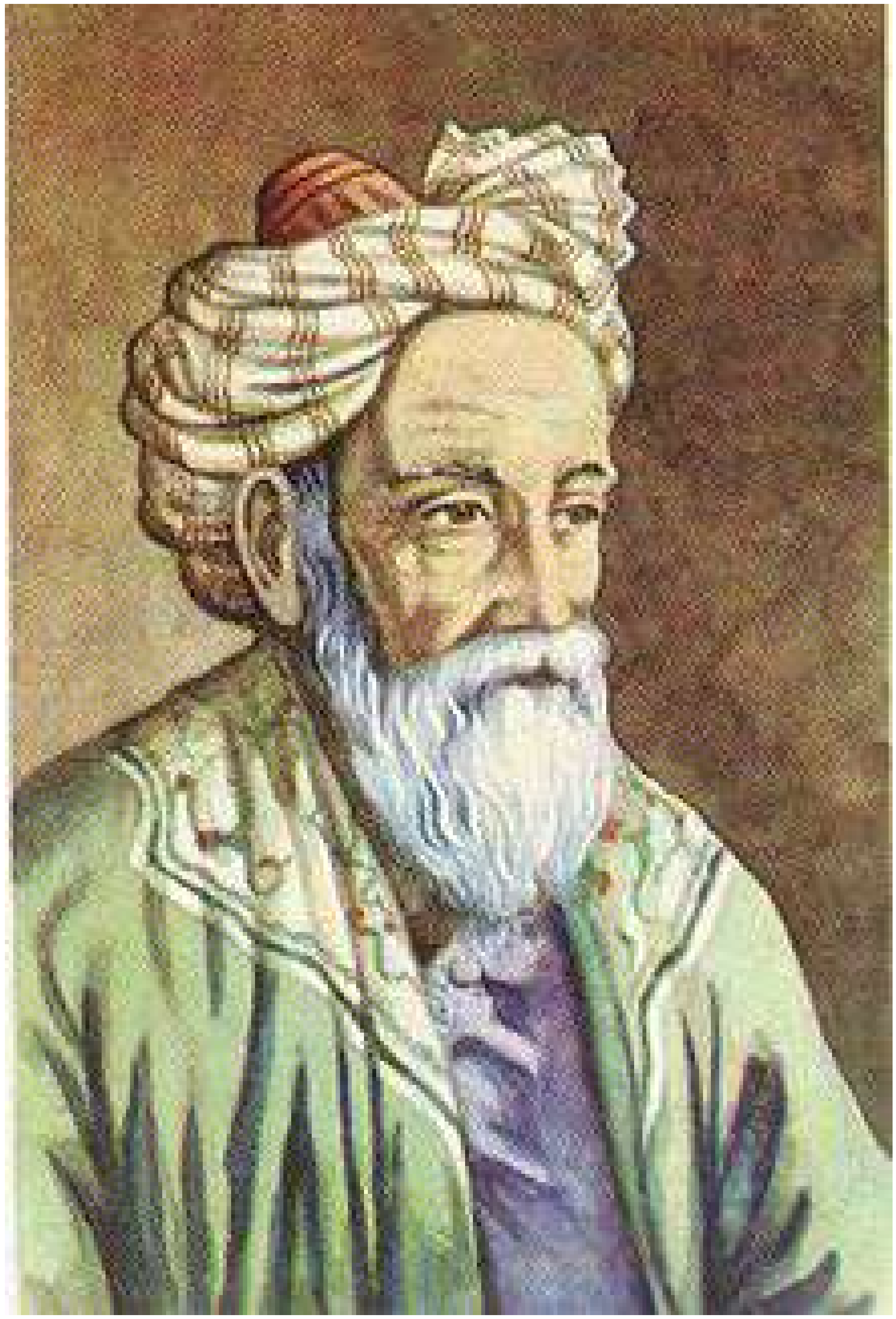

Figure 5.1: **Omar Khayyam was a Persian mathematician, astronomer and poet. His work in mathematics was notable for his solutions to cubic equations, his understanding of the binomial theorem, and his discussions of the axioms of Euclid. As an astronomer, he directed the building of an observatory to reform the Persian calendar. Omar Khayyam's long poem, *Rubaiyat*, is known to western readers through Edward Fitzgerald's brilliant translation.**

Figure 5.2: **Omar Khayyam.**

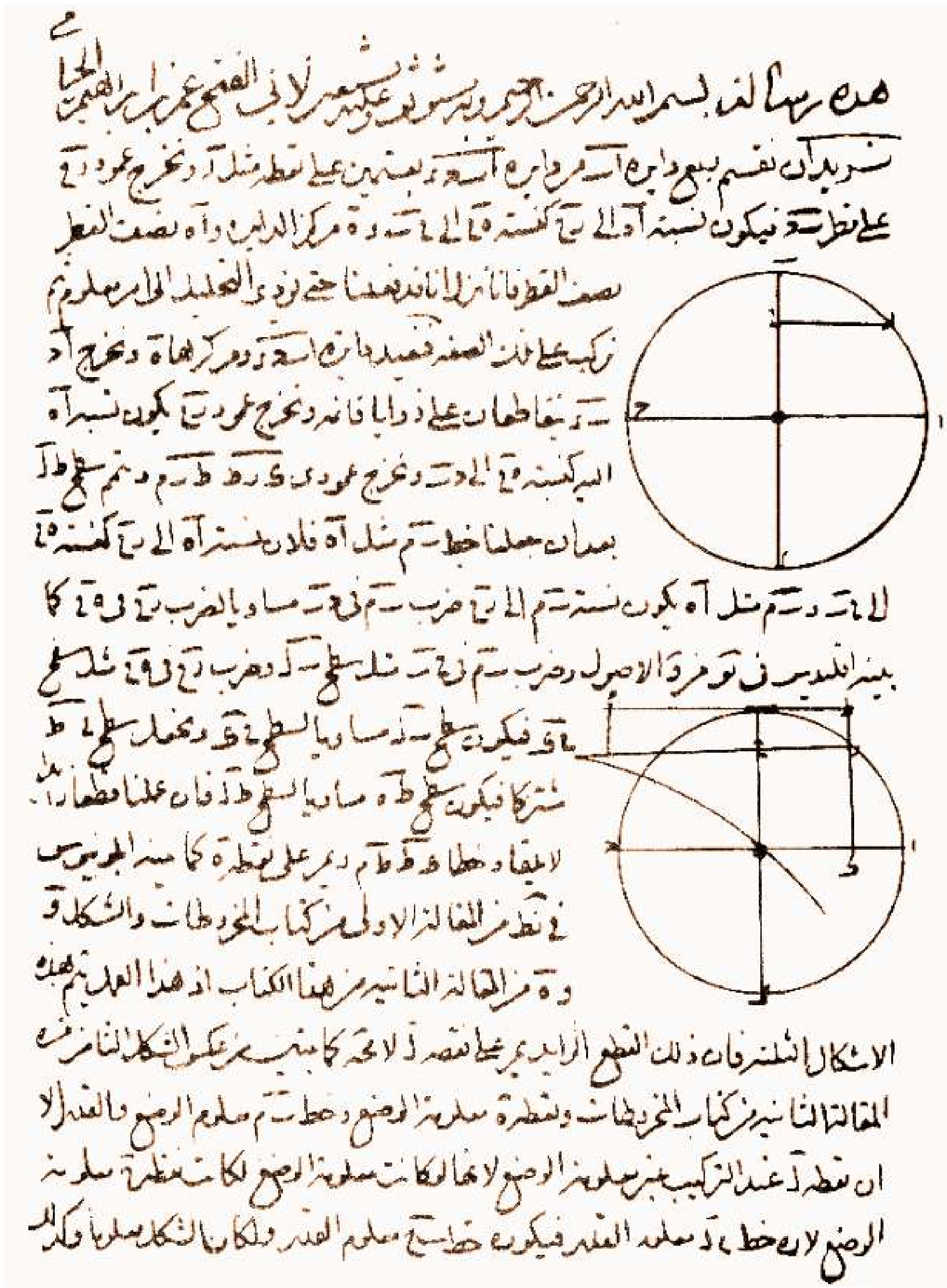

Figure 5.3: **"Cubic equation and intersection of conic sections" the first page of a two-chaptered manuscript kept in Tehran University.**

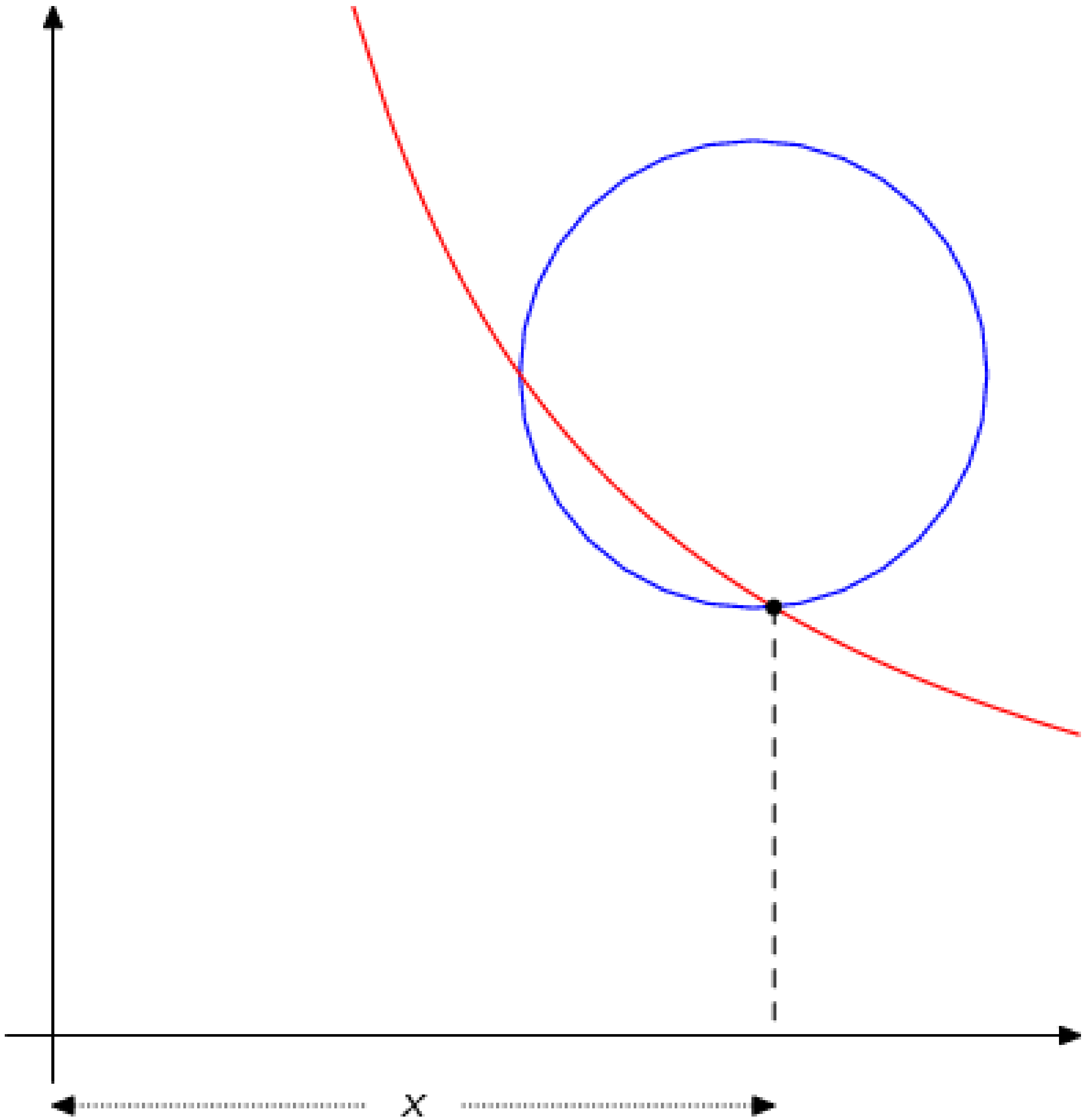

Figure 5.4: **Omar Khayyam's construction of a solution to the cubic equation $x^3+2x = 2x^2+2$. The intersection point produced by the circle and the hyperbola determine the desired segment.**

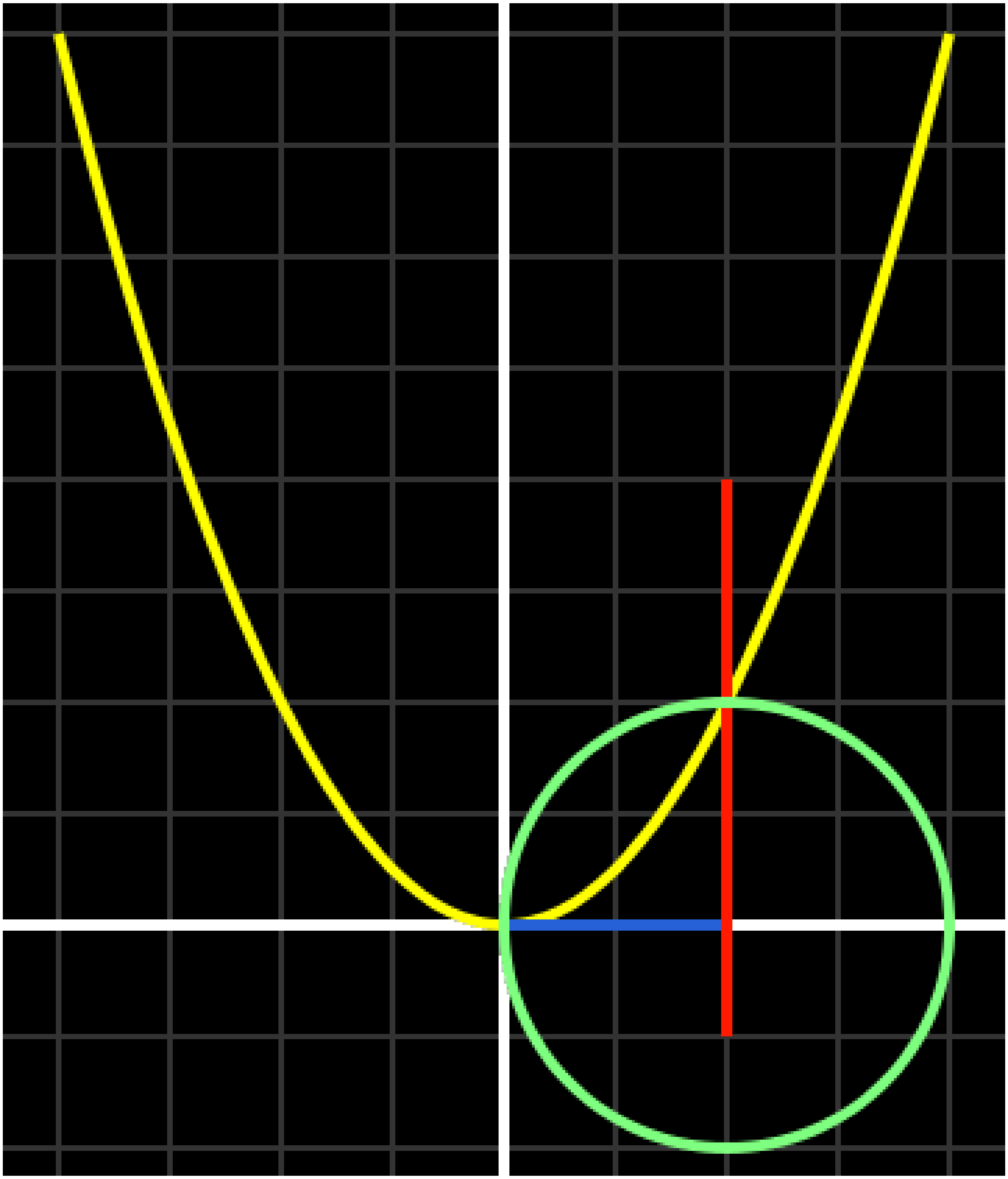

Figure 5.5: **In the language of modern mathematics, Khayyam's solution to the equation $x^3 + a^2x = b$ features a parabola of equation $x^2 = ay$, a circle with diameter b/a^2, and a vertical line through the intersection point. The solution is given by the distance on the x-axis between the origin and the (red) vertical line. Image by Pieter Kuiper.**

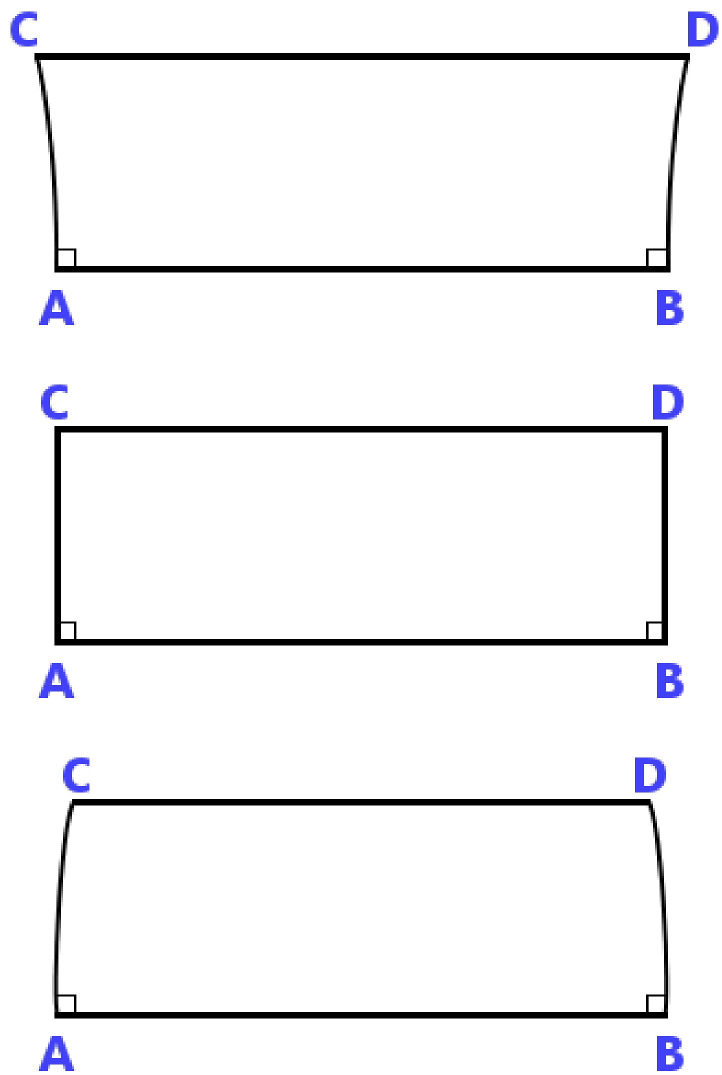

Figure 5.6: **In Omar Khayyam's discussion of Euclid's postulate concerning parallel lines, we see the first glimmering of non-Euclidean geometry. The figure shows one of Khayyam's diagrams. Lines which are locally parallel at one point meet at another point when they are drawn on curved surfaces.**

Figure 5.7: **Statue of Omar Khayyam in Bucharest.**

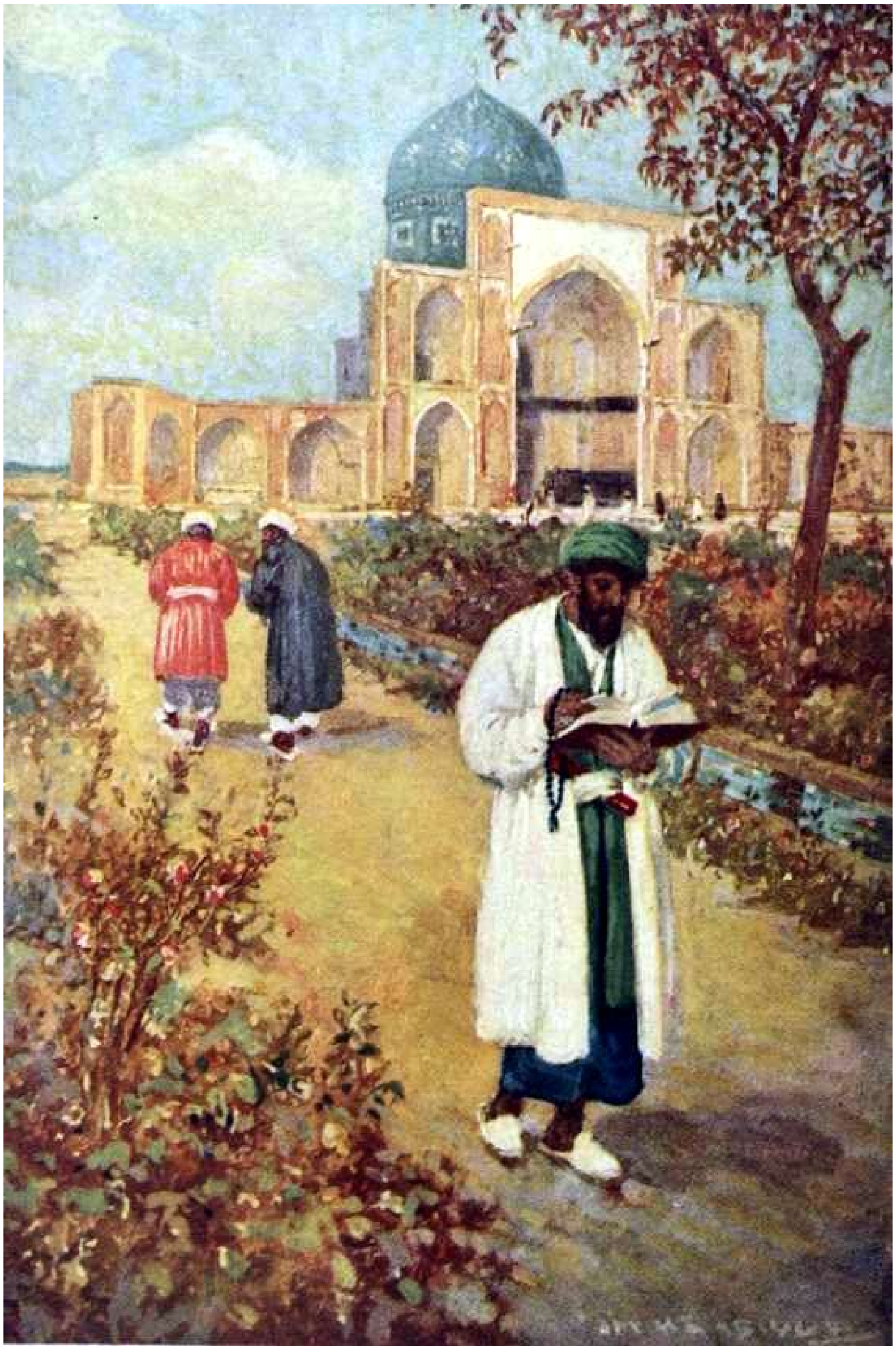

Figure 5.8: **"At the Tomb of Omar Khayyam" by Jay Hambidge (1911).**

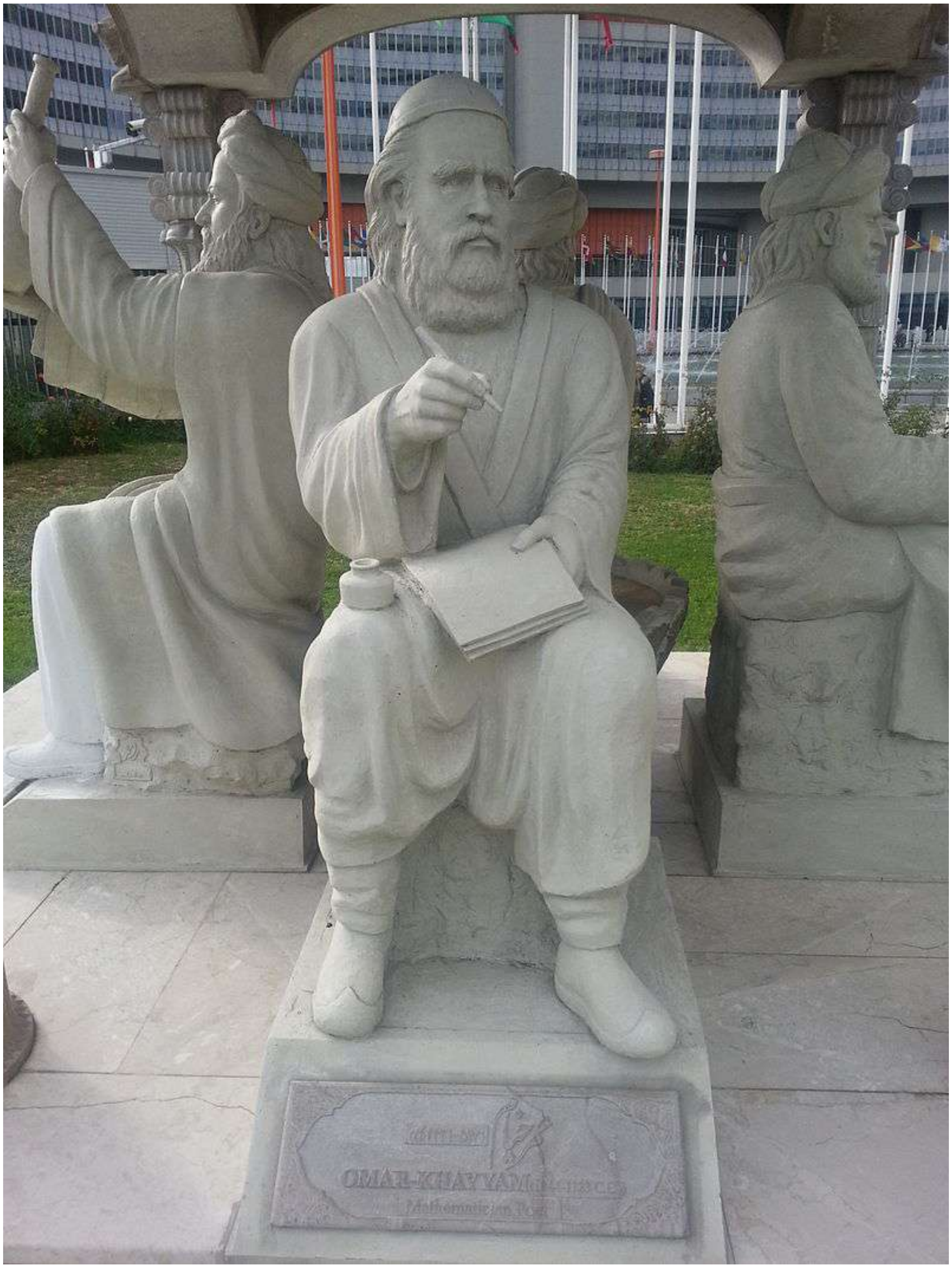

Figure 5.9: **The statue of Khayyam in United Nations Office in Vienna as a part of Persian Scholars Pavilion donated by Iran.**

Suggestions for further reading

1. Edward FitzGerald (translator) *The Rubaiyat of Omar Khayyam* Howard Willford Bell, 1901
2. Victor J. Katz *A History of Mathematics: An Introduction* HarperCollins College Publishers, New York, 1993
3. Roshdi Rashed (Editor) *Encyclopedia of the History of Arabic science* Routledge, 1996
4. *History of Astronomy - Middle East* ephemeris.com, 2003
5. Hazhir Teimourian *Omar Khayyam: Poet, Rebel, Astronomer* The History Press, 2008
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Chapter 6

RENÉ DESCARTES

6.1 Uniting geometry and algebra

Until the night of November 10, 1619, algebra and geometry were separate disciplines. On that autumn evening, the troops of the Elector of Bavaria were celebrating the Feast of Saint Martin at the village of Neuberg in Bohemia. With them was a young Frenchman named René Descartes (1596-1659), who had enlisted in the army of the Elector in order to escape from Parisian society. During that night, Descartes had a series of dreams which, as he said later, filled him with enthusiasm, converted him to a life of philosophy, and put him in possession of a wonderful key with which to unlock the secrets of nature.

The program of natural philosophy on which Descartes embarked as a result of his dreams led him to the discovery of analytic geometry, the combination of algebra and geometry. Essentially, Descartes' method amounted to labeling each point in a plane with two numbers, x and y. These numbers represented the distance between the point and two perpendicular fixed lines, (the coordinate axes). Then every algebraic equation relating x and y generated a curve in the plane.

Descartes realized the power of using algebra to generate and study geometrical figures; and he developed his method in an important book, which was among the books that Newton studied at Cambridge. Descartes' pioneering work in analytic geometry paved the way for the invention of differential and integral calculus by Fermat, Newton and Leibniz. (Besides taking some steps towards the invention of calculus, the great French mathematician, Pierre de Fermat (1601-1665), also discovered analytic geometry independently, but he did not publish this work.)

Analytic geometry made it possible to treat with ease the elliptical orbits which Kepler had introduced into astronomy, as well as the parabolic trajectories which Galileo had calculated for projectiles.

Descartes also worked on a theory which explained planetary motion by means of "vortices"; but this theory was by no means so successful as his analytic geometry, and eventually it had to be abandoned.

Figure 6.1: **Portrait of René Descartes, after Frans Hals.**

Figure 6.2: **Queen Christina (at the table on the right) in discussion with French philosopher René Descartes. (Romanticized painting by Nils Forsberg (1842-1934), after Pierre Louis Dumesnil.**

Figure 6.3: **Queen Christina of Sweden in a portrait by Sébastien Bourdon.**

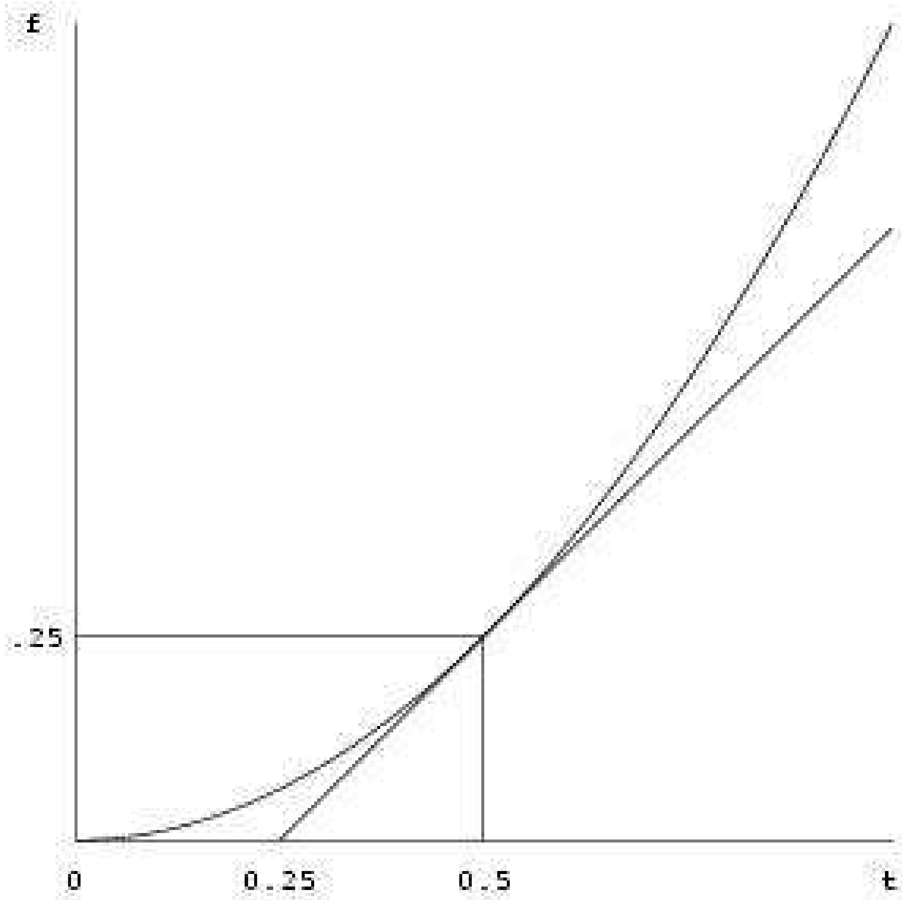

Figure 6.4: **This figure shows the parabola $f = t^2$ plotted using the method of Descartes. Values of f are measured on the vertical axis, while values of t are measured along the horizontal axis. The curve tells us the value of f corresponding to every value of t. For example, when t = 1, f = 1, while when t = 2, f = 4. If we want to know the value of $f = t^2$ corresponding to a particular value of t, we go vertically up to the curve from the horizontal axis, and then horizontally left from the curve to the vertical axis.**

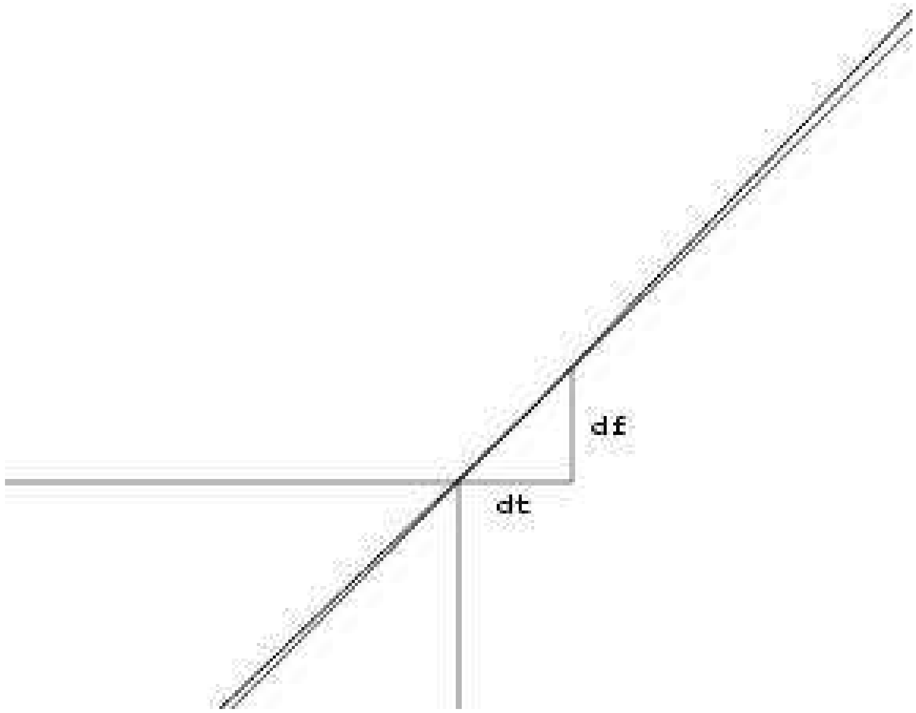

Figure 6.5: **The slope of a curve at a given point t is defined as the limit of the ratio df/dt, when dt becomes infinitesimally small.**

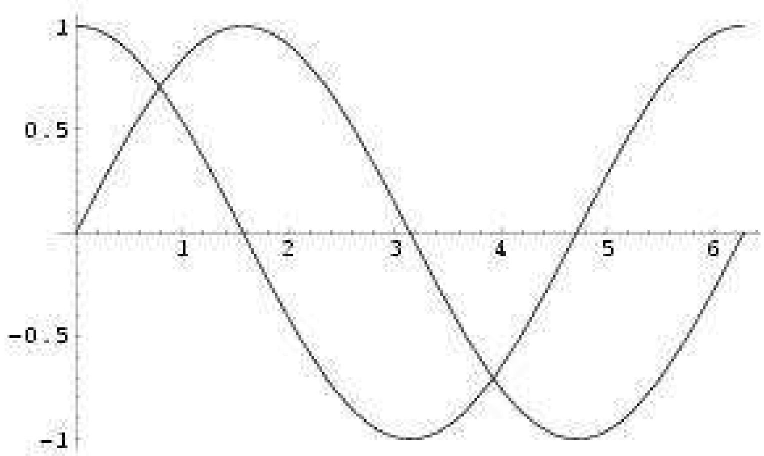

Figure 6.6: **This figure shows the trigonometric functions f = sin(t) and f = cos(t) plotted as functions of t using the method of Descartes. The functions were first tabulated by the Egyptian astronomer Hipparchus.**

6.2 Descartes' work on Optics, physiology and philosophy

Descartes did important work in optics, physiology and philosophy. In philosophy, he is the author of the famous phrase *"Cogito, ergo sum"*, "I think; therefore I exist", which is the starting point for his theory of knowledge. He resolved to doubt everything which it was possible to doubt; and finally he was reduced to knowledge of his own existence as the only real certainty.

René Descartes died tragically through the combination of two evils which he had always tried to avoid: cold weather and early rising. Even as a student, he spent a large portion of his time in bed. He was able to indulge in this taste for a womblike existence because his father had left him some estates in Brittany. Descartes sold these estates and invested the money, from which he obtained an ample income. He never married, and he succeeded in avoiding responsibilities of every kind.

6.3 Descartes' tragic death

Descartes might have been able to live happily in this way to a ripe old age if only he had been able to resist a flattering invitation sent to him by Queen Christina of Sweden. Christina, the intellectual and strong-willed daughter of King Gustav Adolf, was determined to bring culture to Sweden, much to the disgust of the Swedish noblemen, who considered that money from the royal treasury ought to be spent exclusively on guns and fortifications. Unfortunately for Descartes, he had become so famous that Queen Christina wished to take lessons in philosophy from him; and she sent a warship to fetch him from

Holland, where he was staying. Descartes, unable to resist this flattering attention from a royal patron, left his sanctuary in Holland and sailed to the frozen north.

The only time Christina could spare for her lessons was at five o'clock in the morning, three times a week. Poor Descartes was forced to get up in the utter darkness of the bitterly cold Swedish winter nights to give Christina her lessons in a draughty castle library; but his strength was by no means equal to that of the queen, and before the winter was over he had died of pneumonia.

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2. Zev Bechler, *Newton's Physics and the Conceptual Structure of the Scientific Revolution*, Kluwer, Dordrecht, (1991).
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11. Brian Vickers, *English Science, Bacon to Newton*, Cambridge University Press, (1989).
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19. Lesley Murdin, *Under Newton's Shadow; Astronomical Practices in the Seventeenth Century*, Hilger, Bristol, (1985).
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21. Sir Oliver Lodge, *Pioneers of Science*, Dover, New York (1960).

Chapter 7

NEWTON

7.1 Newton's early life

On Christmas day in 1642 (the year in which Galileo died), a recently widowed woman named Hannah Newton gave birth to a premature baby at the manor house of Woolsthorpe, a small village in Lincolnshire, England. Her baby was so small that, as she said later, "he could have been put into a quart mug", and he was not expected to live. He did live, however, and lived to achieve a great scientific synthesis, uniting the work of Copernicus, Brahe, Kepler, Galileo and Descartes.

When Isaac Newton was four years old, his mother married again and went to live with her new husband, leaving the boy to be cared for by his grandmother. This may have caused Newton to become more solemn and introverted than he might otherwise have been. One of his childhood friends remembered him as "a sober, silent, thinking lad, scarce known to play with the other boys at their silly amusements".

7.2 Newton becomes a student at Cambridge

As a boy, Newton was fond of making mechanical models, but at first he showed no special brilliance as a scholar. He showed even less interest in running the family farm, however; and a relative (who was a fellow of Trinity College) recommended that he be sent to grammar school to prepare for Cambridge University.

When Newton arrived at Cambridge, he found a substitute father in the famous mathematician Isaac Barrow, who was his tutor. Under Barrow's guidance, and while still a student, Newton showed his mathematical genius by inventing the binomial theorem.

To understand Newton's work on the binomial theorem, we can begin by thinking of what happens when we multiply the quantity a + b by itself. The result is $a^2 + 2ab + b^2$. Now suppose that we continue the process and multiply $a^2 + 2ab + b^2$ by $a + b$. The result of this second multiplication is $a^3 + 3a^2b + 3ab^2 + b^3$, which can also be written as $(a + b)^3$

. Continuing in this way we can obtain higher powers of a + b:

$$\begin{aligned}(a+b)^1 &= a+b\\ (a+b)^2 &= a^2+2ab+b^2\\ (a+b)^3 &= a^3+3a^b+3b^2a+b^3\\ (a+b)^4 &= a^4+4a^3b+6a^2b^2+4ab^3+b^4\end{aligned} \tag{7.1}$$

and so on. Newton realized that in general, an integral power of a + b can be expressed in the form:

$$(a+b)^n = a^n + \frac{n}{1!}a^{n-1}b + \frac{n(n-1)}{2!}a^{n-2}b^2 + \frac{n(n-1)(n-2)}{3!}a^{n-3}b^3 + \cdots \tag{7.2}$$

where

$$\begin{aligned}0! &\equiv 1\\ 1! &\equiv 1\\ 2! &\equiv 2\times 1 = 2\\ 3! &\equiv 3\times 2\times 1 = 6\\ 4! &\equiv 4\times 3\times 2\times 1 = 24\\ \vdots\ &\ \vdots \qquad \vdots\end{aligned} \tag{7.3}$$

From the definition of n!, it follows that

$$\begin{aligned}n &= \frac{n!}{(n-1)!}\\ n(n-1) &= \frac{n!}{(n-2)!}\\ n(n-1)(n-3) &= \frac{n!}{(n-3)!}\end{aligned} \tag{7.4}$$

so that we can rewrite the equation for $(a+b)^n$ can be rewritten in the form

$$(a+b)^n = \sum_{j=0}^{n} \frac{n!}{j!(n-j)!)} a^{n-j}b^j \tag{7.5}$$

The large Greek letter $\sum$ indicates a sum. In this case, it is taken over all integral values from 0 up to and including to n.

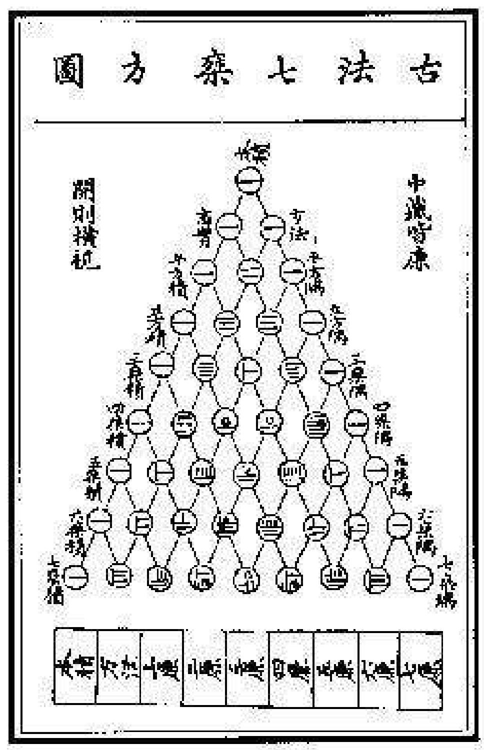

FIGURE 10

Figure 7.1: **Newton's work on binomial coefficients was foreshadowed by that of the French mathematician Blaise Pascal (1623-1662), inventor of "Pascal's triangle". However, Pascal was in turn preceded by the Persian mathematician-poet Omar Khayyam (1048-1131) and by the Chinese mathematician Yanghui, who lived 500 years before Pascal. In the figure we see the Yanghui triangle. The binomial coefficients in each successive row are obtained by adding together coefficients in the previous row. The number above and slightly to the left is added to the number above and slightly to the right, and the sum forms the new coefficient.**

7.3 Differential calculus

In 1665, Cambridge University was closed because of an outbreak of the plague, and Newton returned for two years to the family farm at Woolsthorpe. He was then twenty-three years old. During the two years of isolation, Newton developed his binomial theorem into the beginnings of differential calculus. He imagined Δt to be an extremely small increase in the value of a variable t. For example, t might represent time, in which case Δt would represent an infinitesimal increase in time - a tiny fraction of a split-second. Newton realized that the series

$$(t + \Delta t)^p = t^p + pt^{p-1}\Delta t + + \frac{p(p-1)}{2!} t^{p-2}(\Delta t)^2 + \cdots \tag{7.6}$$

could then be represented to a very good approximation by its first two terms, and in the limit $\Delta t \to 0$, he obtained the result:

$$\begin{matrix}\text{limit} \\ \Delta t \to 0\end{matrix} \left[\frac{f(t+\Delta t) - f(t)}{\Delta t}\right] = pt^{p-1} \tag{7.7}$$

Thus, in the particular case where $f(t) = t^p$ he found that

$$\frac{df}{dt} \equiv \begin{matrix}\text{limit} \\ \Delta t \to 0\end{matrix} \left[\frac{f(t+\Delta t) - f(t)}{\Delta t}\right] = pt^{p-1} \tag{7.8}$$

$\frac{d}{dt}$ can be thought of as an operator which one can apply to a function f (t). Today we call this operation "differentiation", and df/dt is called the function's "first derivative".

The derivative of a function can be interpreted as the slope (at a particular point t) of a curve representing the function. Differential calculus is the branch of mathematics that deals with differentiation, with slopes, with tangents, and with rates of change.

If we differentiate the sum of two functions, we obtain

$$\frac{d}{dt}[f(t) + g(t)] = \begin{matrix}\text{limit} \\ \Delta t \to 0\end{matrix} \left[\frac{f(t+\Delta t) - f(t) + g(t+\Delta t) - g(t)}{\Delta t}\right] \tag{7.9}$$

which can be rewritten as

$$\frac{d}{dt}[f+g] = \frac{df}{dt} + \frac{dg}{dt} \tag{7.10}$$

For example

$$\text{if } f + g = t + t^2, \text{ then } \frac{d}{dt}[f+g] = 1 + 2t \tag{7.11}$$

Differentiating the product of two functions yields

$$\frac{d}{dt}[f(t)g(t)] = \begin{matrix}\text{limit} \\ \Delta t \to 0\end{matrix} \left[\frac{f(t+\Delta t)g(t+\Delta t) - f(t)g(t)}{\Delta t}\right] \tag{7.12}$$

which can be rewritten in the form

$$\frac{d}{dt}[fg] = g\frac{df}{dt} + f\frac{dg}{dt} \tag{7.13}$$

Now suppose that $g(t) = a$ where a is a constant, i.e. independent of t. Then from (7.13) we find that

$$\text{if } a = \text{constant}, \text{ then } \frac{d}{dt}[af] = a\frac{df}{dt} \tag{7.14}$$

Combining these results, we obtain

$$\frac{d}{dt}\left[a_0 + a_1 t + a_2 t^2 + a_3 t^3 + \cdots\right] = a_1 + 2a_2 t + 3a_3 t^2 + 4a_4 t^3 + \cdots \tag{7.15}$$

Differentiating a function gives us a new function, but this new function can also be differentiated, and this process will yield another function, which today is called the "second derivative". In modern notation, the new function obtained by differentiating $f(t)$ twice with respect to t is represented by the symbol $\frac{d^2 f}{dt^2}$, where

$$\frac{d^2 f}{dt^2} \equiv \frac{d}{dt}\left[\frac{df}{dt}\right] \tag{7.16}$$

For example

$$\frac{d^2}{dt^2}\left[a_0 + a_1 t + a_2 t^2 + a_3 t^3 + \cdots\right] = 2a_2 + 6a_3 t + 12a_4 t^2 + \cdots \tag{7.17}$$

We can continue and take the third derivative:

$$\frac{d^3}{dt^3}\left[a_0 + a_1 t + a_2 t^2 + a_3 t^3 + \cdots\right] = 6a_3 + 24a_4 t + 60a_5 t^2 + \cdots \tag{7.18}$$

Continuing to differentiate, we obtain in general

$$\text{if } f = \sum_{n=0}^{\infty} a_n t^n, \text{ then } \left[\frac{d^n f}{dt^n}\right]_{t=0} = n! a_n \tag{7.19}$$

Finally, dividing (7.19) by $n!$ we have

$$\text{if } f = \sum_{n=0}^{\infty} a_n t^n, \text{ then } a_n = \frac{1}{n!}\left[\frac{d^n f}{dt^n}\right]_{t=0} \tag{7.20}$$

Many examples of series obtained using equation (7.20) can be found in the tables of Appendix A. Some important differential relationships are also shown in the tables.

We have used modern notation to go through the reasoning that Newton used to develop his binomial theorem into differential calculus. The quantities that we today call "derivatives", he called "fluxions", i.e. flowing quantities, perhaps because he associated them with a water clock that he had made as a boy - a water-filled jar with a hole in the bottom. If $f(t)$ represents the volume of water in the jar as a function of time, then df/dt represents the rate at which water is flowing out through the hole.

Newton also applied his "method of fluxions" to mechanics. From the three laws of planetary motion discovered by the German astronomer Kepler, Newton had deduced that the force with which the sun attracts a planet must fall off as the square of the distance between the planet and the sun. With great boldness, he guessed that this force is *universal*, and that every object in the universe attracts every other object with a gravitational force that is directly proportional to the product of the two masses, and inversely proportional to the square of the distance between them.

Newton also guessed correctly that in attracting an object outside its surface, the earth acts as though its mass were concentrated at its center. However, he could not construct the proof of this theorem, since it depended on integral calculus, which did not exist in 1666. (Newton himself perfected integral calculus later in his life.)

Referring to the year 1666, Newton wrote later: "I began to think of gravity extending to the orb of the moon; and having found out how to estimate the force with which a globe revolving within a sphere presses the surface of the sphere, from Kepler's rule of the periodical times of the planets being in a sesquialternate proportion of their distances from the centres of their orbs, I deduced that the forces which keep the planets in their orbs must be reciprocally as the squares of the distances from the centres about which they revolve; and thereby compared the force requisite to keep the moon in her orb with the force of gravity at the surface of the earth, and found them to answer pretty nearly."

"All this was in the plague years of 1665 and 1666, for in those days I was in the prime of my age for invention, and minded mathematics and philosophy more than at any time since."

Galileo had studied the motion of projectiles, and Newton was able to build on this work by thinking of the moon as a sort of projectile, dropping towards the earth, but at the same time moving rapidly to the side. The combination of these two motions gives the moon its nearly-circular path.

To see how Newton made this calculation, we can let x, y and z represent the Cartesian position coordinates of a body (for example the moon, or an apple). These are functions of time, and if we assume that the functions can be represented by polynomials in t, we can make use of (7.20) and write

$$x(t) = x_0 + t\left[\frac{dx}{dt}\right]_{t=0} + \frac{t^2}{2!}\left[\frac{d^2x}{dt^2}\right]_{t=0} + \cdots \tag{7.21}$$

$$y(t) = y_0 + t\left[\frac{dy}{dt}\right]_{t=0} + \frac{t^2}{2!}\left[\frac{d^2y}{dt^2}\right]_{t=0} + \cdots \tag{7.22}$$

$$z(t) = z_0 + t\left[\frac{dz}{dt}\right]_{t=0} + \frac{t^2}{2!}\left[\frac{d^2z}{dt^2}\right]_{t=0} + \cdots \tag{7.23}$$

The three Cartesian coordinates of a particle can be the three components of a vector which we can call **r**. or mathematical quantity that has a direction as well the velocity of an object is a vector, since it has a magnitude.)

$$\mathbf{r} \equiv \{x, y, z\} \tag{7.24}$$

The force acting on an object has components in the directions of the three Cartesian coordinates, and thus the force can also be thought of as a vector:

$$\mathbf{F} \equiv \{F_x, F_y, F_z\} \tag{7.25}$$

(We use bold-face type here to denote vectors). In addition to guessing the universal law of gravitation, Newton also postulated that the second derivative of the position vector of a body with respect to time (i.e. its acceleration) is directly proportional to the force acting on it, the constant of proportionality being the inverse of the body's mass:

$$\frac{d^2\mathbf{r}}{dt^2} = \frac{\mathbf{F}}{m} \tag{7.26}$$

Equation (7.26) is Newton's famous third law of motion. It is a vector equaion, and its meaning is that each component of the vector on the left side is equal to the corresponding component of the vector on the right. In other words,

$$\begin{aligned}
\frac{d^2x}{dt^2} &= \frac{F_x}{m} \\
\frac{d^2y}{dt^2} &= \frac{F_y}{m} \\
\frac{d^2z}{dt^2} &= \frac{F_z}{m}
\end{aligned} \tag{7.27}$$

Suppose now that the body is an apple, falling to the ground because of the earth's gravitational attraction. If z represents the vertical height of the apple above the earth's surface, while x and y measure its horizontal position on the surface, and if $-mg$ is the force of gravity acting on the apple, then we can write:

$$\mathbf{F} \equiv \{0, 0, -mg\} \tag{7.28}$$

Combining (7.26) and (7.28), we have

$$\left[\frac{d^2\mathbf{r}}{dt^2}\right]_{t=0} \equiv \{0, 0, -g\} \tag{7.29}$$

The constant g which appears in equation (7.29) is the acceleration due to the earth's gravity acting on an object near to its surface, and it has the value

$$g = 32.174\ \frac{\text{feet}}{\text{sec}^2} = 9.8066\ \frac{\text{meters}}{\text{sec}^2} \tag{7.30}$$

(Newton used the English units, feet and miles. 1 meter = 3.28084 feet. 1 mile = 5280 feet.) Notice that the mass m has now disappeared! The force of gravity in Newton's theory is directly proportional to a body's mass, but the acceleration produced by a force in inversely proportional to it, and therefore the mass cancels out of the equation for gravitational acceleration.

To make the problem of the falling apple a little more complicated, let us suppose that a small boy has climbed the tree and that instead of just dropping the apple, he throws it out horizontally with velocity

$$\left[\frac{d\mathbf{r}}{dt}\right]_{t=0} \equiv \{v_x, 0, 0\} \tag{7.31}$$

Then substituting the initial velocity and acceleration of the apple into the equations of motion, and letting $x_0 = y_0 = 0$, we obtain

$$\begin{aligned} x &= v_x t \\ y &= 0 \\ z &= z_0 - \frac{gt^2}{2} \end{aligned} \tag{7.32}$$

We can use the first of these equations to express t in terms of x and rewrite the equation for z in the form:

$$z = z_0 - g\frac{x^2}{2v_x} \tag{7.33}$$

Thus we see that if it is thrown out horizontally from the tree, the apple will fall to the ground following a parabolic trajectory. Equations (7.32) and (7.33) describe the motions of projectiles and falling bodies. These were already well known to Galileo, who was the first to study such motions experimentally.

Newton boldly postulated that the laws of motion and gravitation that can be observed here on earth extend throughout the universe. To him it seemed that the moon resembles an apple thrown to the side by a small boy sitting in the apple tree. The moon falls towards the earth, but at the same time it moves to the side with the constant velocity v_x. The combination of these two motions gives the moon its nearly-circular orbit. Of course, after it has moved a little, the force of gravitation comes from a different direction, and therefore the moon does not follow a parabolic orbit but an approximately circular one. However, if we consider only a very short period of time, the circle and parabola fit closely together, as is illustrated in Figure 7.2. If we take the origin of our coordinate system to be the center of the earth, then $z_0 = R_m$ where R_m is the radius of the moon's orbit, and the trajectory of the moon through a very short interval of time is given by

$$z = R_m - g'\frac{x^2}{2v_x} \tag{7.34}$$

We use g' instead of g in equation (7.34) because the moon is much more distant from the earth's center than the apple is, and the moon's gravitational acceleration is much less

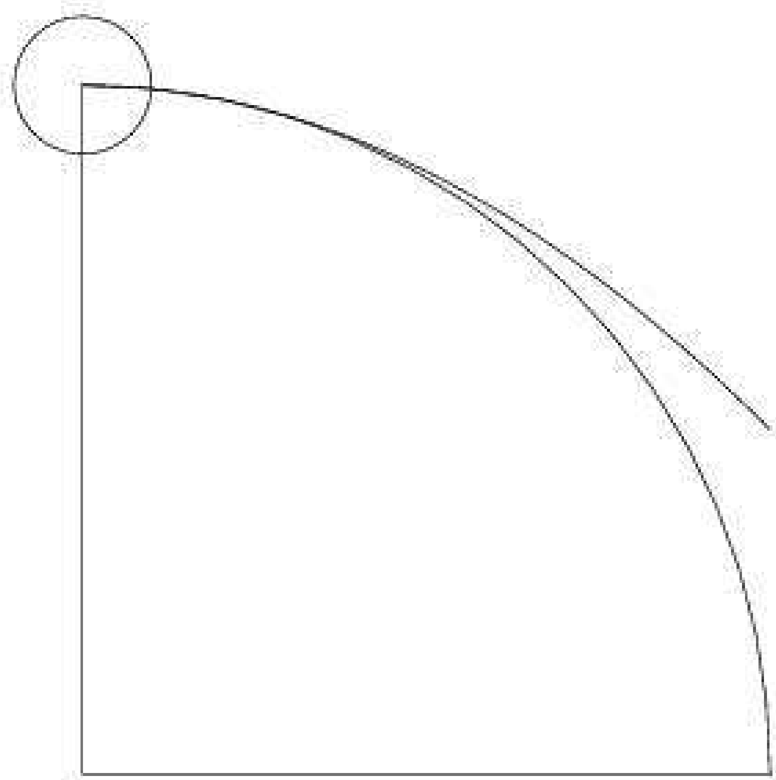

Figure 7.2: **The orbit of the moon is approximately circular in shape. During a very short interval of time, the moon can be thought of as being similar to an object moving horizontally, and at the same time being accelerated in a vertical direction by the force of gravity. The parabolic trajectory of such an object is approximately the same as a circle during that short interval of time, as is shown in the figure.**

than the apple's. Building on Kepler's laws of planetary motion, Newton postulated that the force of gravity exerted by the earth falls off as the reciprocal of the square of the distance from the earth's center. Thus g' and g are related by

$$g' = g\left(\frac{R_e}{R_m}\right)^2 = g\left(\frac{3963\text{ miles}}{238.600\text{ miles}}\right)^2 = .0089\ \frac{\text{feet}}{\text{sec}^2} \tag{7.35}$$

$$z = \sqrt{R:m^2 - x^2} \approx R_m - \frac{x^2}{2R_m} = R_m - g'\frac{x^2}{2v_x} \tag{7.36}$$

$$v_x = \frac{2\pi R_m}{\tau} = 3356\frac{\text{feet}}{\text{sec.}} \tag{7.37}$$

where τ is the period of the moon's orbit.

In this way, Newton "compared the force necessary to keep the moon in her orb with the force of gravity on the earth's surface, and found them to answer pretty nearly."

Newton was not satisfied with this incomplete triumph, and he did not show his calculations to anyone. He not only kept his ideas on gravitation to himself, (probably because of the missing proof), but he also refrained for many years from publishing his work on the calculus. By the time Newton published, the calculus had been invented independently by the great German mathematician and philosopher, Gottfried Wilhelm Leibniz (1646-1716); and the result was a bitter quarrel over priority. However, Newton did publish his experiments in optics, and these alone were enough to make him famous.

7.4 Optics

Newton's famous experiments in optics also date from these years. The sensational experiments of Galileo were very much discussed at the time, and Newton began to think about ways to improve the telescope. Writing about his experiments in optics, Newton says:

"In the year 1666 (at which time I applied myself to the grinding of optic glasses of other figures than spherical), I procured me a triangular prism, to try therewith the celebrated phenomena of colours. And in order thereto having darkened my chamber, and made a small hole in the window shuts to let in a convenient quantity of the sun's light, I placed my prism at its entrance, that it might thereby be refracted to the opposite wall."

"It was at first a very pleasing divertisment to view the vivid and intense colours produced thereby; but after a while, applying myself to consider them more circumspectly, I became surprised to see them in an oblong form, which, according to the received laws of refraction I expected should have been circular."

Newton then describes his crucial experiment. In this experiment, the beam of sunlight from the hole in the window shutters was refracted by two prisms in succession. The first prism spread the light into a rainbow-like band of colors. From this spectrum, he selected a beam of a single color, and allowed the beam to pass through a second prism; but when light of a single color passed through the second prism, the color did not change, nor was the image spread out into a band. No matter what Newton did to it, red light always remained red, once it had been completely separated from the other colors; yellow light remained yellow, green remained green, and blue remained blue.

Newton then measured the amounts by which the beams of various colors were bent by the second prism; and he discovered that red light was bent the least. Next in sequence came orange, yellow, green, blue and finally violet, which was deflected the most. Newton recombined the separated colors, and he found that together, they once again produced white light.

Concluding the description of his experiments, Newton wrote:

"...and so the true cause of the length of the image (formed by the first prism) was detected to be no other than that light is not similar or homogenial, but consists of *deform rays, some of which are more refrangible than others*."

"As rays of light differ in their degrees of refrangibility, so they also differ in their disposition to exhibit this or that particular colour... To the same degree of refrangibility ever belongs the same colour, and to the same colour ever belongs the same degree of refrangibility."

"...The species of colour and the degree of refrangibility belonging to any particular sort of rays is not mutable by refraction, nor by reflection from natural bodies, nor by any other cause that I could yet observe. When any one sort of rays hath been well parted from those of other kinds, it hath afterwards obstinately retained its colour, notwithstanding my utmost endeavours to change it."

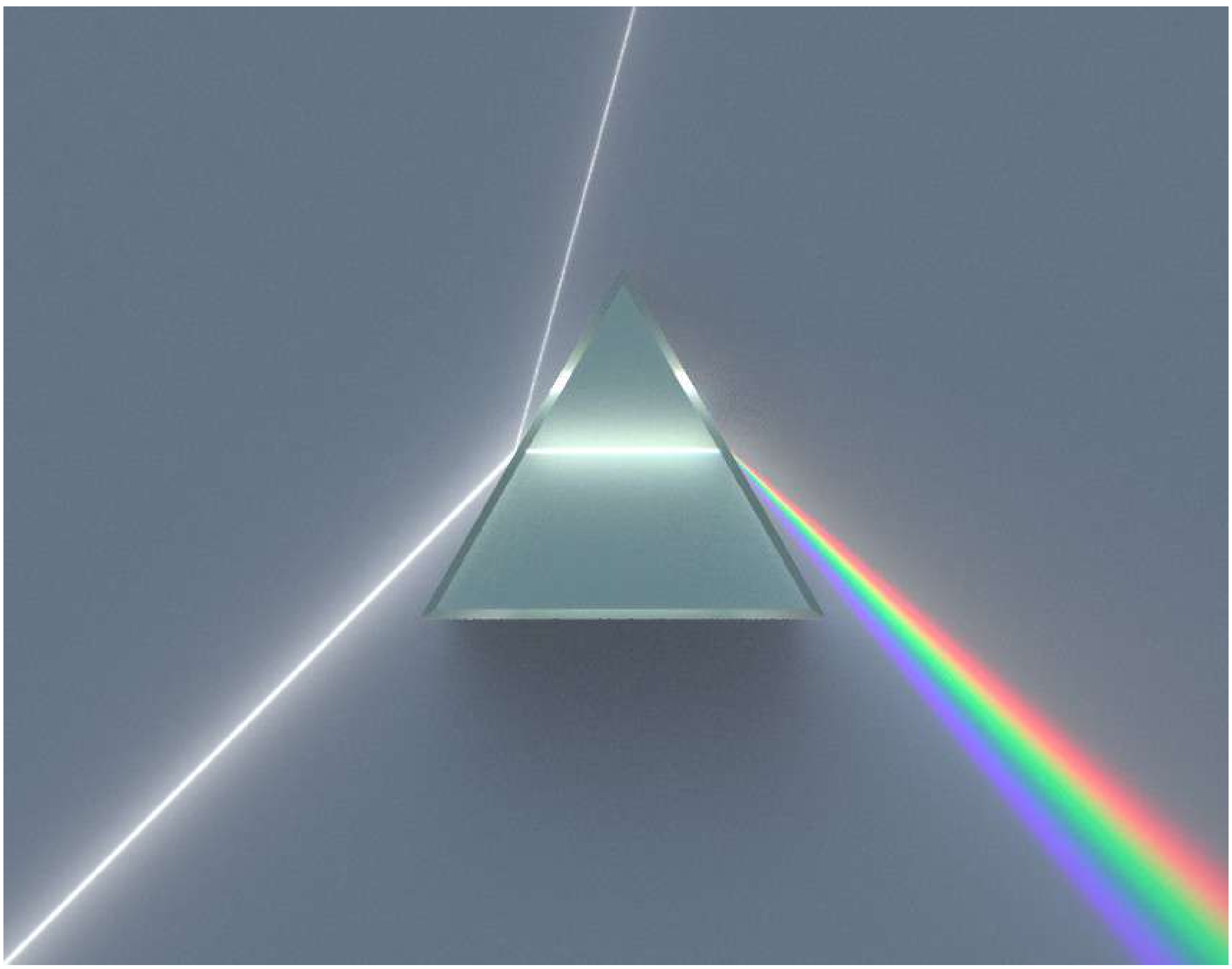

Figure 7.3: **Illustration of a dispersive prism separating white light into the colours of the spectrum, as discovered by Newton.**

Figure 7.4: **Replica of Newton's second reflecting telescope, which he presented to the Royal Society in 1672.**

7.5 Integral calculus

In 1669, Newton's teacher, Isaac Barrow, generously resigned his post as Lucasian Professor of Mathematics so that Newton could have it. Thus, at the age of 27, Newton became the head of the mathematics department at Cambridge. He was required to give eight lectures a year, but the rest of his time was free for research.

Newton worked at this time on developing what he called "the method of inverse fluxions". Today we call his method "integral calculus". What did Newton mean by "inverse fluxions"? By "fluxions" he meant differentials, so we must think of an operation that is the reverse of differentiation.

Suppose that we know from our experience with differentiation that (for example)

$$\text{if and only if } f = t^p + C \text{ then } \frac{df}{dt} = pt^{p-1} \tag{7.38}$$

where C is a constant. Then we also know that

$$\text{if } \frac{df}{dt} = pt^{p-1} \text{ then } f = t^p + C \tag{7.39}$$

In equation (7.39), we know that C is a constant, but we do not know its value. Knowledge of the derivative df/dt allows us to determine the original function $f(t)$ from which it was derived up to an additive constant that must be determined in some other way. The operation of going backwards from the differential of a function to the function itself is called "integration", and the unknown constant C is called the "constant of integration". If we replace p by $p+1$, it follows from (7-39) that

$$\text{if } \frac{df}{dt} = t^p \text{ then } f = \frac{t^p}{p+1} + C \qquad p \neq -1 \tag{7.40}$$

(We have to exclude $p = -1$ in (3.3) to avoid dividing by zero.) It is customary to write this relationship in the form

$$\int dt\ t^p = \frac{t^p}{p+1} + C \qquad p \neq -1 \tag{7.41}$$

Once again the constant of integration, C, is unknown and must be determined in some other way. When $p = 1$, equation (7.41) becomes

$$\int dt\ t = \frac{t^2}{2} + C \tag{7.42}$$

Equations (7.41) and (7.42) are called "indefinite integrals" - indefinite because the constant of integration is unknown. One also speaks of "definite integrals", where knowledge of the derivative df/dt is used to find $f(t_2) - f(t_1)$. If the variable t represents time, then $f(t_2) - f(t_1)$ would represent the difference between the function $f(t)$ evaluated at the time $t = t_2$ minus the same function evaluated at the time $t = t_1$. For example,

$$\text{if } \frac{df}{dt} = t \quad \text{then } f(t_2) - f(t_1) = \frac{t_2^2}{2} - \frac{t_1^2}{2} \tag{7.43}$$

This relationship is written in the form

$$\int_{t_1}^{t_2} dt\ t = \frac{t_2^2}{2} - \frac{t_1^2}{2} \tag{7.44}$$

The integration is said to be taken between the lower limit $t = t_1$ and the upper limit, $t = t_2$. The more general indefinite integral shown in equation (7.41) has a corresponding definite integral of the form:

$$\int_{t_1}^{t_2} dt\ t^p = \frac{t_2^{p+1}}{p+1} - \frac{t_1^{p+1}}{p+1} \qquad p \neq -1 \tag{7.45}$$

When $p = 0$, this becomes

$$\int_{t_1}^{t_2} dt = t_2 - t_1 \tag{7.46}$$

The reason why integrals taken between two limits are called "definite integrals" is that the unknown constant of integration C has cancelled out so no information is missing when we go from the differential of a function to the function itself.

In a previous chapter, we mentioned that Archimedes invented integral calculus and used it to determine the areas of figures bounded by curves. To see how he did this and how Newton, many centuries later, did the same thing, let us begin by multiplying both sides of equation (7.46) by a constant v. This gives us

$$v \int_{t_1}^{t_2} dt = v(t_2 - t_1) \tag{7.47}$$

If we let $t_1 = 0$ we have

$$v \int_{0}^{t_2} dt = vt_2 \tag{7.48}$$

What we have done here. and in Figures 7.5 and 7.6, seems a bit like cracking a peanut with a sledge- hammer. Why have we used such a heavy piece of mathematical hardware to crack a problem that we could have solved in 30 seconds in our heads? However, if the reader will be patient with the first two simple examples, which we have included for the sake of clarity, we will soon go on to problems involving figures bounded by curves, and these cannot be solved without the help of integral calculus.

In the next simple example, we multiply both sides of equation (7.44) with the constant a. This will give us

$$a \int_{t_1}^{t_2} dt\ t = a\left(\frac{t_2^2}{2} - \frac{t_1^2}{2}\right) \tag{7.49}$$

Tables of important indefinite and definite integrals are given in Appendix A.

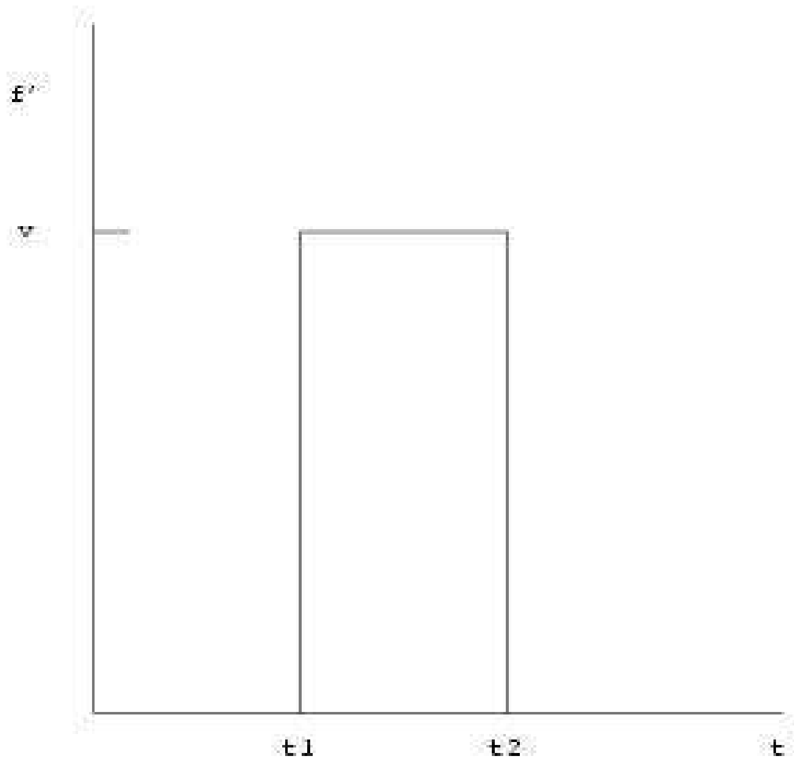

Figure 7.5: **This figure shows a rectangle with height v and base $t_2 - t_1$. The area of the figure is $v(t_2 - t_1)$. If v represents the constant velocity of an object, then the area of the rectangle represents distance that the object moves between the times t_1 and t_2.**

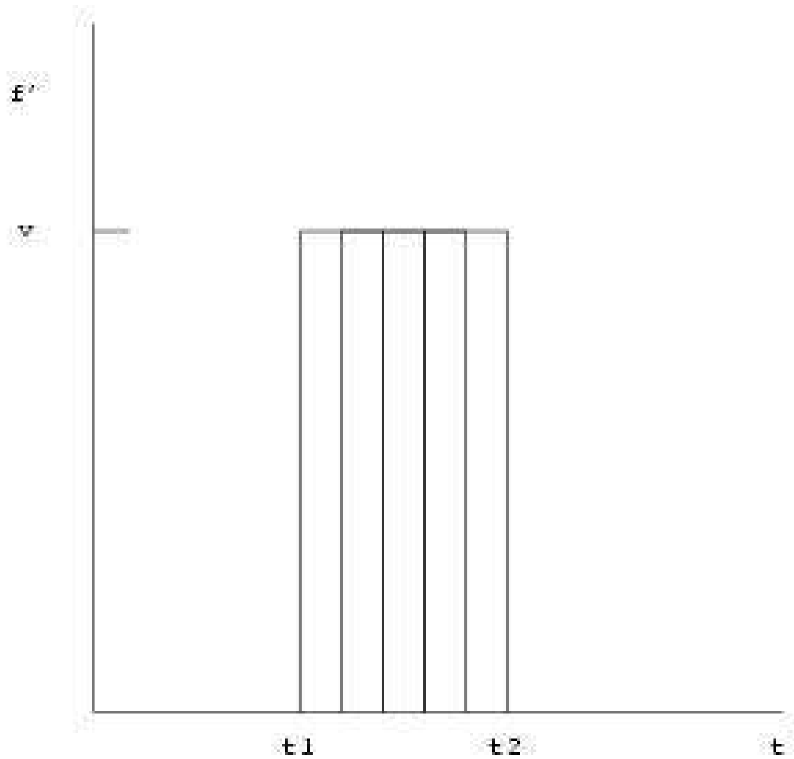

Figure 7.6: **We now divide the large rectangle of Figure 7.5 into five small rectangular strips, each with area $v\Delta t = v(t_2 - t_1)/5$. When we add together the areas of the small strips, we get the same answer for the total area of the rectangle. Physically, $v\Delta t$ can represent the distance that an object with constant velocity v moves in a small interval of time Δt.**

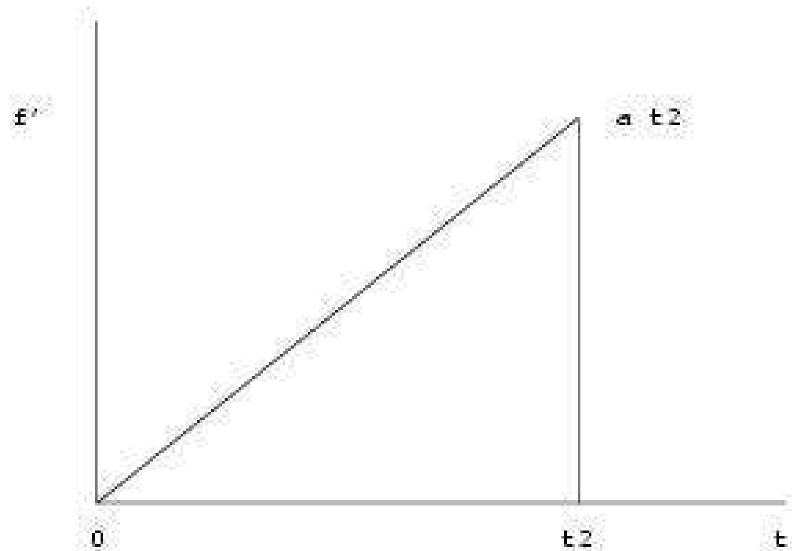

Figure 7.7: **This figure illustrates the geometrical interpretation of equation (7.48). The area under the straight line $v = at$ between the points $t = 0$ and $t = t_2$ is given by $at_2^2/2$, i.e., the height of the triangle, multiplied by half the length of the base. Physically, the area of the triangle can represent the distance moved by an object with constant acceleration a. It's velocity is then given by $v = at$, and the distance travelled is proportional to the square of the elapsed time. Galileo found this law experimentally for falling bodies with constant gravitational acceleration. He observed that the distance travelled by a falling body is proportional to the square of the elapsed time.**

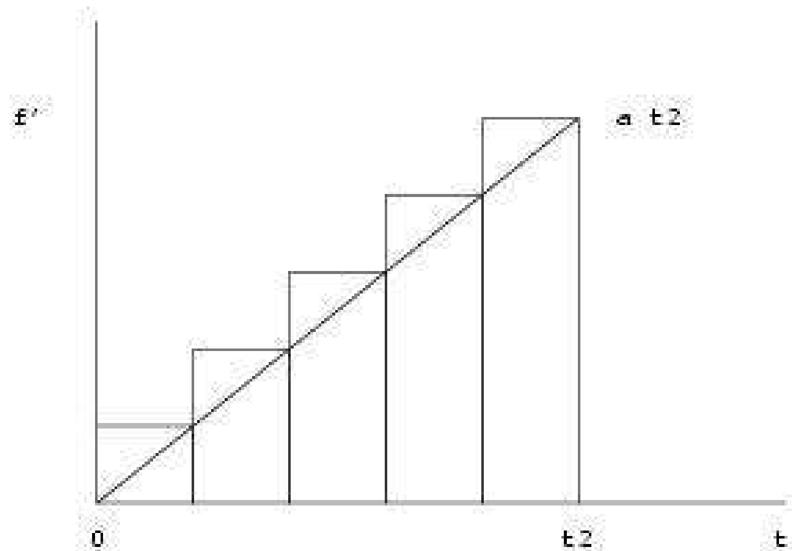

Figure 7.8: **We now divide the triangle of Figure 7.7 into N small rectangular strips. (In the figure, $N = 5$.) The area of the triangle is approximated by the sum of the areas of the small strips. If we increase the number of strips, N , the approximation will become more exact. The area of each of the narrow strips can represent physically the approximate distance that an object with constant acceleration a travels during the interval of time Δt. This distance changes with time because acceleration changes the velocity of the object.**

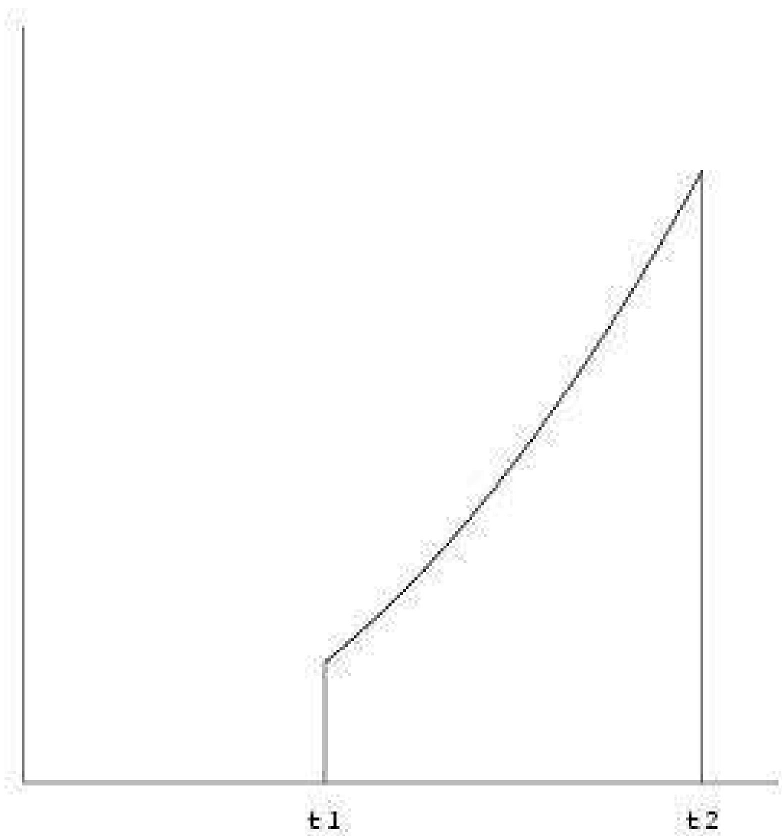

Figure 7.9: **Equation (3.25) tells us how to find the area under the parabola $f(t) = t**22$ between vertical lines drawn at $t = t_1$ and $t = t_2$. The other boundary of the calculation.**

7.6 Halley visits Newton

Newton's prism experiments had led him to believe that the only possible way to avoid blurring of colors in the image formed by a telescope was to avoid refraction entirely. Therefore he designed and constructed the first reflecting telescope. In 1672, he presented a reflecting telescope to the newly-formed Royal Society, which then elected him to membership.

Meanwhile, the problems of gravitation and planetary motion were increasingly discussed by the members of the Royal Society. In January, 1684, three members of the Society were gathered in a London coffee house. One of them was Robert Hooke (1635-1703), author of *Micrographia* and Professor of Geometry at Gresham College, a brilliant but irritable man. He had begun his career as Robert Boyle's assistant, and had gone on to do important work in many fields of science. Hooke claimed that he could calculate the motion of the planets by assuming that they were attracted to the sun by a force which diminished as the square of the distance.

Listening to Hooke were Sir Christopher Wren (1632-1723), the designer of St. Paul's Cathedral, and the young astronomer, Edmund Halley (1656-1742). Wren challenged Hooke to produce his calculations; and he offered to present Hooke with a book worth 40 shillings if he could prove his inverse square force law by means of rigorous mathematics. Hooke tried for several months, but he was unable to win Wren's reward.

Meanwhile, in August, 1684, Halley made a journey to Cambridge to talk with Newton, who was rumored to know very much more about the motions of the planets than he had revealed in his published papers. According to an almost-contemporary account, what happened then was the following:

"Without mentioning his own speculations, or those of Hooke and Wren, he (Halley) at once indicated the object of his visit by asking Newton what would be the curve described by the planets on the supposition that gravity diminished as the square of the distance. Newton immediately answered: an Ellipse. Struck with joy and amazement, Halley asked how he knew it? 'Why', replied he, 'I have calculated it'; and being asked for the calculation, he could not find it, but promised to send it to him."

Newton soon reconstructed the calculation and sent it to Halley; and Halley, filled with enthusiasm and admiration, urged Newton to write out in detail all of his work on motion and gravitation. Spurred on by Halley's encouragement and enthusiasm, Newton began to put his research in order. He returned to the problems which had occupied him during the plague years, and now his progress was rapid because he had invented integral calculus. This allowed him to prove rigorously that terrestrial gravitation acts as though all the earth's mass were concentrated at its center. Newton also had available an improved value for the radius of the earth, measured by the French astronomer Jean Picard (1620-1682). This time, when he approached the problem of gravitation, everything fell into place.

By the autumn of 1684, Newton was ready to give a series of lectures on dynamics, and he sent the notes for these lectures to Halley in the form of a small booklet entitled *On the Motion of Bodies*. Halley persuaded Newton to develop these notes into a larger book, and with great tact and patience he struggled to keep a controversy from developing between Newton, who was neurotically sensitive, and Hooke, who was claiming his share

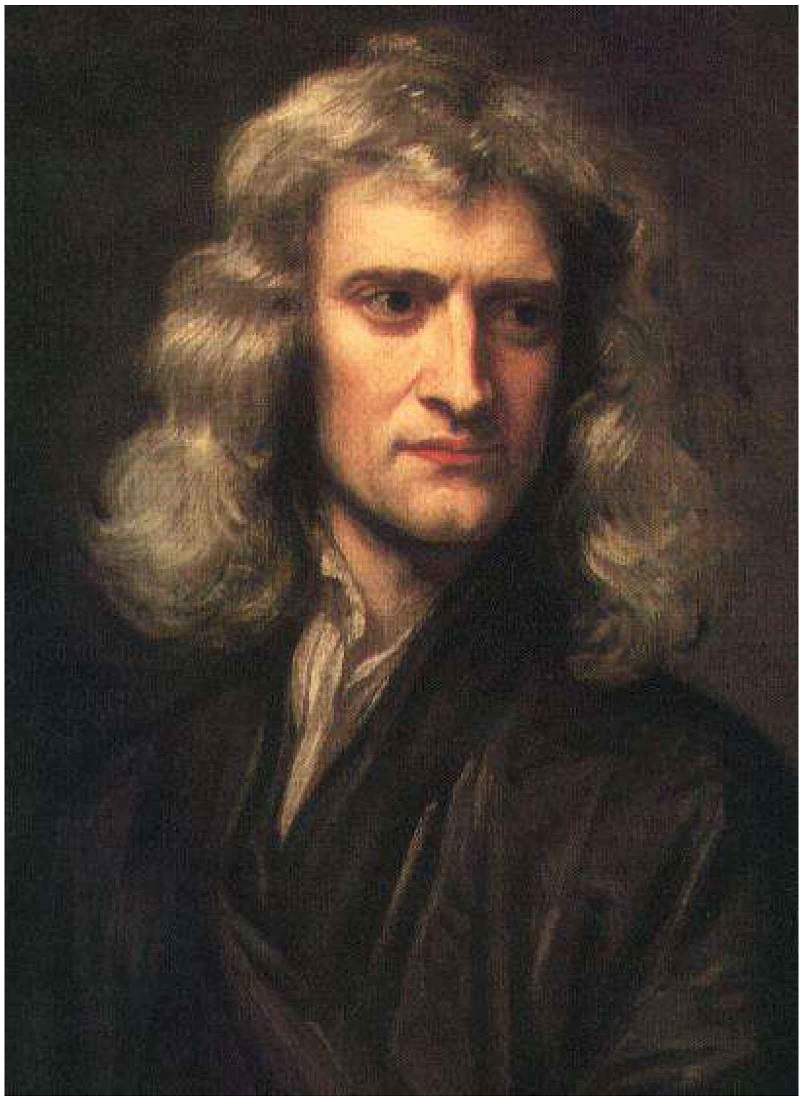

Figure 7.10: **Portrait of Isaac Newton (1642-1727) by Sir Godfrey Kneller.**

of recognition in very loud tones, hinting that Newton was guilty of plagiarism.

Although Newton was undoubtedly the greatest physicist of all time, he had his shortcomings as a human being; and he reacted by striking out from his book every single reference to Robert Hooke. The Royal Society at first offered to pay for the publication costs of Newton's book, but because a fight between Newton and Hooke seemed possible, the Society discretely backed out. Halley then generously offered to pay the publication costs himself, and in 1686 Newton's great book was printed. It is entitled *Philosophae Naturalis Principia Mathematica*, (The Mathematical Principles of Natural Philosophy), and it is divided into three sections.

The first book sets down the general principles of mechanics. In it, Newton states his three laws of motion, and he also discusses differential and integral calculus (both invented by himself).

In the second book, Newton applies these methods to systems of particles and to hydrodynamics. For example, he calculates the velocity of sound in air from the compressibility and density of air; and he treats a great variety of other problems, such as the problem of calculating how a body moves when its motion is slowed by a resisting medium, such as air or water.

The third book is entitled *The System of the World*. In this book, Newton sets out to derive the entire behavior of the solar system from his three laws of motion and from his law of universal gravitation. From these, he not only derives all three of Kepler's laws, but he also calculates the periods of the planets and the periods of their moons; and he explains such details as the flattened, non-spherical shape of the earth, and the slow precession of its axis about a fixed axis in space. Newton also calculated the irregular motion of the moon resulting from the combined attractions of the earth and the sun; and he determined the mass of the moon from the behavior of the tides.

Newton's *Principia* is generally considered to be the greatest scientific work of all time. To present a unified theory explaining such a wide variety of phenomena with so few assumptions was a magnificent and unprecedented achievement; and Newton's contemporaries immediately recognized the importance of what he had done.

The great Dutch physicist, Christian Huygens (1629-1695), inventor of the pendulum clock and the wave theory of light, travelled to England with the express purpose of meeting Newton. Voltaire, who for reasons of personal safety was forced to spend three years in England, used the time to study Newton's *Principia*; and when he returned to France, he persuaded his mistress, Madame du Chatelet, to translate the *Principia* into French; and Alexander Pope, expressing the general opinion of his contemporaries, wrote a famous couplet, which he hoped would be carved on Newton's tombstone:

"Nature and Nature's law lay hid in night.

God said: 'Let Newton be!', and all was light!"

The Newtonian synthesis was the first great achievement of a new epoch in human thought, an epoch which came to be known as the "Age of Reason" or the "Enlightenment". We might ask just what it was in Newton's work that so much impressed the intellectuals of the 18th century. The answer is that in the Newtonian system of the world, the entire evolution of the solar system is determined by the laws of motion and by the positions and velocities of the planets and their moons at a given instant of time. Knowing these, it is possible to predict all of the future and to deduce all of the past.

The Newtonian system of the world is like an enormous clock which has to run on in a predictable way once it is started. In this picture of the world, comets and eclipses are no longer objects of fear and superstition. They too are part of the majestic clockwork of the universe. The Newtonian laws are simple and mathematical in form; they have complete generality; and they are unalterable. In this picture, although there are no miracles or exceptions to natural law, nature itself, in its beautiful works, can be regarded as miraculous.

Newton's contemporaries knew that there were other laws of nature to be discovered besides those of motion and gravitation; but they had no doubt that, given time, all of the laws of nature would be discovered. The climate of intellectual optimism was such that many people thought that these discoveries would be made in a few generations, or at most in a few centuries.

In 1704, Newton published a book entitled *Opticks*, expanded editions of which appeared in 1717 and 1721. Among the many phenomena discussed in this book are the colors produced by thin films. For example, Newton discovered that when he pressed two convex lenses together, the thin film of air trapped between the lenses gave rise to rings of colors ("Newton's rings"). The same phenomenon can be seen in the in the colors of soap bubbles or in films of oil on water.

In order to explain these rings, Newton postulated that "..every ray of light in its passage through any refracting surface is put into a transient constitution or state, which in the progress of the ray returns at equal intervals, and disposes the ray at every return to be easily transmitted through the next refracting surface and between the returns to be easily reflected from it."

Newton's rings were later understood on the basis of the wave theory of light advocated by Huygens and Hooke. Each color has a characteristic wavelength, and is easily reflected when the ratio of the wavelength to the film thickness is such that the wave reflected from the bottom surface of the film interferes constructively with the wave reflected from the top surface. However, although he ascribed periodic "fits of easy reflection" and "fits of easy transmission" to light, and although he suggested that a particular wavelength is associated with each color, Newton rejected the wave theory of light, and believed instead that light consists of corpuscles emitted from luminous bodies.

Newton believed in his corpuscular theory of light because he could not understand on the basis of Huygens' wave theory how light casts sharp shadows. This is strange, because in his *Opticks* he includes the following passage:

"Grimaldo has inform'd us that if a beam of the sun's light be let into a dark room through a very small hole, the shadows of things in this light will be larger than they ought to be if the rays went on by the bodies in straight lines, and that these shadows have three parallel fringes, bands or ranks of colour'd light adjacent to them. But if the hole be enlarg'd, the fringes grow broad and run into one another, so that they cannot be distinguish'd"

After this mention of the discovery of diffraction by the Italian physicist, Francesco

Figure 7.11: **Newton own evaluation of his work was modest. He wrote "I do not know what I may appear to the world, but to myself I seem to have been only like a boy playing on the seashore, and diverting myself in now and then finding a smoother pebble or a prettier shell than ordinary, whilst the great ocean of truth lay all undiscovered before me."**

Marea Grimaldi (1618-1663), Newton discusses his own studies of diffraction. Thus, Newton must have been aware of the fact that light from a very small source does not cast completely sharp shadows!

Newton felt that his work on optics was incomplete, and at the end of his book he included a list of "Queries", which he would have liked to have investigated. He hoped that this list would help the research of others. In general, although his contemporaries were extravagant in praising him, Newton's own evaluation of his work was modest. "I do not know how I may appear to the world", he wrote, "but to myself I seem to have been only like a boy playing on the seashore and diverting myself in now and then finding a smoother pebble or a prettier shell than ordinary, whilst the great ocean of truth lay all undiscovered before me."

7.7 The conflict over priority between Leibniz and Newton

In this chapter, we have used the modern notation, which is much closer to the notation used by the great German mathematician and universal genius, Gottfried Wilhelm von Leibniz than to that used by Newton.

Newton did not publish his work on differential and integral calculus. Slightly later, Leibniz invented these two branches of mathematics independently. Thus a bitter dispute over priority was precipated, from which Leibniz suffered when his patron, the Elector of Hanover, left Germany to become King George I of England.

Huygens and Leibniz

On the continent of Europe, mathematics and physics had been developing rapidly, stimulated by the writings of René Descartes. One of the most distinguished followers of Descartes was the Dutch physicist, Christian Huygens (1629-1695).

Huygens was the son of an important official in the Dutch government. After studying mathematics at the University of Leiden, he published the first formal book ever written about probability. However, he soon was diverted from pure mathematics by a growing interest in physics.

In 1655, while working on improvements to the telescope together with his brother and the Dutch philosopher Benedict Spinoza, Huygens invented an improved method for grinding lenses. He used his new method to construct a twenty-three foot telescope, and with this instrument he made a number of astronomical discoveries, including a satellite of Saturn, the rings of Saturn, the markings on the surface of Mars and the Orion Nebula.

Huygens was the first person to estimate numerically the distance to a star. By assuming the star Sirius to be exactly as luminous as the sun, he calculated the distance to Sirius, and found it to be 2.5 trillion miles. In fact, Sirius is more luminous than the sun, and its true distance is twenty times Huygens' estimate.

Another of Huygens' important inventions is the pendulum clock. Improving on Galileo's studies, he showed that for a pendulum swinging in a circular arc, the period is not precisely independent of the amplitude of the swing. Huygens then invented a pendulum with a modified arc, not quite circular, for which the swing was exactly isochronous. He used this improved pendulum to regulate the turning of cog wheels, driven by a falling weight; and thus he invented the pendulum clock, almost exactly as we know it today.

In discussing Newton's contributions to optics, we mentioned that Huygens opposed Newton's corpuscular theory of light, and instead advocated a wave theory. Huygens believed that the rapid motion of particles in a hot body, such as a candle flame, produces a wave-like disturbance in the surrounding medium; and he believed that this wavelike disturbance of the "ether" produces the sensation of vision by acting on the nerves at the back of our eyes.

In 1678, while he was working in France under the patronage of Louis XIV, Huygens composed a book entitled *Traité de la Lumiere*, (Treatise on Light), in which he says:

"...It is inconceivable to doubt that light consists of the motion of some sort of matter. For if one considers its production, one sees that here upon the earth it is chiefly engendered by fire and flame, which undoubtedly contain bodies in rapid motion, since they dissolve and melt many other bodies, even the most solid; or if one considers its effects, one sees that when light is collected, as by concave mirrors, it has the property of burning as fire does, that is to say, it disunites the particles of bodies. This is assuredly the mark of motion, at least in the true philosophy in which one conceives the causes of all natural effects in terms of mechanical motions..."

Figure 7.12: **Christian Huygens (1629-1695).**

"Further, when one considers the extreme speed with which light spreads on every side, and how, when it comes from different regions, even from those directly opposite, the rays traverse one another without hindrance, one may well understand that when we see a luminous object, it cannot be by any transport of matter coming to us from the object, in the way in which a shot or an arrow traverses the air; for assuredly that would too greatly impugn these two properties of light, especially the second of them. It is in some other way that light spreads; and that which can lead us to comprehend it is the knowledge which we have of the spreading of sound in the air."

Huygens knew the velocity of light rather accurately from the work of the Danish astronomer, Ole Rømer (1644-1710), who observed the moons of Jupiter from the near and far sides of the earth's orbit. By comparing the calculated and observed times for the moons to reach a certain configuration, Rømer was able to calculate the time needed for light to propagate across the diameter of the earth's orbit. In this way, Rømer calculated the velocity of light to be 227,000 kilometers per second. Considering the early date of this first successful measurement of the velocity of light, it is remarkably close to the accepted modern value of 299,792 kilometers per second. Thus Huygens knew that although the speed of light is enormous, it is not infinite.

Huygens considered the propagation of a light wave to be analogous to the spreading of sound, or the widening of the ripple produced when a pebble is thrown into still water. He developed a mathematical principle for calculating the position of a light wave after a short interval of time if the initial surface describing the wave front is known. Huygens considered each point on the initial wave front to be the source of spherical wavelets, moving outward with the speed of light in the medium. The surface marking the boundary between the region outside all of the wavelets and the region inside some of them forms the new wave front.

If one uses Huygens' Principle to calculate the wave fronts and rays for light from a point source propagating past a knife edge, one finds that a part of the wave enters the shadow region. This is, in fact, precisely the effect which was observed by both Grimaldi and Newton, and which was given the name "diffraction" by Grimaldi. In the hands of Thomas Young (1773-1829) and Augustin Jean Fresnel (1788-1827), diffraction effects later became a strong argument in favor of Huygens' wave theory of light.

(You can observe diffraction effects yourself by looking at a point source of light, such as a distant street lamp, through a piece of cloth, or through a small slit or hole. Another type of diffraction can be seen by looking at light reflected at a grazing angle from a phonograph record. The light will appear to be colored. This effect is caused by the fact that each groove is a source of wavelets, in accordance with Huygens' Principle. At certain angles, the wavelets will interfere constructively, the angles for constructive interference being different for each color.)

Interestingly, modern quantum theory (sometimes called wave mechanics) has shown that *both* Huygens' wave theory of light and Newton's corpuscular theory contain aspects of the truth! Light has both wave-like and particle-like properties. Furthermore, quantum theory has shown that small particles of matter, such as electrons, also have wave-like properties! For example, electrons can be diffracted by the atoms of a crystal in a manner

Figure 7.13: **Portrait of Gottfried Wilhelm Leibniz by J.F. Wentzel.**

exactly analogous to the diffraction of light by the grooves of a phonograph record. Thus the difference of opinion between Huygens and Newton concerning the nature of light is especially interesting, since it foreshadows the wave-particle duality of modern physics.

Among the friends of Christian Huygens was the German philosopher and mathematician Gottfried Wilhelm Leibniz (1646-1716). Leibniz was a man of universal and spectacular ability. In addition to being a mathematician and philosopher, he was also a lawyer, historian and diplomat. He invented the doctrine of balance of power, attempted to unify the Catholic and Protestant churches, founded academies of science in Berlin and St. Petersburg, invented combinatorial analysis, introduced determinants into mathematics, independently invented the calculus, invented a calculating machine which could multiply and divide as well as adding and subtracting, acted as advisor to Peter the Great and originated the theory that "this is the best of all possible worlds" (later mercilessly satirized by Voltaire in *Candide*).

Leibniz learned mathematics from Christian Huygens, whom he met while travelling as an emissary of the Elector of Mainz. Since Huygens too was a man of very wide interests, he found the versatile Leibniz congenial, and gladly agreed to give him lessons. Leibniz continued to correspond with Huygens and to receive encouragement from him until the end of the older man's life.

In 1673, Leibniz visited England, where he was elected to membership by the Royal Society. During the same year, he began his work on calculus, which he completed and published in 1684. Newton's invention of differential and integral calculus had been made much earlier than the independent work of Leibniz, but Newton did not publish his discoveries until 1687. This set the stage for a bitter quarrel over priority between the admirers of Newton and those of Leibniz. The quarrel was unfortunate for everyone concerned, especially for Leibniz himself. He had taken a position in the service of the Elector of Hanover, which he held for forty years. However, in 1714, the Elector was called to the throne of England as George I. Leibniz wanted to accompany the Elector to England, but was left behind, mainly because of the quarrel with the followers of Newton. Leibniz died two years later, neglected and forgotten, with only his secretary attending the funeral.

7.8 Political philosophy of the Enlightenment

The 16th, 17th and 18th centuries have been called the "Age of Discovery", and the "Age of Reason", but they might equally well be called the "Age of Observation". On every side, new worlds were opening up to the human mind. The great voyages of discovery had revealed new continents, whose peoples demonstrated alternative ways of life. The telescopic exploration of the heavens revealed enormous depths of space, containing myriads of previously unknown stars; and explorations with the microscope revealed a new and marvelously intricate world of the infinitesimally small.

In the science of this period, the emphasis was on careful observation. This same emphasis on observation can be seen in the Dutch and English painters of the period. The great Dutch masters, such as Jan Vermeer (1632-1675), Frans Hals (1580-1666), Pieter de Hooch (1629-1678) and Rembrandt van Rijn (1606-1669), achieved a careful realism in their paintings and drawings which was the artistic counterpart of the observations of the pioneers of microscopy, Anton van Leeuwenhoek and Robert Hooke. These artists were supported by the patronage of the middle class, which had become prominent and powerful both in England and in the Netherlands because of the extensive world trade in which these two nations were engaged.

Members of the commercial middle class needed a clear and realistic view of the world in order to succeed with their enterprises. (An aristocrat of the period, on the other hand, might have been more comfortable with a somewhat romanticized and out-of-focus vision, which would allow him to overlook the suffering and injustice upon which his privileges were based.) The rise of the commercial middle class, with its virtues of industriousness, common sense and realism, went hand in hand with the rise of experimental science, which required the same virtues for its success.

In England, the House of Commons (which reflected the interests of the middle class), had achieved political power, and had demonstrated (in the Puritan Rebellion of 1640 and the Glorious Revolution of 1688) that Parliament could execute or depose any monarch who tried to rule without its consent. In France, however, the situation was very different.

After passing through a period of disorder and civil war, the French tried to achieve order and stability by making their monarchy more absolute. The movement towards absolute monarchy in France culminated in the long reign of Louis XIV, who became king in 1643 and who ruled until he died in 1715.

The historical scene which we have just sketched was the background against which the news of Newton's scientific triumph was received. The news was received by a Europe which was tired of religious wars; and in France, it was received by a middle class which was searching for an ideology in its struggle against the *ancien régime*.

To the intellectuals of the 18th century, the orderly Newtonian cosmos, with its planets circling the sun in obedience to natural law, became an imaginative symbol representing rationality. In their search for a society more in accordance with human nature, 18th century Europeans were greatly encouraged by the triumphs of science. Reason had shown itself to be an adequate guide in natural philosophy. Could not reason and natural law also be made the basis of moral and political philosophy? In attempting to carry out this program, the philosophers of the Enlightenment laid the foundations of psychology, anthropology, social science, political science and economics.

One of the earliest and most influential of these philosophers was John Locke (1632-1705), a contemporary and friend of Newton. In his *Second Treatise on Government*, published in 1690, John Locke's aim was to refute the doctrine that kings rule by divine right, and to replace that doctrine by an alternative theory of government, derived by reason from the laws of nature. According to Locke's theory, men originally lived together without formal government:

"Men living together according to reason," he wrote, "without a common superior on earth with authority to judge between them, is properly the state of nature... A state also of equality, wherein all the power and jurisdiction is reciprocal, no one having more than another; there being nothing more evident than that creatures of the same species, promiscuously born to all the same advantages of nature and the use of the same facilities, should also be equal amongst one another without subordination or subjection..."

"But though this be a state of liberty, yet it is not a state of licence... The state of nature has a law to govern it, which obliges every one; and reason, which is that law, teaches all mankind who will but consult it, that being equal and independent, no one ought to harm another in his life, health, liberty or possessions."

In Locke's view, a government is set up by means of a social contract. The government is given its powers by the consent of the citizens in return for the services which it renders to them, such as the protection of their lives and property. If a government fails to render these services, or if it becomes tyrannical, then the contract has been broken, and the citizens must set up a new government.

Locke's influence on 18th century thought was very great. His influence can be seen, for example, in the wording of the American Declaration of Independence. In England, Locke's political philosophy was accepted by almost everyone. In fact, he was only codifying

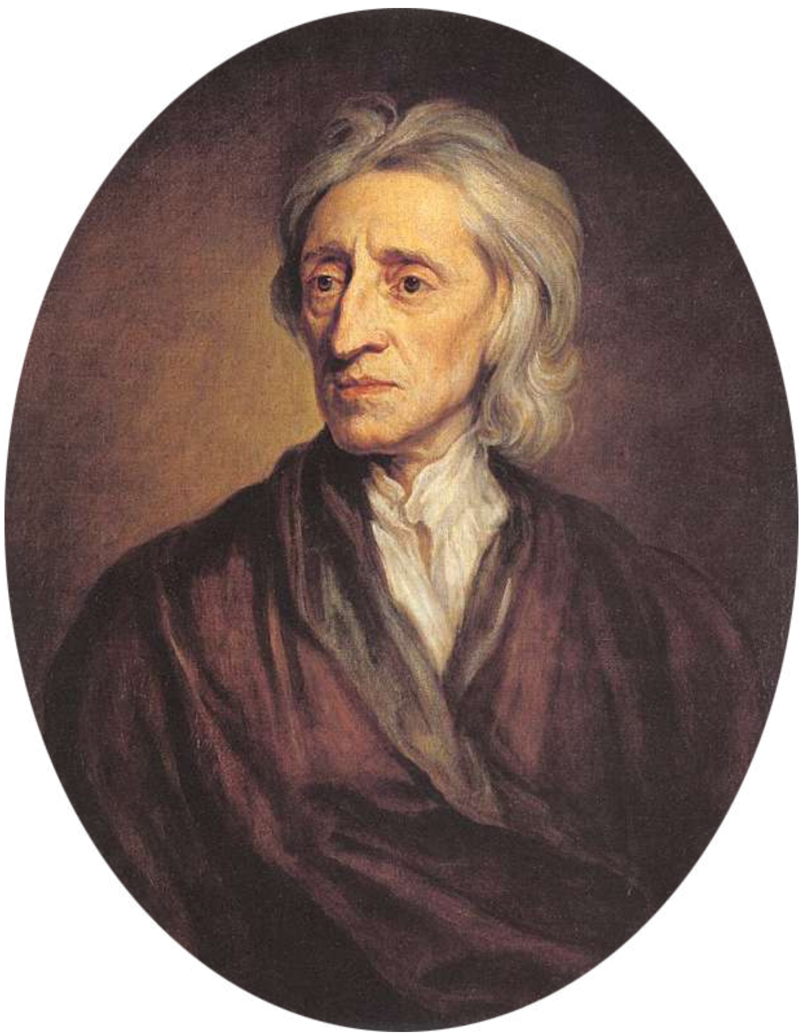

Figure 7.14: **Portrait of John Locke, by Sir Godfrey Kneller.**

ideas which were already in wide circulation and justifying a revolution which had already occurred. In France, on the other hand, Locke's writings had a revolutionary impact.

Credit for bringing the ideas of both Newton and Locke to France, and making them fashionable, belongs to Francois Marie Arouet (1694-1778), better known as "Voltaire". Besides persuading his mistress, Madame de Chatelet, to translate Newton's *Principia* into French, Voltaire wrote an extremely readable commentary on the book; and as a result, Newton's ideas became highly fashionable among French intellectuals. Voltaire lived with Madame du Chatelet until she died, producing the books which established him as the leading writer of Europe, a prophet of the Age of Reason, and an enemy of injustice, feudalism and superstition.

The Enlightenment in France is considered to have begun with Voltaire's return from England in 1729; and it reached its high point with the publication of of the *Encyclopedia* between 1751 and 1780. Many authors contributed to the *Encyclopedia*, which was an enormous work, designed to sum up the state of human knowledge.

Turgot and Montesquieu wrote on politics and history; Rousseau wrote on music, and Buffon on natural history; Quesnay contributed articles on agriculture, while the Baron d'Holbach discussed chemistry. Other articles were contributed by Condorcet, Voltaire and d'Alembert. The whole enterprise was directed and inspired by the passionate faith of Denis Diderot (1713-1784). The men who took part in this movement called themselves *"philosophes"*. Their creed was a faith in reason, and an optimistic belief in the perfectibility of human nature and society by means of education, political reforms, and the scientific method.

The *philosophes* of the Enlightenment visualized history as a long progression towards the discovery of the scientific method. Once discovered, this method could never be lost; and it would lead inevitably (they believed) to both the material and moral improvement of society. The *philosophes* believed that science, reason, and education, together with the principles of political liberty and equality, would inevitably lead humanity forward to a new era of happiness. These ideas were the faith of the Enlightenment; they influenced the French and American revolutions; and they are still the basis of liberal political belief.

7.9 Voltaire and Rousseau

Voltaire (1694-1778)

Francois-Marie Arouet, who later changed his name to Voltaire, was born in Paris. His father was a lawyer and a minor treasury official, while his mother's family was on the lowest rank if the French nobility. He was educated by Jesuits at Collège Louis-le-Grande, where he learned Latin theology and rhetoric. He later became fluent in Italian, Spanish and English.

Despite his father's efforts to make him study law, the young Voltaire was determined to become a writer. He eventually became the author of more than 2,000 books and pamphlets and more than 20,000 letters. His works include many forms of writing, including plays, poems, novels, essays and historical and scientific works. His writings advocated civil liberties, and he used his satirical and witty style of writing to criticize intolerance, religious dogma and absolute monarchy. Because of the intolerance and censorship of his day, he was frequently in trouble and sometimes imprisoned. Nevertheless, his works were very popular, and he eventually became extremely rich, partly through clever investment of money gained through part ownership of a lottery.

During a period of forced exile in England, Voltaire mixed with the English aristocracy, meeting Alexander Pope, John Gay, Jonathan Swift, Lady Mary Wortley Montague, Sarah, Duchess of Marlborough, and many other members of the nobility and royalty. He admired the English system of constitutional monarchy, which he considered to be far superior to the absolutism then prevailing in France. In 1733, he published a book entitled *Letters concerning the English Nation*, in London. When French translation was published in 1734, Voltaire was again in deep trouble. In order to avoid arrest, he stayed in the country château belonging to Émilie du Châtelet and her husband, the Marquis du Châtelet.

As a result, Madame du Châtelet became his mistress and the relationship lasted for 16 years. Her tolerant husband, the Marquis, who shared their intellectual and scientific interests, often lived together with them. Voltaire paid for improvements to the château, and together, the Marquis and Voltaire collected more than 21,000 books, and enormous number for that time. Madame du Châtelet translated Isaac Newton's great book, *Principia Mathematica*, into French, and her translation was destined to be the standard one until modern times. Meanwhile, Voltaire wrote a French explanation of the ideas of the *Principia*, which made these ideas accessible to a wide public in France. Together, the Marquis, his wife and Voltaire also performed many scientific experiments, for example experiments designed to study the nature of fire.

Voltaire's vast literary output is available today in approximately 200 volumes, published by the University of Oxford, where the Voltaire Foundation is now established as a research department.

Rousseau (1712-1778)

In 1754 Rousseau wrote: "The first man who, having fenced in a piece of land, said 'This is mine', and found people naïve enough to believe him, that man was the true founder of civil society. From how many crimes, wars, and murders, from how many horrors and misfortunes might not any one have saved mankind, by pulling up the stakes, or filling up the ditch, and crying to his fellows: Beware of listening to this impostor; you are undone if you once forget that the fruits of the earth belong to us all, and the earth itself to nobody."

Later, he began his influential book *The Social Contract*, published in 1752, with the dramatic words: "Man is born free, and everywhere he is in chains. Those who think themselves the masters of others are indeed greater slaves than they." Rousseau concludes Chapter 3 of this book with the words: "Let us then admit that force does not create right, and that we are obliged to obey only legitimate powers". In other words, the ability to coerce is not a legitimate power, and there is no rightful duty to submit to it. A state has

Figure 7.15: **Voltaire used his satirical and witty style of writing to criticize intolerance, religious dogma and absolute monarchy. He wrote more than 2,000 books and pamphlets and more than 20,000 letters. His writings made a significant contribution to the Enlightenment, and paved the way for revolutions both in France and America.**

Figure 7.16: **The frontpiece of Voltaire's book popularizing Newton's ideas for French readers. Madame du Châtelet appears as a muse, reflecting Newton's thoughts down to Voltaire.**

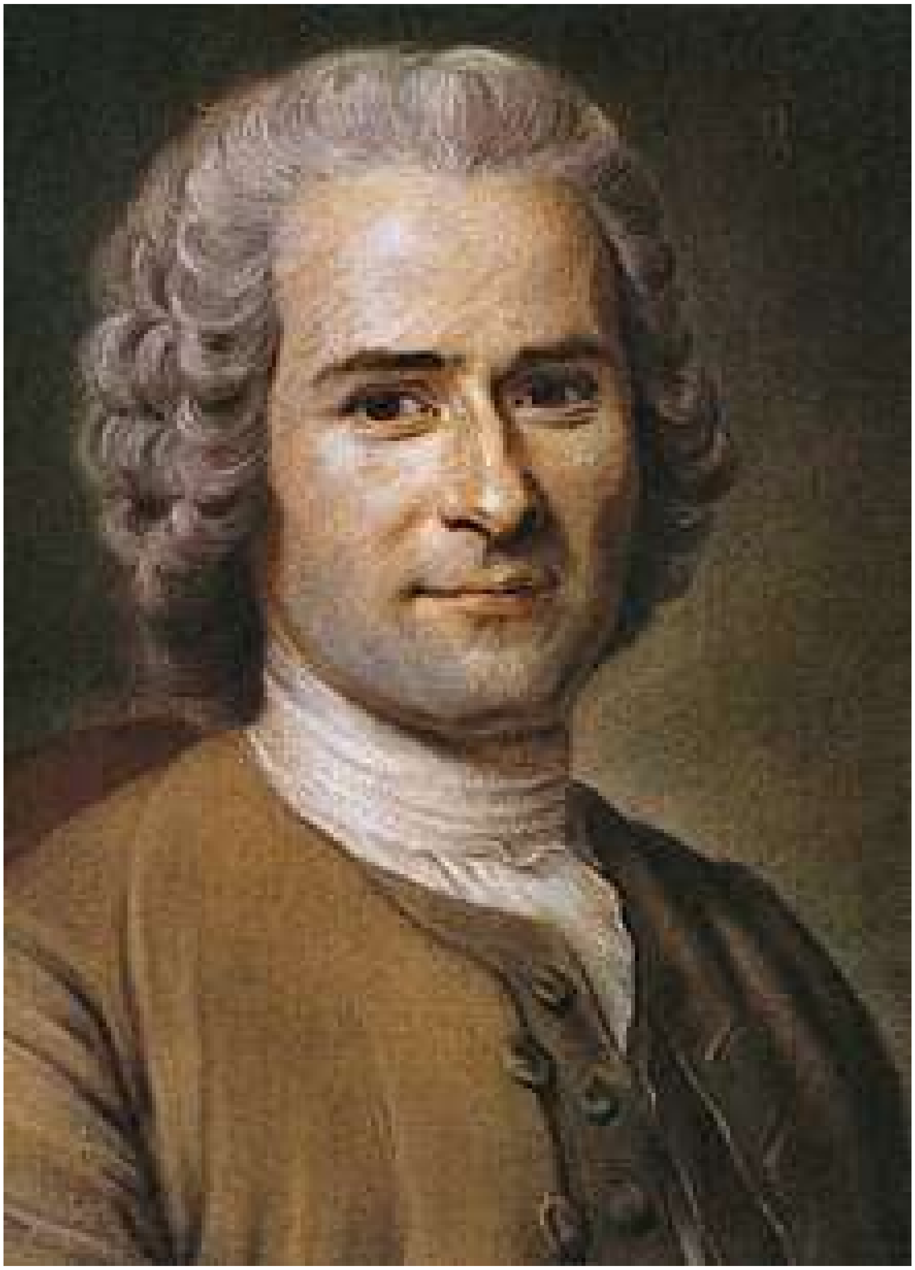

Figure 7.17: **Unlike Voltaire, Rousseau was not an advocate of science, but instead believed in the importance of emotions. He believed that civilization has corrupted humans rather than making them better. Rousseau was a pioneer of the romantic movement. His book, *The Social Contract*, remains influential today.**

no right to enslave a conquered people.

These ideas, and those of John Locke, were reaffirmed in 1776 by the American Declaration of Independence: "We hold these truths to be self-evident: That all men are created equal. That they are endowed by their Creator with certain inaliable rights, and the among these are the rights to life, liberty and the pursuit of happiness; and that to pursue these rights, governments are instituted among men, deriving their just powers from the consent of the governed."

Today, in an era of government tyranny and subversion of democracy, we need to remember that the just powers of any government are not derived from the government's ability to use of force, but exclusively from the consent of the governed.

Suggestions for further reading

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Chapter 8

THE BERNOULLI'S AND EULER

8.1 The Bernoullis and Euler

Among the followers of Leibniz was an extraordinary family of mathematicians called Bernoulli. They were descended from a wealthy merchant family in Basel, Switzerland. The head of the family, Nicolas Bernoulli the Elder, tried to force his three sons, James (1654-1705), Nicolas II (1662-1716) and John (1667-1748) to follow him in carrying on the family business. However, the eldest son, James, had taught himself the Leibnizian form of calculus, and instead became Professor of Mathematics at the University of Basel. His motto was *"Invicto patre sidera verso"* ("Against my father's will, I study the stars").

Nicolas II and John soon caught their brother's enthusiasm, and they learned calculus from him. John became Professor of Mathematics in Gröningen and Nicolas II joined the faculty of the newly-formed Academy of St. Petersburg. John Bernoulli had three sons, Nicolas III (1695-1726), Daniel (1700-1782) and John II (1710-1790), all of whom made notable contributions to mathematics and physics. In fact, the family of Nicolas Bernoulli the Elder produced a total of nine famous mathematicians in three generations!

Daniel Bernoulli's brilliance made him stand out even among the other members of his gifted family. He became professor of mathematics at the Academy of Sciences in St. Petersburg when he was twenty-five. After eight Russian winters however, he returned to his native Basel. Since the chair in mathematics was already occupied by his father, he was given a vacant chair, first in anatomy, then in botany, and finally in physics. In spite of the variety of his titles, however, Daniel's main work was in applied mathematics, and he has been called the father of mathematical physics.

One of the good friends of Daniel Bernoulli and his brothers was a young man named Leonhard Euler (1707-1783). He came to their house once a week to take private lessons from their father, John Bernoulli. Euler was destined to become the most prolific mathematician in history, and the Bernoullis were quick to recognize his great ability. They persuaded Euler's father not to force him into a theological career, but instead to allow him to go with Nicolas III and Daniel to work at the Academy in St. Petersburg.

Euler married the daughter of a Swiss painter and settled down to a life of quiet work, producing a large family and an unparalleled output of papers. A recent edition of Euler's works contains 70 quarto volumes of published research and 14 volumes of manuscripts and letters. His books and papers are mainly devoted to algebra, the theory of numbers, analysis, mechanics, optics, the calculus of variations (invented by Euler), geometry, trigonometry and astronomy; but they also include contributions to shipbuilding science, architecture, philosophy and musical theory!

Euler achieved this enormous output by means of a calm and happy disposition, an extraordinary memory and remarkable powers of concentration, which allowed him to work even in the midst of the noise of his large family. His friend Thiébault described Euler as sitting "..with a cat on his shoulder and a child on his knee - that was how he wrote his immortal works".

In 1771, Euler became totally blind. Nevertheless, aided by his sons and his devoted scientific assistants, he continued to produce work of fundamental importance. It was his habit to make calculations with chalk on a board for the benefit of his assistants, although he himself could not see what he was writing. Appropriately, Euler was making such computations on the day of his death. On September 18, 1783, Euler gave a mathematics lesson to one of his grandchildren, and made some calculations on the motions of balloons. He then spent the afternoon discussing the newly-discovered planet Uranus with two of his assistants. At five o'clock, he suffered a cerebral hemorrhage, lost consciousness, and died soon afterwards. As one of his biographers put it, "The chalk fell from his hand; Euler ceased to calculate, and to live".

In the eighteenth century it was customary for the French Academy of Sciences to propose a mathematical topic each year, and to award a prize for the best paper dealing with the problem. Léonard Euler and Daniel Bernoulli each won the Paris prize more than ten times, and they share the distinction of being the only men ever to do so. John Bernoulli is said to have thrown his son out of the house for winning the Paris prize in a year when he himself had competed for it.

Euler and the Bernoullis did more than anyone else to develop the Leibnizian form of calculus into a workable tool and to spread it throughout Europe. They applied it to a great variety of problems, from the shape of ships' sails to the kinetic theory of gasses. An example of the sort of problem which they considered is the vibrating string.

In 1727, John Bernoulli in Basel, corresponding with his son Daniel in St. Petersburg, developed an approximate set of equations for the motion of a vibrating string by considering it to be a row of point masses, joined together by weightless springs. Then Daniel boldly passed over to the continuum limit, where the masses became infinitely numerous and small.

The result was Daniel Bernoulli's famous wave equation, which is what we would now call a partial differential equation. He showed that the wave equation has sinusoidal solutions, and that the sum of any two solutions is also a solution. This last result, his superposition principle, is a mathematical proof of a property of wave motion noticed by Huygens. The fact that many waves can propagate simultaneously through the same medium without interacting was one of the reasons for Huygens' belief that light is wave-like, since he knew that many rays of light from various directions can cross a given space simultaneously without interacting. Because of their work with partial differential equations, Daniel Bernoulli and Léonard Euler are considered to be the founders of modern theoretical physics.

8.2 Linear ordinary differential equations

Leonhard Euler and all the members of the Bernoulli family were very much interested in differential equations, i.e., in equations relating the differentials of functions to the functions themselves. The simplest example of this type of relationship is the equation:

$$\frac{df}{dt} = kf \tag{8.1}$$

where k is some constant. Equation (8.1) states that the rate of change of some function $f(t)$ is proportional to the function itself. This equation might (for example) describe the rate of growth of money that we have put into the bank, where k is the interest rate. It might also describe the increase or decrease of a population, where k represents the difference between the birth rate and the death rate. In both cases, the rate of change of f is proportional to the amount of f present at a given time. We can try to solve the equation by assuming that the solution can be represented by a series of the form

$$f = \sum_{n=0}^{\infty} a_n t^n = a_0 + a_1 t + a_2 t^2 + a_3 t^3 + a_4 t^4 + \cdots \tag{8.2}$$

where the a_n's are constants that we have to determine. Then the first derivative of the function f with respect to t will be given by

$$\frac{df}{dt} = \sum_{n=0}^{\infty} n a_n t^{n-1} = a_1 + 2a_2 t + 3a_3 t^2 + 4a_4 t^3 + \cdots \tag{8.3}$$

Substituting equations (8.2) and (8.3) into (8.1), we obtain:

$$a_1 + 2a_2 t + 3a_3 t^2 + 4a_4 t^3 + \cdots = ka_0 + ka_1 t + ka_2 t^2 + ka_3 t^3 + ka_4 t^4 + \cdots \tag{8.4}$$

In order for (8.4) to hold for all values of t, we need the following relationships between the constant coefficients a_n:

$$\begin{array}{rcl} a_1 & = & ka_0 \\ 2a_2 & = & ka_1 \\ 3a_3 & = & ka_2 \\ 4a_4 & = & ka_3 \\ 5a_5 & = & ka_4 \\ \vdots & \vdots & \vdots \end{array} \tag{8.5}$$

This set of equations can be solved to give all of the higher coefficients in terms of a_0:

$$\begin{aligned}
a_1 &= \frac{k^2}{1!}a_0 \\
a_2 &= \frac{k^2}{2!}a_0 \\
a_3 &= \frac{k^2}{3!}a_0 \\
a_4 &= \frac{k^2}{4!}a_0 \\
\vdots &\quad \vdots \quad \vdots \\
a_n &= \frac{k^2}{n!}a_0
\end{aligned} \tag{8.6}$$

Substituting these values of the coefficients back into (8.2) and remembering Napier's series definition of e, we obtain

$$f = a_0\left(1 + kt + \frac{(kt)^2}{2!} + \frac{(kt)^3}{3!} + \frac{(kt)^4}{4!} + \cdots\right) \equiv e^{kt} \tag{8.7}$$

In other words, when we differentiate e^{kt} with respect to t, we obtain the same function again, multiplied by k.

8.3 Second-order differential equations

Equation (8.1) is called a "first-order ordinary differential equation" - first-order because it involves only the function itself and its first derivative with no higher derivatives appearing; ordinary because it involves only one variable, t. We will now go on to discuss an example of a second-order ordinary differential equation, where we will see that there are two constants that must be determined by the boundary conditions of the problem.

The harmonic oscillator

As an example of a second-order ordinary differential equation, let us consider the relationship

$$\frac{d^2f}{dt^2} = -\omega_0^2 f \tag{8.8}$$

We can solve this equation by assuming that the function f can be represented by the series shown in equation (8.2), so that its first derivative with respect to t is given by (8.3).

Then, differentiating a second time with respect to t, we have

$$\frac{d^2 f}{dt^2} = \frac{d}{dt}\left(\sum_{n=0}^{\infty} n a_n t^{n-1}\right) = \sum_{n=0}^{\infty} n(n-1) a_n t^{n-2} = -\omega_0^2 \sum_{n=0}^{\infty} a_n t^n \tag{8.9}$$

The requirement that (8.9) must hold for all values of t gives us a set of equations relating the higher even coefficients to a_0:

$$\begin{aligned} a_2 &= -\frac{\omega_0^2}{2!} a_0 \\ a_4 &= -\frac{\omega_0^2}{4!} a_2 \\ a_6 &= -\frac{\omega_0^2}{6!} a_4 \\ \vdots & \quad \vdots \quad \vdots \end{aligned} \tag{8.10}$$

and another set of equations relating the higher odd coefficients to a_1:

$$\begin{aligned} a_3 &= -\frac{\omega_0^2}{3!} a_1 \\ a_5 &= -\frac{\omega_0^2}{5!} a_3 \\ a_7 &= -\frac{\omega_0^2}{7!} a_5 \\ \vdots & \quad \vdots \quad \vdots \end{aligned} \tag{8.11}$$

Thus the solution can be written in the form

$$f = a_1 \left(\omega_0 t - \frac{(\omega_0 t)^3}{3!} + \frac{(\omega_0 t)^5}{5!} - \cdots\right) + a_0 \left(1 - \frac{(\omega_0 t)^2}{2!} + \frac{(\omega_0 t)^4}{4!} - \cdots\right) \tag{8.12}$$

Euler recognized this as being the same as

$$f = a_1 \sin(\omega_0 t) + a_0 \cos(\omega_0 t) \tag{8.13}$$

since series representations of the sine and cosine functions were well known at the time when he was working. He was also able to solve the harmonic oscillator equation in an alternative way by letting

$$f = e^{\pm i\omega_0 t} \tag{8.14}$$

where $i^2 \equiv -1$. This gave Euler two linearly independent solutions, one with the plus sign, and one with the minus sign. Comparing these solutions to the series solutions just discussed, he was led to the formula

$$e^{ix} = \cos(x) + i \sin(x) \tag{8.15}$$

and to the identity

$$e^{i\pi} + 1 = 0 \tag{8.16}$$

8.4 Partial differentiation; Daniel Bernoulli's wave equation

Having discussed differential equations involving only a single variable (ordinary differential equations), let us now turn to differential equations involving several variables. These are called "partial differential equations". The most important pioneer of this branch of mathematics was Daniel Bernoulli.

In 1727, John Bernoulli in Basel, corresponding with his son Daniel in St. Petersburg, developed an approximate set of equations for the motion of a vibrating string by considering it to be a row of point masses, joined together by weightless springs. Then Daniel boldly passed over to the continuum limit, where the masses became infinitely numerous and small.

The result was Daniel Bernoulli's famous wave equation, which is what we would now call a partial differential equation. But what is a partial differential equation? What is partial differentiation?

Daniel Bernoulli developed his wave equation to describe the motion of a vibrating string, for example a violin string, and in this problem there are two variables: x, which represents the distance along the string, and t, which represents time. The displacement of the string from its equilibrium position is represented by $f(x,t)$. In other words, the displacement is a function of two variables, position and time. To deal with this problem, Daniel Bernoulli defined partial differentials in much the same way that Isaac Newton defined ordinary differentials. He introduced the definitions:

$$\frac{\partial f}{\partial x} \equiv \begin{array}{c}\text{limit}\\ \Delta x \to 0\end{array} \left[\frac{f(x+\Delta x, t) - f(x,t)}{\Delta x}\right] \tag{8.17}$$

and

$$\frac{\partial f}{\partial t} \equiv \begin{array}{c}\text{limit}\\ \Delta t \to 0\end{array} \left[\frac{f(x, t+\Delta t) - f(x,t)}{\Delta t}\right] \tag{8.18}$$

The rules for partial differentiation are the same as for ordinary differentiation, except that we must add an extra rule: When performing partial differentiation with respect to one variable, all other variables must be regarded as constants. Second partial derivatives are defined similarly. For example, to find

$$\frac{\partial^2 f}{\partial x^2} \equiv \frac{\partial}{\partial x}\left[\frac{\partial f}{\partial x}\right] \tag{8.19}$$

and similarly

$$\frac{\partial^2 f}{\partial t^2} \equiv \frac{\partial}{\partial t}\left[\frac{\partial f}{\partial t}\right] \tag{8.20}$$

It is also possible to define mixed partial derivatives, and it turns out that in the mixed second partial derivative the order of differentiation does not matter.

$$\frac{\partial^2 f}{\partial x \partial t} \equiv \frac{\partial}{\partial x}\left[\frac{\partial f}{\partial t}\right] = \frac{\partial}{\partial t}\left[\frac{\partial f}{\partial x}\right] \tag{8.21}$$

In the notation that we have been discussing, Daniel Bernoulli's wave equation has the form

$$\left[\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right] f(x,t) = 0 \tag{8.22}$$

where c is a constant. Bernoulli was able to show that in the case of a vibrating string,

$$c = \sqrt{\frac{T}{\mu}} \tag{8.23}$$

where T is the tension in the string and where μ is the mass per unit length. Daniel Bernoulli solved his wave equation by assuming that a solution could be written in the form

$$f(x,t) = \phi(x)\left[\cos(\omega t) + a_1 \sin(\omega t)\right] \tag{8.24}$$

where the constant a_1 is determined by the initial conditions of the problem. Then, since

$$-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\left[\cos(\omega t) + a_1 \sin(\omega t)\right] = -\omega^2\left[\cos(\omega t) + a_1 \sin(\omega t)\right] \tag{8.25}$$

The x-dependent part of the solution had to satisfy

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\omega^2}{c^2}\right)\phi(x) = \left(\frac{\partial^2}{\partial x^2} + k^2\right)\phi(x) = 0 \tag{8.26}$$

where

$$k^2 \equiv \frac{\omega^2}{c^2} \tag{8.27}$$

Daniel Bernoulli showed that (8.26) has sinusoidal solutions of the form

$$\phi(x) = A_1 \sin(kx) + A_2 \cos(kx) \tag{8.28}$$

where the constants A_1 and A_2 as well as the value of k are determined by the boundary conditions. For example, if the vibrating string is clamped at the positions $x = 0$ and $x = L$, then we know that $A_2 = 0$ (since $\cos(0) = 0$), and that

$$\phi(L) = \sin(kL) = 0 \tag{8.29}$$

The boundary condition shown in equation (8.29) determines the allowed values of k; they must such that kL is an integral multiple of π, and thus the only allowed values are

$$k = \frac{n\pi}{L} \qquad n = 1, 2, 3, 4, \cdots \tag{8.30}$$

Only positive integers need be considered, because although the negative integers would satisfy the boundary conditions, they do not yield any new independent solutions. Thus Daniel Bernoulli's wave equation, with the boundary conditions f (0, t) = 0 and f (L, t) = 0, can be satisfied by any function of the form

$$f_n(x,t) = A_n \sin(kx) \left[\cos(kct) + a_n \sin(kct)\right] \qquad k = \frac{n\pi}{L} \tag{8.31}$$

where n is an integer.

8.5 Daniel Bernoulli's superposition principle

Daniel Bernoulli realized that the sum of any two solutions to his wave equation is also a solution. This is easy to prove: We know that if $f_n(x,t)$ has the form shown in equation (8.31), then

$$\left[\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right] f_n(x,t) = 0 \tag{8.32}$$

Then a function of the form

$$\Phi(x,t) = \sum_n f_n(x,t) \tag{8.33}$$

will also be a solution, since

$$\left[\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right] \Phi(x,t) = \sum_n \left[\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right] f_n(x,t) = 0 \tag{8.34}$$

Daniel Bernoulli's superposition principle is a mathematical proof of a property of wave motion noticed by Huygens. The fact that many waves can propagate simultaneously through the same medium without interacting was one of the reasons for Huygens' belief that light is wavelike, since he knew that many rays of light from various directions can cross a given space simultaneously without interacting.

8.6 The argument between Bernoulli and Euler

Leonhard Euler and Daniel Bernoulli were both such great mathematicians and great friends that it is strange to think that there could ever have been a disagreement between them. Nevertheless, a long argument between these two geniuses began as a result of their independent solutions to the wave equation. The argument was by no means sterile, however, and eventually it led to the foundation of a new branch of mathematics - Fourier analysis.

We have just seen Bernoulli's solution to the wave equation. Leonhard Euler also solved it, and in a completely different way. Euler showed that if F and G are any two well-behaved functions of a single variable, then

$$\left[\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right] F(x+ct) = 0 \tag{8.35}$$

and

$$\left[\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right] G(x-ct) = 0 \tag{8.36}$$

For example, when

$$F(x+ct) = (x+ct)^2 = x^2 + 2xct + c^2t^2 \tag{8.37}$$

then

$$\frac{\partial^2}{\partial x^2} F(x+ct) = \frac{\partial^2}{\partial x^2}\left[x^2 + 2xct + c^2t^2\right] = 2 \tag{8.38}$$

while

$$-\frac{1}{c^2}\frac{\partial^2}{\partial t^2} F(x+ct) = -\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\left[x^2 + 2xct + c^2t^2\right] = -2 \tag{8.39}$$

Adding (10-38) to (8.39) yields (8.35). Notice that in carrying out the partial differentiations with respect to x, we regard t as a constant, while when we differentiate with respect to t, we hold x constant.

Leonhard Euler was able to show that if F is a function of some variable w, then

$$\frac{\partial}{\partial x} F(w) = \frac{\partial F}{\partial w}\frac{\partial w}{\partial x} \qquad\qquad \frac{\partial}{\partial t} F(w) = \frac{\partial F}{\partial w}\frac{\partial w}{\partial t} \tag{8.40}$$

and using these relationships he was able to prove that equations (8.35) and (8.36) hold in general, no matter what the functions F and G might be.

Meanwhile, Daniel Bernoulli had derived his own solutions to the wave equation, the ones shown in equation (8.31), and he had also shown that if these solutions are added together, with various values of the constants A_n and a_n , the result is also a solution. Euler and Bernoulli wrote letters to each other about their work on the wave equation, and being great mathematicians, they were able draw the logical conclusion that followed from their results: If they were both right, it had to follow that by choosing the constants A_n in the right way it would be possible to construct series such that

$$f(x) = \sum_{n=0}^{\infty} A_n \sin\left(\frac{n\pi x}{L}\right) \qquad n = 1, 2, 3, 4, \cdots \tag{8.41}$$

regardless of the form of $f(x)$, the only restriction being that f should be single-valued, continuous and differentiable and that it should obey the boundary conditions $f(0) = 0$ and $f(L) = 0$. Euler found this hard to believe, and to the end of his life he continued to think that there must be something wrong. Euler believed the he himself had found the most general solutions to the wave equation, and that his friend Daniel's set of solutions was somehow incomplete - not sufficiently general. This famous argument between the two great mathematicians led to a whole new branch of mathematics - Fourier analysis.

Together with Joseph-Louis Lagrange (1736-1813), Leonhard Euler pioneered another new branch of matematics, variational calculus, which we will discuss in detail in the chapter on Lagrange.

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Chapter 9

FOURIER

9.1 A poor taylor's son becomes Napoleon's friend

The controversy about the completeness of Bernoulli's solutions was still raging when Jean-Baptiste Joseph Fourier (1768-1830) arrived on the scene. Although he began life as the orphaned son of a poor tailor, Fourier later achieved distinction as Professor of Mathematics at Napoleon's École Normale, and he even became a personal friend of the emperor.

Fourier was orphaned at the age of nine, but through a recommendation to the Bishop of Auxerre, he was educated by the Benedictine Order of the Convent of St. Mark, where he soon exhibited many signs of genius. After graduating, Fourier became a military lecturer in mathematics. During the French Revolution, he played a prominent role in his own district, serving on the Revolutionary Committee. He was imprisoned briefly during Robespierre's Terror. After his release, Joseph Fourier was appointed to the École Normale, and afterwards, he rose to become the successor to Joseph-Louis Lagrange at the École Polytechnique.

Fourier followed Napoleon to Egypt, where he helped to set up the Egyptian Institute, and where he made estimates of the ages of the pyramids and other monuments. Napoleon finally appointed Fourier as the Prefect of a district in southern France in the vicinity of Grenoble. Fourier worked hard at this job, supervising (for example) the draining of swamps to eliminate malaria. Nevertheless, he continued his mathematical research, and during his time in Grenoble he composed a monumental study of heat conduction, his *Mémoir sur la Chaleur*. In this work, he made use of a method that later became known as Fourier analysis.

9.2 Fourier's studies of heat

The diffusion equation, which governs heat flow, is similar to the wave equation except that it involves only first-order differentiation with respect to time. For the case of heat flow in a metal rod, the equation for the temperature as a function of both position and time has the form

$$\frac{\partial}{\partial t}T(x,t) = C\frac{\partial^2}{\partial x^2}T(x,t) \tag{9.1}$$

Here T is the temperature, x and t are position and time respectively and C is a constant which depends on the material.. To simplify the problem, we have considered only one space dimension. Equation (9.1) might, for example, describe heat flow in an iron bar.

9.3 Fourier analysis

Fourier was able to use a slightly modified version of Daniel Bernoulli's methods to find solutions to the diffusion equation, and given the initial temperature distribution, he was able to calculate the temperature distribution at any future time. To do this, he needed to determine the constants A_n in series such as the one shown in equation (10.41). (Today, this type of series is called a Fourier series.) One of the equations that Fourier used to determine these constants had the form

$$\frac{2}{L}\int_0^L dx \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right) = \begin{cases} 0 \text{ if } n \neq m \\ \\ 1 \text{ if } n = m \end{cases} \tag{9.2}$$

where both n and m are integers. From equation (9.2) it follows that

$$\frac{2}{L}\int_0^L dx \sin\left(\frac{n\pi x}{L}\right) f(x) = \frac{2}{L}\int_0^L dx \sin\left(\frac{n\pi x}{L}\right)\sum_{m=0}^{\infty} A_m \sin\left(\frac{m\pi x}{L}\right) = A_n \tag{9.3}$$

Fourier was able to substitute the A_n's calculated from (9.3) back into the series for f (x). For example, suppose that

$$f(x) = \begin{cases} 1 \text{ if } x < L/2 \\ \\ 0 \text{ if } x > L/2 \end{cases} \tag{9.4}$$

Then

$$\begin{aligned} A_n &= \frac{2}{L}\int_0^L dx \sin\left(\frac{n\pi x}{L}\right) f(x) \\ &= \frac{2}{L}\int_0^{L/2} dx \sin\left(\frac{n\pi x}{L}\right) \\ &= \frac{2}{n\pi}\left[1 - \cos\left(\frac{n\pi x}{L}\right)\right] \end{aligned} \tag{9.5}$$

When Fourier submitted his *Mémoir sur la Chaleur* to the Academy of Sciences in Paris, it was severely criticized and it failed to win the annual prize set by the Academy.

Figure 9.1: **Engraved portrait of French mathematician Jean Baptiste Joseph Fourier (1768-1830). He founded a branch of mathematics now known as Fourier analysis. Its generalizations have great importance for many branches of theoretical science and engineering.**

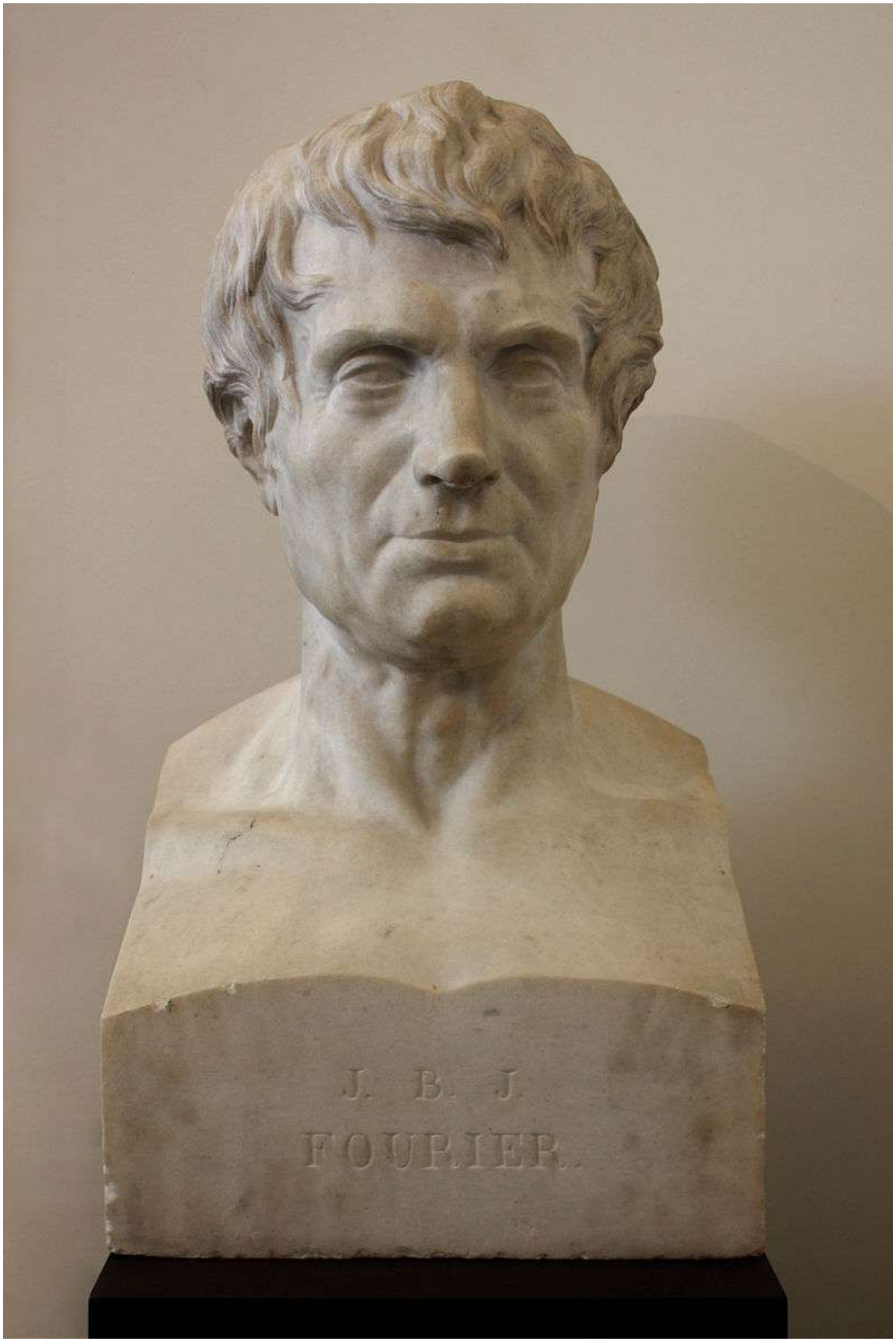

Figure 9.2: **Bust of Fourier in Grenoble.**

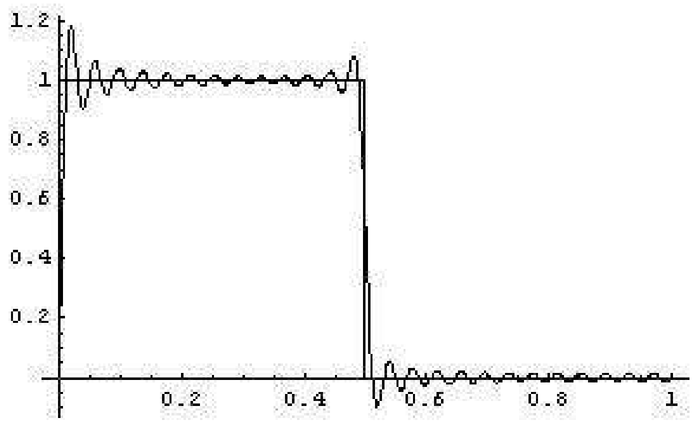

Figure 9.3: **This figure shows the Fourier series representation of the function defined by equation (9.4) compared with the function itself. The slowly convergent series has been truncated after 50 terms, and thus it fails to represent the function with complete accuracy. However, if an infinite number of terms had been included, the Fourier series would be completely accurate. "Square waves" of the kind shown here are sometimes used to test high fidelity electronic amplifiers, because very high frequencies are needed to accurately reproduce the sharp corners of the square wave.**

The jury consisted of three of the most eminent mathematicians of the period, Joseph-Louis Lagrange (1736-1813), Pierre-Simon Laplace (1749-1827) and Adrien-Marie Legendre (1749-1827). Lagrange, Laplace and Legendre objected that although Fourier's methods worked extremely well in practice, he had not really overcome Euler's objections, i.e. he had not really shown that every continuous, single-valued and differentiable function f (x) obeying the boundary conditions $f(0) = 0$ and $f(L) = 0$ can be represented by the series shown in equation (10.41). (This property of the set of functions in the series is called "completeness", and it was not proved until much later.) Undeterred by the criticism, Fourier published his book without any changes. Both parties were right. Fourier was right in believing his set of functions to be complete, and the jury was right in pointing out that he had not proved it. The generalizations of Fourier's methods are extremely powerful, and they form the basis for many branches of theoretical science and engineering.

9.4 Fourier transforms

Notation and basic properties

Let us introduce the abbreviated notation:

$$\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \cdots \int_{-\infty}^{\infty} dx_d \; f(x_1, x_2, \ldots, x_d) \equiv \int d\mathbf{x} \; f(\mathbf{x}) \tag{9.6}$$

and

$$e^{i(p_1x_1+p_2x_2+\cdots+p_dx_d)} \equiv e^{i\mathbf{p}\cdot\mathbf{x}} \tag{9.7}$$

Then the d-dimensional Fourier transform of the function $f(\mathbf{x})$ is given by

$$f^t(\mathbf{p}) = \frac{1}{(2\pi)^{d/2}} \int d\mathbf{x}\ e^{-i\mathbf{p}\cdot\mathbf{x}}\ f(\mathbf{x}) \tag{9.8}$$

while the inverse transform is

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}} \int d\mathbf{p}\ e^{i\mathbf{p}\cdot\mathbf{x}}\ f^t(\mathbf{p}) \tag{9.9}$$

We would like to show that the scalar product of two functions in direct space is equal to the scalar product of their Fourier transforms in reciprocal space. From (9.9) we have

$$g(\mathbf{x})^* = \frac{1}{(2\pi)^{d/2}} \int d\mathbf{p}'\ e^{-i\mathbf{p}'\cdot\mathbf{x}}\ g^t(\mathbf{p}')^* \tag{9.10}$$

so that

$$\int d\mathbf{x}\ g(\mathbf{x})^* f(\mathbf{x}) = \frac{1}{(2\pi)^d} \int d\mathbf{p} \int d\mathbf{p}'\ g^t(\mathbf{p}')^* f^t(\mathbf{p}) \int d\mathbf{x}\ e^{i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{x}} \tag{9.11}$$

However,

$$\frac{1}{(2\pi)^d} \int d\mathbf{x}\ e^{i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{x}} = \delta(\mathbf{p}-\mathbf{p}') \tag{9.12}$$

so that

$$\int d\mathbf{x}\ g(\mathbf{x})^* f(\mathbf{x}) = \int d\mathbf{p}\ g^t(\mathbf{p})^* f^t(\mathbf{p}) \tag{9.13}$$

Equation (9.13) implies that if we have an orthonormal set of functions $\{\phi_j(\mathbf{x})\}$ in direct space, so that

$$\int d\mathbf{x}\ \phi^*_{j'}(\mathbf{x})\phi_j(\mathbf{x}) = \delta_{j',j} \tag{9.14}$$

then their Fourier transforms form an orthonormal set in reciprocal space:

$$\int d\mathbf{p}\ \phi^{t*}_{j'}(\mathbf{p})\phi^t_j(\mathbf{p}) = \delta_{j',j} \tag{9.15}$$

From (9.13) it also follows that

$$\int d\mathbf{x}\ \phi^*_{j'}(\mathbf{x})V(\mathbf{x})\phi_j(\mathbf{x}) = \int d\mathbf{p}\ \phi^{t*}_{j'}(\mathbf{p})(V\phi_j)^t(\mathbf{p}) \tag{9.16}$$

where

$$(V\phi_j)^t(\mathbf{p}) \equiv \frac{1}{(2\pi)^{d/2}} \int d\mathbf{x}\; e^{-i\mathbf{p}\cdot\mathbf{x}}\; V(\mathbf{x})\phi_j(\mathbf{x}) \tag{9.17}$$

Also, from (9.9) and (9.13) we have

$$\int d\mathbf{p}\; \phi_{j'}^{t*}(\mathbf{p})\; \Delta\phi_j^t(\mathbf{p}) = -\int d\mathbf{p}\; \phi_{j'}^{t*}(\mathbf{p})\; p^2\phi_j^t(\mathbf{p}) \tag{9.18}$$

where

$$p^2 \equiv \mathbf{p}\cdot\mathbf{p} \tag{9.19}$$

Expansion of a plane wave

Suppose that we have a complete set of orthonormal functions $\{\phi_j(\mathbf{x})\}$ in a d-dimensional space. The completeness condition (in the sense of distributions) can be written in the form

$$\sum_j \phi_j^*(\mathbf{x})\phi_j(\mathbf{x}') = \delta(\mathbf{x}-\mathbf{x}') \tag{9.20}$$

Multiplying both sides of (9.20) by $e^{-i\mathbf{p}\cdot\mathbf{x}'}$ and integrating over $d\mathbf{x}'$, we obtain:

$$\sum_j \phi_j^*(\mathbf{x}) \int d\mathbf{x}'\; e^{-i\mathbf{p}\cdot\mathbf{x}'}\; \phi_j(\mathbf{x}') = \int d\mathbf{x}'\; e^{-i\mathbf{p}\cdot\mathbf{x}'}\; \delta(\mathbf{x}-\mathbf{x}') = e^{-i\mathbf{p}\cdot\mathbf{x}} \tag{9.21}$$

so that

$$\begin{aligned} e^{-i\mathbf{p}\cdot\mathbf{x}} &= \sum_j \phi_j^*(\mathbf{x}) \int d\mathbf{x}'\; e^{-i\mathbf{p}\cdot\mathbf{x}'}\; \phi_j(\mathbf{x}') \\ &= (2\pi)^{d/2} \sum_j \phi_j^*(\mathbf{x})\phi_j^t(\mathbf{p}) \end{aligned} \tag{9.22}$$

Then

$$\begin{aligned} f^t(\mathbf{p}) &= \frac{1}{(2\pi)^{d/2}} \int d\mathbf{x}\; e^{-i\mathbf{p}\cdot\mathbf{x}} f(\mathbf{x}) \\ &= \sum_j \phi_j^t(\mathbf{p}) \int d\mathbf{x}\; \phi_j^*(\mathbf{x}) f(\mathbf{x}) \end{aligned} \tag{9.23}$$

and

$$\begin{aligned} f(\mathbf{x}) &= \frac{1}{(2\pi)^{d/2}} \int d\mathbf{p}\; e^{i\mathbf{p}\cdot\mathbf{x}} f^t(\mathbf{p}) \\ &= \sum_j \phi_j(\mathbf{x}) \int d\mathbf{p}\; \phi_j^*(\mathbf{p}) f^t(\mathbf{p}) \end{aligned} \tag{9.24}$$

It follows from (9.22) that if the set of functions $\{\phi_j(\mathbf{x})\}$ is chosen in such a way that they are basis functions of irreducible representations of a group G, and if I_γ^ν is the set of indices j such that $\phi_j(\mathbf{x})$ transforms like the νth basis function of the γth irreducible representation of G, then

$$P_\gamma^\nu\left[e^{-i\mathbf{p}\cdot\mathbf{x}}\right] = (2\pi)^{d/2} \sum_{j \in I_\gamma^\nu} \phi_j^*(\mathbf{x})\phi_j^t(\mathbf{p}) \tag{9.25}$$

If we multiply (9.22) on the left by $e^{i\mathbf{p}'\cdot\mathbf{x}}$ and integrate over dx, we obtain

$$\begin{aligned} \int d\mathbf{x}\ e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{x}} &= (2\pi)^{d/2} \sum_j \int d\mathbf{x}\ e^{i\mathbf{p}'\cdot\mathbf{x}} \phi_j^*(\mathbf{x})\phi_j^t(\mathbf{p}) \\ &= (2\pi)^d \sum_j \phi_j^{*t}(\mathbf{p}')\phi_j^t(\mathbf{p}) \end{aligned} \tag{9.26}$$

so that (in the sense of distributions)

$$\sum_j \phi_j^{*t}(\mathbf{p}')\phi_j^t(\mathbf{p}) = \delta(\mathbf{p}-\mathbf{p}') \tag{9.27}$$

Let us now try to make the meaning of completeness relations like (9.20) and (9.27) a little more precise: Suppose that there exists a Hilbert space H with an orthonormal basis $\{\phi_j(\mathbf{x})\}$. Then, for any $f \in H$, we can write

$$f(\mathbf{x}) = \sum_j \phi_j(\mathbf{x}) \int d\mathbf{x}'\ \phi_j^*(\mathbf{x}')f(\mathbf{x}') \tag{9.28}$$

But we could equally well have written

$$f(\mathbf{x}) = \int d\mathbf{x}'\ f(\mathbf{x}')\ \delta(\mathbf{x}-\mathbf{x}') \tag{9.29}$$

Thus we can see that the sum on the left-hand side of (9.20) is acting like a Dirac delta function; but the relationship is only known to hold within H. Similar considerations hold for (9.27). In the discussion above, we imagined the set of functions $\{\phi_j(\mathbf{x})\}$ to be symmetry-adapted, and we let I_γ^ν stand for a domain within which all the functions transform like the νth basis function of the γth irreducible representation of the symmetry group G. Then if

$$P_\gamma^\nu\left[f(\mathbf{x})\right] = \sum_{j \in I_\gamma^\nu} \phi_j(\mathbf{x}) \int d\mathbf{x}'\ \phi_j^*(\mathbf{x}')f(\mathbf{x}') = f(\mathbf{x}) \tag{9.30}$$

we can conclude that $f(\mathbf{x})$ lies entirely within the domain I_γ^ν and that it transforms like the νth basis function of the γth irreducible representation of G. What about its Fourier transform, $f_n^t(\mathbf{x})$?. From (9.23),

$$\begin{aligned} f_n^t(\mathbf{p}) &= \sum_j \phi_j^t(\mathbf{p}) \int d\mathbf{x}' \ \phi_j^*(\mathbf{x}') f_n(\mathbf{x}') \\ &= \sum_{j \in I_\gamma^\nu} \phi_j^t(\mathbf{p}) \int d\mathbf{x}' \ \phi_j^*(\mathbf{x}') f_n(\mathbf{x}') \end{aligned} \tag{9.31}$$

The second line of (9.31) follows from the fact the the $d\mathbf{x}'$ integral vanishes unless $\phi_j^*(\mathbf{x}')$ lies within the domain I_γ^ν. Thus, if $f_n(\mathbf{x})$ lies within the domain I_γ^ν, then $f_n^t(\mathbf{p})$ will lie within the corresponding domain in reciprocal space. One can express this by saying that symmetry properties are preserved under Fourier transformation.

9.5 The Fourier convolution theorem

Let

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}} \int d\mathbf{p}' \ e^{i\mathbf{p}'\cdot\mathbf{x}} \ f^t(\mathbf{p}') \tag{9.32}$$

and

$$g(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}} \int d\mathbf{p}'' \ e^{i\mathbf{p}''\cdot\mathbf{x}} \ g^t(\mathbf{p}'') \tag{9.33}$$

Then we can write

$$\begin{aligned} &\int d\mathbf{x} \ e^{-i\mathbf{p}\cdot\mathbf{x}} f(\mathbf{x}) g(\mathbf{x}) \\ =& \frac{1}{(2\pi)^d} \int d\mathbf{p}' \int d\mathbf{p}'' f^t(\mathbf{p}') g^t(\mathbf{p}'') \int d\mathbf{x} \ e^{i(\mathbf{p}'+\mathbf{p}''-\mathbf{p})\cdot\mathbf{x}} \\ =& \int d\mathbf{p}' \int d\mathbf{p}'' f^t(\mathbf{p}') g^t(\mathbf{p}'') \ \delta(\mathbf{p}'+\mathbf{p}''-\mathbf{p}) \end{aligned} \tag{9.34}$$

so that

$$\int d\mathbf{x} \ e^{-i\mathbf{p}\cdot\mathbf{x}} f(\mathbf{x}) g(\mathbf{x}) = \int d\mathbf{p}' \ f^t(\mathbf{p}') g^t(\mathbf{p}-\mathbf{p}') \tag{9.35}$$

Thus we see that in a d-dimensional space, the Fourier convolution theorem has exactly the same form as in 3 dimensions. In a similar way, it is easy to show that

$$\int d\mathbf{p} \ e^{i\mathbf{p}\cdot\mathbf{x}} f^t(\mathbf{p}) g^t(\mathbf{p}) = \int d\mathbf{x}' \ f(\mathbf{x}') g(\mathbf{x}-\mathbf{x}') \tag{9.36}$$

9.6 Harmonic analysis for non-Euclidean spaces

It is interesting to ask whether something analogous to Fourier transform theory can be developed for spaces whose metric is non-Euclidean. For example, we might think of the surface of a very large hypersphere of hyperradius r, embedded in a d-dimensional space. Since the hyperradius is very large, the surface is locally almost flat, but nevertheless it has a slight curvature. On this surface, the unit vector $\mathbf{u} \equiv \mathbf{x}/r$ plays the role which $\mathbf{x}$ would play in a Euclidean space. Just as we can write

$$f(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}} \int d\mathbf{p}\ e^{i\mathbf{p}\cdot\mathbf{x}}\ f^t(\mathbf{p}) \tag{9.37}$$

where

$$f^t(\mathbf{p}) = \frac{1}{(2\pi)^{d/2}} \int d\mathbf{x}\ e^{-i\mathbf{p}\cdot\mathbf{x}}\ f(\mathbf{x}) \tag{9.38}$$

in a Euclidean space, so, on our very large hypersphere, we can write

$$f(\mathbf{u}) = \sum_{\lambda,\mu} Y_{\lambda,\mu}(\mathbf{u})\ a_{\lambda,\mu} \tag{9.39}$$

where. from the orthonormality of the hyperspherical harmonics, we have

$$a_{\lambda,\mu} = \int d\Omega_d\ Y^*_{\lambda,\mu}(\mathbf{u}) f(\mathbf{u}) \tag{9.40}$$

Provided that $f(\mathbf{u})$ can be expanded as a polynomial, our general hyperangular integration theorem can be used to carry out the integration in 9.40. More generally, we can try to find the set of hyperspherical harmonics appropriate for any non-Euclidean space, and these can be used as a plane-wave-like basis for an analogue to Fourier transform theory.

9.7 Fourier's discovery of the greenhouse effect

Fourier calculated that an object the size of the earth at the earthÃ¸s distance from the sun ought to be considerably cooler than the earth's actual temperature. Among the possible explanations that he proposed for this anomaly, was what we now call the "greenhouse effect". Fourier realized that the earth's atmosphere could contribute to the planet's anomalously high temperature. In a paper proposing this idea, published in 1827, he referred to the experiments of Horace Bénédict de Saussure (1740-1799), who demonstrated the effect using a vase under sheets of glass, and lined with blackened cork.

Suggestions for further reading

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Chapter 10

JOSEPH-LOUIS LAGRANGE

10.1 A professor at the age of 19!

Joseph-Louis Lagrange (1736-1813) was born in Turin, Italy and baptized with his Italian name, Giuseppe Lodovico Lagrangia. His father was the Treasurer in the Office of Public Works, and his mother was the daughter of a physician.

Lagrange was originally educated at the College of Turin with the intention that he should become a lawyer. However, after reading Edmond Halley's book on the use of algebra in optics, he became interested in mathematics.

Working by himself, and largely self-taught. Lagrange began to develop the field of mathematics that we now call variational calculus. He applied this to the problem of finding the tautochrone, the curve an object sliding without friction would always reach the bottom after the same interval of time, regardless of the object's starting point. In 1755, he sent this calculations to Euler, who was then in Berlin. Euler was extremely impressed by the work of the young Italian mathematician, and although he was only 19 years old, Lagrange was appointed Professor of Mathematics at the Royal Artillery School in Turin.

10.2 Successor to Euler at the Berlin Academy

In 1756, Lagrange sent to Euler a set of calculations in which he applied the calculus of variations to mechanics. Euler recognized these calculations as a generalization of the results that he himself had obtained. Full of admiration for the young mathematical genius, Euler consulted with his colleague Maupertius, and then invited Lagrange to accept a position at the Academy in Berlin. However, afraid of being distracted from his work by the move, Lagrange initially refused. Instead he became a founding member of the Academy if Sciences of Turin, and began the publication of a journal in French and Latin entitled *Mélanges de Turin*. Much of this journal was devoted to Lagrange's own mathematical papers.

Finally, in 1766, Euler returned to St. Petersburg in Russia, and the King of Prussia

Frederick II (Frederick the Great) himself offered Lagrange the post of Director of Mathematics at the Berlin Academy, at a very generous salary. This time, Lagrange accepted the invitation to Berlin, and he remained there for twenty years as Euler's successor, producing a monumental volume of work on mechanics, variational calculus, number theory and many other topics. Some of his work on the roots of equations anticipated the work of Galois which led to group theory.

10.3 Lagrange is called to Paris

In 1786, Lagrange's great patron, Frederick II died. and Lagrange's position in Berlin became less happy. He then accepted an invitation to come to Paris, where he became a member of the French Academy, and part of a committee to go over to the metric system and the decimal system for weights and measures. Lagrange survived during the dangerous times of the French Revolution by conforming to whatever regulations were current. While his great friend, Lavoisier, was guillotined in Robespierre's Terror, Lagrange not only survived but was made a Senator.

Napoleon named Lagrange to the Legion of Honour and Count of the Empire in 1808. On 3 April 1813, a week before his death, he was awarded the Grand Croix of the Ordre Impérial de la Réunion.

10.4 The calculus of variations

In a typical problem of the calculus of variations, one considers an integral of the form

$$\delta S \equiv \delta \int L\left(x^1, x^2, \cdots, x^d, \frac{dx^1}{dt}, \frac{dx^2}{dt}, \cdots, \frac{dx^d}{dt},\right) dt = 0 \tag{10.1}$$

L is some function of the coordinates, $x^1, \cdots, x^d$ and their t-derivatives. The problem is to find the coordinates as functions of t which will give a minimum or maximum value to the integral S. For example, the principle of Pierre Fermat (1601-1665) states that *in geometrical optics, the actual path of a ray of light is the one that takes the least time.* The infinitesimal time dt required for the light signal to move an infinitesimal distance dl along its path is

$$dt = \frac{n(\mathbf{x})}{c} dl \tag{10.2}$$

where c is the velocity of light in a vacuum and $n(\mathbf{x})$ is the index of refraction. From the Pythagorean Theorem we have

$$\begin{aligned} dl &= \sqrt{dx^2 + dy + dz^2} = \sqrt{d\mathbf{x} \cdot d\mathbf{x}} \\ &= \sqrt{\frac{d\mathbf{x}}{dl} \cdot \frac{d\mathbf{x}}{dl}}\, dl = \frac{d\mathbf{x}}{dl} \cdot \frac{d\mathbf{x}}{dl}\, dl \end{aligned} \tag{10.3}$$

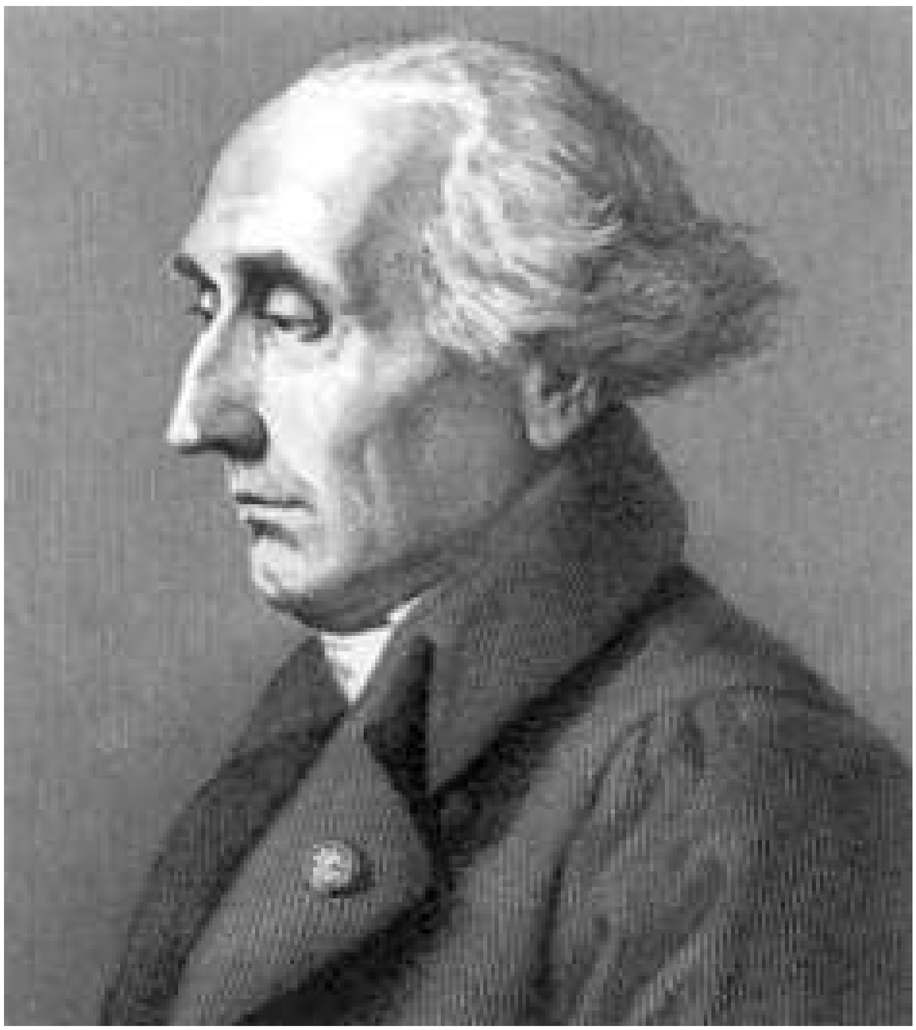

Figure 10.1: **Portrait of Lagrange.**

Figure 10.2: **Another portrait of Joseph-Louis Lagrange.**

Figure 10.3: **A commemorative French Stamp.**

Figure 10.4: **Lagrange's patron during his twenty-year stay in Berlin, Frederick the Great of Prussia. The portrait shows him at the age of 68. His court and Academy featured many of the leading intellectuals of the time.**

Thus we can write Fermat's principle in the form:

$$S = \int L\left(x, y, z, \frac{dx}{dl}, \frac{dy}{dl}, \frac{dz}{dl}\right) dl = \text{minimum} \tag{10.4}$$

where

$$L = n(\mathbf{x})\frac{d\mathbf{x}}{dl} \cdot \frac{d\mathbf{x}}{dl} \tag{10.5}$$

A similar principle was discovered by the great Irish mathematician Sir William Rowan Hamilton (1805-1865). In 1835, he showed that for a system of particles whose state in Newtonian mechanics is specified at a given time by the coordinates $x^1, x^2, \cdots, x^d$, and the velocities $dx^1/dt, dx^2/dt, \cdots, dx^d/dt$. the integral

$$S = \int L\ dt = \int (T - V)\ dt \tag{10.6}$$

is an extremum, where T is the kinetic energy

$$T = \frac{1}{2}\sum_{i=1}^{d}\sum_{j=1}^{d} m_{i,j}\frac{dx^i}{dt}\frac{dx^j}{dt} \equiv \frac{1}{2}\sum_{i=1}^{d}\sum_{j=1}^{d} m_{i,j}\dot{x}^i\dot{x}^j \tag{10.7}$$

and where $V(x^1, x^2, \cdots, x^d)$ is the potential energy. Leonhard Euler (1707-1783) and Joseph-Louis Lagrange (1736-1813), who developed the calculus of variations, had shown that if the coordinates and their time derivatives obey the differential equations

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}^i} - \frac{\partial L}{\partial x^i} = 0 \qquad i = 1, 2, \cdots, d \tag{10.8}$$

Then the integral $S = \int L\ dt$ will be an extremum, and vice versa. The way that they showed this was as follows: Suppose that we have found the true path, $x^i(t)$, for which $S = \int L\ dt$ is an extremum. Now consider what happens to S when we wander slightly away from the true path. The situation is analogous to calculating the change of a function as we move very slightly away from one of its maxima or minima. If we are at the top of a mountain, or at the bottom of a valley, then taking a very slight step in any direction will not change our altitude, since at that point the ground is level. In the same way, if we alter the path by an amount δx^i, the resulting alteration in $\int L\ dt$ will be zero:

$$\delta \int L\ dt = \int \delta L\ dt = 0 \tag{10.9}$$

The variation of the Lagrangian function L resulting directly from the variation of the coordinates, or indirectly through the consequent variation of the velocities is

$$\delta L = \sum_{i=1}^{d}\left[\frac{\partial L}{\partial x^i}\delta x^i + \frac{\partial L}{\partial \dot{x}^i}\frac{d}{dt}(\delta x^i)\right] \tag{10.10}$$

We next integrate by parts using the relationship

$$\int_a^b u\ dv = [uv]_a^b - \int_a^b v\ du \tag{10.11}$$

This give us the relationship

$$\int_a^b \sum_{i=1}^d \frac{\partial L}{\partial \dot{x}^i} \frac{d}{dt}(\delta x^i)\ dt = \left[\sum_{i=1}^d \frac{\partial L}{\partial \dot{x}^i} \delta x^i\right]_a^b - \int_a^b \sum_{i=1}^d \frac{d}{dt} \frac{\partial L}{\partial \dot{x}^i} \delta x^i\ dt \tag{10.12}$$

Since the slightly altered path must still reach the end points a and b, the variation from the true path must vanish at those points, and therefore

$$\left[\sum_{i=1}^d \frac{\partial L}{\partial \dot{x}^i} \delta x^i\right]_a^b = 0 \tag{10.13}$$

Finally, combining equations (10.10), (10.12) and (10.13). we obtain

$$\int_a^b \delta L\ dt = \int_a^b \sum_{i=1}^d \left[-\frac{d}{dt}\frac{\partial L}{\partial \dot{x}^i} + \frac{\partial L}{\partial x^i}\right] \delta x^i\ dt = 0 \tag{10.14}$$

To ensure that the integral in (10.14) will vanish for an arbitrary slight variation of path δx^i, it is necessary that

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}^i} - \frac{\partial L}{\partial x^i} = 0 \qquad i = 1, 2, \cdots, d \tag{10.15}$$

Therefore the Euler-Lagrange equations (10.8) are a consequence of action principle (10.1).

10.5 Cyclic coordinates

The Lagrangian formalism allows us to obtain conservation laws with great ease. As an example, we can think of a single particle moving in a central potential, $V(r)$. This is a case where it is convenient to express the particle's Lagrangian in terms of spherical polar coordinates. Let

$$\begin{aligned} x &= r\sin\theta\cos\phi \\ y &= r\sin\theta\sin\phi \\ z &= r\cos\theta \end{aligned} \tag{10.16}$$

In Cartesian coordinates, the element of length is given by

$$dl^2 = dx^2 + dy^2 + dz^2 \tag{10.17}$$

Combining (10.16) and (10.17) we find that in spherical polar coordinates, the element of length is

$$dl^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2\theta \; d\phi^2 \tag{10.18}$$

We can now write down the Lagrangian of the particle in terms of r, θ and ϕ:

$$L = \frac{1}{2}m\left[\left(\frac{dr}{dt}\right)^2 + r^2\left(\frac{d\theta}{dt}\right)^2 + r^2\sin^2\theta\left(\frac{d\phi}{dt}\right)^2\right] - V(r) \tag{10.19}$$

The Euler-Lagrange equations of the particle then become

$$\begin{aligned}
\frac{d}{dt}\frac{\partial L}{\partial \dot r} = \frac{\partial L}{\partial r} \qquad &\rightarrow \qquad m\frac{d^2 r}{dt^2} = mr\dot\theta^2 + mr\sin^2\theta\dot\phi^2 - \frac{\partial V}{\partial r} \\
\frac{d}{dt}\frac{\partial L}{\partial \dot\theta} = \frac{\partial L}{\partial \theta} \qquad &\rightarrow \qquad \frac{d}{dt}\left(mr^2\frac{d\theta}{dt}\right) = mr^2\sin\theta\cos\theta\dot\phi^2 \\
\frac{d}{dt}\frac{\partial L}{\partial \dot\phi} = \frac{\partial L}{\partial \phi} \qquad &\rightarrow \qquad \frac{d}{dt}\left(mr^2\sin^2\theta\frac{d\phi}{dt}\right) = 0
\end{aligned} \tag{10.20}$$

The second and third of the equations in this array are conservation laws. In fact, if the coordinate system is chosen in such a way that $\dot\phi = 0$, the second equation is Kepler's second law. When a coordinate does not appear in the Lagrangian, but only its time derivative, that coordinate is said to be *cyclic*. For each cyclic coordinate, there is a conservation law. The momentum conjugate to a coordinate is defined to be the partial derivative of the Lagrangian with respect to the time derivative of that coordinate. In the example which we are considering here, the momenta conjugate to the coordinates r, θ and ϕ are

$$\begin{aligned}
p_r &\equiv \frac{\partial L}{\partial \dot r} = m\frac{dr}{dt} \\
p_\theta &\equiv \frac{\partial L}{\partial \dot\theta} = mr^2\frac{d\theta}{dt} \\
p_\phi &\equiv \frac{\partial L}{\partial \dot\phi} = mr^2\sin^2\theta\frac{d\phi}{dt}
\end{aligned} \tag{10.21}$$

We can see from this example that the momenta which are conjugate to cyclic coordinates are conserved. The Euler-Lagrange equations ensure that this is true in general. We can also see that transformation to coordinates, as many as possible of which are cyclic, is a big step towards solving the equations of motion of a system.

As a second example of a transformation to coordinates, some of which are cyclic, we can think of a two particles interacting through a potential which depends only on the distance between them. In that case, the Lagrangian, expressed in Cartesian coordinates, is given by

$$L = \frac{1}{2}m_1\frac{d\mathbf{x}_1}{dt}\cdot\frac{d\mathbf{x}_1}{dt} + \frac{1}{2}m_2\frac{d\mathbf{x}_2}{dt}\cdot\frac{d\mathbf{x}_2}{dt} - V(|\mathbf{x}_1 - \mathbf{x}_2|) \tag{10.22}$$

The Lagrangian formulation allows us to introduce a new set of coordinates which are much more convenient. Let

$$\begin{aligned} \mathbf{X}_{c.m.} &\equiv \frac{m_1\mathbf{x}_1 + m_2\mathbf{x}_2}{m_1+m_2} \\ \mathbf{X}_{12} &\equiv \mathbf{x}_1 - \mathbf{x}_2 \end{aligned} \tag{10.23}$$

In terms of the center of mass coordinates $\mathbf{X}_{c.m.}$ and the relative position coordinates $\mathbf{X}_{12}$, the Lagrangian of the system becomes:

$$\begin{aligned} L &= \frac{1}{2}(m_1+m_2)\frac{d\mathbf{X}_{c.m.}}{dt}\cdot\frac{d\mathbf{X}_{c.m.}}{dt} + \frac{1}{2}\left(\frac{m_1m_2}{m_1+m_2}\right)\frac{d\mathbf{X}_{12}}{dt}\cdot\frac{d\mathbf{X}_{12}}{dt} \\ &- V(|\mathbf{X}_{12}|) \end{aligned} \tag{10.24}$$

Since the Lagrangian does not depend on $\mathbf{X}_{c.m}$, the center of mass coordinates are cyclic, and the momenta conjugate to them are conserved:

$$\frac{d}{dt}(\mathbf{p}_{c.m.}) = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\mathbf{X}}_{c.m.}}\right) = \frac{d}{dt}\left((m_1+m_2)\frac{d\mathbf{X}_{c.m.}}{dt}\right) = 0 \tag{10.25}$$

Since the potential energy does not depend on the orientation of the vector $\mathbf{X}_{12}$, but only on its magnitude, we could complete our transformation to cyclic coordinates by expressing $\mathbf{X}_{12}$ in terms of spherical polar coordinates. Then the only non-cyclic coordinate would be $r_{12} \equiv |\mathbf{X}_{12}|$. It is a general rule that if the Lagrangian is independent of some generalized coordinate X^μ, i.e if

$$\frac{\partial L}{\partial X^\mu} = 0 \tag{10.26}$$

then the momentum conjugate to it is conserved:

$$p_\mu \equiv \frac{\partial L}{\partial \dot{X}^\mu} = \text{constant} \tag{10.27}$$

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Chapter 11

CONDORCET

In France the Marquis de Condorcet had written an equally optimistic book, *Esquisse d'un Tableau Historique des Progrès de l'Esprit Humain.* Condorcet's optimism was unaffected even by the fact that at the time when he was writing he was in hiding, under sentence of death by Robespierre's government. Like Godwin's *Political Justice*, this book offers an optimistic vision of of how human society can be improved. Together, the two books provoked Malthus to write his book on population.

11.1 Condorcet becomes a mathematician

Marie-Jean-Antoine-Nicolas Caritat, Marquis de Condorcet, was born in 1743 in the town of Ribemont in southern France. He was born into an ancient and noble family of the principality of Orange but there was nothing in his background to suggest that he might one day become a famous scientist and social philosopher. In fact, for several generations before, most of the men in the family had followed military or ecclesiastical careers and none were scholars.

After an initial education received at home from his mother, Condorcet was sent to his uncle, the Bishop of Lisieux, who provided a Jesuit tutor for the boy. In 1758 Condorcet continued his studies with the Jesuits at the College of Navarre. After he graduated from the College, Condorcet's powerful and independent intelligence suddenly asserted itself. He announced that he intended to study mathematics. His family was unanimously and violently opposed to this idea. The privileges of the nobility were based on hereditary power and on a static society. Science, with its emphasis on individual talent and on progress, undermined both these principles. The opposition of Condorcet's family is therefore understandable but he persisted until they gave in.

From 1765 to 1774, Condorcet focused on science. In 1765, he published his first work on mathematics entitled *Essai sur le calcul intégral*, which was well received, launching his career as a mathematician. He would go on to publish many more papers, and in 1769, at the age of 26, he was elected to the Academie royale des Sciences (French Royal Academy of Sciences)

Condorcet worked with Leonhard Euler and Benjamin Franklin. He soon became an honorary member of many foreign academies and philosophic societies including the Royal Swedish Academy of Sciences (1785), Foreign Honorary Member of the American Academy of Arts and Sciences (1792), and also in Prussia and Russia.

11.2 Human rights and scientific sociology

In 1774, at the age of 31, Condorcet was appointed Inspector-General of the Paris Mint by his friend, the economist Turgot. From this point on, Condorcet shifted his focus from the purely mathematical to philosophy and political matters. In the following years, he took up the defense of human rights in general, and of women's and blacks' rights in particular (an abolitionist, he became active in the Society of the Friends of the Blacks in the 1780s). He supported the ideals embodied by the newly formed United States, and proposed projects of political, administrative and economic reforms intended to transform France.

The year 1785 saw the publication of Condorcet's highly original mathematical work, *Essai sur l'application de l'analyse à la probabilité des décisions rendues à la pluralité des voix*, in which he pioneered the application of the theory of probability in the social sciences. A later, much enlarged, edition of this book extended the applications to games of chance. Through these highly original works, Condorcet became a pioneer of scientific sociology.

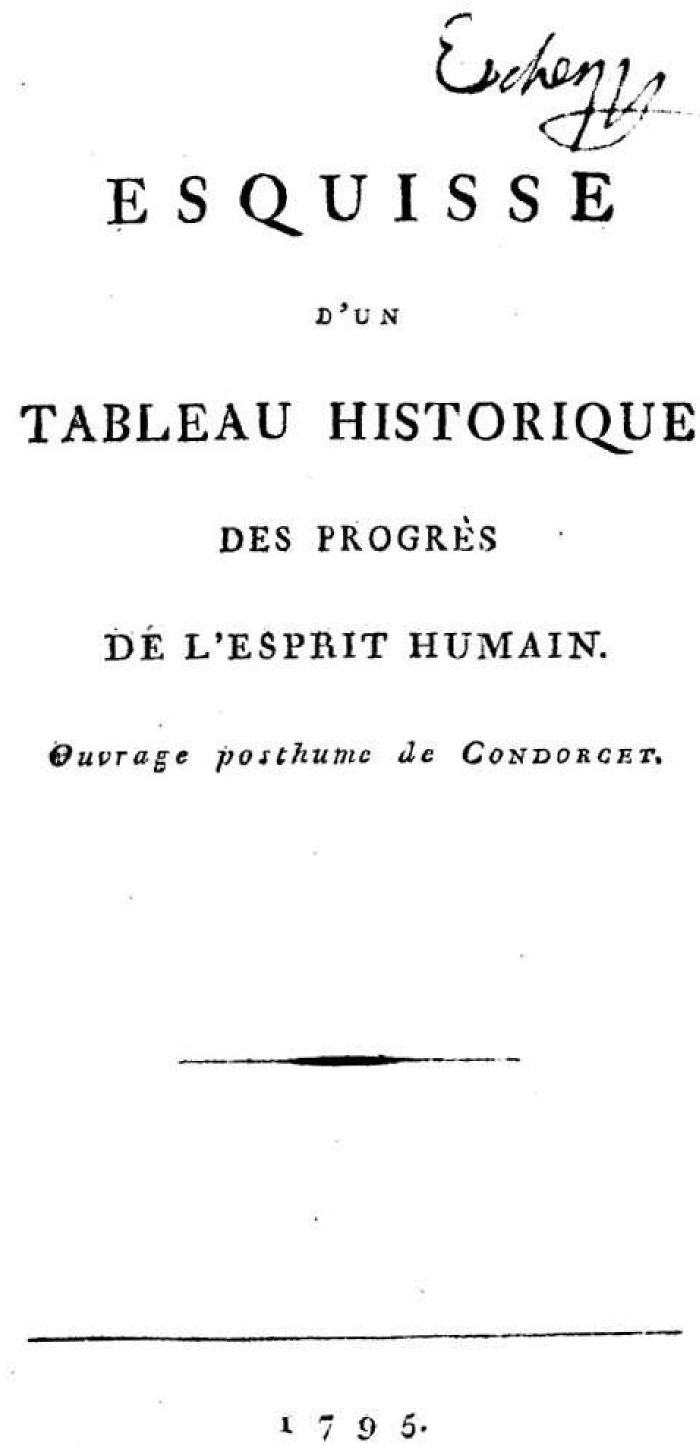
In 1786, Condorcet married one of the most beautiful women of the time, Sophie de Grouchy (1764-1822). Condorcet's position as Inspector-General of the Mint meant that they lived at the Hotel des Monnaies. Mme Condorcet's salon there was famous.

Figure 11.1: **The Marquis de Condorcet.**

Figure 11.2: **A commerative French stamp.**

Figure 11.3: **Condorcet's wife, Sophie de Gauchy.**

Figure 11.4: **The French economist Turgot was Condorcet's mentor and friend.**



ESQUISSE

D'UN

TABLEAU HISTORIQUE

DES PROGRÈS

DE L'ESPRIT HUMAIN.

Ouvrage posthume de CONDORCET.

1795.

Figure 11.5: **The frontpage of Condorcet's famous book, in which he defined the idea of human progress, and anticipated Darwin's theory of evolution.**

11.3 The French Revolution

Ever since the age of 17, Condorcet had thought about questions of justice and virtue and especially about how it is in our own interest to be both just and virtuous. Very early in his life he had been occupied with the idea of human perfectibility. He was convinced that the primary duty of every person is to contribute as much as possible to the development of mankind, and that by making such a contribution, one can also achieve the greatest possible personal happiness. When the French Revolution broke out in 1789 he saw it as an unprecedented opportunity to do his part in the cause of progress and he entered the arena wholeheartedly.

Condorcet was first elected as a member of the Municipality of Paris; and then, in 1791, he became one of the six Commissioners of the Treasury. Soon afterwards he was elected to the Legislative Assembly, of which he became first the Secretary and finally the President. In 1792, Condorcet proposed to the Assembly that all patents of nobility should be burned. The motion was carried unanimously; and on 19 June his own documents were thrown on a fire with the others at the foot of a statue of Louis XIV.

Condorcet was one of the chief authors of the proclamation which declared France to be a republic and which summoned a National Convention. As he remained above the personal political quarrels that were raging at the time, Condorcet was elected to the National Convention by five different constituencies. When the Convention brought Louis XVI to trial, Condorcet maintained that, according to the constitution, the monarch was inviolable and that the Convention therefore had no legal right to try the King. When the King was tried despite these protests, Condorcet voted in favor of an appeal to the people.

11.4 Drafting a new constitution for France

In October 1792, when the Convention set up a Committee of Nine to draft a new constitution for France, Condorcet sat on this committee as did the Englishman, Thomas Paine. Under sentence of death in England for publishing his pamphlet *The Rights of Man*, Paine had fled to France and had become a French citizen. He and Condorcet were the chief authors of a moderate (Gerondist) draft of the constitution. However, the Jacobin leader, Robespierre, bitterly resented being excluded from the Committee of Nine and, when the Convention then gave the responsibility for drafting the new constitution to the Committee for Public Safety, which was enlarged for this purpose by five additional members. The result was a hastily produced document with many glaring defects. When it was presented to the Convention, however, it was accepted almost without discussion. This was too much for Condorcet to stomach and he published anonymously a letter entitled Advice to the French on the New Constitution, in which he exposed the defects of the Jacobin constitution and urged all Frenchmen to reject it.

11.5 Hiding from Robespierre's Terror

Condorcet's authorship of this letter was discovered and treated as an act of treason. On 8 July 1793, Condorcet was denounced in the Convention; and an order was sent out for his arrest. The officers tried to find him, first at his town house and then at his house in the country but, warned by a friend, Condorcet had gone into hiding.

The house where Condorcet took refuge was at Rue Servandoni, a small street in Paris leading down to the Luxembourg Gardens, and it was owned by Madame Vernet, the widow of a sculptor. Madame Vernet, who sometimes kept lodgings for students, had been asked by Condorcet's friends whether she would be willing to shelter a proscribed man. 'Is he a good man?', she had asked; and when assured that this was the case, she had said, 'Then let him come at once. You can tell me his name later. Don't waste even a moment. While we are speaking, he may be arrested.' She did not hesitate, although she knew that she risked death, the penalty imposed by the Convention for sheltering a proscribed man.

11.6 Condorcet writes the *Esquisse*

Although Robespierre's agents had been unable to arrest him, Condorcet was sentenced to the guillotine *in absentia*. He knew that in all probability he had only a few weeks or months to live and he began to write his last thoughts, racing against time. Hidden in the house at Rue Servandoni, and cared for by Madame Vernet, Condorcet returned to a project which he had begun in 1772, a history of the progress of human thought, stretching from the remote past to the distant future. Guessing that he would not have time to complete the full-scale work he had once planned, he began a sketch or outline: *Esquisse d'un Tableau Historique des progrés de l'Esprit Humain*.

Condorcet's *Esquisse*, is an enthusiastic endorsement of the idea of infinite human perfectibility which was current among the philosophers of the 18th century, and in this book, Condorcet anticipated many of the evolutionary ideas of Charles Darwin. He compared humans with animals, and found many common traits. Condorcet believed that animals are able to think, and even to think rationally, although their thoughts are extremely simple compared with those of humans. He also asserted that humans historically began their existence on the same level as animals and gradually developed to their present state.

Since this evolution took place historically, he reasoned, it is probable, or even inevitable, that a similar evolution in the future will bring mankind to a level of physical, mental and moral development which will be as superior to our own present state as we are now superior to animals.

In his *Esquisse*, Condorcet called attention to the unusually long period of dependency which characterize the growth and education of human offspring. This prolonged childhood is unique among living beings. It is needed for the high level of mental development of the human species; but it requires a stable family structure to protect the young during their long upbringing. Thus, according to Condorcet, biological evolution brought into existence a moral precept, the sanctity of the family.

Similarly, Condorcet maintained, larger associations of humans would have been impossible without some degree of altruism and sensitivity to the suffering of others incorporated into human behavior, either as instincts or as moral precepts or both; and thus the evolution of organized society entailed the development of sensibility and morality.

Condorcet believed that ignorance and error are responsible for vice; and he listed what he regarded as the main mistakes of civilization: hereditary transmission of power, inequality between men and women, religious bigotry, disease, war, slavery, economic inequality, and the division of humanity into mutually exclusive linguistic groups.

Condorcet believed the hereditary transmission of power to be the source of much of the tyranny under which humans suffer; and he looked forward to an era when republican governments would be established throughout the world. Turning to the inequality between men and women, Condorcet wrote that he could see no moral, physical or intellectual basis for it. He called for complete social, legal, and educational equality between the sexes.

Condorcet predicted that the progress of medical science would free humans from the worst ravages of disease. Furthermore, he maintained that since perfectibility (i.e. evolution) operates throughout the biological world, there is no reason why mankind's physical structure might not gradually improve, with the result that human life in the remote future could be greatly prolonged. Condorcet believed that the intellectual and moral facilities of man are capable of continuous and steady improvement; and he thought that one of the most important results of this improvement will be the abolition of war.

At the end of his *Esquisse*, Condorcet said that any person who has contributed to the progress of mankind to the best of his ability becomes immune to personal disaster and suffering. He knows that human progress is inevitable and can take comfort and courage from his inner picture of the epic march of mankind, through history, towards a better future.

Shortly after Condorcet completed the *Esquisse*, he received a mysterious warning that soldiers of the Convention were on their way to inspect Madame Vernet's house. Wishing to spare his generous hostess from danger, he disguised himself as well as he could and slipped past the portress. However, Condorcet had only gone a few steps outside the house when he was recognized by Madame Verdet's cousin, who risked his life to guide Condorcet past the sentinels at the gates of Paris, and into the open country beyond.

Condorcet wandered for several days without food or shelter, hiding himself in quarries and thickets. Finally, on 27 March 1794, hunger forced him to enter a tavern at the village of Clamart, where he ordered an omelette. When asked how many eggs it should contain, the exhausted and starving philosopher replied without thinking, 'twelve'. This reply, together with his appearance, excited suspicion. He was asked for his papers and, when it was found that he had none, soldiers were sent for and he was arrested. He was taken to a prison at Bourg-la-Reine, but he was so weak that he was unable to walk there, and had to be carried in a cart. The next morning, Condorcet was found dead on the floor of his cell. The cause of his death is not known with certainty. It was listed in official documents as congestion sanguine, congestion of the blood but the real cause may have been cold, hunger, exhaustion or poison. Many historians believe that Condorcet was murdered by Robespierre's agents, since he was so popular that a public execution would have been impossible.

After Condorcet's death the currents of revolutionary politics shifted direction. Robespierre, the leader of the Terror, was himself soon arrested. The execution of Robespierre took place on 25 July 1794, only a few months after the death of Condorcet.

Condorcet's *Esquisse d'un Tableau Historique des Progrès de l'Esprit Humain* was published posthumously in 1795. In the post-Thermidor reconstruction, the Convention voted funds to have it printed in a large edition and distributed throughout France, thus adopting the *Esquisse* as its official manifesto. Condorcet's name will always be linked with this small prophetic book. It was destined to establish the form in which the eighteenth-century idea of progress was incorporated into Western thought.

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Chapter 12

HAMILTON

Sir William Rowan Hamilton (1805-1865) made many extremely important contributions both to mathematics and to physics. He was a remarkable child prodigy. At the age of three, he was given to his uncle, James Hamilton, to be educated. His uncle was a linguist, and by the time William was thirteen years old, he had acquired as many languages as he had years of age. Besides all the classical and modern European languages, these included Persian, Arabic, Hindustani, Sanskrit, and even Marathi and Malay. In those days, Hamilton slept in a room next to his uncle with a string tied to the back of his nightshirt. The string went through a hole in the wall to his uncle's room. When the uncle thought that it was time for his nephew to wake up and work, he pulled the string.

Figure 12.1: **Sir William Rowan Hamilton (1805-1865).**

Figure 12.2: **Irish commemorative coin celebrating the 200th Anniversary of Hamilton's birth.**

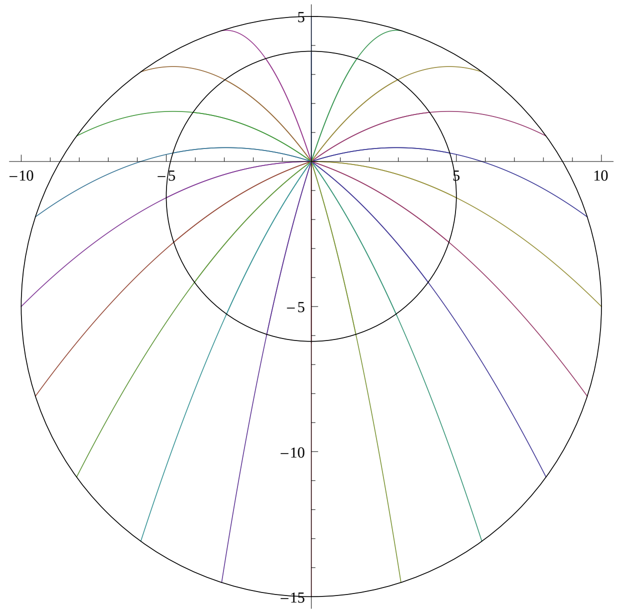

Figure 12.3: **This figure shows a system of particle trajectories of the kind visualized by Hamilton. Here the system might be produced by the fragments of an exploding sky-rocket, assuming that they are all of equal mass and are thrown out with equal velocities. At various times after the explosion, the fragments will reach points given by spheres drawn around the falling center of mass.**

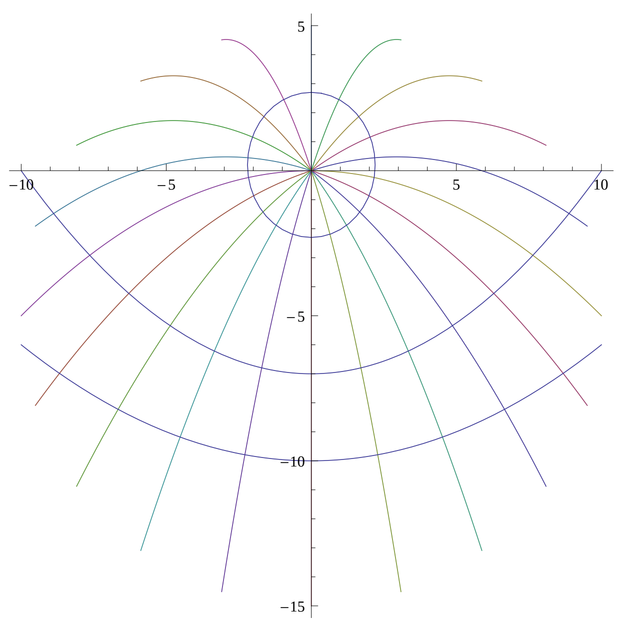

Figure 12.4: **This figure shows surfaces corresponding to constant values of Hamilton's characteristic function S. These surfaces are everywhere perpendicular to the trajectories discussed in the previous figure.**

12.1 Uniting optics and mechanics

Hamilton retained his knowledge of languages until the end of his life, and often read books in Persian and Arabic for pleasure. Fortunately, however, this orgy of linguistics was not continued and Hamilton became strongly interested in mathematics. At the age of 18, he submitted a *Memoir on Systems of Rays* for publication. It caused the Astronomer Royal of Ireland to exclaim, "This young man, I do not say *will be* but *is* the first mathematician of his age!"

With remarkable intuition, Hamilton anticipated both quantum theory and the general theory of relativity. He saw the close analogy between geometrical optics and the classical trajectories of Newtonian mechanics. In geometrical optics, the rays of light are perpendicular to wave fronts. Hamilton introduced a function that yielded wave fronts for mechanics, thus anticipating wave mechanics, a field that lay a century ahead in time. His reformulation of Newtonian mechanics also anticipated general relativity by showing that the trajectories of objects can be viewed as the shortest paths in a space with a special metric. The Hamiltonian reformulation of Newtonian mechanics has proved to be the a key to the development of modern physics.

12.2 Professor of Astronomy at the age of 21

Hamilton entered Trinity College, Dublin, where his scholastic record was remarkable. At the age of 21, while still an undergraduate, he was appointed to be Andrews Professor of Astronomy and Royal Astronomer of Ireland. He then moved into Dunsink Observatory, where he spent the remainder of his life. He married a clergyman's daughter, and they had three children together, but she could not stand the strain of living with him and returned to live with her parents.

Hamilton was the close friend of the poets Coleridge and Wordsworth, and his life had a profligate poetic quality. His lectures on astronomy attracted many scholars and poets, and even ladies, which at that time was unusual. One of his lectures inspired the poet Felicia Hermans to write *The Prayer of a Lonely Student*.

Hamilton drank a great deal, and the heaps of papers in his study were in a state of disorder. During the last part of his life, he was often alone, cared for by the house-keeper of the observatory. He had no regular meals, but from time to time, the house-keeper would hand him a mutton chop, which he would accept without a word, and without looking up from his work. After Hamilton's death, dozens of partly-eaten mutton chops were found among his mounds of papers.

12.3 Hamilton's unified formulation

As we mentioned above, the work of Sir William Rowan Hamilton (1805-1865) contains some remarkably modern insights, foreshadowing quantum mechanics and relativity theory. His treatment of mechanics and optics unified the two disciplines in a manner that foreshadows wave mechanics. In his first paper on systems of rays in geometrical optics, he considered rays coming from a point source which flashes on at a certain instant of time. If the light is propagating in a uniform medium, the rays will form system of straight lines, pointing outward from the point source of the light. Perpendicular to these lines, will be a set of concentric spherical surfaces, which represent the maximum distance that can be reached at any given time. In a non-uniform medium, the system of rays will not be straight lines, and surfaces will not be spheres, but nevertheless, the lines representing rays will always be perpendicular to the surfaces representing wave fronts. Hamilton introduced the integral

$$S(\mathbf{x}) = \int dt = \frac{1}{c}\int n(\mathbf{x})\ dl \tag{12.1}$$

This integral, taken along the path of a ray, gives the time needed for the wave front of a flash to reach a particular point $\mathbf{x}$. Hamilton called $S(\mathbf{x})$ the *eikonal function*, taking the name from the Greek word for "image", and he showed that it satisfies the differential equation

$$\frac{1}{[2n(\mathbf{x})]^2}\left[\left(\frac{\partial S}{\partial x}\right)^2 + \left(\frac{\partial S}{\partial y}\right)^2 + \left(\frac{\partial S}{\partial z}\right)^2\right] = 1 \tag{12.2}$$

Equation (12.2) follows from Fermat's principle, which states that the actual path of a ray of light is the one that takes the least time:

$$S(\mathbf{x}) = \int dt = \frac{1}{c}\int n(\mathbf{x})\ dl = \frac{1}{c}\int n(\mathbf{x})\frac{d\mathbf{x}}{dl}\cdot\frac{d\mathbf{x}}{dl}\ dl = \text{minimum} \tag{12.3}$$

The Euler-Lagrange equations corresponding to (12.3) are

$$\frac{d}{dl}\left[\frac{\partial L}{\partial\left(\frac{dx^i}{dl}\right)}\right] - \frac{\partial L}{\partial x^i} = 0 \tag{12.4}$$

so that

$$\begin{aligned} \frac{\partial S}{\partial x^i} &= \int \frac{\partial L}{\partial x^i}\ dt = \int \frac{d}{dl}\left[\frac{\partial L}{\partial\left(\frac{dx^i}{dl}\right)}\right]\ dl = \frac{\partial L}{\partial\left(\frac{dx^i}{dl}\right)} \\ L &= n(\mathbf{x})\frac{d\mathbf{x}}{dl}\cdot\frac{d\mathbf{x}}{dl} \end{aligned} \tag{12.5}$$

Thus

$$\frac{\partial S}{\partial x^i} = 2n(\mathbf{x})\frac{dx^i}{dl} \qquad\qquad i = 1, 2, 3 \tag{12.6}$$

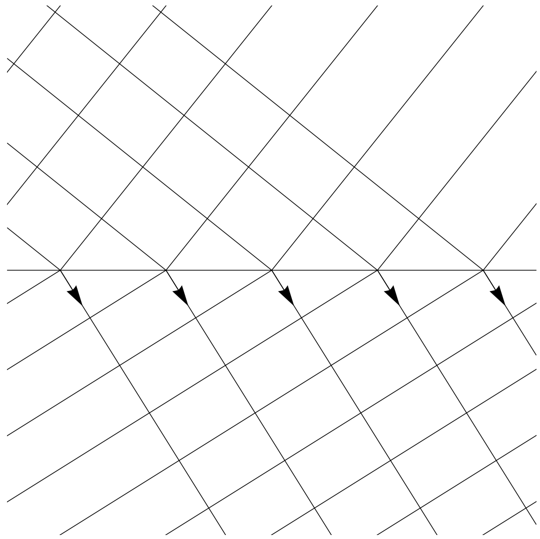

Figure 12.5: **This figure shows a system of parallel light rays entering a medium with a different index of refraction. The rays of light are perpendicular to the wave fronts at all points in space. The wave fronts correspond to surfaces with constant values of Hamilton's eikonal function.**

By combining (12.6) with the relation

$$\frac{d\mathbf{x}}{dl} \cdot \frac{d\mathbf{x}}{dl} = 1 \tag{12.7}$$

we obtain Hamilton's eikonal equation, (12.2). With remarkable intuition, Hamilton saw the analogy between the rays of geometrical optics and the trajectories of point masses in classical mechanics. His next step was to put mechanics on the same footing as optics by defining what he called the *characteristic function* for a system of trajectories. We can obtain an understanding of Hamilton's characteristic function by thinking of the fragments of an exploding skyrocket. If all of the fragments leave the point of the explosion with equal velocity, then they will form the sort of system which Hamilton studied. The upward-moving fragments are decelerated by gravity, while the downward-moving ones are accelerated. The positions of the fragments at successive instants of time are on spheres drawn around the falling center of mass of the system. Hamilton defined the characteristic function $S(\mathbf{x})$ by the relationship

$$S(\mathbf{x}) = \int_{\mathbf{x_0}}^{\mathbf{x}} L\ dt \tag{12.8}$$

taken along the system of trajectories. From the Euler-Lagrange equations, it follows that

$$\frac{\partial S}{\partial x^i} = \int \frac{\partial L}{\partial x^i}\ dt = \int \frac{d}{dt}\frac{\partial L}{\partial \dot{x}^i}\ dt = \frac{\partial L}{\partial \dot{x}^i} = p_i \tag{12.9}$$

Hamilton used this relationship to show that his characteristic function satisfies a differential equation similar to his eikonal equation (12.2). He first defined the total energy function (we call it the Hamiltonian) of a mechanical system as

$$H = \sum_i p_i \dot{x}^i - L \tag{12.10}$$

It follows from equation (12.10) that

$$\frac{dp_i}{dt} \equiv \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}^i}\right) = \frac{\partial L}{\partial x^i} = -\frac{\partial H}{\partial x^i} \tag{12.11}$$

From (12.10) it also follows that

$$\frac{\partial H}{\partial p_i} = \dot{x}^i \tag{12.12}$$

Equations (12.11) and (12.12) are called Hamilton's equations of motion. From these equations, it follows that for systems where the potential energy is independent of time and where there are no velocity-dependent forces, the Hamiltonian function (12.10) is a constant of the motion. For such *conservative systems*, H is a constant of the motion.

$$\begin{aligned}\frac{dH}{dt} &= \frac{\partial H}{\partial t} + \sum_i \left[\frac{\partial H}{\partial p_i}\frac{dp_i}{dt} + \frac{\partial H}{\partial x^i}\frac{dx^i}{dt}\right] \\ &= \sum_i \left[-\frac{\partial H}{\partial p_i}\frac{\partial H}{\partial x^i} + \frac{\partial H}{\partial x^i}\frac{\partial H}{\partial p_i}\right] = 0 \end{aligned} \tag{12.13}$$

Thus

$$H(x^i, p_i) = E \tag{12.14}$$

where E is a constant. Hamilton then substituted $\partial S/\partial x^i$ for p_i. In this way he obtained an equation which has become known as the *Hamiltonian-Jacobi equation*:

$$H\left(x^i, \frac{\partial S}{\partial x^i}\right) = E \tag{12.15}$$

For example, in the case where the mechanical system is a single point mass moving in the potential $V(\mathbf{x})$, the Hamiltonian of the system is

$$H = \frac{m}{2}\frac{d\mathbf{x}}{dt} \cdot \frac{d\mathbf{x}}{dt} + V(\mathbf{x}) = \frac{1}{2m}\mathbf{p} \cdot \mathbf{p} + V(\mathbf{x}) \tag{12.16}$$

and the Hamilton-Jacobi equation is

$$\frac{1}{2m}\left[\left(\frac{\partial S}{\partial x}\right)^2 + \left(\frac{\partial S}{\partial y}\right)^2 + \left(\frac{\partial S}{\partial z}\right)^2\right] + V(\mathbf{x}) = E \tag{12.17}$$

which is analogous to Hamilton's eikonal equation, (12.2).

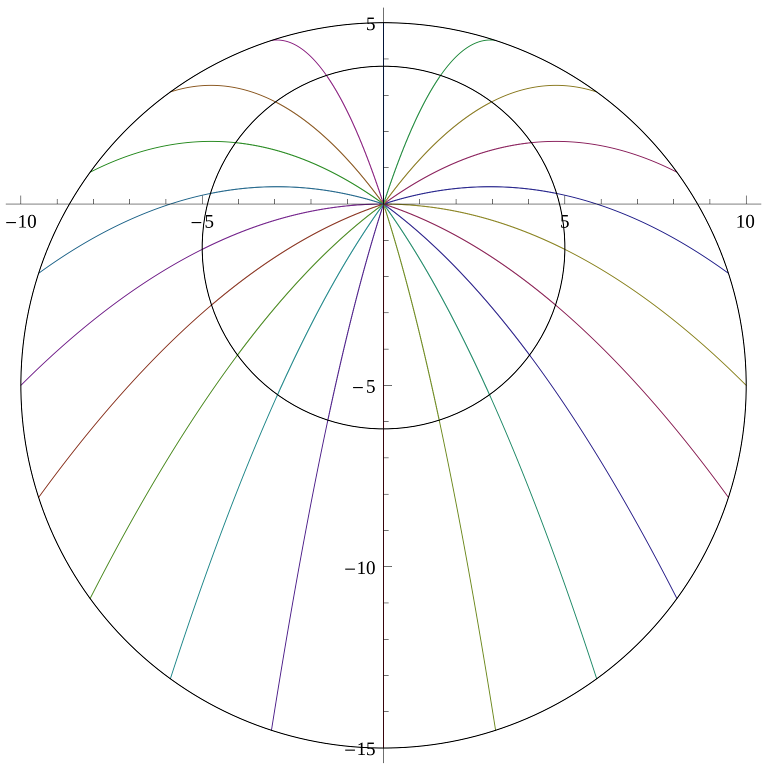

Figure 12.6: **This figure shows a system of particle trajectories of the kind visualized by Hamilton. Here the system might be produced by the fragments of an exploding sky-rocket, assuming that they are all of equal mass and are thrown out with equal velocities. At various times after the explosion, the fragments will reach points given by spheres drawn around the falling center of mass.**

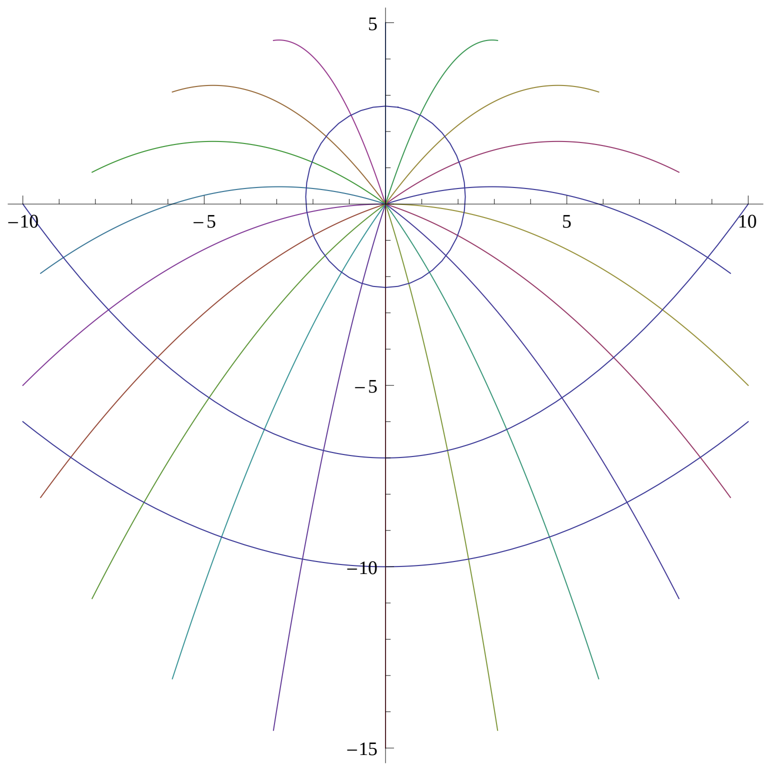

Figure 12.7: **This figure shows surfaces corresponding to constant values of Hamilton's characteristic function S. These surfaces are everywhere perpendicular to the trajectories discussed in the previous figure.**

12.4 Quaternions

On October 16, 1843, Hamilton was walking beside a canal with his wife, He was on his way to a meeting of the Council of the Royal Irish Academy. His wife spoke to him now and then, but he hardly heard her because he was so deep in thought. Breaking the barrier of tradition he proposed the introduction of non-commutative algebraic entities, to which he gave the name "quaternions".

Hamilton described his discovery of quaternions, hypercomplex numbers and non-commutative algebra in the following words:

"And here there dawned on me the notion that we must admit, in some sense, a fourth dimension of space for the purpose of calculating with triples ... An electric circuit seemed to close, and a spark flashed forth."

He later carved the formula

$$i^2 = j^2 = k^2 = ijk = -1 \tag{12.18}$$

on the stone of the bridge that he and his wife had passed when the discovery flashed through his mind.

Hamilton spent the remainder of his life working on non-commutative algebra, and he considered it to be very important, writing:

"I still must assert that this discovery appears to me to be as important for the middle of the nineteenth century as the discovery of fluxions [the calculus] was for the close of the seventeenth."

The Pauli spin matrices, introduced much later in quantum theory, obey non-commutative equations closely similar to those that Hamilton proposed for quaternions.

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Chapter 13

ABEL AND GALOIS

Niels Henrik Abel (1802-1829) and Éveriste Galois (1811-1832), both mathematicians of genius, and both tragically short-lived, contributed to the development of group theory. both Abel and Galois were interested in the question of whether general roots could be found for fourth-order and fifth-order polynomials. This question led them to study what we now call the group of permutations. Today group theory, to whose foundation Abel and Galois contributed, is of great importance in mathematics, physics and chemistry.

The political events of the time during which Abel and Galois lived greatly affected their lives. Norway, which was Abel's home, was then a part of Denmark, and when Denmark was blockaded by the English during the Napoleonic Wars, Norway also suffered under this blockade. Unable to export timber and to import grain. Norwegians suffered great hardship during this period. Abel's life was marked by poverty, and he died very young from tuberculosis, which he probably would not have acquired if he had not been so poor.

The life of Galois was also marked by the political events of this period. In the case of Galois, it was revolutionary politics which affected his life, and which led to his early death.

Figure 13.1: **Niels Henrik Abel.**

Figure 13.2: **Christine Kemp, Abel's fiancé.**

Figure 13.3: **Statue of Niels Henrik Abel in Oslo (former Christiania).**

Figure 13.4: **Niels Henrik Abel memorial in Gjerstad.**

Figure 13.5: **A Norwegian stamp.**

Figure 13.6: **Portrait of Éveriste Galois.**

Figure 13.7: **Augustin-Louis Cauchy reviewed Galois' early mathematical papers.**

Figure 13.8: **Battle for the Town Hall by Jean-Victor Schnetz. Galois, as a staunch Republican, would have wanted to participate in the July Revolution of 1830 but was prevented by the director of the École Normale.**

Figure 13.9: **A drawing done in 1848 from memory by Evariste's brother.**

Figure 13.10: **A French stamp.**

13.1 Group theory

The definition of a finite group

A finite group is defined by the following conditions:

1. If any two elements belonging to the group are multiplied together, the product is another element belonging to the group.
2. There is an identity element.
3. Each element has an inverse.
4. Multiplication of the elements is associative[1], but necessarily commutative.
5. The group contains g elements, where g is a finite positive integer called the *order* of the group.

As a simple example, we might think of a molecule which is symmetric with respect to rotations through an angle of $2\pi/3$ about some axis but which has no other symmetry. Then the set of geometrical operations that leave the molecule invariant form a group containing 3 elements: the identity element; a rotation through an angle $2\pi/3$ about the axis of symmetry, and a rotation through an angle $4\pi/3$ about the same axis. Let us denote these operations respectively by E, C_3, and C_3^{-1}. We can easily construct a multiplication table for the group. If we do so, *each element of the group will appear once and only once in any row or column of the multiplication table.* This follows from the fact that $AX = B$ has one and only one solution among the group elements. Since A^{-1} and B belong to the group, and since the product of any two elements belongs to the group, $X = A^{-1}B$ is also a uniquely-defined element. Now suppose that the element B appears more than once in the Ath row of the multiplication table. Then $AX = B$ will have more than one solution which is impossible. Since no element can appear more than once, each element must appear once because there are g elements and g places in the row, all of which have to be filled.

Representations of geometrical symmetry groups

The elements of a geometrical symmetry group are linear coordinate transformations. Such transformations have the form

$$X^i = \sum_{j=1}^{d} \frac{\partial X^i}{\partial x^j} x^j + b^i \tag{13.1}$$

where $\partial X^i/\partial x^j$ and b^i are constants.

[1] A(BC)=(AB)C

Now consider a set of functions Φ_1, Φ_2, ..., Φ_M. We can use equation (13.1) to express $\Phi_1(\mathbf{x})$ as a function of $\mathbf{X}$. If we then expand the resulting function of $\mathbf{X}$ in terms of the other Φ_n's, we shall obtain a relation of the form

$$\Phi_n(\mathbf{x}) = \sum_{n'} \Phi_{n'}(\mathbf{X}) D_{n',n} \tag{13.2}$$

If we denote the coordinate transformation in equation (13.1) by the symbol G, we can rewrite equations (13-1) and (13.2) in the form:

$$\begin{aligned} \mathbf{X} &= G_j \mathbf{x} \\ \Phi_n(\mathbf{x}) &\equiv \Phi_n(G_j^{-1}\mathbf{X}) \equiv G_j \Phi_n(\mathbf{X}) \\ &= \sum_{n'} \Phi_{n'}(\mathbf{X}) D_{n',n}(G) \end{aligned} \tag{13.3}$$

In this sense, the coordinate transformation defines an operator G_j, and $D_{n',n}(G_j)$ is a matrix representing G_j. Is can easily be shown that the matrices representing a set of operators G_1, G_2,...,G_g in a given basis, obey the same multiplication table as the operators themselves. For example, if we know that

$$C_3 C_3^{-1} = E \tag{13.4}$$

and that

$$\begin{aligned} C_3 \Phi_n &= \sum_{n'} \Phi_{n'} D_{n',n}(C_3) \\ C_3^{-1} \Phi_n &= \sum_{n'} \Phi_{n'} D_{n',n}(C_3^{-1}) \\ E \Phi_n &= \sum_{n'} \Phi_{n'} D_{n',n}(E) \end{aligned} \tag{13.5}$$

then it follows that:

$$\begin{aligned} C_3 C_3^{-1} \Phi_n &= \sum_{n'} C_3 \Phi_{n'} D_{n',n}(C_3^{-1}) \\ &= \sum_{n''} \Phi_{n''} \left\{ \sum_{n'} D_{n'',n'}(C_3) D_{n',n}(C_3^{-1}) \right\} \\ &= E\Phi_n = \sum_{n''} \Phi_{n''} D_{n'',n}(E) \end{aligned} \tag{13.6}$$

so that we must have

$$D_{n'',n}(E) = \sum_{n'} D_{n'',n'}(C_3) D_{n',n}(C_3^{-1}) \tag{13.7}$$

Thus *given any set of basis functions* Φ_1, Φ_2, ..., Φ_M *which mix together under the elements of a group* G_1, G_2,...,G_g, *we can obtain a set of matrices* $D_{n',n}(G_j)$ *defined by the relationships*

$$G_j\Phi_n = \sum_{n'} \Phi_{n'} D_{n',n}(G_j) \qquad j = 1, 2, ..., g \tag{13.8}$$

These matrices will obey the same multiplication table as the operators G_1, G_2,...,G_g, *and they are said to form a matrix representation of the group.*

Besides finite groups, there are also continuous groups, such as the group of rotations in space, and the group of translations in space.

Group theory allows us to study symmetry in a systematic way. For this reason, it has proved to be of great importance for modern theoretical physics and theoretical chemistry. Both exact symmetries and approximate symmetries are extremely important in modern particle physics. Group theory is also much used in theoretical chemistry, where it is used to explain the observed properties of molecules. It is also used to choose optimal basis sets in quantum chemical calculations. Group theory is also very useful in X-ray crystallography.

An extensive discussion of the theory of finite groups can be found in Appendix C of this book.

13.2 Abel's family and education

Niels Henrik Abel (1802-1829) was the second son of Pastor Søren Abel, of Gjerstad Church, near the town of Risør in Norway. His mother, Anne Marie Simonsen, came from a family of well-to-do ship owners. She enjoyed arranging social events, and took little interest in her children's education.

Besides being a pastor, with degrees in theology and philosophy, Søren Abel had some importance in Norwegian politics. With the coming of Norwegian independence, he was elected to the Storting, the supreme legislature of Norway. It met in Oslo, at the Cathedral School, and in this way, Søren Abel's attention was attracted to the school. Two of his sons, Niels Henrik Abel and his elder brother Hans were sent there to study.

The Cathedral School had at one time been excellent. However, the school's best teachers were transferred to the University by the time that the Abel brothers arrived, and thus the teaching was mediocre.

This situation changed with the arrival of the mathematician Bernt Michael Holmboe, who immediately recognized Niels Henrik Abel's outstanding abilities in mathematics, and gave him both encouragement and private lessons. Under Holmboe's guidance, Abel began to study the works of Euler, Newton, Lalande, d'Alembert, Lagrange and Laplace.

Meanwhile, Søren Abel had become involved in two controversies. The first of these was a theological argument, which was widely reported in the Norwegian press. The second was a scandal resulting from Søren's insults to Carsten Anker, the host of the Norwegian

Constituent Assembly. Søren Abel returned to Gjerstad in disgrace, his political career in ruins. He began drinking heavily, and died two years later at the age of 48.

13.3 Abel's travels in Europe

The death of Søren Abel was a tragedy for his son Niels. There was now no money from home to support his studies. However, Niels Henrik Abel's mentor and friend, Bernt Michael Holmboe, raised money to help his talented student to finish the Cathedral school and to enter the Royal Frederick University in Oslo. By the time that he entered the university, Abel was already the most knowlegable mathematician in Norway.

While still a student at the university, Abel wrote a paper on the solution to quintic equations, i.e. the roots of 5th-order polynomials. He sent the paper to the mathematician Ferdinand Degen, for publication by the Royal Society of Copenhagen. Degen asked Abel for a numerical example, and while working to provide an example, Abel discovered a mistake in his calculation. He later proved that the exact algebraic solution of quintic equations equations, and equations of higher order than quintic, is impossible.

Degen advised Abel to turn his attention to another outstanding problem. "... whose development would have the greatest consequences for analysis and mechanics. I refer to elliptic integrals. A serious investigator with suitable qualifications for research of this kind would by no means be restricted to the many beautiful properties of these most remarkable functions, but could discover a Strait of Magellan leading into wide expanses of a tremendous analytic ocean." Abel later followed Degen's advice and did important work on elliptic integrals.

While a student at the Royal Frederick University in Oslo, Abel found another friend and supporter in the Professor of Astronomy, Christopher Hansteen, who gave him encouragement, financial support, and a place to live. Hansteen's wife cared for Abel as though he were her own son. In 1823, the 21 year old Abel published a paper entitled *Solutions of some problems by means of definite integrals* in Norway's first scientific journal, journal, "Magazin for Naturvidenskaberne", which had been founded by Hansteen. Abel's paper contained the first solution of an integral equation.

Abel obtained a grant to visit Degen and other mathematicians in Copenhagen. While there, he met his future fiancé, Christine Kemp. He also applied for funds to travel in Europe to meet mathematicians such as Gauss, but because he was not fluent in French and German, permission to travel was delayed for two years so that he could study these languages.

Finally, in September, 1825, Abel set out for the continent of Europe together with four friends from the university. In Copenhagen, Abel had been given a letter of introduction to the mathematician August Crelle, and he met Crelle in Berlin. Crell was the publisher of a journal devoted to mathematical research, and Abel began to contribute many papers to Crelle's journal.

Wikipedia gives the following description of Abel's travels;

"From Berlin Abel also followed his friends to the Alps. He went to Leipzig and Freiberg to visit Georg Amadeus Carl Friedrich Naumann and his brother the mathematician August Naumann. In Freiberg Abel did research in the theory of functions, particularly, elliptic, hyperelliptic, and a new class now known as abelian functions.

"From Freiberg they went on to Dresden, Prague, Vienna, Trieste, Venice, Verona, Bolzano, Innsbruck, Luzern and Basel. From July 1826 Abel traveled on his own from Basel to Paris. Abel had sent most of his work to Berlin to be published in Crelle's Journal, but he had saved what he regarded as his most important work for the French Academy of Sciences, a theorem on addition of algebraic differentials. With the help of a painter, Johan Gorbitz, he found an apartment in Paris and continued his work on the theorem. He finished in October 1826 and submitted it to the academy. It was to be reviewed by Augustin-Louis Cauchy. Abel's work was scarcely known in Paris, and his modesty restrained him from proclaiming his research. The theorem was put aside and forgotten until his death.

"Abel's limited finances finally compelled him to abandon his tour in January 1827. He returned to Berlin, and was offered a position as editor of Crelle's Journal, but opted out. By May 1827 he was back in Norway. His tour abroad was viewed as a failure.[by whom?] He had not visited Gauss in Göttingen and he had not published anything in Paris. His scholarship was therefore not renewed and he had to take up a private loan in Norges Bank of 200 spesidaler. He never repaid this loan. He also started tutoring. He continued to send most of his work to Crelle's Journal. But in mid-1828 he published, in rivalry with Carl Jacobi, an important work on elliptic functions in Astronomische Nachrichten in Altona."

Abel died of tuberculosis, which he contracted in Paris. On his way to visit his fiancé, Christine Kemp, in Finland, at Christmas 1928, he became seriously ill. He recovered somewhat, and the couple enjoyed the holiday together; but soon afterwards the illness worsened severely and he died at the early age of 27.

After Abel's death, news arrived that Crelle had succeeded in obtaining a professorship for him in Berlin, but it was too late to help.

The Abel Prize

In 1899, the Norwegian mathematician Sophus Lie learned that no Nobel Prize would be awarded in mathematics, and he proposed that such a prize should be awarded by Norway. In 1902. King Oscar II of Sweden and Norway expressed his willingness to establish and finance such a prize. However, the establishment of the prize, which was named in honor of Niels Henrik Abel, was delayed until 2001 by the dissolution of the political bond between Sweden and Norway. Today the Abel Prize honors outstanding mathematicians, as well as commemorating Abel's life and work. A twice-yearly Abel symposium was also established.

13.4 A list of mathematical topics to which Abel contributed

- Abel's binomial theorem
- Abelian variety
- Abel equation
- Abel equation of the first kind
- Abelian extension
- Abel function
- Abelian group
- Abel's identity
- Abel's inequality
- Abel's irreducibility theorem
- Abel-Jacobi map
- Abel-Plana formula
- Abel-Ruffini theorem
- Abelian means
- Abel's summation formula
- Abelian and tauberian theorems
- Abel's test
- Abel's theorem
- Abel transform
- Abel transformation
- Abelian variety
- Abelian variety of CM-type
- Dual abelian variety

13.5 The life and work of Éveriste Galois

Éveriste Galois was born in 1811 in a district of Paris called Bourg-la-Reine. His father was an important man in this community, and was elected mayor of Bourg-la-Reine.

Éveriste Galois's mother was well educated, especially in languages such as Latin and Greek, and for his first twelve years it was she who educated her son Éveriste. After this, he entered the Lycée Louis-le-Grande. At the age of 14 he became enormously interested in mathematics, reading books by Legendre and Lagrange as though they were novels, and mastering them after a first reading.

After graduating from Lycée Louis-le-Grande, Galois wanted to enter the École Polytechnique, but failed his entrance examination, probably because he was awkward at explaining his thoughts to the examiners. He was forced to enter the École Normale instead, which was much less good for the study of mathematics. Nevertheless, the followin year, Galois published a a paper on continued fractions. He soon produced two important papers on the theory of polynomial equations, which he sent to the mathematician Augustin-Louis

Cauchy. It seems that Cauchy considered the work to be excellent and suggested that the two papers be combined and sent to the French Academy as an entry for the Academy's annual prize. However, for some reason, Galois' papers were never combined and submitted.

In 1829, Galois' father committed suicide. The parish priest had forged Mayor Galois' name on malicious forged epigrams directed at Galois' own relatives. Overcome by the ensuing scandal, Mayor Galois hanged hiself. His father's death was a terrible blow to Éveriste, who never recovered emotionally from the loss.

Évariste Galois was arrested and imprisoned for his political activities during the revolutionary period in which he lived. Although eventually released from prison, he was killed in a duel at the age of 20. The reasons for the duel are not known with certainty, but the daughter of the prison doctor may have been involved. Galois was searching for love to replace the loss of his beloved father.

13.6 Mathematical contributions of Galois

Galois Theory deals with the properties of mathematical fields.

Definition of a field in mathematics

Physicists and mathematicians have very different definitions of the word *field*. In mathematics, a *field* is defined to be a set which is mapped on itself by two binary operations called *addition* and *multiplication*.

If a. b and c are elements in the field F, then the mathematical definition of a field requires

- Associativity of addition and multiplication: $a+(b+c) = (a+b)+c$, and $a \cdot (b \cdot c) = (a \cdot b) \cdot c$.
- Commutativity of addition and multiplication: $a + b = b + a$, and $a \cdot b = b \cdot a$.
- Additive and multiplicative identity: there exist two different elements 0 and 1 in F such that $a + 0 = a$ and $a \cdot 1 = a$.
- Additive inverses: for every a in F, there exists an element in F, denoted $-a$, called the additive inverse of a, such that $a + (-a) = 0$.
- Multiplicative inverses: for every $a \neq 0$ in F, there exists an element in F, denoted by a^{-1} or $1/a$, called the multiplicative inverse of a, such that $a \cdot a^{-1} = 1$.
- Distributivity of multiplication over addition: $a \cdot (b + c) = (a \cdot b) + (a \cdot c)$.

Examples of fields include the rational numbers, the real numbers, and the complex numbers.

For the rational numbers, we have

$$\frac{a}{b} \cdot \frac{b}{a} = \frac{ab}{ba} = 1 \tag{13.9}$$

so that an inverse exits under multiplication. The distributive requirement can also be demonstrated:

$$
\begin{aligned}
&\frac{a}{b} \cdot \left(\frac{c}{d} + \frac{e}{f}\right) \\
&= \frac{a}{b} \cdot \left(\frac{c}{d} \cdot \frac{f}{f} + \frac{e}{f} \cdot \frac{d}{d}\right) \\
&= \frac{a}{b} \cdot \left(\frac{cf}{df} + \frac{ed}{fd}\right) = \frac{a}{b} \cdot \frac{cf+ed}{df} \\
&= \frac{a(cf+ed)}{bdf} = \frac{acf}{bdf} + \frac{aed}{bdf} = \frac{ac}{bd} + \frac{ae}{bf} \\
&= \frac{a}{b} \cdot \frac{c}{d} + \frac{a}{b} \cdot \frac{e}{f}
\end{aligned} \tag{13.10}
$$

which proves the distributive property. In general the requirements of a field can be recognized as known properties of the rational numbers.

Éveriste Galois is remembered for exploring the relationships between field theory and group theory, (where field theory is defined in the mathematical rather than physical sense).

Fields with a finite number of elements are called Galois fields. An interesting example of a mathematical field with only four elements is given in the following tables:

Table 13.1: **Addition**

+	0	I	A	B
0	0	I	A	B
I	I	0	B	A
A	A	B	0	I
B	B	A	I	0

Table 13.2: **Multiplication**

·	0	I	A	B
0	0	0	0	0
I	0	I	A	B
A	0	A	B	I
B	0	B	I	A

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Chapter 14

GAUSS AND RIEMANN

14.1 Gauss contributed to many fields

Johann Carl Friedrich Gauss was born in 1777 in Brunswick, now a part of Lower Saxony, Germany. His parents were not wealthy, and his mother was illiterate, but Gauss soon showed himself to be a child prodigy. At the age of three, he corrected an error that his father had made in summing up his accounts.

Another story is told about the precocity of Gauss: At the age of seven, he amazed his school teacher who was in the habit of giving his students the problem of summing all the integers from 1 to 100. His young student Gauss almost instantly gave him the correct answer, having realized that the sum could be expressed as 50 pairs of numbers, each with the sum, 101.

Continuing in this way, Gauss made important mathematical discoveries as a teenager. His great ability attracted the attention of the Duke of Brunswick, who arranged for Gauss to be sent to the Collegium Carolinium, today known as the Braunschweig University of Technology.Later, the Duke also supported the studies of Gauss at the University of Göttingen.

While still a student at Göttingen, Gauss discovered how to construct a seventeen-sided polygon with a compass and ruler. He was so pleased with this discovery that he decided to make mathematics his career, instead of his previous choice, philosophy.

Gauss returned from Göttingen to Brunswick, where he received a degree. The Duke of Brunswick agreed to continue his stipend, and he requested that Gauss should submit a doctoral dissertation to the University of Helmstedt. The dissertation which Gauss submitted discussed the fundamental theorem of algebra.

Supported by the Duke of Brunswick's stipend, Gauss was able to devote himself completely to research. In 1801, at the age of 24, he published an important book entitled *Disquisitiones Arithmeticae.* Most of the chapters were devoted to number theory.

Contributions to astronomy

In 1801 the astronomer Zach discovered the small planet Ceres, later reclassified as an asteroid. He was only able to track it for a short time, before it disappeared behind the sun. Many astronomers tried to calculate where Ceres would re-appear. Gauss also made a calculation, which turned out to be by far the most accurate. He had used his methods of least squares and normal distributions, which will be discussed below. The astronomer Olbers suggested that Gauss be made director of the proposed new astronomical observatory, but no action was taken at the time.

The year 1805 was both happy and sad for Gauss. In that year, he married Johanna Ostoff, and his personal life became happy. However, 1805 was also the year in which his great patron, the Duke of Brunswick, was killed in a war. In 1807, Gauss left Brunswick to take up the position of director of the new astronomical observatory in Göttingen.

In 1808, Gauss was again hit by tragedy. Both his father and his wife died. Johanna died in childbirth, and her newly-born son died soon afterward. Although emotionally shattered by these personal losses, Gauss continued to work. and a year later he married Johanna's best friend, Minna. In 1809 he published a second important book, *Theoria motus corporum coelestium in sectionibus conicis Solem ambientium.* This two-volume work discusses differential equations, conic sections, and the motion of celestial bodies. He showed how to estimate the orbits of planets, and how to refine the estimates. This book was his most important contribution to theoretical astronomy, but he continued to make astronomical observations until the age of 70.

The geodesic survey

In 1818, Gauss was asked to work on a geodesic survey of his country, and he accepted the task with pleasure. For this purpose, he invented the heliotrope, which reflected the sun's light, and which made use of mirrors and a small telescope. Gauss published over 70 papers related to the survey.

Differential geometry

In 1828, Gauss published *Disquisitiones generales circa superficies curva*, an important paper which discusses geodesics and total curvature. Today, Gaussian curvature is an important topic in differential geometry.

Work on terrestrial magnetism

In 1831, Wilhelm Weber became the Professor of Physics at Göttingen University, and the following year, he and Gauss began a collaborative study of terrestrial magnetism. By 1840, Gauss had written three important papers on the subject: *Intensitas vis magneticae terrestris ad mensuram absolutam revocata* (1832), *Allgemeine Theorie des Erdmagnetismus* (1839) and *Allgemeine Lehrsätze in Beziehung auf die im verkehrten Verhältnisse* *des Quadrats der Entfernung wirkenden Anziehungs- und Abstossungskräfte* (1840).

Gauss and Weber invented the first electromagnetic telegraph in 1933. It was capable of sending messages over a distance of 5,000 feet between the Göttingen Observatory and the Institute of Physics. Gauss also established the unit of magnetism in terms of mass, charge and time. In this period he also derived Gauss' law, which states that the flux of electric field out of any region of space is proportional to to the electric charge contained within the region. This law laster became one of the four equations on which James Clerk Maxwell based his general theory of electromagnetism.

Gauss was able to show that the earth could have only two magnetic poles. He contributed greatly to Alexander von Humboldt's efforts to map the earth's magnetic field.

14.2 Normal distributions in probability theory

Figure 14.8 shows a Gaussian distribution function of the form

$$\varphi(x) = \sqrt{\frac{\sigma^2}{2\pi}} e^{-\sigma^2(x-\mu)^2/2} \tag{14.1}$$

In his 1809 book, *Theoria motus corporum coelestium in sectionibus conicis solem ambientium*, Gauss addressed the problem of finding a way to make use of several measurements of the same quantity to achieve the best possible estimate of the quantity's actual value. This led him to introduce what we now call the gaussian distribution function or alternatively the normal distribution function.

Gaussians have many useful properties, The Fourier transform of a gaussian is a gaussian in reciprocal space, and he product of two 3-dimensional Cartesian gaussian functions, is another Cartesian gaussian. This last property has led to the widespread use of Cartesian gaussians as basis functions in quantum chemical calculations, to facilitate the calculation of many-center Coulomb and exchange integrals.

14.3 Bernhard Riemann's life and work

Georg Friedrich Bernhard Riemann (1826-1866) was the son of a German Lutheran pastor. He was born in a village near Dannenberg in the Kingdom of Hanover.From an early age he showed exceptional mathematical ability, coupled with poor health, extreme shyness and fear of public speaking.

In 1846, Bernhard Riemann's father gathered enough money to send him to the University of Göttingen, where it was intended that he should study theology. While at the university, however, Riemann attracted the attention of Gauss, who recognized Riemann's great mathematical ability and recommended that he should change the topic of his studies to mathematics. Permission to do so was fortunately granted by Bernhard Riemann's father.

At that time, the University of Berlin was famous for its mathematical faculty, and Riemann studied there for two years before returning to Göttingen.

In order to become a lecturer at the University of Göttingen, Riemann was required to deliver a qualifying lecture. He prepared three, on different topics, and to his surprise, Gauss chose topic that he least expected: *On the hypotheses that underlie geometry.* This lecture turned out to be a milestone in the history of mathematics.

The main point of Riemann's lecture was the definition of the curvature tensor; but he also posed deep questions concerning the physical space in which we live. Riemann was too far ahead of his time to be appreciated by most of his audience, but Gauss was deeply impressed. According to Monastyrsky, "Among Riemann's audience, only Gauss was able to appreciate the depth of Riemann's thoughts. ... The lecture exceeded all his expectations and greatly surprised him. Returning to the faculty meeting, he spoke with the greatest praise and rare enthusiasm to Wilhelm Weber about the depth of the thoughts that Riemann had presented."

The pioneering work on the metric tensor by Riemann later formed the basis for Einstein's general theory of relativity. Freudenthal writes that "The general theory of relativity splendidly justified his work. In the mathematical apparatus developed from Riemann's address, Einstein found the frame to fit his physical ideas, his cosmology, and cosmogony: and the spirit of Riemann's address was just what physics needed: the metric structure determined by data."

In 1859, Riemann became the head of the mathematics department at the University of Göttingen.

Riemann's death from tuberculosis

Throughout his life, Riemann's health had never been good. He contracted tuberculosis, and was forced to go to Italy for the sake of his health. However, the illness worsened and he died in Italy. Throughout his life, Riemann had been a devout Christian, and he died while reciting the Lord's Prayer together with his wife.

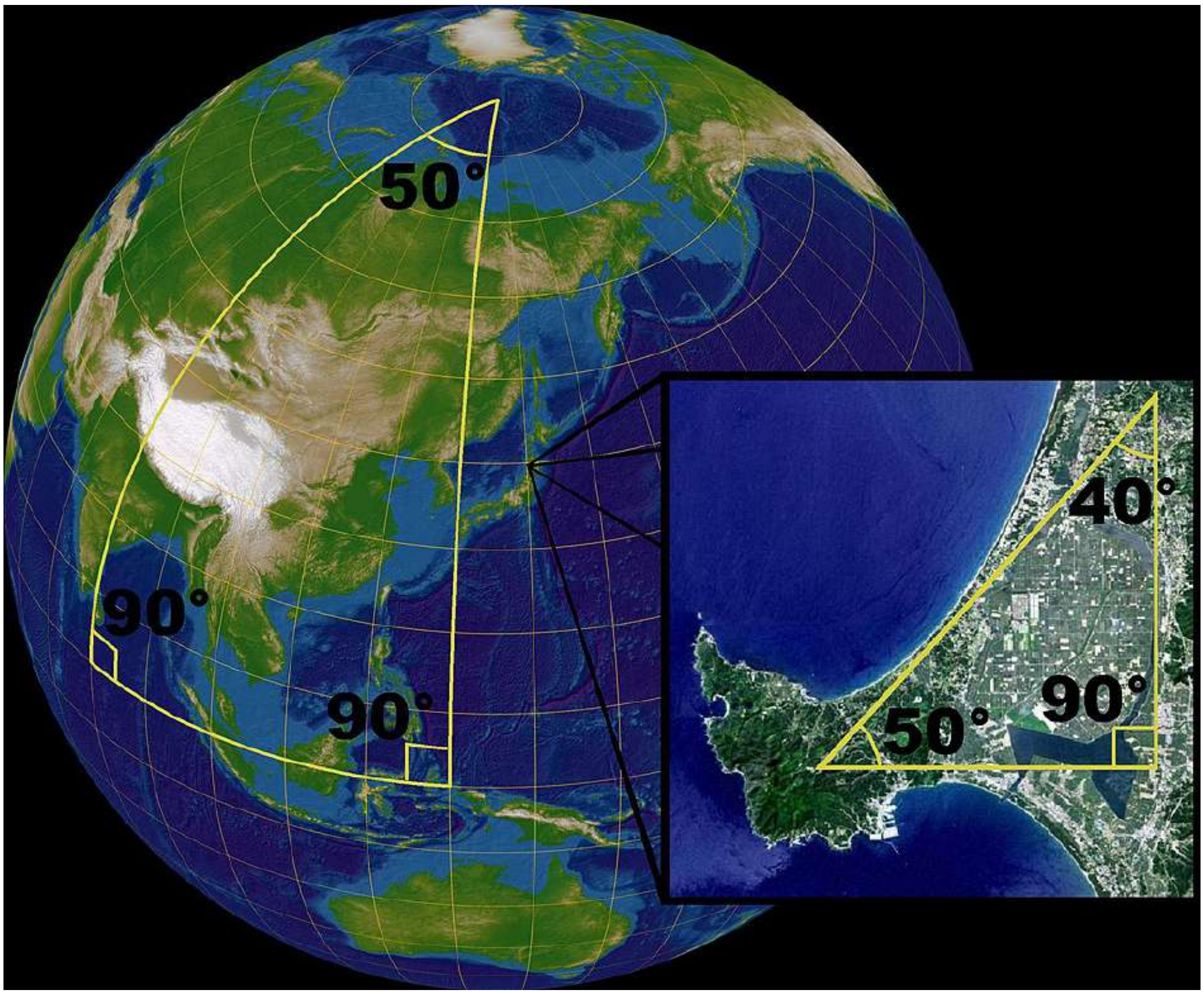

Figure 14.1: **On a sphere, the sum of the angles of a triangle is not equal to 180^o. The surface of a sphere is not a Euclidean space, but locally the laws of the Euclidean geometry are good approximations. In a small triangle on the face of the earth, the sum of the angles is very nearly 180^o.**

Figure 14.2: **János Bolyai. (1802-1860), from Hungary, sent Gauss his work on non-Euclidean geometry. Gauss wrote to a friend, "I regard this young geometer Bolyai as a genius of the first order." However, to Bolyai himself, he wrote (regarding the paper that Bolyai had sent to him) "To praise it would amount to praising myself. For the entire content of the work...coincides almost exactly with my own meditations which have occupied my mind for the past thirty or thirty-five years."**

Figure 14.3: **The Russian mathematician Nikolai Ivanovich Lobachevsky (1792-1856) independently worked on non-Euclidean geometry.**

Figure 14.4: **Portrait of Carl Friedrich Gauss (1777-1855).**

Figure 14.5: **Portrait of Gauss published in *Astronomische Nachrichten* (1828).**

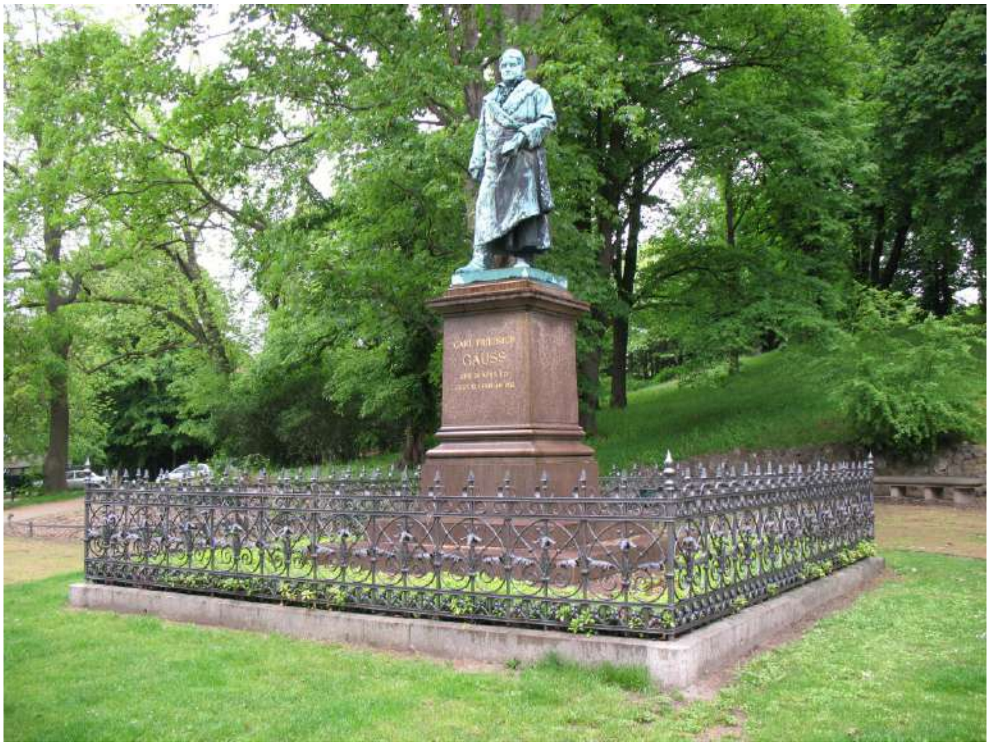

Figure 14.6: **Statue of Gauss at his birthplace, Brunswick.**

Figure 14.7: **German 10-Deutsche Mark Banknote (1993) featuring Gauss.**

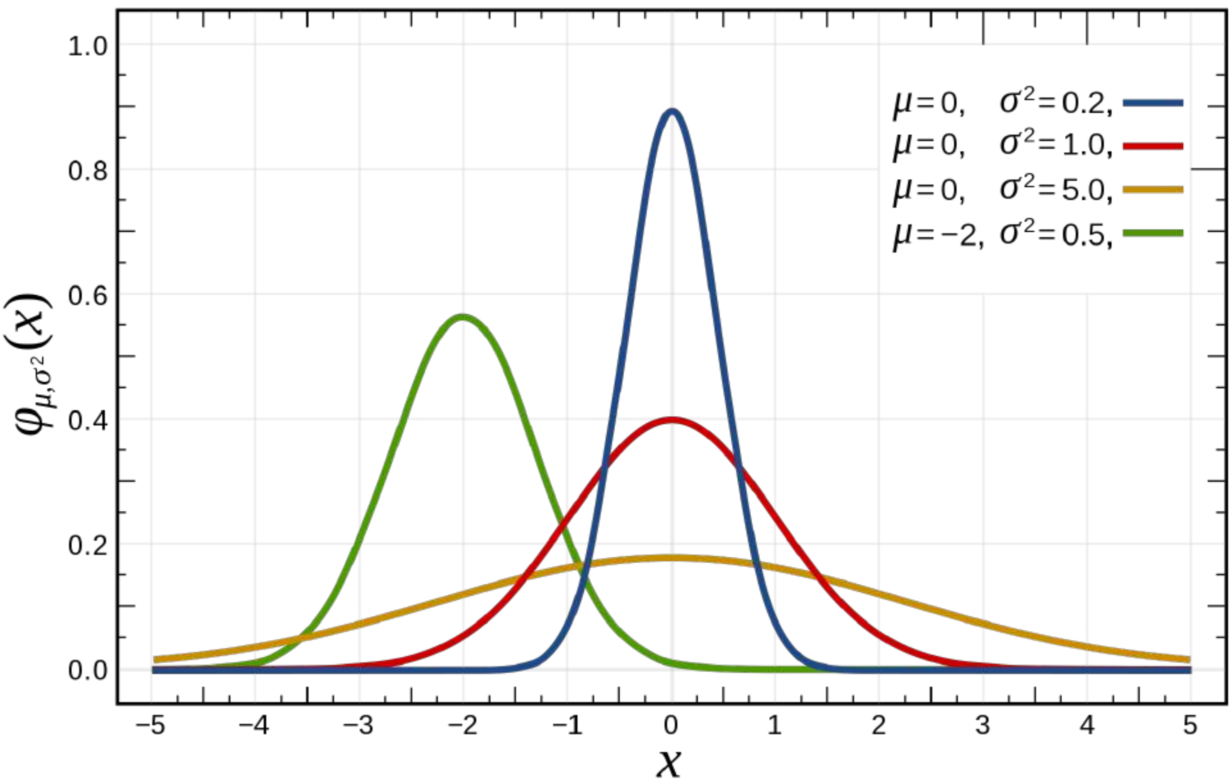

Figure 14.8: **Four normal distributions. In 1809 Gauss published his monograph *Theoria motus corporum coelestium in sectionibus conicis solem ambientium* where among other things he introduces several important statistical concepts, such as the method of least squares, the method of maximum likelihood, and the normal distribution.**

Figure 14.9: **Gauss and Weber, two pioneers in the study of electromagnetism. Together, they invented the first electromagnetic telegraph, and mapped the earths magnetic field. The unit of magnetic field strength is named after Gauss, while the unit of magnetic flux is named after Weber. In 1856, Weber demonstrated that the ratio of electric to magnetic units was equal to the velocity of light, a finding that led James Clerk Maxwell to believe correctly that light is an electromagnetic wave. In 1865, Maxwell published his epoch-making book *A Dynamical Theory of the Electromagnetic Field*, which was based on the observations of Gauss and Weber, and those of Michael Faraday. Maxwell's book achieved, after Newton's *Principia*, the second great unification in physics, and it paved the way for much of modern technology - electrical power generation, radio, television, computers, and so on.**

Figure 14.10: **A photograph of Georg Friedrich Bernhard Riemann taken in 1863. In a famous lecture in 1854, he founded Riemanian geometry, discussing infinitely differentiable manifolds, and curvature.**

Figure 14.11: **Another image of Riemann.**

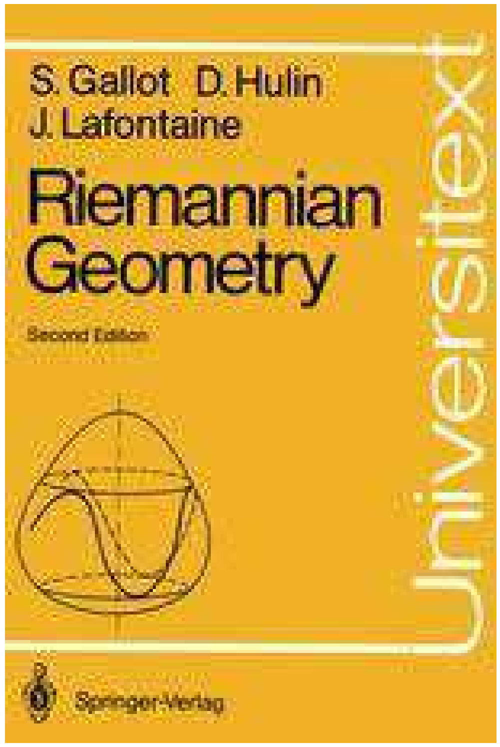

Figure 14.12: **Riemannian Geometry.**

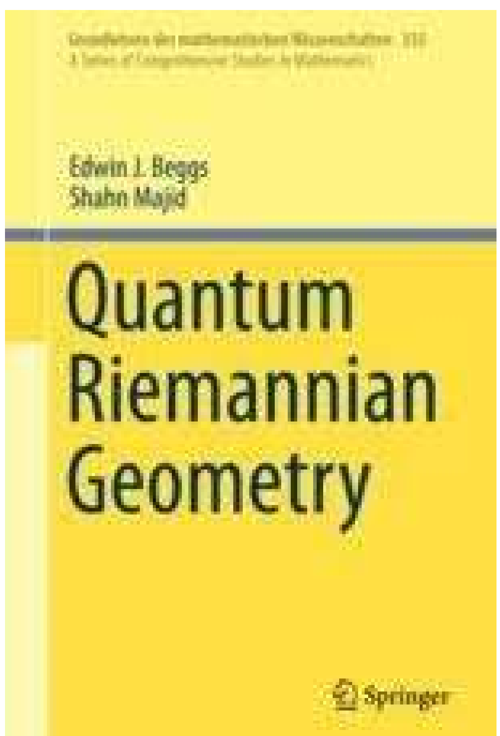

Figure 14.13: **Quantum Riemannian Geometry.**

14.4 Functions of a complex variable

The Cauchy-Riemann equations

Let $z = x + iy$ be a complex variable, and let

$$f(z) = u(x, y) + iv(x, y) \tag{14.2}$$

be a function of z, where u and v are real functions of x and y. Then the Cauchy-Riemann equations are

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \tag{14.3}$$

and

$$\frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x} \tag{14.4}$$

In regions of the complex plane where the Cauchy-Riemann equations are satisfied, the function $f(z)$ is said to be *analytic*. For example, the function

$$f(z) = z^2 \tag{14.5}$$

is analytic everywhere in the complex plane. while the function

$$f(z) = \frac{1}{(x + iy)(x - iy)} \tag{14.6}$$

is analytic everywhere in the complec plane except at two points, $z = \pm iy$.

The Cauchy-Riemann equations can be used to evaluate definite integrals. It cam be shown that the integral taken around a contour in the complex plane is equal to the sum of the *residues* contained at the singularities of the function within the contour. This method of evaluating definite integrals is usually called *Riemannian integration*

Riemannian surfaces

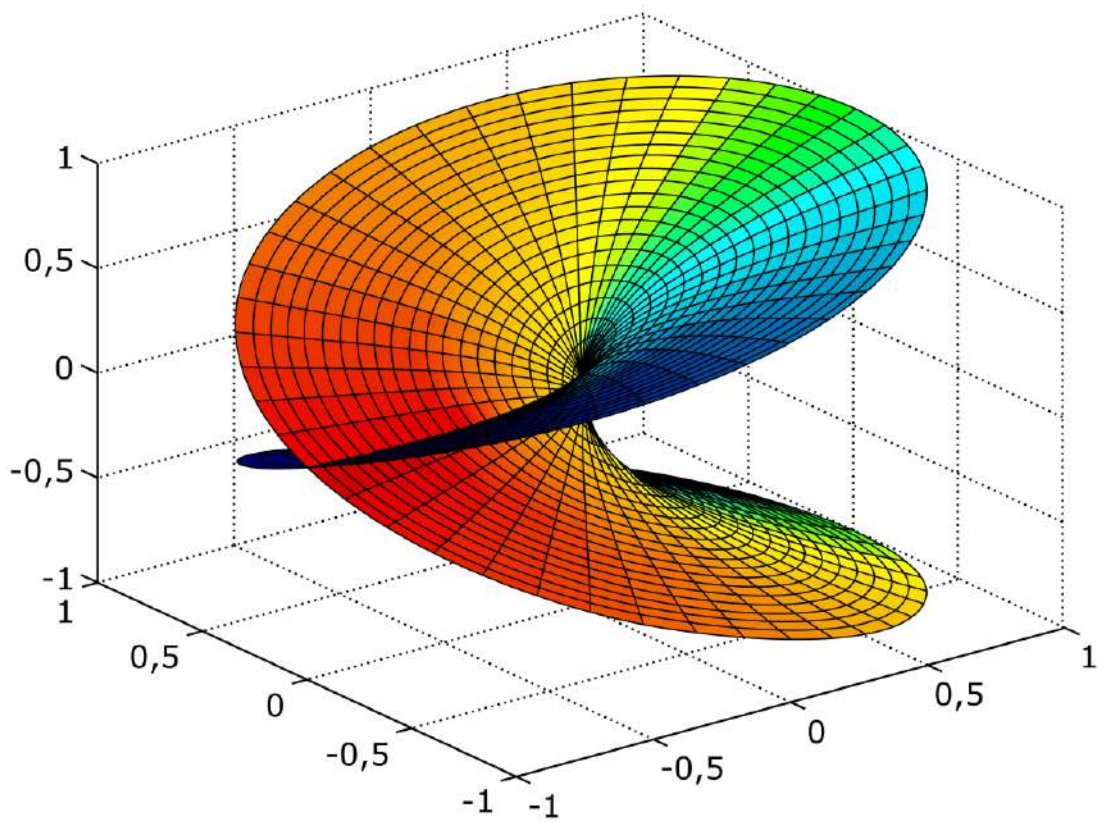

Figure 14.14: **Riemann surface for the function $f(z) = \sqrt{z}$. The two horizontal axes represent the real and imaginary parts of z, while the vertical axis represents the real part of $\sqrt{z}$. The imaginary part of $\sqrt{z}$ is represented by the coloration of the points.**

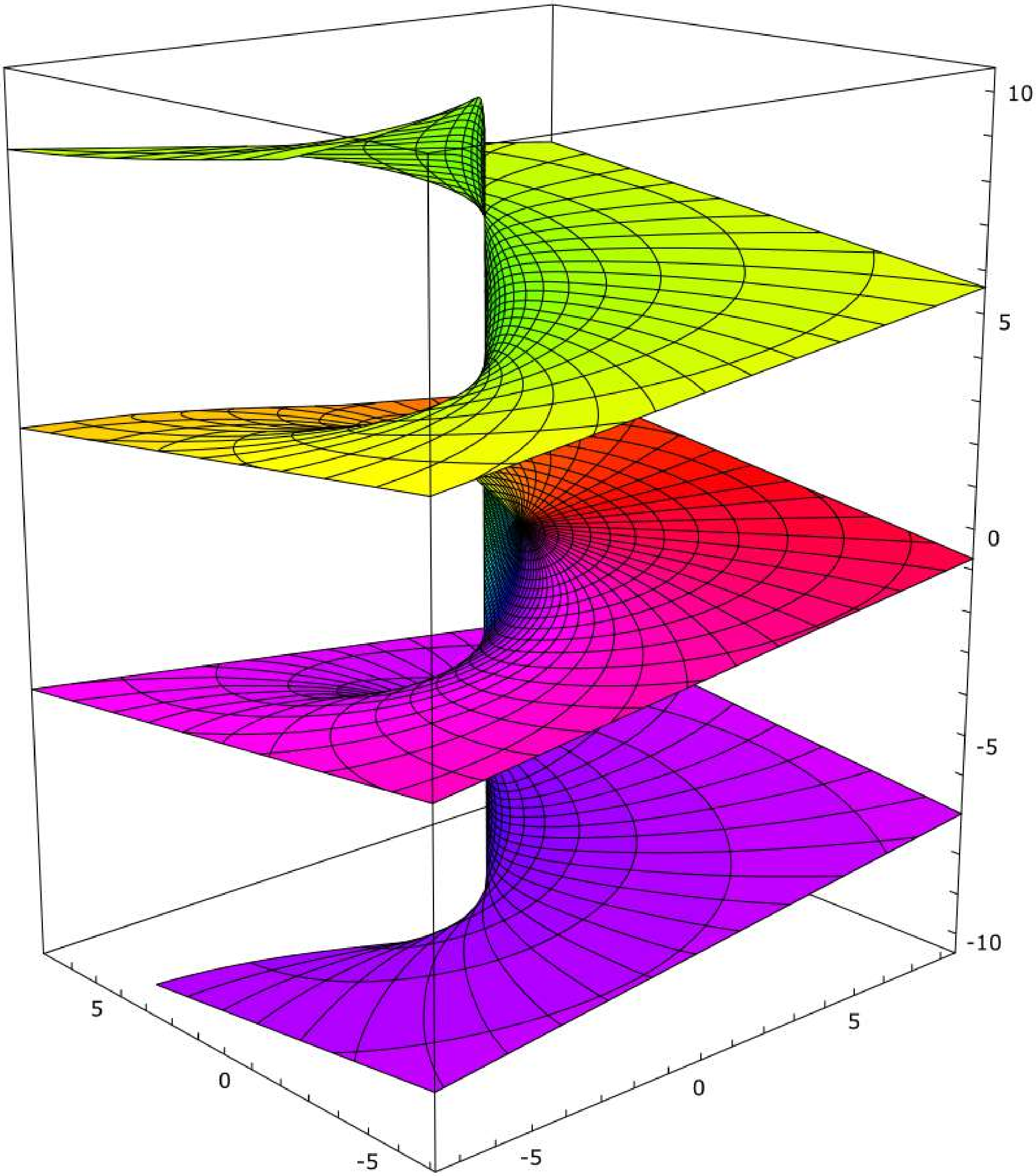

Figure 14.15: $f(z) = \log(z)$

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Chapter 15

HILBERT

15.1 David Hilbert's life and work

David Hilbert (1862-1943) was born in or near to Kömogsberg in the Kingdom of Prussia. His father, Otto Hilbert, was a county judge, while his mother, Maria, was the daughter of a Königsberg merchant. She was greatly interested in philosophy, astronomy and prime numbers. and it was she who taught her son. David, for his first eight years, before he entered school.

Later, at the gymnasium stage of his education, David Hilbert was at first enrolled in a gymnasium that emphasized the classics. He was unhappy there, and did poorly. For his final year, however, he transferred to the Wilhelm Gymnasium, where there was more emphasis on mathematics. There, he received top grades for mathematics. His final report stated that "For mathematics he always showed a very lively interest and a penetrating understanding: he mastered all the material taught in the school in a very pleasing manner and was able to apply it with sureness and ingenuity."

In the autumn of 1880, at the age of 18, he entered the University of Königsberg, where he took courses on integral calculus, the theory of determinants, the curvature of surfaces. and number theory.

In 1882, another student, Hermann Minkowsky. arrived at the University of Königsberg. He and David Hilbert became lifelong friends, and they greatly influenced each other's mathematical thoughts. They were later to become two of the four masters of the Mathematical Institute at the University of Göttingen: Klein, Runge, Minkowsi and Hilbert.

In 1884, Hilbert presented a defense of his doctoral thesis. It was entitled *Über invariante Eigenschaften specieller binärer Formen, insbesondere der Kugelfunctionen*, and it dealt with the invariant properties of sets of spherical harmonics.

Hilbert was encouraged by Felix Klein to travel to Paris and to meet the most important French mathematicians. He did so and was received in Paris in a very friendly way. The French mathematicians spoke to him in German out of politeness, but not being entirely fluent in German, they were sometimes not able to communicate their ideas adequately.

Klein advised Hilbert that the University of Königsberg was a backwater, but Hilbert decided to stay and teach there anyway, writing to Klein, "I am content and full of joy to have decided myself for Königsberg. The constant association with Professor Lindemann and, above all, with Hurwitz is not less interesting than it is advantageous to myself and stimulating. The bad part about Königsberg being so far away from things I hope I will be able to overcome by making some trips again next year, and perhaps then I will get to meet Herr Gordan."

Hilbert taught at Königsberg from 1886 to 1895, finally rising to the rank of Full Professor. In 1895, Felix Klein succeeded in having Hilbert appointed to a vacant chair at the University of Göttingen, and Hilbert remained there for the rest of his career, becoming one of the four masters of the Mathematical Institute.

In 1899, Hilbert published an influential book entitled *Grundlagen der Geometrie*, which put geometry on a formal axiomatic basis, and later another influential book entitled *Grundlagen der Mathematik*.

In August, 1900, David Hilbert gave a lecture at the International Congress of Mathematicians in Paris, in which he proposed 23 outstanding problems for the mathematical community to solve. Some of these problems remain challenging even today.

In 1912, Hilbert changed his focus from pure mathematics to mathematical physics. He arranged to have a tutor in physics for himself, and he gave a number of seminars on the work of Albert Einstein. Hilbert invited Einstein to visit Göttingen, and talks between the two helped Einstein to formulate his general theory of relativity in a mathematically correct way. After Einstein's visit, Hilbert also made contributions to the general theory of relativity.

In 1930, Hilbert retired from the University of Göttingen, but he continued to give lectures there occasionally. Shortly afterwards, the Nazis came to power and Jewish professors were purged from the university, together with professors who had Jewish wives. After this happened, Hilbert was seated next to Bernhard Rust, the new Minister of Education at a dinner. The minister asked "Did the Mathematical Institute really suffer so much from the departure of the Jews?". Hilbert replied, "Suffer? It no longer exists!"

Illness and death

Starting in 1925, Hilbert began to exhibit signs of exhaustion. His illness was diagnosed as pernicious anemia, which was at that time untreatable. He died in 1943.

15.2 Hilbert space

Hilbert space, or function space, is an infinite-dimensional Euclidian space in which functions play the role of unit vectors. In discussing Hilbert space, it is convenient to use the bra and ket notation later introduced by P.A.M. Dirac. In this notation, a set of orthonormal functions

$$\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \phi_3(\mathbf{x}), \phi_4(\mathbf{x}), \cdots \tag{15.1}$$

is represented by a set of *kets*:

$$|1\rangle, |2\rangle, |3\rangle, |4\rangle, \cdots \tag{15.2}$$

Their conjugate functions are represented by the set of *bras*

$$\langle 1|, \langle 2|, \langle 3|, \langle 4|, \cdots \tag{15.3}$$

The scalar product of two members of this set is represented by

$$\int d\mathbf{x}\ \phi^*(\mathbf{x})\phi(\mathbf{x}) \rightarrow \langle i|j\rangle = \delta_{i,j} \equiv \begin{cases} 1 & \text{if } i = j \\ \\ 0 & \text{if } i \neq j \end{cases} \tag{15.4}$$

This scalar product is closely analogous to the scalar product of two unit vectors in a Euclidian vector space. Because of orthonormality, the scalar product is zero unless $i = j$.

15.3 Generalized Fourier analysis

Let us now consider some function, $f(\mathbf{x})$. David Hilbert showed that we can represent any well-behaved single-valued function by an infinite series of the form

$$f(\mathbf{x}) = \sum_{j=1}^{\infty} a_j \phi_j(\mathbf{x}) \tag{15.5}$$

where

$$a_j = \int d\mathbf{x}\ \phi^*(\mathbf{x}) f(\mathbf{x}) \tag{15.6}$$

In bra and ket notation, this becomes

$$|f\rangle = \sum_{j=1}^{\infty} |j\rangle\langle j|f\rangle \tag{15.7}$$

15.4 Projection operators

The quantity

$$P_A = \sum_{j \in A} |j\rangle\langle j| \tag{15.8}$$

is called a *projection operator*. When acting on any function, P_A projects out that part of the function which is contained in the domain A of Hilbert space. Projection more than once gives the same result as projecting a single time. In other words.

$$P_A = P_A P_A = P_A P_A P_A = P_A P_A P_A P_A \cdots \tag{15.9}$$

If the domains A and B have no elements in common, then

$$P_A P_B = 0 \qquad A \notin B \tag{15.10}$$

The completeness property of a set of functions requires that

$$\sum_{j=1}^{\infty} |j\rangle\langle j| = I \tag{15.11}$$

where I is the identity operator.

Matrix representation of operators

Let H be some operator, for example the quantum mechanical Hamiltonian of a particle. Then in the bra and ket notation, the matrix representation of an operator is given by

$$\int d\mathbf{x}\ \phi_i^*(\mathbf{x}) H \phi_j(\mathbf{x}) \to \langle i|H|j\rangle \equiv H_{i,j} \tag{15.12}$$

where the operator acts on everything to its right. Using his studies of the matrix representation of operators, David Hilbert was able to show that the seemingly different representations of quantum theory given by Heisenberg and Schrödinger are actually just two forms of the same theory.

15.5 Some quotations from David Hilbert

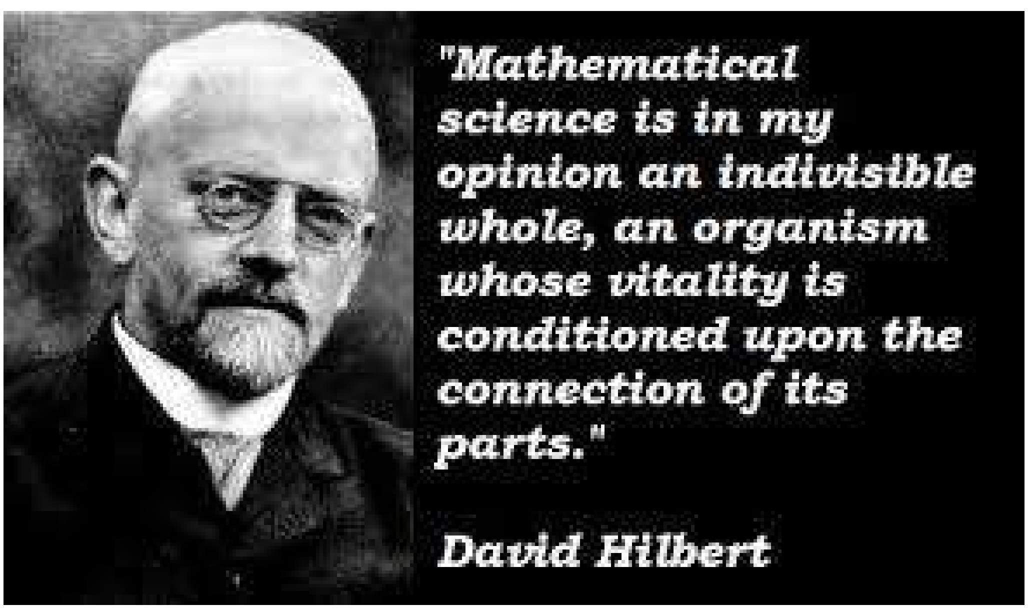
- **“We must know! We will know!”**
- **“Before beginning I should put in three years of intensive study, and I haven’t that much time to squander on a probable failure.” [On why he didn’t try to solve Fermat’s last theorem]**
- **“Galileo was no idiot. Only an idiot could believe that science requires martyrdom - that may be necessary in religion, but in time a scientific result will establish itself.”**
- **“I have tried to avoid long numerical computations, thereby following Riemann’s postulate that proofs should be given through ideas and not voluminous computations.”**
- **“Mathematics is a game played according to certain simple rules with meaningless marks on paper.”**
- **“How thoroughly it is ingrained in mathematical science that every real advance goes hand in hand with the invention of sharper tools and simpler methods which, at the same time, assist in understanding earlier theories and in casting aside some more complicated developments.”**
- **“The art of doing mathematics consists in finding that special case which contains all the germs of generality.”**

- **"The further a mathematical theory is developed, the more harmoniously and uniformly does its construction proceed, and unsuspected relations are disclosed between hitherto separated branches of the science."**
- **"One can measure the importance of a scientific work by the number of earlier publications rendered superfluous by it."**
- **"Mathematics knows no races or geographic boundaries; for mathematics, the cultural world is one country."**
- **"The infinite! No other question has ever moved so profoundly the spirit of man."**
- **"No one shall expel us from the paradise that Cantor has created for us."**
- **"He who seeks for methods without having a definite problem in mind seeks in the most part in vain."**
- **"If one were to bring ten of the wisest men in the world together and ask them what was the most stupid thing in existence, they would not be able to discover anything so stupid as astrology."**
- **"Physics is becoming too difficult for the physicists."**
- **"Meine Herren, der Senat ist doch keine Badeanstalt. The faculty is not a pool changing room." [On the proposed appointment of Emmy Noether as the first woman professor.]**
- **"Who of us would not be glad to lift the veil behind which the future lies hidden; to cast a glance at the next advances of our science and at the secrets of its development during future centuries? What particular goals will there be toward which the leading mathematical spirits of coming generations will strive? What new methods and new facts in the wide and rich field of mathematical thought will the new centuries disclose?" (Opening of his speech to the 1900 Congress in Paris.)**
- **"Every mathematical discipline goes through three periods of development: the naive, the formal, and the critical."**
- **"In mathematics ... we find two tendencies present. On the one hand, the tendency towards abstraction seeks to crystallise the logical relations inherent in the maze of materials ... being studied, and to correlate the material in a systematic and orderly manner. On the other hand, the tendency towards intuitive understanding fosters a more immediate grasp of the objects one studies, a live rapport with them, so to speak, which stresses the concrete meaning of their relations." Geometry and the imagination (New York, 1952).**
- **"No other question has ever moved so profoundly the spirit of man; no other idea has so fruitfully stimulated his intellect; yet no other concept stands in greater need of clarification than that of the infinite."**
- **"A mathematical theory is not to be considered complete until you have made it so clear that you can explain it to the first man whom you meet on the street."**

- **"If I were to awaken after having slept for a thousand years, my first question would be: Has the Riemann hypothesis been proven?"**
- **"Mathematical science is in my opinion an indivisible whole, an organism whose vitality is conditioned upon the connection of its parts."**
- **"Mathematics knows no races or geographic boundaries; for mathematics, the cultural world is one country."**
- **(On Cantor's set theory:) "The finest product of mathematical genius and one of the supreme achievements of purely intellectual human activity."**
- **"The art of doing mathematics consists in finding that special case which contains all the germs of generality."**
- **"The further a mathematical theory is developed, the more harmoniously and uniformly does its construction proceed, and unsuspected relations are disclosed between hitherto separated branches of the science."**

Figure 15.1: **David Hilbert.**

Figure 15.2: **The Mathematical Institute in Göttingen. Its new building, constructed with funds from the Rockefeller Foundation, was opened by Hilbert and Courant in 1930.**



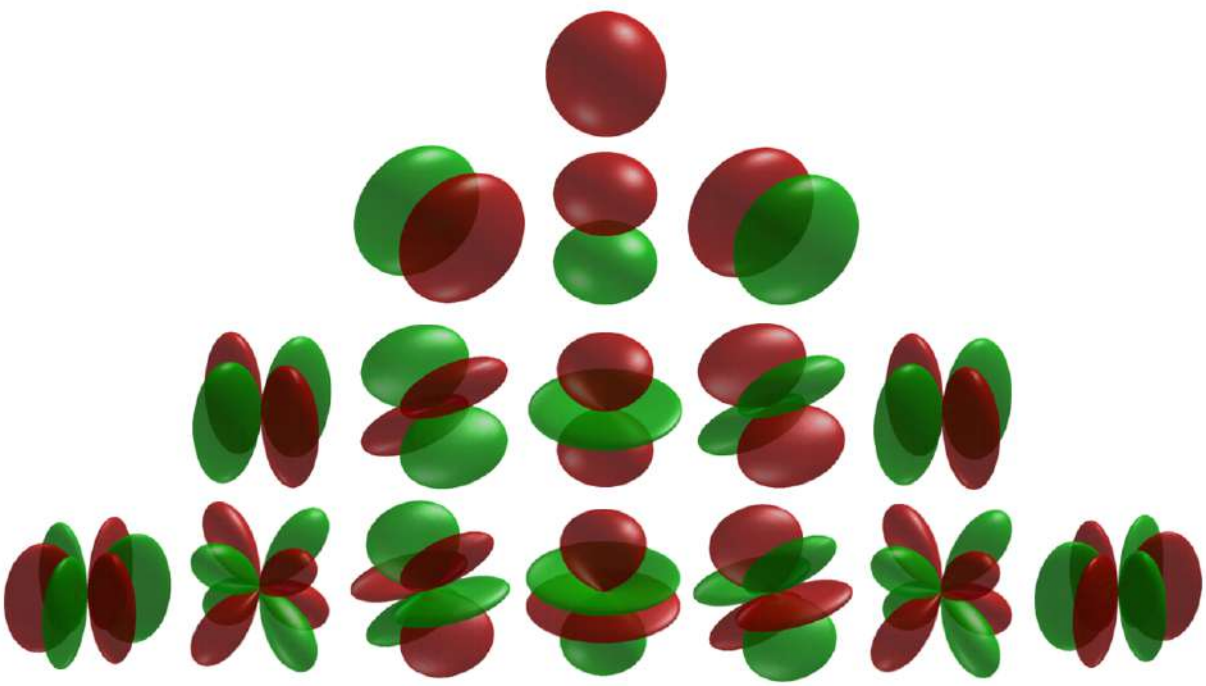


Figure 15.3: **Spherical harmonics, an orthonormal basis for the Hilbert space of square-integrable functions on the sphere, shown graphed along the radial direction.**

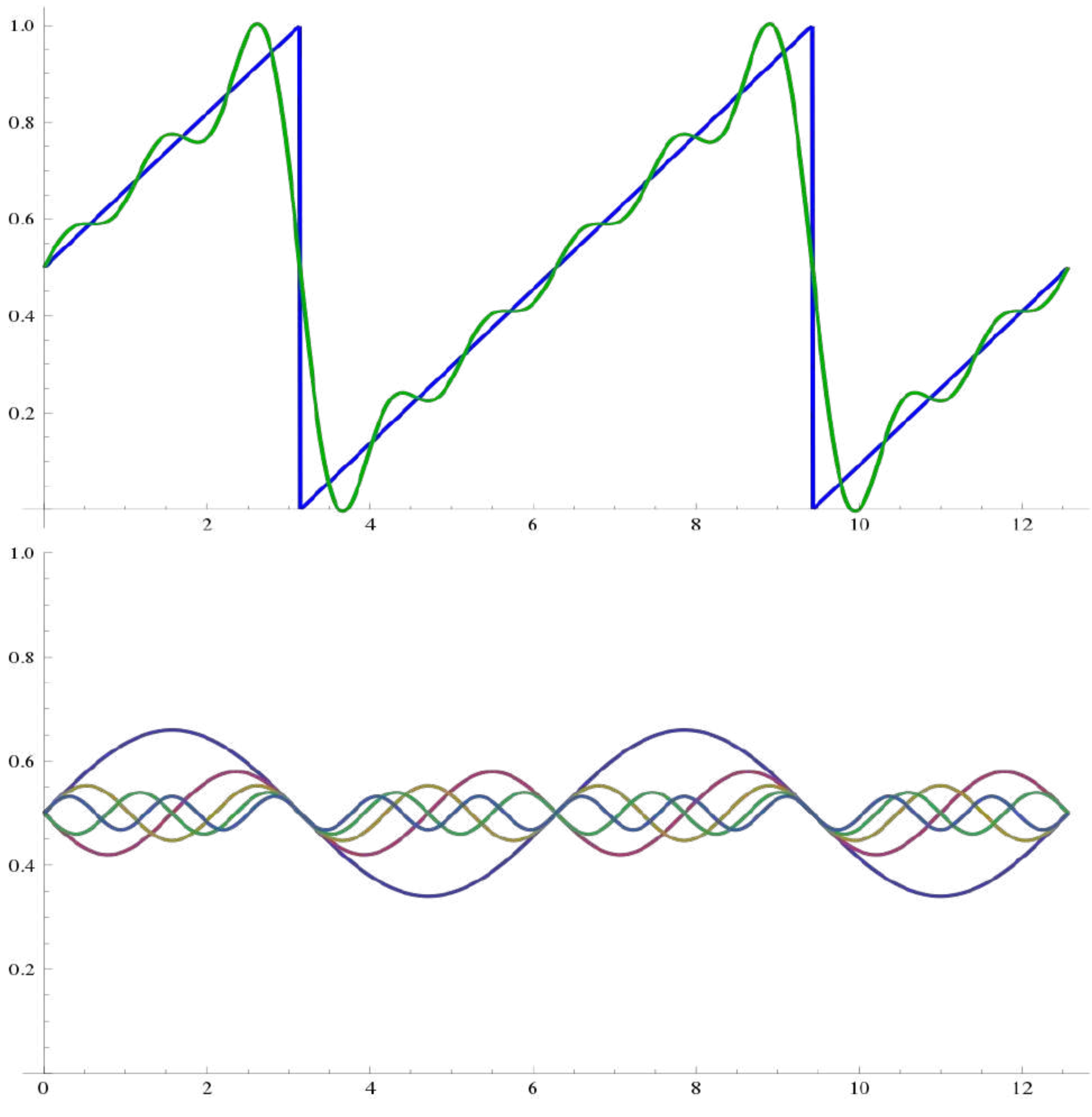


Figure 15.4: **Superposition of sinusoidal wave basis functions (bottom) to form a sawtooth wave (top).**

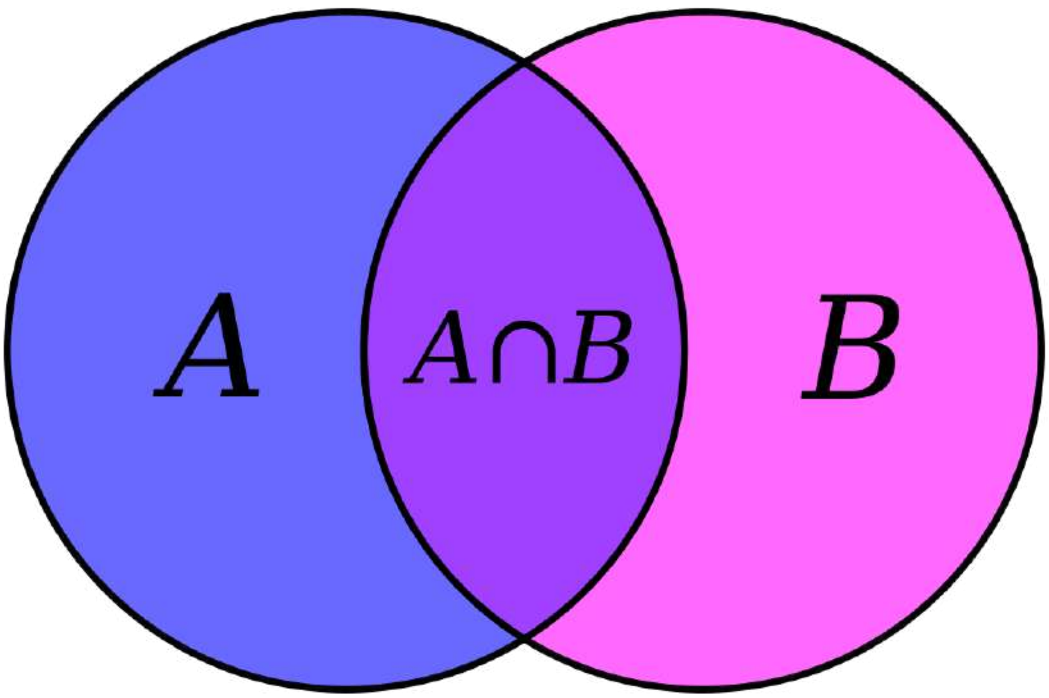


Figure 15.5: **A Venn diagram illustrating the intersection of two sets. The sets might, for example, represent sets of unit vectors in a Hilbert space. In that case, if $P_A = \sum_{j \in A} |j\rangle\langle j|$ and $P_B = \sum_{k \in B} |k\rangle\langle k|$, then $P_A P_B = P_C$, where P_C is the projection operator corresponding to the intersection of A and B.**

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Chapter 16

EINSTEIN

"The unleashed power of the atom has changed everything except our ways of thinking, and thus we drift towards unparalleled catastrophes."

"I don't know what will be used in the next world war, but the 4th will be fought with stones."

Albert Einstein (1879-1955)

Besides being one of the greatest physicists of all time, Albert Einstein was a lifelong pacifist, and his thoughts on peace can speak eloquently to us today. We need his wisdom today, when the search for peace has become vital to our survival as a species.

16.1 Family background

Albert Einstein was born in Ulm, Germany, in 1879. He was the son of middle-class, irreligious Jewish parents, who sent him to a Catholic school. Einstein was slow in learning to speak, and at first his parents feared that he might be retarded; but by the time he was eight, his grandfather could say in a letter: "Dear Albert has been back in school for a week. I just love that boy, because you cannot imagine how good and intelligent he has become."

Remembering his boyhood, Einstein himself later wrote: "When I was 12, a little book dealing with Euclidean plane geometry came into my hands at the beginning of the school year. Here were assertions, as for example the intersection of the altitudes of a triangle in one point, which, though by no means self-evident, could nevertheless be proved with such certainty that any doubt appeared to be out of the question. The lucidity and certainty made an indescribable impression on me."

When Albert Einstein was in his teens, the factory owned by his father and uncle began to encounter hard times. The two Einstein families moved to Italy, leaving Albert alone and miserable in Munich, where he was supposed to finish his course at the gymnasium. Einstein's classmates had given him the nickname "Beidermeier", which means something like "Honest John"; and his tactlessness in criticizing authority soon got him into trouble. In Einstein's words, what happened next was the following: "When I was in the seventh grade at the Lutpold Gymnasium, I was summoned by my home-room teacher, who expressed the wish that I leave the school. To my remark that I had done nothing wrong, he replied only, 'Your mere presence spoils the respect of the class for me'."

Einstein left gymnasium without graduating, and followed his parents to Italy, where he spent a joyous and carefree year. He also decided to change his citizenship. "The over-emphasized military mentality of the German State was alien to me, even as a boy", Einstein wrote later. "When my father moved to Italy, he took steps, at my request, to have me released from German citizenship, because I wanted to be a Swiss citizen."

The financial circumstances of the Einstein family were now precarious, and it was clear that Albert would have to think seriously about a practical career. In 1896, he entered the famous Zürich Polytechnic Institute with the intention of becoming a teacher of mathematics and physics. However, his undisciplined and nonconformist attitudes again got him into trouble. His mathematics professor, Hermann Minkowski (1864-1909), considered Einstein to be a "lazy dog"; and his physics professor, Heinrich Weber, who originally had gone out of his way to help Einstein, said to him in anger and exasperation: "You're a clever fellow, but you have one fault: You won't let anyone tell you a thing! You won't let anyone tell you a thing!"

Einstein missed most of his classes, and read only the subjects which interested him. He was interested most of all in Maxwell's theory of electro-magnetism, a subject which was too "modern" for Weber. There were two major examinations at the Zürich Polytechnic Institute, and Einstein would certainly have failed them had it not been for the help of his loyal friend, the mathematician Marcel Grossman.

Grossman was an excellent and conscientious student, who attended every class and took meticulous notes. With the help of these notes, Einstein managed to pass his examinations; but because he had alienated Weber and the other professors who could have helped him, he found himself completely unable to get a job. In a letter to Professor F. Ostwald on behalf of his son, Einstein's father wrote: "My son is profoundly unhappy because of his present joblessness; and every day the idea becomes more firmly implanted in his mind that he is a failure, and will not be able to find the way back again."

From this painful situation, Einstein was rescued (again!) by his friend Marcel Grossman, whose influential father obtained for Einstein a position at the Swiss Patent Office: Technical Expert (Third Class). Anchored at last in a safe, though humble, position, Einstein married one of his classmates. He learned to do his work at the Patent Office very efficiently; and he used the remainder of his time on his own calculations, hiding them guiltily in a drawer when footsteps approached.

In 1905, this Technical Expert (Third Class) astonished the world of science with five papers, written within a few weeks of each other, and published in the Annalen der Physik. Of these five papers, three were classics: One of these was the paper in which Einstein applied Planck's quantum hypothesis to the photoelectric effect. The second paper discussed "Brownian motion", the zig-zag motion of small particles suspended in a liquid and hit

Figure 16.1: **Einstein at the age of three in 1882.**

Figure 16.2: **Albert Einstein in 1893 (age 14).**

Figure 16.3: **Albert Einstein in 1904 (age 25).**

Figure 16.4: **Olympia Academy founders: Conrad Habicht, Maurice Solovine and Einstein.**

Figure 16.5: **Albert and Mileva Einstein, 1912.**

Figure 16.6: **Einstein with his second wife, Elsa, in 1921.**

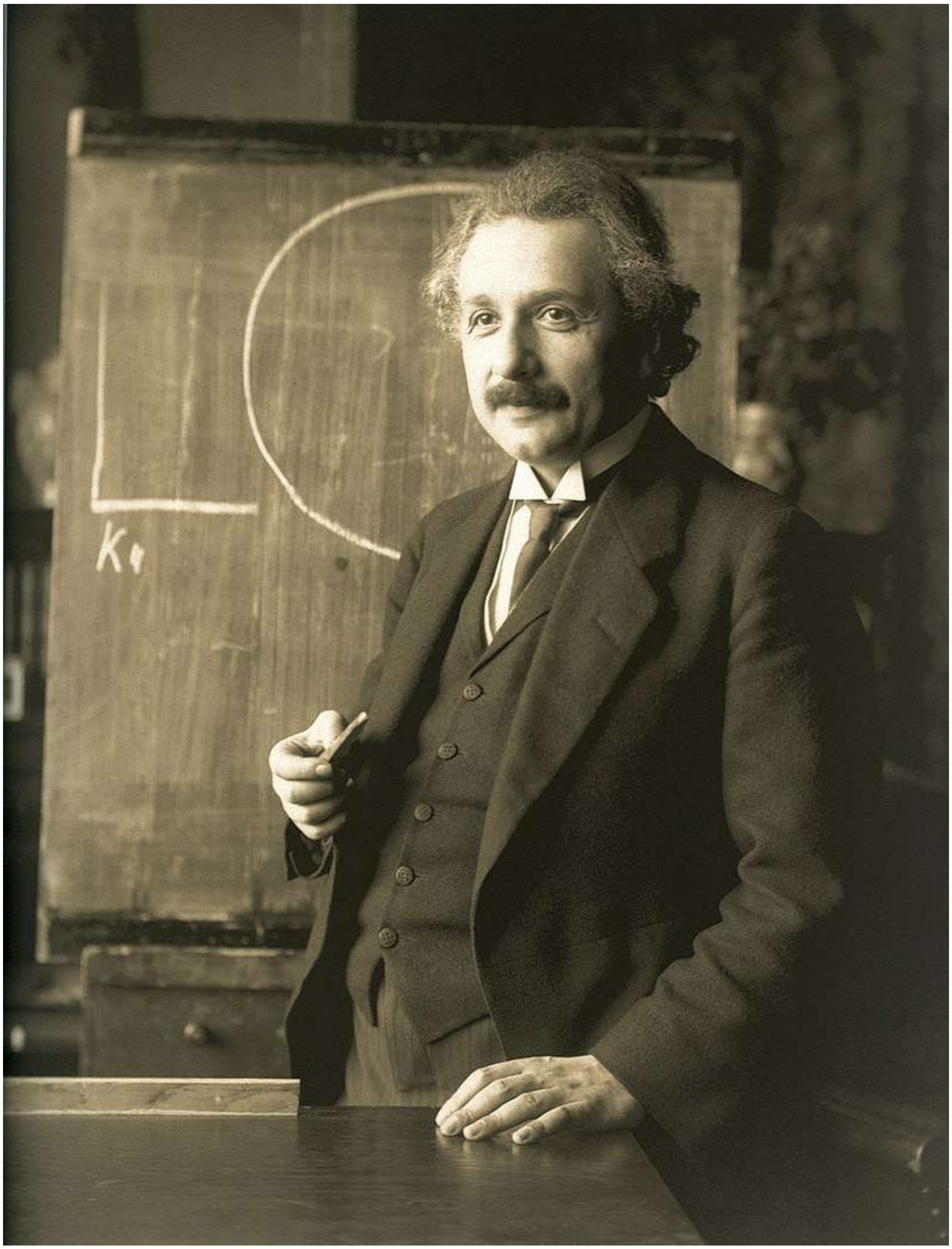

Figure 16.7: **Albert Einstein during a lecture in Vienna in 1921.**

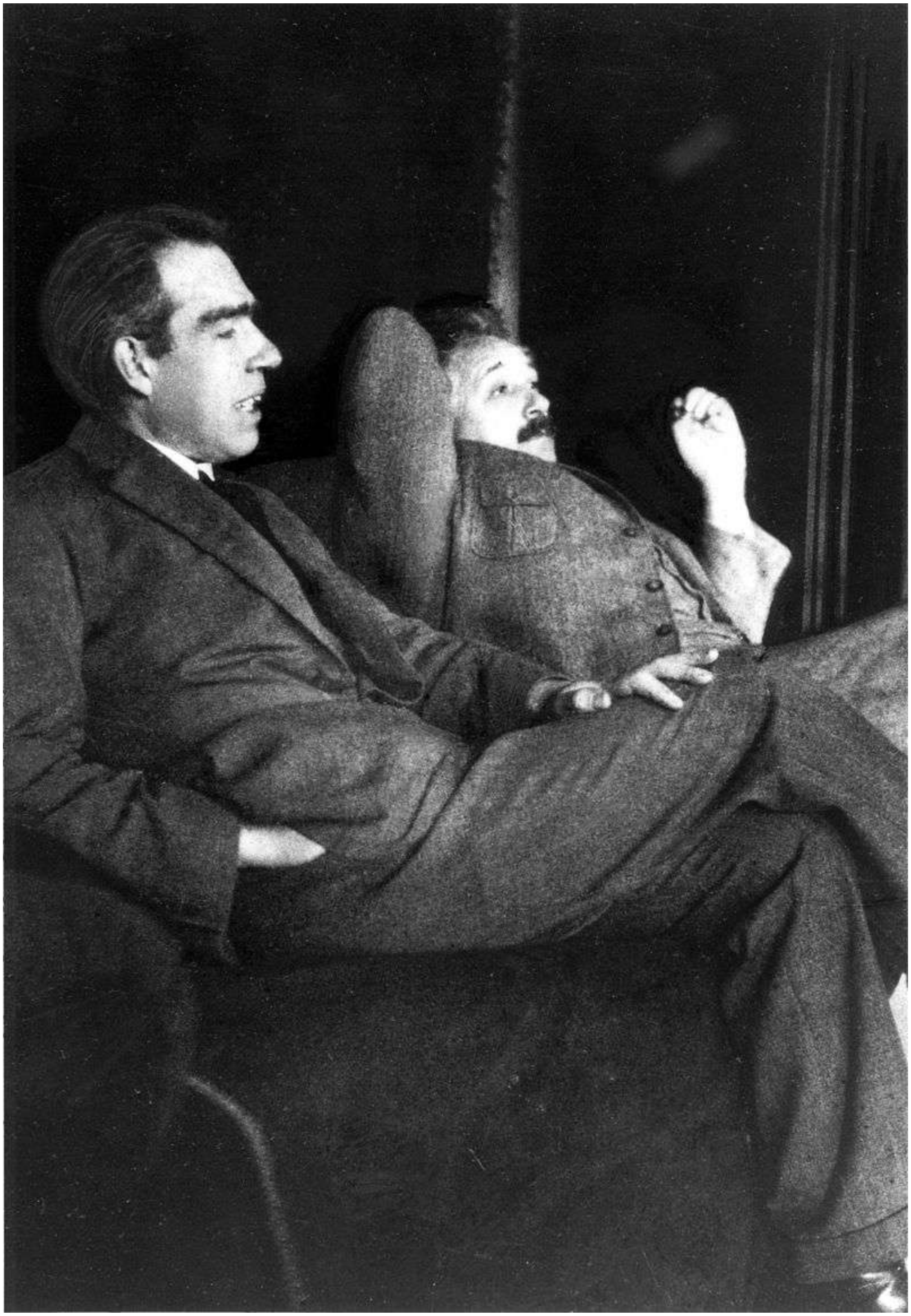

Figure 16.8: **Einstein and Niels Bohr, 1925.**

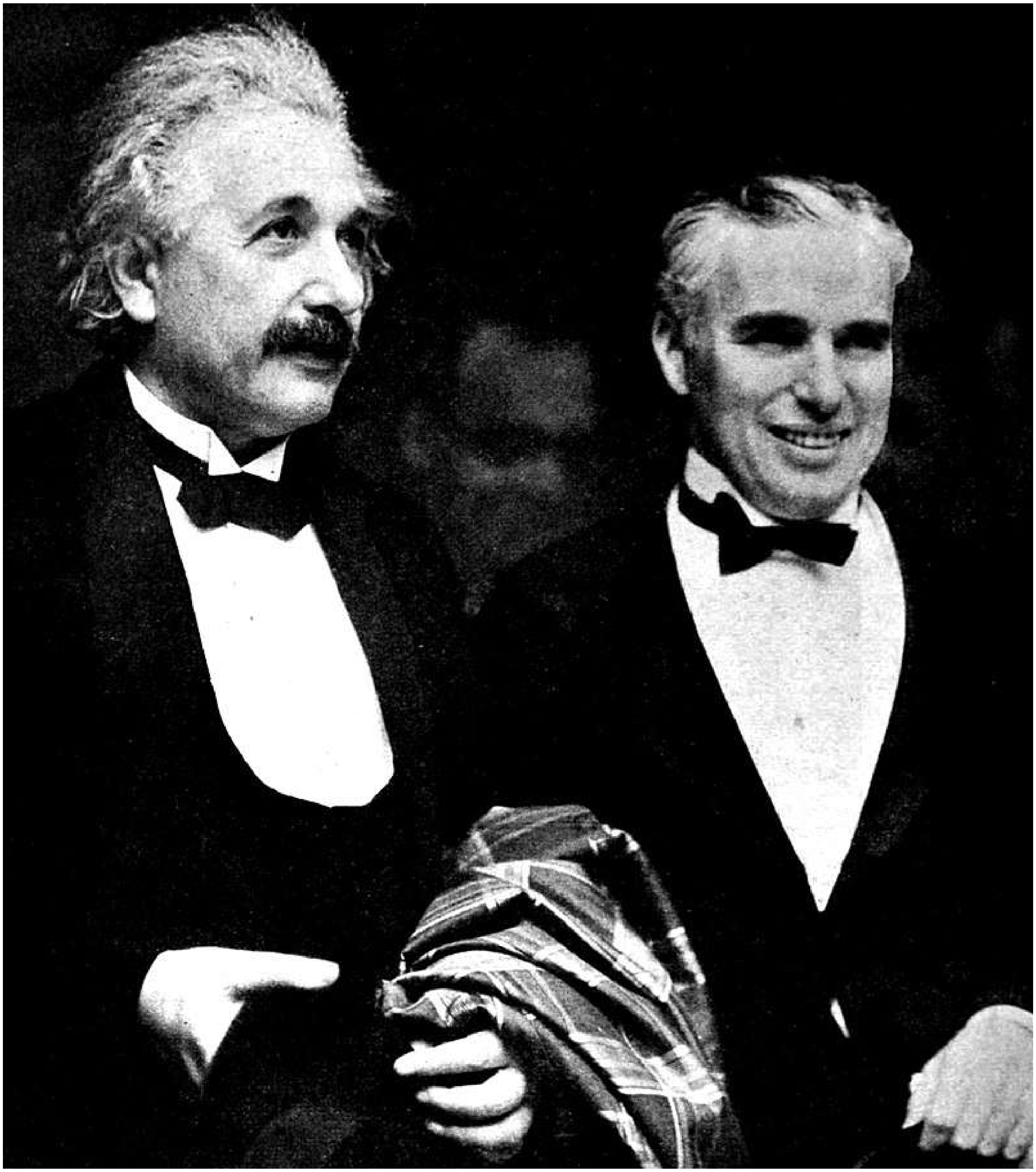

Figure 16.9: **Einstein (left) and Charlie Chaplin at the Hollywood premiere of City Lights, January 1931.**

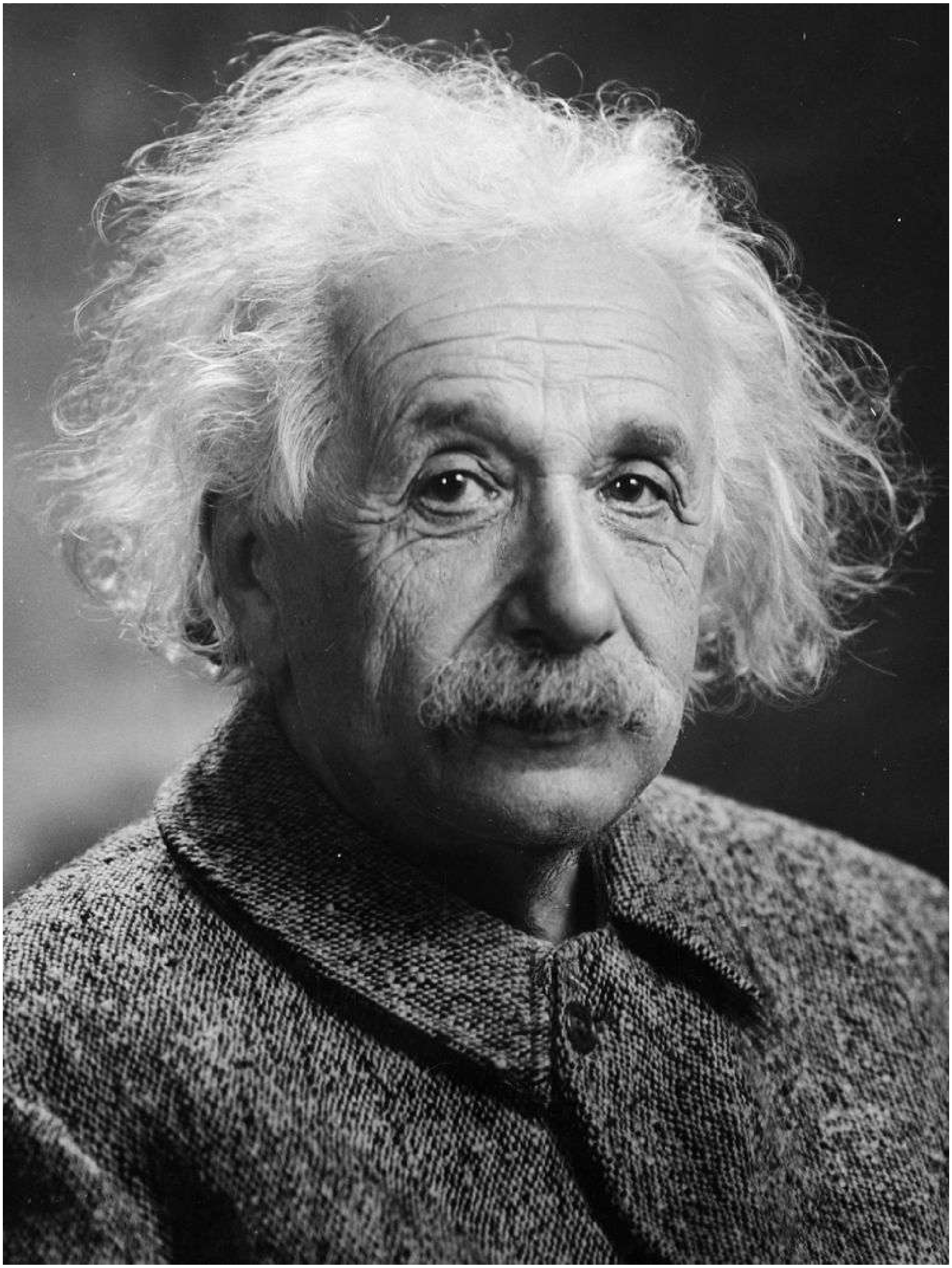

Figure 16.10: **Einstein in 1947.**

randomly by the molecules of the liquid. This paper supplied a direct proof of the validity of atomic ideas and of Boltzmann's kinetic theory. The third paper was destined to establish Einstein's reputation as one of the greatest physicists of all time. It was entitled "On the Electrodynamics of Moving Bodies", and in this paper, Albert Einstein formulated his special theory of relativity. Essentially, this theory maintained that all of the fundamental laws of nature exhibit a symmetry with respect to rotations in a 4-dimensional space-time continuum.

16.2 Special relativity theory

The theory of relativity grew out of problems connected with Maxwell's electromagnetic theory of light. Ever since the wavelike nature of light had first been demonstrated, it had been supposed that there must be some medium to carry the light waves, just as there must be some medium (for example air) to carry sound waves. A word was even invented for the medium which was supposed to carry electromagnetic waves: It was called the "ether".

By analogy with sound, it was believed that the velocity of light would depend on the velocity of the observer relative to the "ether". However, all attempts to measure differences in the velocity of light in different directions had failed, including an especially sensitive experiment which was performed in America in 1887 by A.A. Michelson and E.W. Morley.

Even if the earth had, by a coincidence, been stationary with respect to the "ether" when Michelson and Morley first performed their experiment, they should have found an "ether wind" when they repeated their experiment half a year later, with the earth at the other side of its orbit. Strangely, the observed velocity of light seemed to be completely independent of the motion of the observer!

In his famous 1905 paper on relativity, Einstein made the negative result of the Michelson-Morley experiment the basis of a far-reaching principle: He asserted that no experiment whatever can tell us whether we are at rest or whether we are in a state of uniform motion. With this assumption, the Michelson-Morley experiment of course had to fail, and the measured velocity of light had to be independent of the motion of the observer.

Einstein's Principle of Special Relativity had other extremely important consequences: He soon saw that if his principle were to hold, then Newtonian mechanics would have to be modified. In fact, Einstein's Principle of Special Relativity required that *all* fundamental physical laws exhibit a symmetry between space and time. The three space dimensions, and a fourth dimension, ict, had to enter every fundamental physical law in a symmetrical way. (Here i is the square root of -1, c is the velocity of light, and t is time.)

When this symmetry requirement is fulfilled, a physical law is said to be "Lorentz-invariant" (in honor of the Dutch physicist H.A. Lorentz, who anticipated some of Einstein's ideas). Today, we would express Einstein's principle by saying that every fundamental physical law must be Lorentz-invariant (i.e. symmetrical in the space and time coordinates). The law will then be independent of the motion of the observer, provided that the observer is moving uniformly.

Einstein was able to show that, when properly expressed, Maxwell's equations are already Lorentz-invariant; but Newton's equations of motion have to be modified. When the needed modifications are made, Einstein found, then the mass of a moving particle appears to increase as it is accelerated. A particle can never be accelerated to a velocity greater than the velocity of light; it merely becomes heavier and heavier, the added energy being converted into mass.

From his 1905 theory, Einstein deduced his famous formula equating the energy of a system to its mass multiplied by the square of the velocity of light. As we shall see, his formula was soon used to explain the source of the energy produced by decaying uranium and radium; and eventually it led to the construction of the atomic bomb. Thus Einstein, a lifelong pacifist, who renounced his German citizenship as a protest against militarism, became instrumental in the construction of the most destructive weapon ever invented - a weapon which casts an ominous shadow over the future of humankind.

Just as Einstein was one of the first to take Planck's quantum hypothesis seriously, so Planck was one of the first physicists to take Einstein's relativity seriously. Another early enthusiast for relativity was Hermann Minkowski, Einstein's former professor of mathematics. Although he once had characterized Einstein as a "lazy dog", Minkowski now contributed importantly to the mathematical formalism of Einstein's theory; and in 1907, he published the first book on relativity. In honor of Minkowski's contributions to relativity, the 4-dimensional space-time continuum in which we live is sometimes called "Minkowski space".

In 1908, Minkowski began a lecture to the Eightieth Congress of German Scientists and Physicians with the following words:

" From now on, space by itself, and time by itself, are destined to sink completely into the shadows; and only a kind of union of both will retain an independent existence."

Gradually, the importance of Einstein's work began to be realized, and he was much sought after. He was first made Assistant Professor at the University of Zürich, then full Professor in Prague, then Professor at the Zürich Polytechnic Institute; and finally, in 1913, Planck and Nernst persuaded Einstein to become Director of Scientific Research at the Kaiser Wilhelm Institute in Berlin. He was at this post when the First World War broke out

While many other German intellectuals produced manifestos justifying Germany's invasion of Belgium, Einstein dared to write and sign an anti-war manifesto. Einstein's manifesto appealed for cooperation and understanding among the scholars of Europe for the sake of the future; and it proposed the eventual establishment of a League of Europeans. During the war, Einstein remained in Berlin, doing whatever he could for the cause of peace, burying himself unhappily in his work, and trying to forget the agony of Europe, whose civilization was dying in a rain of shells, machine-gun bullets, and poison gas.

16.3 General relativity

The work into which Einstein threw himself during this period was an extension of his theory of relativity. He already had modified Newton's equations of motion so that they exhibited the space-time symmetry required by his Principle of Special Relativity. However, Newton's law of gravitation. remained a problem.

Obviously it had to be modified, since it disagreed with his Special Theory of Relativity; but how should it be changed? What principles could Einstein use in his search for a more correct law of gravitation? Certainly whatever new law he found would have to give results very close to Newton's law, since Newton's theory could predict the motions of the planets with almost perfect accuracy. This was the deep problem with which he struggled.

In 1907, Einstein had found one of the principles which was to guide him, the Principle of Equivalence of inertial and gravitational mass. After turning Newton's theory over and over in his mind, Einstein realized that Newton had used mass in two distinct ways: His laws of motion stated that the force acting on a body is equal to the mass of the body multiplied by its acceleration; but according to Newton, the gravitational force on a body is also proportional to its mass. In Newton's theory, gravitational mass, by a coincidence, is equal to inertial mass; and this holds for all bodies. Einstein decided to construct a theory in which gravitational and inertial mass necessarily have to be the same.

He then imagined an experimenter inside a box, unable to see anything outside it. If the box is on the surface of the earth, the person inside it will feel the pull of the earth's gravitational field. If the experimenter drops an object, it will fall to the floor with an acceleration of 32 feet per second per second. Now suppose that the box is taken out into empty space, far away from strong gravitational fields, and accelerated by exactly 32 feet per second per second. Will the enclosed experimenter be able to tell the difference between these two situations? Certainly no difference can be detected by dropping an object, since in the accelerated box, the object will fall to the floor in exactly the same way as before.

With this "thought experiment" in mind, Einstein formulated a general Principle of Equivalence: He asserted that no experiment whatever can tell an observer enclosed in a small box whether the box is being accelerated, or whether it is in a gravitational field. According to this principle, gravitation and acceleration are locally equivalent, or, to say the same thing in different words, gravitational mass and inertial mass are equivalent.

Einstein soon realized that his Principle of Equivalence implied that a ray of light must be bent by a gravitational field. This conclusion followed because, to an observer in an accelerated frame, a light beam which would appear straight to a stationary observer, must necessarily appear very slightly curved. If the Principle of Equivalence held, then the same slight bending of the light ray would be observed by an experimenter in a stationary frame in a gravitational field.

Another consequence of the Principle of Equivalence was that a light wave propagating upwards in a gravitational field should be very slightly shifted to the red. This followed because in an accelerated frame, the wave crests would be slightly farther apart than they normally would be, and the same must then be true for a stationary frame in a gravitational field. It seemed to Einstein that it ought to be possible to test experimentally both the gravitational bending of a light ray and the gravitational red shift.

This seemed promising; but how was Einstein to proceed from the Principle of Equivalence to a formulation of the law of gravitation? Perhaps the theory ought to be modeled after Maxwell's electromagnetic theory, which was a field theory, rather than an "action at a distance" theory. Part of the trouble with Newton's law of gravitation was that it allowed a signal to be propagated instantaneously, contrary to the Principle of Special Relativity. A field theory of gravitation might cure this defect, but how was Einstein to find such a theory? There seemed to be no way.

From these troubles Albert Einstein was rescued (a third time!) by his staunch friend Marcel Grossman. By this time, Grossman had become a professor of mathematics in Zürich, after having written a doctoral dissertation on tensor analysis and non-Euclidean geometry, the very things that Einstein needed. The year was then 1912, and Einstein had just returned to Zürich as Professor of Physics at the Polytechnic Institute. For two years, Einstein and Grossman worked together; and by the time Einstein left for Berlin in 1914, the way was clear. With Grossman's help, Einstein saw that the gravitational field could be expressed as a curvature of the 4-dimensional space-time continuum.

In 1919, a British expedition, headed by Sir Arthur Eddington, sailed to a small island off the coast of West Africa. Their purpose was to test Einstein's prediction of the bending of light in a gravitational field by observing stars close to the sun during a total eclipse. The observed bending agreed exactly with Einstein's predictions; and as a result he became world-famous. The general public was fascinated by relativity, in spite of the abstruseness of the theory (or perhaps because of it). Einstein, the absent-minded professor, with long, uncombed hair, became a symbol of science. The world was tired of war, and wanted something else to think about.

Einstein met President Harding, Winston Churchill and Charlie Chaplin; and he was invited to lunch by the Archbishop of Canterbury. Although adulated elsewhere, he was soon attacked in Germany. Many Germans, looking for an excuse for the defeat of their nation, blamed it on the pacifists and Jews; and Einstein was both these things.

16.4 Metric tensors

Let us consider a coordinate system $x^1, x^2, \cdots, x^d$ labelling the points in a d-dimensional space. We can label the points in a different way by going to a new coordinate system $X^1, X^2, \cdots, X^d$ where the new coordinates are expressed as functions of the old ones.

$$\begin{aligned} X^1 &= X^1(x^1, x^2, \cdots, x^d) \\ X^2 &= X^2(x^1, x^2, \cdots, x^d) \\ \vdots \; & \; \vdots \qquad\quad \vdots \\ X^d &= X^d(x^1, x^2, \cdots, x^d) \end{aligned} \tag{16.1}$$

For example, (16.1) might represent a transformation from Cartesian coordinates to spherical polar coordinates. If we have an equation written in terms of the old coordinates, we might ask how to rewrite it in terms of the new ones. More generally, we can try to write a physical equation in such a way that it will look the same in every coordinate system. Suppose that the space is Euclidean (flat), so that in terms of the Cartesian coordinates $x^1, x^2, \cdots, x^d$, the infinitesimal element of length separating two points is given by the Pythagorean rule:

$$ds^2 = \delta_{i,j} dx^i dx^j \equiv g_{i,j} dx^i dx^j \tag{16.2}$$

(In equation (16.2) and in the remainder of this section, we use the Einstein convention, in which a sum over repeated indices is understood, although not written explicitly.) The symbol $g_{i,j}$ which appears in the definition of the infinitesimal length ds^2 is called the *covariant metric tensor*, and for Cartesian coordinates in a Euclidean space, it is just the Kronecker delta function. Using the identity

$$dx^i = \frac{\partial x^i}{\partial X^\mu} dX^\mu \tag{16.3}$$

we can rewrite (16.2) as

$$ds^2 = \delta_{i,j} \frac{\partial x^i}{\partial X^\mu} \frac{\partial x^j}{\partial X^\nu} dX^\mu dX^\nu \equiv G_{\mu,\nu} dX^\mu dX^\nu \tag{16.4}$$

where

$$G_{\mu,\nu} \equiv g_{i,j} \frac{\partial x^i}{\partial X^\mu} \frac{\partial x^j}{\partial X^\nu} \tag{16.5}$$

The quantity $G_{\mu,\nu}$ which appears in equations (16.4) and (16.5) is the covariant metric tensor in the new coordinate system. In any space, whether Euclidean or not, the covariant metric tensor is defined by the expression which yields ds^2, the square of the infinitesimal distance between two points, as in equation (16.2) or (16.4). The word *tensor* refers to the way in which a quantity transforms under changes in the coordinate system. The *rank* of a tensor is the number of indices. The covariant metric tensor is the prototype of a covariant tensor of second rank. Any physical quantity which must be transformed according to the rule

$$A_{\mu,\nu} = a_{i,j} \frac{\partial x^i}{\partial X^\mu} \frac{\partial x^j}{\partial X^\nu} \tag{16.6}$$

under the coordinate transformation $x^1, x^2, \cdots, x^d \rightarrow X^1, X^2, \cdots, X^d$ is said to be a covariant tensor of second rank. The d-component entity

$$dX^\mu = \frac{\partial X^\mu}{\partial x^i} dx^i \tag{16.7}$$

is the prototype of a contravariant tensor of first rank. Any quantity that transforms according to the rule

$$A^\mu = \frac{\partial X^\mu}{\partial x^i} a^i \tag{16.8}$$

is said to be a contravariant tensor of first rank (or contravariant vector). The distance element ds is the prototype of an invariant or *scalar*. Any quantity ϕ which is invariant under coordinate transformations is said to be a scalar. The gradient of a scalar

$$\frac{\partial \phi}{\partial X^\mu} = \frac{\partial x^i}{\partial X^\mu}\frac{\partial \phi}{\partial x^i} \tag{16.9}$$

is the prototype of a covariant tensor of first rank, or covariant vector. Any quantity which transforms according to the rule

$$A_\mu = \frac{\partial x^i}{\partial X^\mu} a_i \tag{16.10}$$

is said to be a covariant vector. We can also define tensors of higher rank. For example,

$$A^{\mu\nu\sigma} = \frac{\partial X^\mu}{\partial x^i}\frac{\partial X^\nu}{\partial x^j}\frac{\partial X^\sigma}{\partial x^k} a^{ijk} \tag{16.11}$$

is said to be a contravariant tensor of third rank. A covariant vector and a contravariant vector can be *contracted* into a scalar:

$$A_\mu B^\mu = \frac{\partial x^i}{\partial X^\mu}\frac{\partial X^\mu}{\partial x^j} a_i b^j = \delta^i_j a_i b^j = a_i b^i \tag{16.12}$$

Similarly, if we contract a contravariant vector with the covariant metric tensor, we obtain a covariant vector:

$$\begin{aligned} G_{\mu\nu} A^\nu &= A_\mu \\ g_{ij} a^i &= a_i \end{aligned} \tag{16.13}$$

It is useful to define a quantity called the *contravariant metric tensor*, which gives the Kronecker δ-function when it is contracted with the covariant metric tensor:

$$\begin{aligned} G^{\mu\nu} G_{\nu\sigma} &= \delta^\mu_\sigma \\ g^{ij} g_{jk} &= \delta^i_k \\ G^{\mu\nu} &= \frac{\partial X^\mu}{\partial x^i}\frac{\partial X^\nu}{\partial x^j} g^{ij} \end{aligned} \tag{16.14}$$

If we contract a covariant vector with the contravariant metric tensor, we obtain a contravariant vector:

$$G^{\mu\nu} A_\nu = A^\mu \tag{16.15}$$

In a similar way, we can raise or lower the indices of a tensor of higher rank. For example, it is easy to show that

$$G_{\mu\nu} A^{\nu\sigma\rho} = A_\mu^{\sigma\rho} \tag{16.16}$$

In a Cartesian coordinate system with unit metric we are accustomed to writing the volume element as

$$dv = dx^1 dx^2 \cdots dx^d \tag{16.17}$$

This is obviously unsatisfactory from the standpoint of tensor analysis, since the right-hand side of equation (16.17) appears to be a contravariant tensor of rank d (or rather a particular component of such a tensor), while the left-hand side has no indices at all. In order to write the volume element in an invariant way, the Italian mathematician Tulio Levi-Civita (1873-1941) introduced a totally antisymmetric covariant tensor of rank d. In a Cartesian coordinate system, for a flat space, the Levi-Civita tensor is given by

$$e_{ijkl\cdots} = \begin{cases} (-1)^\sigma & \text{if } ijkl\cdots = \sigma(1234\cdots) \\ \\ 0 & \text{otherwise} \end{cases} \tag{16.18}$$

In other words, the Levi-Civita tensor is ± 1 if $ijkl\cdots$ is a permutation of $1234\cdots$, with the sign depending on whether the permutation is even or odd, and it is zero otherwise. In terms of this tensor, the volume element of equation (16.17) becomes

$$dv = \frac{1}{d!} e_{ijkl\cdots} dx^i dx^j dx^k dx^l \cdots \tag{16.19}$$

while in a transformed coordinate system it is

$$dV = \frac{1}{d!} E_{\mu\nu\sigma\rho\cdots} dX^\mu dX^\nu dX^\sigma dX^\rho \cdots \tag{16.20}$$

where

$$E_{\mu\nu\sigma\cdots} = e_{ijk\cdots} \frac{\partial x^i}{\partial X^\mu} \frac{\partial x^j}{\partial X^\nu} \frac{\partial x^k}{\partial X^\sigma} \cdots \tag{16.21}$$

In this way, Levi-Civita used the formalism of tensor calculus to re-derive the previous result of the German mathematician Carl Gustav Jacobi (1804-1851), who had shown that in a curvilinear coordinate system, the volume element is given by

$$dV = \left| \frac{\partial x^i}{\partial X^\mu} \right| dX^1 dX^2 \cdots dX^d \tag{16.22}$$

where $|\partial x^i / \partial X^\mu|$ is the determinant of the $d \times d$ square matrix of transformation coefficients from Cartesian coordinates to curvilinear coordinates. This determinant is called the *Jacobian* of the transformation. From the relationship

$$G_{\mu,\nu} = \frac{\partial x^i}{\partial X^\mu} \delta_{ij} \frac{\partial x^j}{\partial X^\nu} \tag{16.23}$$

one can show that the Jacobian

$$\sqrt{|G_{\mu\nu}|} \equiv \left|\frac{\partial x^i}{\partial X^\mu}\right| \equiv \sqrt{|G|} \tag{16.24}$$

is the square root of the determinant of the covariant metric tensor. The Jacobian is usually represented by the symbol $\sqrt{|G|}$. Levi-Civita's book *Absolute Differential Calculus* has been translated into many languages. It is still in print, and it remains one of the best textbooks in the field, along with Schrödinger's *Space-Time Structure*, Brillouin's *Les Tenseurs* and Landau and Lifshitz's *The Classical Theory of Fields*.

The Jacobian, $\sqrt{|G|}$, is the prototype of a *scalar density*. We can construct *tensor densities* by multiplying tensors by the Jacobian appropriate for the coordinate system. When a tensor density is transformed to another coordinate system, the Jacobian has to be recalculated from the transformed covariant metric tensor. *Tensor capacities* can be constructed by dividing tensors by the Jacobian. Now consider a scalar function ψ. Its gradient is a covariant vector, and therefore

$$G^{\mu\nu}\frac{\partial\psi}{\partial X^\mu}\frac{\partial\psi}{\partial X^\nu} = \text{scalar} \tag{16.25}$$

It follows that if we let

$$\mathcal{L} = \sqrt{|G|}\left[G^{\mu\nu}\frac{\partial\psi}{\partial X^\mu}\frac{\partial\psi}{\partial X^\nu} + \kappa\psi^2\right] \tag{16.26}$$

where κ is a constant, then the variational principle

$$\delta\int\int\cdots\int \mathcal{L}\; dX^1 dX^2\cdots dX^d = 0 \tag{16.27}$$

will be invariant under a curvilinear coordinate transformation. As we saw above, the Euler-Lagrange equations that follow from this variational principle are

$$\frac{\partial}{\partial X^\mu}\frac{\partial\mathcal{L}}{\partial\left(\partial\psi/\partial X^\mu\right)} - \frac{\partial\mathcal{L}}{\partial\psi} = 0 \tag{16.28}$$

With the Lagrangian density of equation (16.26), this becomes

$$\frac{1}{\sqrt{|G|}}\frac{\partial}{\partial X^\mu}\sqrt{|G|}\; G^{\mu\nu}\frac{\partial\psi}{\partial X^\nu} = \kappa\;\psi \tag{16.29}$$

16.5 The Laplace-Beltrami operator

The operator

$$\Delta = \sum_{\mu=1}^{d}\sum_{\nu=1}^{d}\frac{1}{\sqrt{|G|}}\frac{\partial}{\partial X^\mu}\sqrt{|G|}\; G^{\mu\nu}\frac{\partial}{\partial X^\nu} \tag{16.30}$$

is the generalized Laplacian operator, which plays such an important role in the theory of hyperspherical harmonics, but here it is written in a form due to Eugenio Beltrami (1835-1899), which is invariant under coordinate transformations. (In equation (16.29), we have abandoned the Einstein convention, and have re-introduced explicit sums.) To illustrate this equation, let us consider some examples. In a d-dimensional space, we can let

$$\begin{aligned}
x^1 &= r\ \sin\theta_1 \sin\theta_2 ... \sin\theta_{d-2} \cos\theta_{d-1} \\
x^2 &= r\ \sin\theta_1 \sin\theta_2 ... \sin\theta_{d-2} \sin\theta_{d-1} \\
x^3 &= r\ \sin\theta_1 \sin\theta_2 ... \cos\theta_{d-2} \\
\vdots\ &\ \vdots\ \ \vdots \\
x^{d-1} &= r\ \sin\theta_1 \cos\theta_2 \\
x^d &= r\ \cos\theta_1
\end{aligned} \tag{16.31}$$

while

$$\begin{aligned}
X^1 &= r \\
X^2 &= \theta_1 \\
X^3 &= \theta_2 \\
\vdots\ &\ \vdots\ \ \vdots \\
X^{d-1} &= \theta_{d-2} \\
X^d &= \theta_{d-1}
\end{aligned} \tag{16.32}$$

Then the Jacobians for various values of d are

$$\begin{array}{lrcl}
d=3 & \sqrt{|G|} &=& r^2 \sin\theta_1 \\
d=4 & \sqrt{|G|} &=& r^3 \sin^2\theta_1 \sin\theta_2 \\
d=5 & \sqrt{|G|} &=& r^4 \sin^3\theta_1 \sin^2\theta_2 \sin\theta_3 \\
d=6 & \sqrt{|G|} &=& r^5 \sin^4\theta_1 \sin^3\theta_2 \sin^2\theta_3 \sin\theta_4 \\
 & \vdots &\vdots& \qquad\vdots \\
d=d & \sqrt{|G|} &=& r^{d-1} \sin^{d-2}\theta_1 \sin^{d-3}\theta_2 ... \sin^2\theta_{d-3} \sin\theta_{d-2}
\end{array} \tag{16.33}$$

The covariant metric tensor for $d=3$ is

$$G_{\mu,\nu} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & r^2 \sin^2\theta_1 \end{pmatrix} \tag{16.34}$$

while for $d=4$

$$G_{\mu,\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & r^2 & 0 & 0 \\ 0 & 0 & r^2 \sin^2\theta_1 & 0 \\ 0 & 0 & 0 & r^2 \sin^2\theta_1 \sin^2\theta_2 \end{pmatrix} \tag{16.35}$$

and so on. Combining these results, we obtain the Laplace-Beltrami operators:

$$\begin{aligned}
&\sum_{\nu} G^{\mu,\nu}\frac{\partial}{\partial X^{\nu}} \\
= &\left(\frac{\partial}{\partial r}, \frac{1}{r^2}\frac{\partial}{\partial \theta_1}, \frac{1}{r^2\sin^2\theta_1}\frac{\partial}{\partial \theta_2}, \frac{1}{r^2\sin^2\theta_1\sin^2\theta_2}\frac{\partial}{\partial \theta_3}, \ldots\right)
\end{aligned} \tag{16.36}$$

For $d = 3$,

$$\begin{aligned}
&\sum_{\nu=1}^{3}\sqrt{|G|}\; G^{\mu,\nu}\frac{\partial}{\partial X^{\nu}} \\
= \; & r^2\sin\theta_1\left(\frac{\partial}{\partial r}, \frac{1}{r^2}\frac{\partial}{\partial \theta_1}, \frac{1}{r^2\sin^2\theta_1}\frac{\partial}{\partial \theta_2}\right)
\end{aligned} \tag{16.37}$$

$$\begin{aligned}
&\sum_{\mu=1}^{3}\sum_{\nu=1}^{3}\frac{1}{\sqrt{|G|}}\frac{\partial}{\partial X^{\mu}}\sqrt{|G|}\; G^{\mu,\nu}\frac{\partial}{\partial X^{\nu}} \\
= \; & \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2\sin\theta_1}\frac{\partial}{\partial \theta_1}\sin\theta_1\frac{\partial}{\partial \theta_1} + \frac{1}{r^2\sin^2\theta_1}\frac{\partial^2}{\partial \theta_2^2}
\end{aligned} \tag{16.38}$$

For $d = 4$,

$$\begin{aligned}
&\sum_{\nu=1}^{4}\sqrt{|G|}\; G^{\mu,\nu}\frac{\partial}{\partial X^{\nu}} \\
= \; & r^3\sin^2\theta_1\sin\theta_2\left(\frac{\partial}{\partial r}, \frac{1}{r^2}\frac{\partial}{\partial \theta_1}, \frac{1}{r^2\sin^2\theta_1}\frac{\partial}{\partial \theta_2}, \frac{1}{r^2\sin^2\theta_1\sin^2\theta_2}\frac{\partial}{\partial \theta_3}\right)
\end{aligned} \tag{16.39}$$

$$\begin{aligned}
&\sum_{\mu=1}^{4}\sum_{\nu=1}^{4}\frac{1}{\sqrt{|G|}}\frac{\partial}{\partial X^{\mu}}\sqrt{|G|}\; G^{\mu,\nu}\frac{\partial}{\partial X^{\nu}} \\
= \; & \frac{1}{r^3}\frac{\partial}{\partial r}r^3\frac{\partial}{\partial r} + \frac{1}{r^2\sin^2\theta_1}\frac{\partial}{\partial \theta_1}\sin^2\theta_1\frac{\partial}{\partial \theta_1} \\
+ \; & \frac{1}{r^2\sin^2\theta_1\sin\theta_2}\frac{\partial}{\partial \theta_2}\sin\theta_2\frac{\partial}{\partial \theta_2} + \frac{1}{r^2\sin^2\theta_1\sin^2\theta_2}\frac{\partial^2}{\partial \theta_3^2}
\end{aligned} \tag{16.40}$$

For general values of d,

$$\begin{aligned}
&\sum_{\nu=1}^{d}\sqrt{|G|}\; G^{\mu,\nu}\frac{\partial}{\partial X^{\nu}} \\
= \; & r^{d-1}\sin^{d-2}\theta_1\sin^{d-3}\theta_2\cdots\sin\theta_{d-2} \\
\times \; & \left(\frac{\partial}{\partial r}, \frac{1}{r^2}\frac{\partial}{\partial \theta_1}, \frac{1}{r^2\sin^2\theta_1}\frac{\partial}{\partial \theta_2}, \ldots, \frac{1}{r^2\sin^2\theta_1\sin^2\theta_2\cdots\sin^2\theta_{d-2}}\frac{\partial}{\partial \theta_{d-1}}\right)
\end{aligned} \tag{16.41}$$

$$
\begin{aligned}
&\sum_{\mu=1}^{d}\sum_{\nu=1}^{d}\frac{1}{\sqrt{|G|}}\frac{\partial}{\partial X^\mu}\sqrt{|G|}\;G^{\mu,\nu}\frac{\partial}{\partial X^\nu} \\
= \quad & \frac{1}{r^{d-1}}\frac{\partial}{\partial r}r^{d-1}\frac{\partial}{\partial r}+\frac{1}{r^2\sin^{d-2}\theta_1}\frac{\partial}{\partial\theta_1}\sin^{d-2}\theta_1\frac{\partial}{\partial\theta_1} \\
+ \quad & \frac{1}{r^2\sin^2\theta_1\sin^{d-3}\theta_2}\frac{\partial}{\partial\theta_2}\sin^{d-3}\theta_2\frac{\partial}{\partial\theta_2}+\cdots \\
+ \quad & \frac{1}{r^2\sin^2\theta_1\sin^2\theta_2\sin^2\theta_3\cdots\sin\theta_{d-2}}\frac{\partial}{\partial\theta_{d-2}}\sin\theta_{d-2}\frac{\partial}{\partial\theta_{d-2}} \\
+ \quad & \frac{1}{r^2\sin^2\theta_1\sin^2\theta_2\cdots\sin^2\theta_{d-2}}\frac{\partial^2}{\partial\theta_{d-1}^2}
\end{aligned}
\tag{16.42}
$$

As we saw in equation (**??**), the Laplace-Beltrami operator in hyperspherical coordinates can be written as

$$
\Delta=\frac{1}{r^{d-1}}\frac{\partial}{\partial r}r^{d-1}\frac{\partial}{\partial r}-\frac{\Lambda^2}{r^2}
\tag{16.43}
$$

where r is the hyperradius and where Λ^2 is the generalized angular momentum operator. Comparing this with the results that we have just been discussing, we can see that for $d=3$,

$$
-\Lambda^2=\frac{1}{\sin\theta_1}\frac{\partial}{\partial\theta_1}\sin\theta_1\frac{\partial}{\partial\theta_1}+\frac{1}{\sin^2\theta_1}\frac{\partial^2}{\partial\theta_2^2}
\tag{16.44}
$$

while for $d=4$,

$$
\begin{aligned}
-\Lambda^2 \quad = \quad & \frac{1}{\sin^2\theta_1}\frac{\partial}{\partial\theta_1}\sin^2\theta_1\frac{\partial}{\partial\theta_1} \\
+ \quad & \frac{1}{\sin^2\theta_1\sin\theta_2}\frac{\partial}{\partial\theta_2}\sin\theta_2\frac{\partial}{\partial\theta_2}+\frac{1}{\sin^2\theta_1\sin^2\theta_2}\frac{\partial^2}{\partial\theta_3^2}
\end{aligned}
\tag{16.45}
$$

and for $d=5$,

$$
\begin{aligned}
-\Lambda^2 \quad = \quad & \frac{1}{\sin^3\theta_1}\frac{\partial}{\partial\theta_1}\sin^3\theta_1\frac{\partial}{\partial\theta_1}+\frac{1}{\sin^2\theta_1\sin^2\theta_2}\frac{\partial}{\partial\theta_2}\sin^2\theta_2\frac{\partial}{\partial\theta_2} \\
+ \quad & \frac{1}{\sin^2\theta_1\sin^2\theta_2\sin\theta_3}\frac{\partial}{\partial\theta_3}\sin\theta_3\frac{\partial}{\partial\theta_3}+\frac{1}{\sin^2\theta_1\sin^2\theta_2\sin^2\theta_3}\frac{\partial^2}{\partial\theta_4^2}
\end{aligned}
\tag{16.46}
$$

For general values of d, we have

$$
\begin{aligned}
-\Lambda^2 \quad = \quad & \frac{1}{\sin^{d-2}\theta_1}\frac{\partial}{\partial\theta_1}\sin^{d-2}\theta_1\frac{\partial}{\partial\theta_1} \\
+ \quad & \frac{1}{\sin^2\theta_1\sin^{d-3}\theta_2}\frac{\partial}{\partial\theta_2}\sin^{d-3}\theta_2\frac{\partial}{\partial\theta_2}+\cdots \\
+ \quad & \frac{1}{\sin^2\theta_1\sin^2\theta_2\sin^2\theta_3\cdots\sin\theta_{d-2}}\frac{\partial}{\partial\theta_{d-2}}\sin\theta_{d-2}\frac{\partial}{\partial\theta_{d-2}} \\
+ \quad & \frac{1}{\sin^2\theta_1\sin^2\theta_2\cdots\sin^2\theta_{d-2}}\frac{\partial^2}{\partial\theta_{d-1}^2}
\end{aligned}
\tag{16.47}
$$

We have until now been considering spaces that are intrinsically flat, but a d-dimensional hyperspherical surface embedded in a $d+1$-dimensional space has intrinsic curvature. If the hyperradius r is regarded as a constant, then the Laplace-Beltrami operator for such a surface is given by

$$\Delta = -\frac{\Lambda^2}{r^2} \tag{16.48}$$

while the covariant metric tensor on the surface is

$$G_{\mu,\nu} = \begin{pmatrix} r^2 & 0 & 0 & 0 & \cdots \\ 0 & r^2 \sin^2\theta_1 & 0 & 0 & \cdots \\ 0 & 0 & r^2\sin^2\theta_1 \sin^2\theta_2 & 0 & \cdots \\ 0 & 0 & 0 & r^2 \sin^2\theta_1 \sin^2\theta_2 \sin^2\theta_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \tag{16.49}$$

The infinitesimal element of length on the surface, ds is given by

$$\begin{aligned} ds^2 &= \sum_{\mu=1}^{d}\sum_{\nu=1}^{d} G_{\mu,\nu} dX^\mu dX^\nu \\ &= r^2\left(d\theta_1^2 + \sin^2\theta_1 d\theta_2^2 + \sin^2\theta_1 \sin^2\theta_2 d\theta_3^2 + \cdots\right) \end{aligned} \tag{16.50}$$

16.6 Geodesics

In the geometry of curved spaces, *geodesics* play the role that straight lines play in Euclidean geometry. The geodesic curves are local minima of path length. The *minimal geodesics* between two points are the shortest paths through the curved space, and play an important role when analyzing physical systems in curved space. They can be determined by the variational principle

$$\begin{aligned} s &= \int ds = \int \sqrt{\sum_{\mu=1}^{d}\sum_{\nu=1}^{d} G_{\mu,\nu}\frac{dX^\mu}{ds}\frac{dX^\nu}{ds}}\; ds \\ &= \int \sum_{\mu=1}^{d}\sum_{\nu=1}^{d} G_{\mu,\nu}\frac{dX^\mu}{ds}\frac{dX^\nu}{ds}\; ds = \text{minimum} \end{aligned} \tag{16.51}$$

The Euler-Lagrange equations which follow from this variational principle are

$$\frac{d}{ds}\frac{\partial L}{\partial(dX^\mu/ds)} - \frac{\partial L}{\partial X^\mu} = 0 \qquad \mu = 1, 2, \cdots, d \tag{16.52}$$

with

$$L = \sum_{\mu=1}^{d}\sum_{\nu=1}^{d} G_{\mu,\nu}(\mathbf{X})\frac{dX^\mu}{ds}\frac{dX^\nu}{ds} \tag{16.53}$$

The Euler-Lagrange equations for geodesics can be written in the form

$$\frac{d^2X^\sigma}{ds} = \Gamma^\sigma_{\mu\nu}\frac{dX^\mu}{ds}\frac{dX^\sigma}{ds} \tag{16.54}$$

Here $\Gamma^\sigma_{\mu\nu}$ is a Christoffel symbol, which is related to the metric tensors by

$$\Gamma^\sigma_{\mu\nu} = \frac{1}{2}G^{\sigma\rho}\left(\frac{\partial G_{\rho\mu}}{\partial X^\nu} + \frac{\partial G_{\rho\nu}}{\partial X^\mu} - \frac{\partial G_{\mu\nu}}{\partial X^\rho}\right) \tag{16.55}$$

In general relativity theory, the trajectories of particles are geodesics in a space-time continuum, whose metric is affected by the presence of other masses.

16.7 Einstein's letter to Freud: Why war?

Because of his fame, Einstein was asked to make several speeches at the Reichstag. and in all these speeches he condemned violence and nationalism, urging that these be replaced by and international cooperation and law under an effective international authority. He also wrote many letters and articles pleading for peace and for the renunciation of militarism and violence.

Einstein believed that the production of armaments is damaging, not only economically, but also spiritually. In 1930 he signed a manifesto for world disarmament sponsored by the Womens International League for Peace and Freedom. In December of the same year, he made his famous statement in New York that if two percent of those called for military service were to refuse to fight, governments would become powerless, since they could not imprison that many people. He also argued strongly against compulsory military service and urged that conscientious objectors should be protected by the international community. He argued that peace, freedom of individuals, and security of societies could only be achieved through disarmament, the alternative being "slavery of the individual and annihilation of civilization".

In letters, and articles, Einstein wrote that the welfare of humanity as a whole must take precedence over the goals of individual nations, and that we cannot wait until leaders give up their preparations for war. Civil society, and especially public figures, must take the lead. He asked how decent and self-respecting people can wage war, knowing how many innocent people will be killed.

In 1931, the International Institute for Intellectual Cooperation invited Albert Einstein to enter correspondence with a prominent person of his own choosing on a subject of importance to society. The Institute planned to publish a collection of such dialogues. Einstein accepted at once, and decided to write to Sigmund Freud to ask his opinion about how humanity could free itself from the curse of war. A translation from German of part of the long letter that he wrote to Freud is as follows:

"Dear Professor Freud, The proposal of the League of Nations and its International Institute of Intellectual Cooperation at Paris that I should invite a person to be chosen by myself to a frank exchange of views on any problem that I might select affords me a very

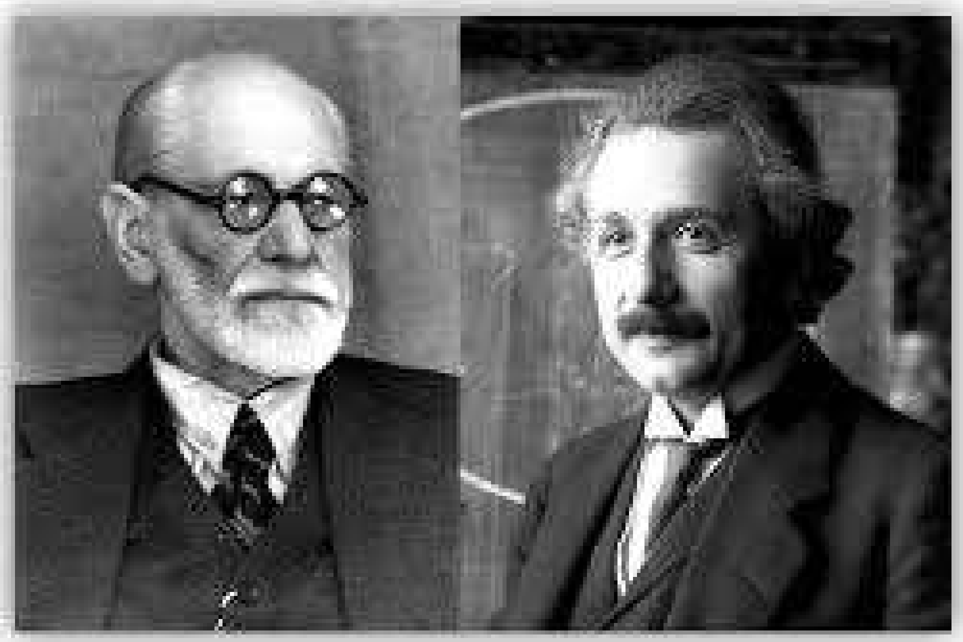

Figure 16.11: **Sigmund Freud and Albert Einstein (public domain). Their exchange of letters entitled "Why War?" deserves to be read by everyone concerned with the human future.**

welcome opportunity of conferring with you upon a question which, as things are now, seems the most important and insistent of all problems civilization has to face. This is the problem: Is there any way of delivering mankind from the menace of war? It is common knowledge that, with the advance of modern science, this issue has come to mean a matter of life or death to civilization as we know it; nevertheless, for all the zeal displayed, every attempt at its solution has ended in a lamentable breakdown."

"I believe, moreover, that those whose duty it is to tackle the problem professionally and practically are growing only too aware of their impotence to deal with it, and have now a very lively desire to learn the views of men who, absorbed in the pursuit of science, can see world-problems in the perspective distance lends. As for me, the normal objective of my thoughts affords no insight into the dark places of human will and feeling. Thus in the enquiry now proposed, I can do little more than seek to clarify the question at issue and, clearing the ground of the more obvious solutions, enable you to bring the light of your far-reaching knowledge of man's instinctive life upon the problem.."

"As one immune from nationalist bias, I personally see a simple way of dealing with the superficial (i.e. administrative) aspect of the problem: the setting up, by international consent, of a legislative and judicial body to settle every conflict arising between nations... But here, at the outset, I come up against a difficulty; a tribunal is a human institution which, in proportion as the power at its disposal is... prone to suffer these to be deflected by extrajudicial pressure..."

Freud replied with a long and thoughtful letter in which he said that a tendency towards conflict is an intrinsic part of human emotional nature, but that emotions can be overridden by rationality, and that rational behavior is the only hope for humankind.

16.8 The fateful letter to Roosevelt

Albert Einstein's famous relativistic formula, relating energy to mass, soon yielded an understanding of the enormous amounts of energy released in radioactive decay. Marie and Pierre Curie had noticed that radium maintains itself at a temperature higher than its surroundings. Their measurements and calculations showed that a gram of radium produces roughly 100 gram-calories of heat per hour. This did not seem like much energy until Rutherford found that radium has a half-life of about 1,000 years. In other words, after a thousand years, a gram of radium will still be producing heat, its radioactivity only reduced to one-half its original value. During a thousand years, a gram of radium produces about a million kilocalories, an enormous amount of energy in relation to the tiny size of its source! Where did this huge amount of energy come from? Conservation of energy was one of the most basic principles of physics. Would it have to be abandoned?

The source of the almost-unbelievable amounts of energy released in radioactive decay could be understood through Einstein's formula equating the energy of a system to its mass multiplied by the square of the velocity of light, and through accurate measurements of atomic weights. Einstein's formula asserted that mass and energy are equivalent. It was realized that in radioactive decay, neither mass nor energy is conserved, but only a quantity more general than both, of which mass and energy are particular forms. Scientists in several parts of the world realized that Einstein's discovery of the relationship between mass and energy, together with the discovery of fission of the heavy element uranium meant that it might be possible to construct a uranium-fission bomb of immense power.

Meanwhile night was falling on Europe. In 1929, an economic depression had begun in the United States and had spread to Europe. Without the influx of American capital, the postwar reconstruction of the German economy collapsed. The German middle class, which had been dealt a severe blow by the great inflation of 1923, now received a second heavy blow. The desperate economic chaos drove German voters into the hands of political extremists.

On January 30, 1933, Adolf Hitler was appointed Chancellor and leader of a coalition cabinet by President Hindenburg. Although Hitler was appointed legally to this post, he quickly consolidated his power by unconstitutional means: On May 2, Hitler's police seized the headquarters of all trade unions, and arrested labor leaders. The Communist and Socialist parties were also banned, their assets seized and their leaders arrested. Other political parties were also smashed. Acts were passed eliminating Jews from public service; and innocent Jewish citizens were boycotted, beaten and arrested. On March 11, 1938, Nazi troops entered Austria.

On March 16, 1939, the Italian physicist Enrico Fermi (who by then was a refugee in America) went to Washington to inform the Office of Naval Operations that it might be possible to construct an atomic bomb; and on the same day, German troops poured into Czechoslovakia.

A few days later, a meeting of six German atomic physicists was held in Berlin to discuss the applications of uranium fission. Otto Hahn, the discoverer of fission, was not present, since it was known that he was opposed to the Nazi regime. He was even said to have exclaimed: "I only hope that you physicists will never construct a uranium bomb! If Hitler ever gets a weapon like that, I'll commit suicide."

The meeting of German atomic physicists was supposed to be secret; but one of the participants reported what had been said to Dr. S. Flügge, who wrote an article about uranium fission and about the possibility of a chain reaction. Flügge's article appeared in the July issue of Naturwissenschaften, and a popular version in the Deutsche Allgemeine Zeitung. These articles greatly increased the alarm of American atomic scientists, who reasoned that if the Nazis permitted so much to be printed, they must be far advanced on the road to building an atomic bomb.

In the summer of 1939, while Hitler was preparing to invade Poland, alarming news reached the physicists in the United States: A second meeting of German atomic scientists had been held in Berlin, this time under the auspices of the Research Division of the German Army Weapons Department. Furthermore, Germany had stopped the sale of uranium from mines in Czechoslovakia.

The world's most abundant supply of uranium, however, was not in Czechoslovakia, but in Belgian Congo. Leo Szilard, a refugee Hungarian physicist who had worked with Fermi to measure the number of neutrons produced in uranium fission, was deeply worried that the Nazis were about to construct atomic bombs; and it occurred to him that uranium from Belgian Congo should not be allowed to fall into their hands.

Szilard knew that his former teacher, Albert Einstein, was a personal friend of Elizabeth, the Belgian Queen Mother. Einstein had met Queen Elizabeth and King Albert of Belgium at the Solvay Conferences, and mutual love of music had cemented a friendship between them. When Hitler came to power in 1933, Einstein had moved to the Institute of Advanced Studies at Princeton; and Szilard decided to visit him there. Szilard reasoned that because of Einstein's great prestige, and because of his long-standing friendship with the Belgian Royal Family, he would be the proper person to warn the Belgians not to let their uranium fall into the hands of the Nazis. Einstein agreed to write to the Belgian king and queen.

On August 2, 1939, Szilard again visited Einstein, accompanied by Edward Teller and Eugene Wigner, who (like Szilard) were refugee Hungarian physicists. By this time, Szilard's plans had grown more ambitious; and he carried with him the draft of another letter, this time to the American President, Franklin D. Roosevelt. Einstein made a few corrections, and then signed the fateful letter, which reads (in part) as follows:

"Some recent work of E. Fermi and L. Szilard, which has been communicated to me in manuscript, leads me to expect that the element uranium may be turned into an important source of energy in the immediate future. Certain aspects of the situation seem to call for watchfulness and, if necessary, quick action on the part of the Administration. I believe, therefore, that it is my duty to bring to your attention the following.."

"It is conceivable that extremely powerful bombs of a new type may be constructed. A single bomb of this type, carried by boat and exploded a port, might very well destroy the whole port, together with some of the surrounding territory.."

The letter also called Roosevelt's attention to the fact that Germany had already stopped the export of uranium from the Czech mines under German control. After making a few corrections, Einstein signed it. On October 11, 1939, three weeks after the defeat of Poland, Roosevelt's economic adviser, Alexander Sachs, personally delivered the letter to the President. After discussing it with Sachs, the President commented,"This calls for action." Later, when atomic bombs were dropped on civilian populations in an already virtually-defeated Japan, Einstein bitterly regretted having signed Szilard's letter to Roosevelt. He said repeatedly that signing the letter was the greatest mistake of his life, and his remorse was extreme.

Throughout the remainder of his life, in addition to his scientific work, Einstein worked tirelessly for peace, international understanding and nuclear disarmament. His last public act, only a few days before his death in 1955, was to sign the Russell-Einstein Manifesto, warning humankind of the catastrophic consequences that would follow from a war with nuclear weapons.

A few more things that Einstein said about peace:

We cannot solve our problems with the same thinking that we used when we created them.

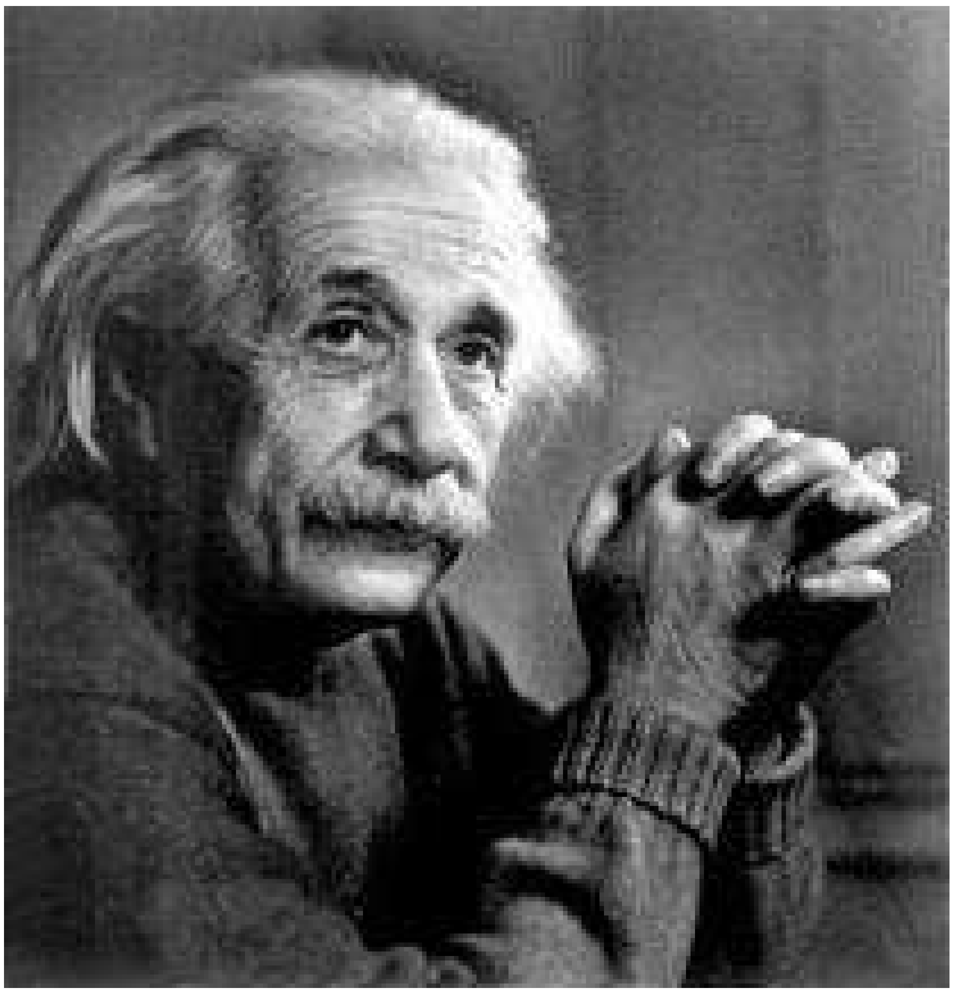

Figure 16.12: **Signing the Russell-Einstein declaration was the last public act of Einstein's life.**

It has become appallingly obvious that our technology has exceeded our humanity.

Peace cannot be kept by force; it can only be achieved by understanding.

The world is a dangerous place to live; not because of the people who are evil, but because of the people who don't do anything about it.

Insanity: doing the same thing over and over again and expecting to get different results.

Nothing will end war unless the people themselves refuse to go to war.

Past thinking and methods did not prevent world wars. Future thinking must prevent war.

You cannot simultaneously prevent and prepare for war.

Never do anything against conscience, even if the state demands it.

Taken as a whole, I would believe that Gandhi's views were the most enlightened of all political men of our time.

Without ethical culture, there is no salvation for humanity.

War seems to me to be a mean, contemptible thing: I would rather be hacked in pieces than take part in such an abominable business. And yet so high, in spite of everything, is my opinion of the human race that I believe this bogey would have disappeared long ago, had the sound sense of the nations not been systematically corrupted by commercial and political interests acting through the schools and the Press.

16.9 The Russell-Einstein Manifesto

In March, 1954, the US tested a hydrogen bomb at the Bikini Atoll in the Pacific Ocean. It was 1000 times more powerful than the Hiroshima bomb. The Japanese fishing boat, Lucky Dragon, was 130 kilometers from the Bikini explosion, but radioactive fallout from the test killed one crew member and made all the others seriously ill.

In England, Prof. Joseph Rotblat, a Polish scientist who had resigned from the Manhattan Project for for moral reasons when it became clear that Germany would not develop nuclear weapons, was asked to appear on a BBC program to discuss the Bikini test. He

Figure 16.13: **Joseph Rotblat believed that the Bikini bomb was of a fission-fusion-fission type. Besides producing large amounts of fallout, such a bomb can be made enormously powerful at very little expense.**

was asked to discuss the technical aspects of H-bombs, while the Archbishop of Canterbury and the philosopher Lord Bertrand Russell were asked to discuss the moral aspects.

Rotblat had became convinced that the Bikini bomb must have involved a third stage, where fast neutrons from the hydrogen thermonuclear reaction produced fission in a casing of ordinary uranium. Such a bomb would produce enormous amounts of highly dangerous radioactive fallout, and Rotblat became extremely worried about the possibly fatal effect on all living things if large numbers of such bombs were ever used in a war. He confided his worries to Bertrand Russell, whom he had met on the BBC program.

After discussing the Bikini test and its radioactive fallout with Joseph Rotblat, Lord Russell became concerned for the future of the human gene pool if large numbers of such bombs should ever be used in a war. After consultations with Albert Einstein and others, he drafted a document warning of the grave dangers presented by fission-fusion-fission bombs. On July 9, 1955, with Rotblat in the chair, Russell read the Manifesto to a packed press conference.

The document contains the words: **"Here then is the problem that we present to you, stark and dreadful and inescapable: Shall we put an end to the human**

Figure 16.14: **Lord Russell devoted much of the remainder of his life to working for the abolition of nuclear weapons. Here he is seen in 1962 in Trafalgar Square, London, addressing a meeting of the Campaign for Nuclear Disarmament.**

race, or shall mankind renounce war?... There lies before us, if we choose, continual progress in happiness, knowledge and wisdom. Shall we, instead, choose death because we cannot forget our quarrels? We appeal as human beings to human beings: Remember your humanity, and forget the rest. If you can do so, the way lies open to a new Paradise; if you cannot, there lies before you the risk of universal death."

In 1945, with the horrors of World War II fresh in everyone's minds, the United Nations had been established with the purpose of eliminating war. A decade later, the Russell-Einstein Manifesto reminded the world that war *must* be abolished as an institution because of the constantly increasing and potentially catastrophic power of modern weapons.

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Chapter 17

ERWIN SCHRÖDINGER

17.1 A wave equation for matter

In 1926, the difficulties surrounding the "old quantum theory" of Max Planck, Albert Einstein and Niels Bohr were suddenly solved, and its true meaning was understood. Two years earlier, a French aristocrat, Louis de Broglie, writing his doctoral dissertation at the Sorbonne in Paris, had proposed that very small particles, such as electrons, might exhibit wavelike properties. The ground state and higher excited states of the electron in Bohr's model of the hydrogen atom would then be closely analogous to the fundamental tone and higher overtones of a violin string.

Almost the only person to take de Broglie's proposal seriously was Albert Einstein, who mentioned it in one of his papers. Because of Einstein's interest, de Broglie's matter-waves came to the attention of other physicists. The Austrian theoretician, Erwin Schrödinger, working at Zürich, searched for the underlying wave equation which de Broglie's matter-waves obeyed.

Schrödinger's gifts as a mathematician were so great that it did not take him long to solve the problem. The Schrödinger wave equation for matter is now considered to be more basic than Newton's equations of motion. The wavelike properties of matter are not apparent to us in our daily lives because the wave-lengths are extremely small in comparison with the sizes of objects which we can perceive. However, for very small and light particles, such as electrons moving in their orbits around the nucleus of an atom, the wavelike behavior becomes important.

Schrödinger was able to show that Niels Bohr's atomic theory, including Bohr's seemingly arbitrary quantization of angular momentum, can be derived by solving the wave equation for the electrons moving in the attractive field of the nucleus. The allowed orbits of Bohr's theory correspond in Schrödinger's theory to harmonics, similar to the fundamental harmonic and higher overtones of an organ pipe or a violin string. (If Pythagoras had been living in 1926, he would have rejoiced to see the deepest mysteries of matter explained in terms of harmonics!)

Bohr himself believed that a complete atomic theory ought to be able to explain the

Figure 17.1: **Bust of Erwin Schrödinger in the courtyard arcade of the main building, University of Vienna.**

chemical properties of the elements in Mendeléev's periodic system. Bohr's 1913 theory failed to pass this test, but the new de Broglie-Schrödinger theory succeeded! Through the work of Pauli, Heitler, London, Slater, Pauling, Hund, Mulliken, Hückel and others, who applied Schrödinger's wave equation to the solution of chemical problems, it became apparent that the wave equation could indeed (in principle) explain all the chemical properties of matter.

Strangely, the problem of developing the fundamental quantum theory of matter was solved not once, but three times in 1926! At the University of Göttingen in Germany, Max Born (1882-1970) and his brilliant young students Werner Heisenberg and Pascal Jordan solved the problem in a completely different way, using matrix methods. At the same time, a theory similar to the "matrix mechanics" of Heisenberg, Born and Jordan was developed independently at Cambridge University by a 24 year old mathematical genius named Paul Adrian Maurice Dirac. At first, the Heisenberg-Born-Jordan-Dirac quantum theory seemed to be completely different from the Schrödinger theory; but soon the Göttingen mathematician David Hilbert (1862-1943) was able to show that the theories were really identical, although very differently expressed.

17.2 Felix Bloch's story about Schrödinger

There is an interesting story about Erwin Schrödinger's derivation of his famous wave equation. According to the solid state physicist Felix Bloch, Peter Debye was chairing a symposium in Zürich, Switzerland, at which de Broglie's waves were being discussed. At one point during the symposium, Debye said: "Well, if there are waves associated with every particle, there must be a wave equation." Then, turning to Schrödinger, he said: "You, Erwin. You're not doing anything important at the moment. Why don't you find the wave equation obeyed by de Broglie's waves?"

During the following weekend, the whole group started off for a skiing trip. "Come with us, Erwin!", they said, but Schrödinger replied: "No, forgive me, I think I will stay here and work." By the end of the weekend he had derived his famous non-relativistic wave equation. He had first tried a relativistic equation (now known as the Klein-Gordon equation), but had rejected it because he believed that the equation had to be first-order in time.

Later, Felix Bloch asked Peter Debye, "Aren't you sorry that you didn't derive the wave equation yourself, instead of giving the job to Schrödinger?" Debye replied wistfully, "At least I was right about the need for a wave equation, wasn't I?"

Schrödinger's non-relativistic wave equation

The non-relativistic relationship between energy and momentum is given by

$$E = c\sqrt{p^2 + m^2c^2} + V \approx \frac{p^2}{2m} + V \qquad m^2c^2 >> p^2 \tag{17.1}$$

Schrödinger's non-relativistic wave equation,

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = E\psi \tag{17.2}$$

can be derived by making the substitutions

$$p_j \quad \rightarrow \quad \frac{\hbar}{i}\frac{\partial}{\partial x_j} \qquad j = 1, 2, 3 \tag{17.3}$$

If the wave function ψ has time-dependence of the form

$$\psi(\mathbf{x}, t) = \psi(\mathbf{x})e^{iEt/\hbar} \tag{17.4}$$

then we can write

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi \tag{17.5}$$

where

$$H \equiv \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right) \tag{17.6}$$

17.3 Separation of the equation

The Schrödinger equation for hydrogenlike (1-electron) atoms is

$$\left(-\frac{\hbar^2}{2m_e}\nabla^2 - \frac{e^2 Z^2}{r}\right)\psi(\mathbf{x}) = E\psi(\mathbf{x}) \tag{17.7}$$

If we let

$$\psi(\mathbf{x}) = R(r)Y_{l,m}(\theta, \varphi) \tag{17.8}$$

the Schrödinger equation for hydrogenlike (one electron) atoms is separable:

$$\nabla^2 R(r)Y_{l,m}(\theta, \varphi) \quad = \quad \left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right)R(r)Y_{l,m}(\theta, \varphi) \tag{17.9}$$

Dividing both sides by $Y_{l,m}(\theta, \varphi)$, we find that the radial part of the Schrödinger equation for one-electron atoms must obey the equation

$$\left(-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{e^2 Z^2}{r} + \frac{l(l+1)}{r^2}\right)R(r) = ER(r) \tag{17.10}$$

where we have made use of the relationship

$$\nabla^2 Y_{l,m}(\theta, \varphi) = -\frac{l(l+1)}{r^2}Y_{l,m}(\theta, \varphi) \tag{17.11}$$

and where we have replaced partial derivatives in the radial equation by ordinary derivatives, since we now have a differential equation in a single variable.

17.4 Solutions to the radial equation

If we let

$$\rho \equiv Zr \tag{17.12}$$

and

$$\epsilon = \frac{2E}{Z^2} \tag{17.13}$$

then the radial equation becomes:

$$\left[\frac{1}{\rho^2}\frac{d}{d\rho}\rho^2\frac{d}{d\rho} - \frac{l(l+1)}{\rho^2} + \frac{2}{\rho} + \epsilon\right] R_{n,l}(\rho) = 0 \tag{17.14}$$

Equation (17.14) has solutions of the form

$$R_{n,l}(\rho) = N_{n,l}\ \rho^l\ e^{-\rho/(n)} F\ [\ l+1-n\ |\ 2l+2\ |\ 2\rho/n)\ ] \tag{17.15}$$

where

$$N_{n,l} = \frac{Z^{3/2}}{2(2l+1)!}\left(\frac{(l+n)!}{(n-1-l)!}\right)^{1/2}\left(\frac{2}{n}\right)^{l+2} \tag{17.16}$$

and where $F[a|b|x]$ is a confluent hypergeometric function:

$$F[a|b|x] \equiv 1 + \frac{ax}{b} + \frac{a(a+1)x^2}{b(b+1)2!} + \frac{a(a+1)(a+2)x^3}{b(b+1)(b+2)3!} + ... \tag{17.17}$$

The confluent hypergeometric series terminates and reduces to a polynomial when a is a negative integer. In our case this means that $l+1-n$ must be a negative integer, and thus, for the series to terminate, as is required for finiteness at large values of r, l cannot exceed $n-1$. A table of the first few radial wave functions for hydrogenlike atoms is shown below:

Table 17.1: Radial wave functions for hydrogenlike atoms

n	l	$R_{nl}(r)$
1	0	$e^{-Zr}Z^{3/2}$
2	0	$\frac{e^{-Zr/2}Z^{3/2}\left(1-\frac{Zr}{2}\right)}{\sqrt{2}}$
2	1	$\frac{e^{-Zr/2}Z^{3/2}Zr}{2\sqrt{6}}$
3	0	$\frac{2e^{-Zr/3}Z^{3/2}\left(\frac{(2Z)r^2}{27}-\frac{2Zr}{3}+1\right)}{3\sqrt{3}}$
3	1	$\frac{4}{27}\sqrt{\frac{2}{3}}e^{-Zr/3}Z^{3/2}\left(1-\frac{Zr}{6}\right)Zr$
3	2	$\frac{2}{81}\sqrt{\frac{2}{15}}e^{-Zr/3}Z^{3/2}(Zr)^2$

17.5 Fock's momentum-space treatment of hydrogen

In a brilliant 1935 paper, the Russian physicist V. Fock was able to show that a relationship exists between 4-dimensional hyperspherical harmonics and the solutions to the Fourier transformed Schrödinger for hydrogenlike (1-electron) atoms. In direct space, the Schrödinger equation (in atomic units) for an electron moving in the potential $V(\mathbf{x})$ is

$$\left[-\frac{1}{2}\nabla^2 + V(\mathbf{x})\right]\psi(\mathbf{x}) = E\psi(\mathbf{x}) \tag{17.18}$$

We can let

$$\psi(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}}\int d^3p\ e^{i\mathbf{p}\cdot\mathbf{x}}\psi^t(\mathbf{p}) \tag{17.19}$$

where

$$\psi^t(\mathbf{p}) = \frac{1}{(2\pi)^{3/2}}\int d^3x\ e^{-i\mathbf{p}\cdot\mathbf{x}}\psi(\mathbf{x}) \tag{17.20}$$

Substituting (17.19) into (17.18), we have

$$\frac{1}{(2\pi)^{3/2}}\int d^3p\ \left[\frac{p^2}{2} + V(\mathbf{x}) - E\right] e^{i\mathbf{p}\cdot\mathbf{x}}\psi^t(\mathbf{p}) = 0 \tag{17.21}$$

We now multiply on the left by $e^{-i\mathbf{p}'\cdot\mathbf{x}}$ and integrate over d^3x. This gives:

$$\left[\frac{p'^2}{2} - E\right]\psi^t(\mathbf{p}') = \frac{-1}{(2\pi)^{3/2}}\int d^3p\ V^t(\mathbf{p}'-\mathbf{p})\ \psi^t(\mathbf{p}) \tag{17.22}$$

which is the 1-particle Schrödinger equation in reciprocal space. For hydrogenlike atoms,

$$V(\mathbf{x}) = -\frac{Z}{r} \tag{17.23}$$

so that from (**??**),

$$V^t(\mathbf{p}) = -\sqrt{\frac{2}{\pi}}\frac{Z}{p^2} \tag{17.24}$$

Letting

$$-2E = k^2 \tag{17.25}$$

and combining (17.22), (17.23) and (17.24), we obtain

$$\left[p'^2 + k^2\right]\psi^t(\mathbf{p}') = \frac{Z}{\pi^2}\int d^3p\ \frac{1}{|\mathbf{p}'-\mathbf{p}|^2}\ \psi^t(\mathbf{p}) \tag{17.26}$$

Fock then made the transformation:

$$\begin{aligned} u_1 &= \frac{2kp_1}{k^2+p^2} \equiv \sin\chi\ \sin\theta\ \cos\varphi \\ u_2 &= \frac{2kp_2}{k^2+p^2} \equiv \sin\chi\ \sin\theta\ \sin\varphi \\ u_3 &= \frac{2kp_3}{k^2+p^2} \equiv \sin\chi\ \cos\theta \\ u_4 &= \frac{k^2-p^2}{k^2+p^2} \equiv \cos\chi \end{aligned} \tag{17.27}$$

Here θ and φ are the polar angles of the vector $\mathbf{p}$:

$$\begin{aligned} p_1 &= p\ \sin\theta\ \cos\varphi \\ p_2 &= p\ \sin\theta\ \sin\varphi \\ p_3 &= p\ \cos\theta \end{aligned} \tag{17.28}$$

while

$$\chi \equiv \cos^{-1}\left(\frac{k^2-p^2}{k^2+p^2}\right) = \sin^{-1}\left(\frac{2kp}{k^2+p^2}\right) \tag{17.29}$$

is an angle introduced by Fock in order to transform the integral d^3p into an integral over solid angle in a 4-dimensional space. Fock's transformation maps the 3-dimensional p-space onto the surface of a unit sphere in a 4-dimensional space. It is easy to verify from (17.27) that

$$u_1^2 + u_2^2 + u_3^2 + u_4^2 = 1 \tag{17.30}$$

From the Jacobian of the transformation from Cartesian coordinates to 4-dimensional hyperspherical coordinates, one finds that the element of solid angle in the 4-dimensional space is given by

$$\begin{aligned} d\Omega &= \sin^2\chi\ \sin\theta\ d\chi d\theta d\varphi \\ &= \left(\frac{2kp}{k^2+p^2}\right)^2 \sin\theta\ d\chi d\theta d\varphi \end{aligned} \tag{17.31}$$

Comparing this with

$$d^3p = p^2 dp\ \sin\theta\ d\theta d\varphi \tag{17.32}$$

and making use of the fact that

$$\frac{d\chi}{dp} = \frac{2k}{k^2+p^2} \tag{17.33}$$

we have

$$\begin{aligned} d\Omega &= \left(\frac{2k}{k^2+p^2}\right)^3 d^3p \\ d^3p &= \left(\frac{k^2+p^2}{2k}\right)^3 d\Omega \end{aligned} \tag{17.34}$$

Also, from (17.27), we have:

$$\begin{aligned} \mathbf{p}\cdot\mathbf{p}' &= \frac{4k^2}{(k^2+p^2)(k^2+p'^2)(\mathbf{u}\cdot\mathbf{u}' - u_4u_4')} \\ \frac{1}{|\mathbf{p}-\mathbf{p}'|^2} &= \frac{4k^2}{(k^2+p^2)(k^2+p'^2)}\frac{1}{|\mathbf{u}-\mathbf{u}'|^2} \end{aligned} \tag{17.35}$$

Inserting (17.34) and (17.35) into (17.26), we obtain:

$$\left[p'^2+k^2\right]^2\psi^t(\mathbf{p}') = \frac{Z}{2k\pi^2}\int d\Omega\,\frac{(k^2+p^2)^2}{|\mathbf{u}'-\mathbf{u}|^2}\,\psi^t(\mathbf{p}) \tag{17.36}$$

We now let

$$\psi^t(\mathbf{p}) = \frac{4k^{5/2}}{(k^2+p^2)^2}\,\varphi(\Omega) \tag{17.37}$$

(As shown in Section 5.3 below, the factor $4k^{5/2}$ in the numerator is needed to normalize $\psi^t(\mathbf{p})$). Equation (17.36) then takes on the simple form

$$\varphi(\Omega') = \frac{Z}{2k\pi^2}\int d\Omega\,\frac{1}{|\mathbf{u}'-\mathbf{u}|^2}\,\varphi(\Omega) \tag{17.38}$$

From equation (**??**), with $d = 4$ and $\alpha = d/2 - 1 = 1$, we have

$$\frac{1}{|\mathbf{u}'-\mathbf{u}|^2} = \sum_{\lambda=0}^{\infty} C_\lambda^1(\mathbf{u}\cdot\mathbf{u}') \tag{17.39}$$

so that (17.38) becomes

$$\varphi(\Omega') = \frac{Z}{2k\pi^2}\sum_{\lambda=0}^{\infty}\int d\Omega\; C_\lambda^1(\mathbf{u}\cdot\mathbf{u}')\;\varphi(\Omega) \tag{17.40}$$

Remembering equation (**??**) we can rewrite this in the form

$$\varphi(\Omega') = \frac{Z}{2k\pi^2}\sum_{\lambda=0}^{\infty} K_\lambda\; O_\lambda[\varphi(\Omega)] \tag{17.41}$$

For $d = 4$,

$$K_\lambda = \frac{I(0)}{\lambda+1} = \frac{2\pi^2}{\lambda+1} \tag{17.42}$$

so that equation (17.41) becomes:

$$\varphi(\Omega') = \frac{Z}{k}\sum_{\lambda=0}^{\infty}\frac{1}{\lambda+1}\;O_\lambda[\varphi(\Omega')] \tag{17.43}$$

If $\varphi(\Omega)$ is an eigenfunction of Λ^2. so that

$$O_{\lambda'}[\varphi(\Omega')] = \delta_{\lambda'\lambda}\varphi(\Omega) \tag{17.44}$$

then (17.43) will be satisfied provided that

$$\frac{Z}{k(\lambda+1)} = 1 \tag{17.45}$$

or, from (17.25),

$$E = -\frac{k^2}{2} = -\frac{Z^2}{2(\lambda+1)^2} = -\frac{Z^2}{2n^2} \qquad \lambda = 0,1,2... \qquad n = 1,2,3... \tag{17.46}$$

where we have made the identification $\lambda + 1 = n$. We can see that Fock's treatment gives the usual energy levels for hydrogenlike atoms. For the transformed wave function $\varphi(\Omega)$, any 4-dimensional hyperspherical harmonic will do, but for most applications, it is convenient to use hyperspherical harmonics of the type shown in Table 2.1. Thus we obtain the Fourier transformed hydrogenlike orbitals:

$$\begin{aligned} \psi^t_{n,l,m}(\mathbf{p}) &= \frac{4k^{5/2}}{(k^2+p^2)^2}Y_{n-1,l,m}(\Omega_4) \equiv M(p)Y_{n-1,l,m}(\Omega_4) \\ M(p) &\equiv \frac{4k^{5/2}}{(k^2+p^2)^2} \end{aligned} \tag{17.47}$$

For the first few values of n, l and m, 17.47 yields:

$$\begin{aligned} \psi^t_{1,0,0}(\mathbf{p}) &= \frac{2\sqrt{2}\;k^{5/2}}{(k^2+p^2)^2\pi} \\ \psi^t_{2,0,0}(\mathbf{p}) &= \frac{4\sqrt{2}\;k^{5/2}(k^2-p^2)}{(k^2+p^2)^3\pi} \\ \psi^t_{2,1,-1}(\mathbf{p}) &= -\frac{8ik^{7/2}(p_1-ip_2)}{(k^2+p^2)^3\pi} \\ \psi^t_{2,1,0}(\mathbf{p}) &= -\frac{8i\sqrt{2}\;k^{7/2}}{(k^2+p^2)\pi} \\ \psi^t_{2,1,1}(\mathbf{p}) &= \frac{8ik^{7/2}(p_1+ip_2)}{(k^2+p^2)^3\pi} \\ &\vdots \qquad \vdots \qquad \vdots \end{aligned} \tag{17.48}$$

To see how Fock's reciprocal space solutions to the hydrogenlike wave equation are related to the familiar hydrogenlike orbitals, we can make a table of hydrogenlike orbitals with Z/n replaced by the constant k. The radial functions become

$$\begin{aligned}
R'_{1,0}(r) &= 2k^{3/2}e^{-kr} \\
R'_{2,0}(r) &= 2k^{3/2}(1-kr)e^{-kr} \\
R'_{2,1}(r) &= \frac{2k^{3/2}}{\sqrt{3}}\, kr\ e^{-kr} \\
R'_{3,0}(r) &= 2k^{3/2}\left(1-2kr+\frac{2k^2r^2}{3}\right)e^{-kr} \\
\vdots \quad & \quad \vdots \quad\quad \vdots
\end{aligned} \tag{17.49}$$

and so on, and the corresponding wave functions will be

$$\chi_{n,l,m}(\mathbf{x}) = R'_{n,l}(r)Y_{l,m}(\Omega_3) \tag{17.50}$$

As you can verify, taking the Fourier transforms of the wave functions defined by equations (17.49) and (17.50), and making the substitutions shown in equation (17.27), we obtain the Fourier transformed solutions of V. Fock, equation (17.47). But this set of solutions is not quite the same as a set of familiar hydrogenlike orbitals because Z/n is everywhere replaced by the constant k. A set of Fock's solutions corresponding to a particular value of k is called a set of *Coulomb Sturmians*. Such a set obeys a potential-weighted orthonormality relation, as we will discuss in detail in Chapters 6 and 7.

17.6 The Pauli exclusion principle and the periodic table

Bohr himself believed that a complete atomic theory ought to be able to explain the chemical properties of the elements in Mendeléev's periodic system. Bohr's 1913 theory failed to pass this test, but the new de Broglie-Schrödinger theory succeeded! Through the work of Pauli, Heitler, London, Slater, Pauling, Hund, Mulliken, Hückel and others, who applied Schrödinger's wave equation to the solution of chemical problems, it became apparent that the wave equation could indeed (in principle) explain all the chemical properties of matter.

The solutions to Schrödinger's wave equation for an electron moving in the field of a nucleus are called *atomic orbitals*, and the first few of them are shown in Figure 11.6.They are analogous to the harmonics of a violin string or an organ pipe, except the they are three-dimensional. The electron had been shown to have a magnetic moment, and in a magnetic field, it was found to orient itself either in the direction of an applied magnetic field, or in the opposite direction - either "spin-up" or "spin-down". This effect could be observed in the splitting of the lines in atomic spectra in the presence of an applied magnetic field. The "spin" and magnetic moment of electrons were completely explained in 1928 by P.A.M. Dirac's relativistic wave equation.

Meanwhile, the Austrian physicist Wolfgang Pauli proposed his famous *exclusion principle*, which explained the periodic table and the chemical properties of the elements. According to the Pauli exclusion principle, in the lowest energy state of an atom, the electrons fill the atomic orbitals in the order (1s), (2p), (3d), ... Two electrons are allowed in each linearly independent orbital, one with spin up and the other with spin down. This leads to the following electron configurations for the elements:

- Hydrogen; (1s); very active metal; valence=1
- Helium; $(1s)^2$; noble (inert) gas; valence=0
- Lithium; $(1s)^2(2p)^1$; very active metal; valence=1
- Beryllium; $(1s)^2(2p)^2$; metal; valence=2
- Boron; $(1s)^2(2p)^3$; less active metal; valence=3
- Carbon; $(1s)^2(2p)^4$; intermediate; valence=4
- Nitrogen; $(1s)^2(2p)^5$; less active nonmetal; valence=5
- Oxygen; $(1s)^2(2p)^6$; nonmetal; valence=6
- Fluorine; $(1s)^2(2p)^7$; very active nonmetal; valence=7
- Neon; $(1s)^2(2p)^8$; noble gas; valence=0
- Sodium; $(1s)^2(2p)^8(2s)^1$; very active metal; valence=1

In chemical reactions, the metals tend to give away their outer-shell electrons, while the non-metals tend to accept electrons. The most active metals, hydrogen, lithium, sodium, potassium, rubidium and cesium, all have a single electron in their outer shell, and they tend to give this electron away. The most active nonmetals, fluorine, chlorine, bromine and iodine, all are missing a single electron to complete their outer shell. We can notice that common table salt, is a cubic crystal structure formed from Na^+ ions and Cl^- ions. When it is dissolved in water, the sodium-chloride crystal dissociates into Na^+ ions, complexed with water molecules and Cl^- ions, also forming complexes with water. We see here the strong tendency of very active metals to give up their outer shell electron and to form positive ions, while very active nonmetals have an equally strong tendency to form negative ions. Helium, neon, argon, krypton, and radon, all with completely filled outer shell, are unreactive noble gases, with no tendency at all to give away or accept electrons or to form ions.

The Hartree-Fock equations

The application of the Schrödinger equation to our understanding of chemical reactivity and the periodic table was made quantitative through the work of Douglas Hartree (1897-1958) and Vladimir A. Fock (1898-1974).

Douglas Hartree was born in Cambridge, England, where his father was a professor of engineering at Cambridge University and his mother was the mayor of the city. In his work on the electronic structure of atoms, Hartree visualized the electrons moving

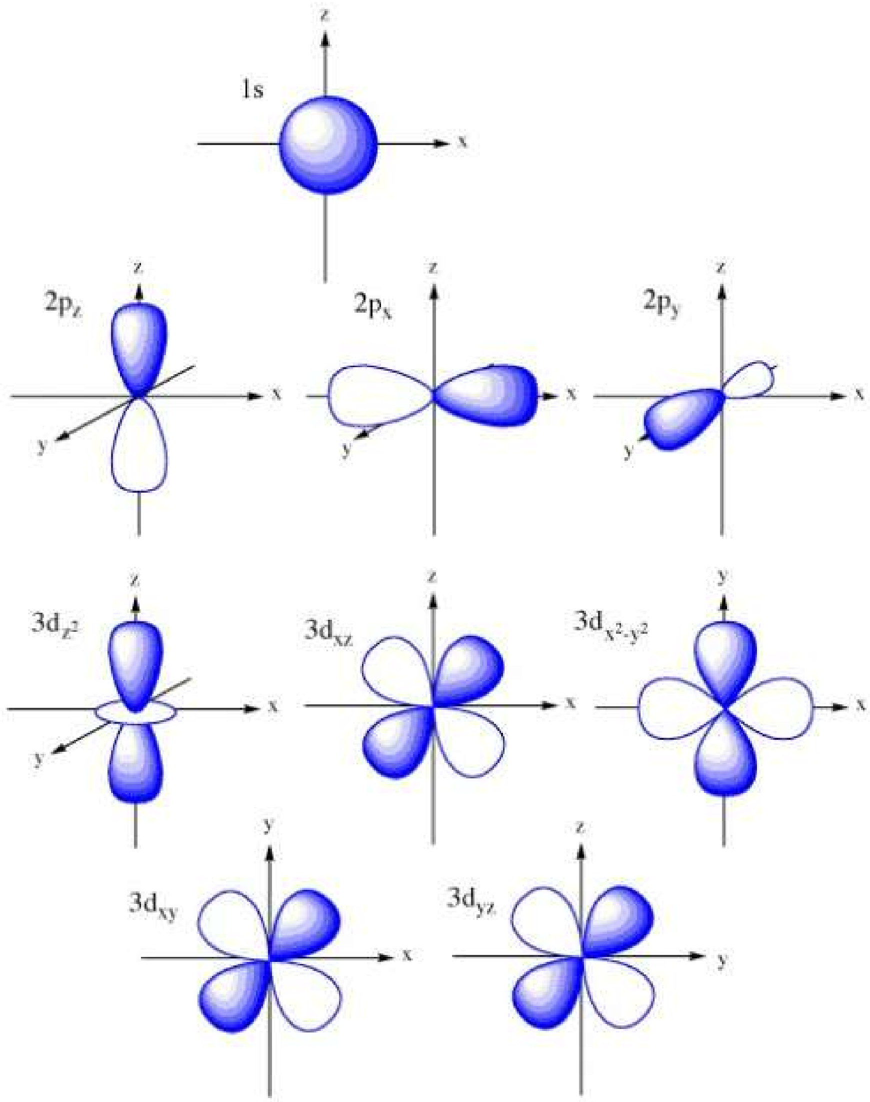

Figure 17.2: **Atomic orbitals.**

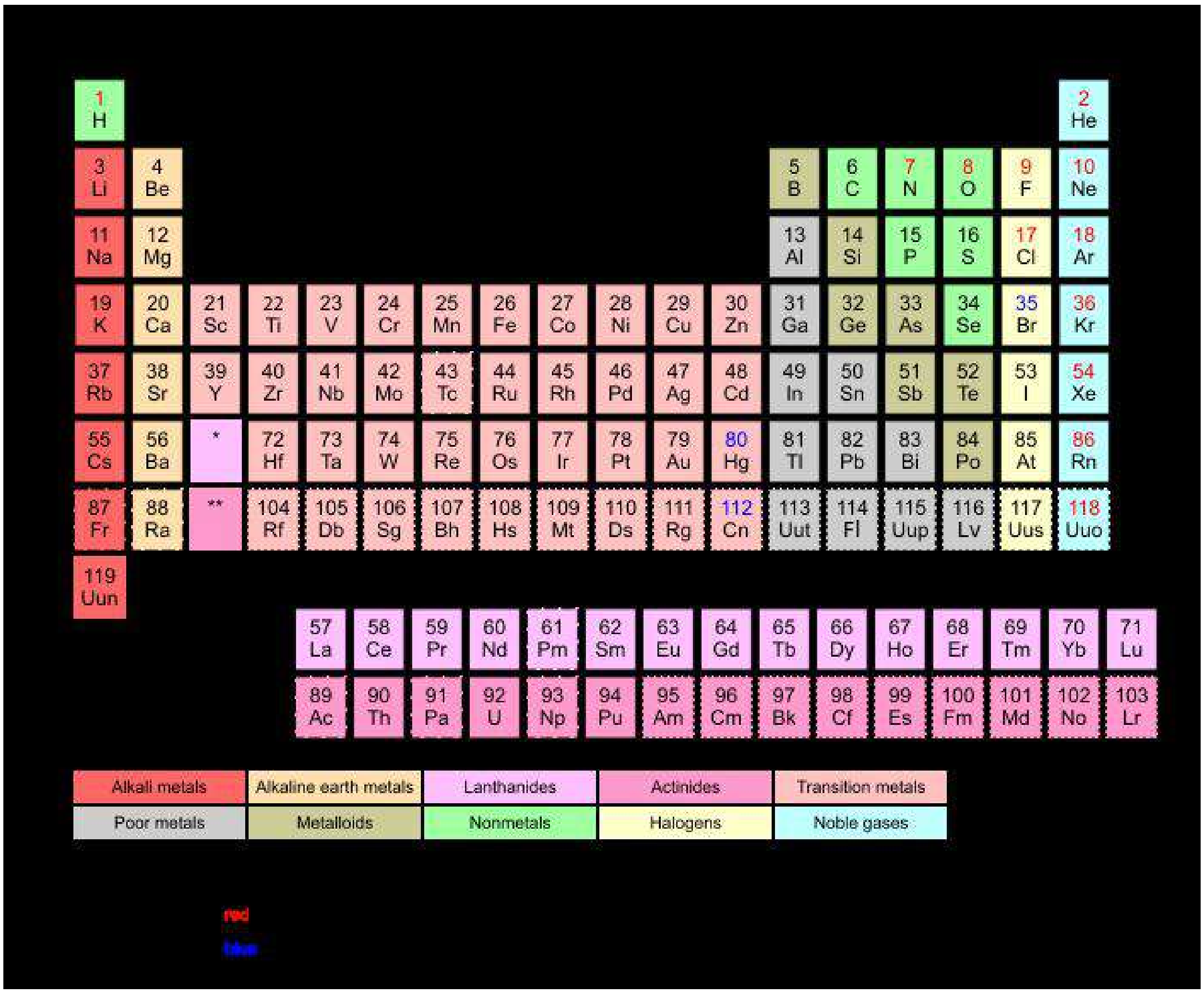

Figure 17.3: **The periodic table of the elements.**

in both the attractive field of the atomic nucleus and in a repulsive potential produced collectively by all the electrons. Hartree's method for treating this problem was to make an initial guess of the size of the atomic orbitals (Figure 11.6) occupied by the electrons. He then calculated the repulsive potential that would result, and combined it with the nuclear attraction potential. Solving the Schrödinger equation for the an electron moving in this new potential, he obtained a set of improved atomic orbitals, and from these he could calculate an improved total potential. He continued to iterate this process until the change resulting from successive iterations became very small, at which point he described the electrical field in which the electrons moved as being *self-consistent*. Hartree called his procedure the Self-Consistent-Field (or SCF) Method. He published his first results in 1927, only a year after Schrödinger's discovery of his wave equation.

The Russian physicist Vladimir A. Fock was able to refine Hartree's method by postulating that the total electronic wave function of an atom or molecule had to be antisymmetric with respect to the exchange of the coordinates of any two electrons in the system. When spin was included in the wave function, this requirement led in a natural way to the exclusion principle postulated by Wolfgang Pauli. When combined with Hartree's SCF method, Fock's antisymmetry requirement led to more accurate results and better agreement between theory and experiment. However, the Hartree-Fock SCF equations were much more difficult to solve. Later Clemens C.J. Roothaan (1918-2019) converted the Hartree-Fock equations into a matrix form suitable for solution by digital computers. The method in use today is thus known as the Hartree-Fock-Roothaan SCF Method. When applied to molecules, it is called the Hartree-Fock-Roothaan LCAO SCF Method. The LCAO in the name stands for the fact that molecular orbitals are represented as Linear Combinations of Atomic Orbitals.

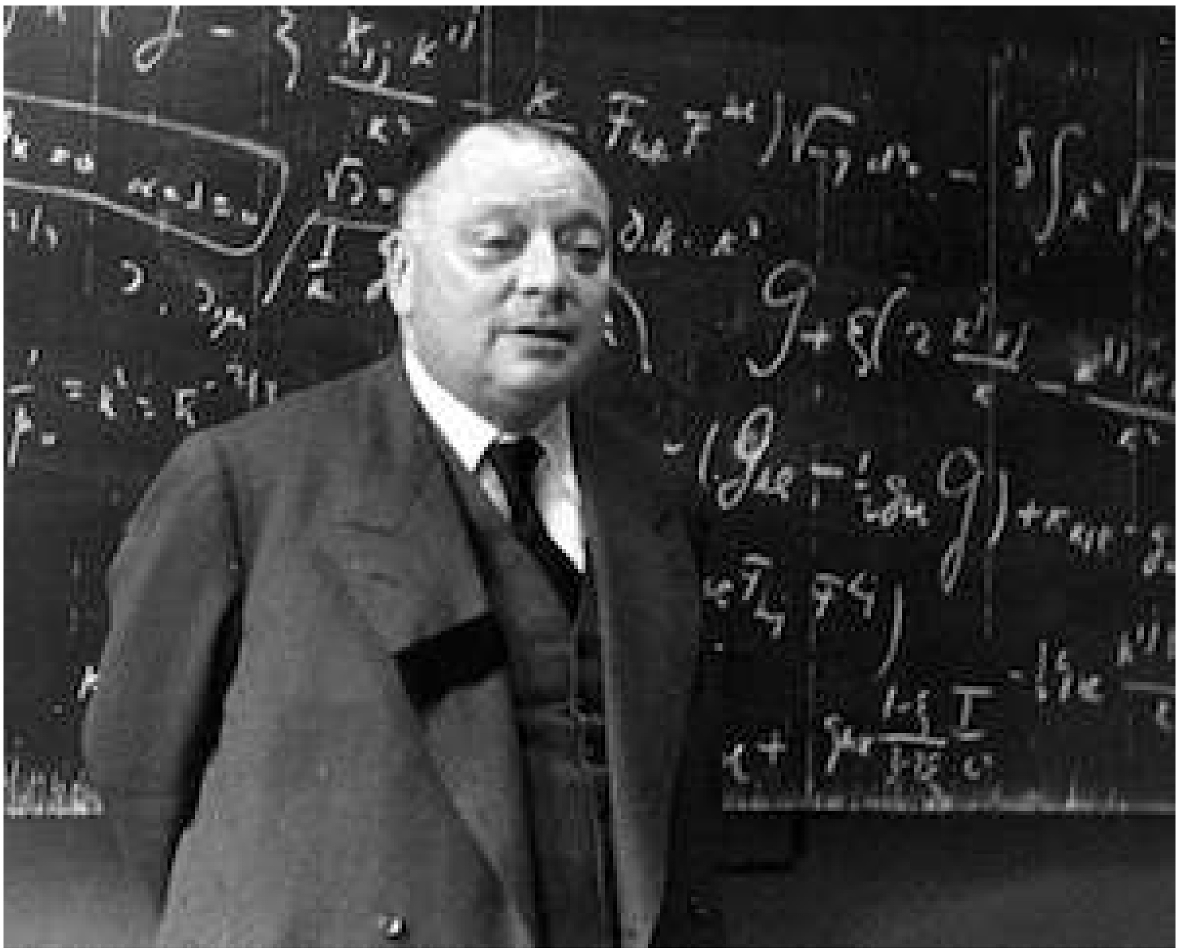

Figure 17.4: **Wolfgang Pauli (1900-1958).**

Figure 17.5: **Douglas Hartree (1897-1958).**

Figure 17.6: **Vladimir A. Fock (1898-1974).**

Figure 17.7: **Louis Victor Pierre Raymond, duc de Broglie, (1892-1987).**

Figure 17.8: **Heisenberg in 1933**

Figure 17.9: **Niels Bohr, Werner Heisenberg and Wolfgang Pauli, c. 1935.**

Figure 17.10: **Peter Debye, (1884-1966).**

17.7 Valence bond theory

17.8 What is life?

What is Life? That was the title of a small book published by the physicist Erwin Schrödinger in 1944. Schrödinger (1887-1961) was born and educated in Austria. In 1926 he shared the Nobel Prize in Physics[1] for his contributions to quantum theory (wave mechanics). Schrödinger's famous wave equation is as fundamental to modern physics as Newton's equations of motion are to classical physics.

When the Nazis entered Austria in 1938, Schrödinger opposed them, at the risk of his life. To escape arrest, he crossed the Alps on foot, arriving in Italy with no possessions except his knapsack and the clothes which he was wearing. He traveled to England; and in 1940 he obtained a position in Ireland as Senior Professor at the Dublin Institute for Advanced Studies. There he gave a series of public lectures upon which his small book is based.

In his book, *What is Life?*, Schrödinger developed the idea that a gene is a very large information-containing molecule which might be compared to an aperiodic crystal. He also examined in detail the hypothesis (due to Max Delbrück) that X-ray induced mutations of the type studied by Hermann Muller can be thought of as photo-induced transitions from one isomeric conformation of the genetic molecule to another. Schrödinger's book has great historic importance, because Francis Crick (whose education was in physics) was one of the many people who became interested in biology as a result of reading it. Besides discussing what a gene might be in a way which excited the curiosity and enthusiasm of Crick, Schrödinger devoted a chapter to the relationship between entropy and life.

"What is that precious something contained in our food which keeps us from death? That is easily answered," Schrodinger wrote, "Every process, event, happening - call it what you will; in a word, everything that is going on in Nature means an increase of the entropy of the part of the world where it is going on. Thus a living organism continually increases its entropy - or, as you may say, produces positive entropy, which is death. It can only keep aloof from it, i.e. alive, by continually drawing from its environment negative entropy - which is something very positive as we shall immediately see. What an organism feeds upon is negative entropy. Or, to put it less paradoxically, the essential thing in metabolism is that the organism succeeds in freeing itself from all the entropy it cannot help producing while alive..."[2]

"Entropy, taken with a negative sign, is itself a measure of order. Thus the device by which an organism maintains itself stationary at a fairly high level of orderliness (= fairly low level of entropy) really consists in continually sucking orderliness from its environment. This conclusion is less paradoxical than it appears at first sight. Rather it could be blamed

[1] with P.A.M. Dirac

[2] The Hungarian-American biochemist Albert Szent-Györgyi, who won a Nobel prize for isolating vitamin C, and who was a pioneer of bioenergetics, expressed the same idea in the following words: "We need energy to fight against entropy".

for triviality. Indeed, in the case of higher animals we know the kind of orderliness they feed upon well enough, viz. the extremely well-ordered state of matter state in more or less complicated organic compounds which serve them as foodstuffs. After utilizing it, they return it in a very much degraded form - not entirely degraded, however, for plants can still make use of it. (These, of course, have their most powerful source of 'negative entropy' in the sunlight.)" At the end of the chapter, Schrödinger added a note in which he said that if he had been writing for physicists, he would have made use of the concept of free energy; but he judged that this concept might be difficult or confusing for a general audience.

In the paragraphs which we have quoted, Schrodinger focused on exactly the aspect of life which is the main theme of the present book: All living organisms draw a supply of thermodynamic information from their environment, and they use it to "keep aloof" from the disorder which constantly threatens them. In the case of animals, the information-containing free energy comes in the form of food. In the case of green plants, it comes primarily from sunlight. The thermodynamic information thus gained by living organisms is used by them to create configurations of matter which are so complex and orderly that the chance that they could have arisen in a random way is infinitesimally small.

John von Neumann invented a thought experiment which illustrates the role which free energy plays in creating statistically unlikely configurations of matter. Von Neumann imagined a robot or automaton, made of wires, electrical motors, batteries, etc., constructed in such a way that when floating on a lake stocked with its component parts, it will reproduce itself.[3] The important point about von Neumann's automaton is that it requires a source of free energy (i.e., a source of energy from which work can be obtained) in order to function. We can imagine that the free energy comes from electric batteries which the automaton finds in its environment. (These are analogous to the food eaten by animals.) Alternatively we can imagine that the automaton is equipped with photocells, so that it can use sunlight as a source of free energy, but it is impossible to imagine the automaton reproducing itself without some energy source from which work can be obtained to drive its reproductive machinery. If it could be constructed, would von Neumann's automaton be alive? Few people would say yes. But if such a self-reproducing automaton could be constructed, it would have some of the properties which we associate with living organisms.

The autocatalysts which are believed to have participated in molecular evolution had some of the properties of life. They used "food" (i.e., energy-rich molecules in their environments) to reproduce themselves, and they evolved, following the principle of natural selection. The autocatalysts were certainly precursors of life, approaching the borderline between non-life and life.

Is a virus alive? We know, for example, that the tobacco mosaic virus can be taken to pieces. The proteins and RNA of which it is composed can be separated, purified, and stored in bottles on a laboratory shelf. At a much later date, the bottles containing the separate components of the virus can be taken down from the shelf and incubated together, with the result that the components assemble themselves in the correct way,

[3] In Chapter 8 we will return to von Neumann's self-replicating automaton and describe it in more detail.

guided by steric and electrostatic complementarity. New virus particles are formed by this process of autoassembly, and when placed on a tobacco leaf, the new particles are capable of reproducing themselves. In principle, the stage where the virus proteins and RNA are purified and placed in bottles could be taken one step further: The amino acid sequences of the proteins and the base sequence of the RNA could be determined and written down.

Later, using this information, the parts of the virus could be synthesized from amino acids and nucleotides. Would we then be creating life? Another question also presents itself: At a certain stage in the process just described, the virus seems to exist only in the form of information - the base sequence of the RNA and the amino acid sequence of the proteins. Can this information be thought of as the idea of the virus in the Platonic sense? (Pythagoras would have called it the "soul" of the virus.) Is a computer virus alive? Certainly it is not so much alive as a tobacco mosaic virus. But a computer virus can use thermodynamic information (supplied by an electric current) to reproduce itself, and it has a complicated structure, containing much cybernetic information.

Under certain circumstances, many bacteria form spores, which do not metabolize, and which are able to exist without nourishment for very long periods - in fact for millions of years. When placed in a medium containing nutrients, the spores can grow into actively reproducing bacteria. There are examples of bacterial spores existing in a dormant state for many millions of years, after which they have been revived into living bacteria. Is a dormant bacterial spore alive?

Clearly there are many borderline cases between non-life and life; and Aristotle seems to have been right when he said, "Nature proceeds little by little from lifeless things to animal life, so that it is impossible to determine either the exact line of demarcation, or on which side of the line an intermediate form should lie." However, one theme seems to characterize life: It is able to convert the thermodynamic information contained in food or in sunlight into complex and statistically unlikely configurations of matter. A flood of information-containing free energy reaches the earth's biosphere in the form of sunlight. Passing through the metabolic pathways of living organisms, this information keeps the organisms far away from thermodynamic equilibrium ("which is death"). As the thermodynamic information flows through the biosphere, much of it is degraded into heat, but part is converted into cybernetic information and preserved in the intricate structures which are characteristic of life. The principle of natural selection ensures that as this happens, the configurations of matter in living organisms constantly increase in complexity, refinement and statistical improbability. This is the process which we call evolution, or in the case of human society, progress.

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Chapter 18

DIRAC

18.1 Dirac's relativistic wave equation

In 1928, P.A.M. Dirac derived a relativistic wave equation that was first-order in time. To do this, he made use of a set of four anticommuting matrices. Solutions to the Dirac equation in the absence of external fields also obey the Klein-Gordon equation, which is second-order in time, the equation that Schrödinger first tried and then abandoned. Dirac's relativistic equation explained for the first time many details of the spectrum of hydrogen, but critics complained that it predicted the existence of negative energy states, and they asked, "Why don't the positive energy electrons fall down into these states?" Dirac replied "Because the negative energy states are all occupied." 'But then", the critics said, "an extremely energetic photon could create an electron-hole pair!" "Keep looking", Dirac answered, "and you will find that it sometimes happens." Thus, an astonishing consequence of Dirac's relativistic wave equation was the prediction of the existence of antimatter!

Years passed. Then, in 1932, the physicist Carl David Anderson observed in a cosmic ray photographic plate an event that confirmed Dirac's prediction of the existence of antimatter. A highly-energetic photon was annihilated, and converted into an electron-antielectron pair. The antielectron was given the name "positron". Since that time, the antiparticles of other particles have been discovered, created in high-energy events where a photon is annihilated and a particle-antiparticle pair created.

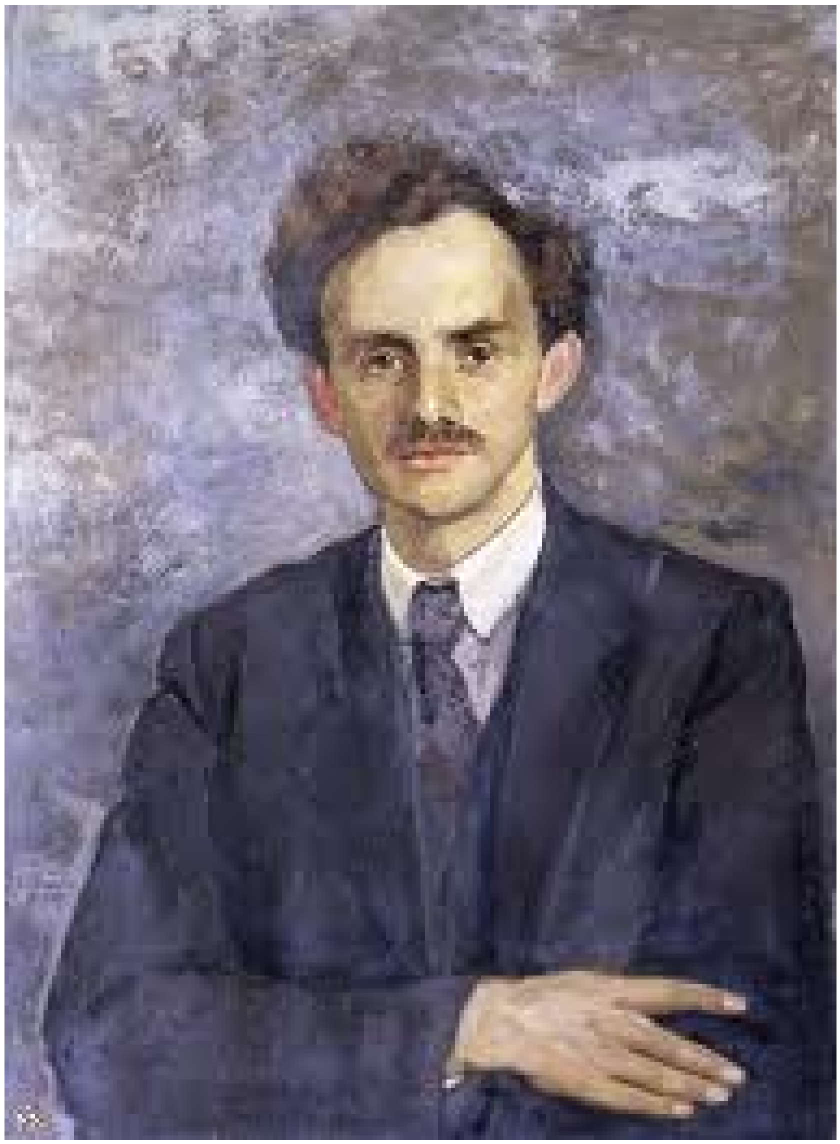

Figure 18.1: **P.A.M. Dirac, the greatest British physicist of the 20th century. A memorial inscribed with his relativistic wave equation stands in Westminister Cathedral, near to the statue of Newton.**

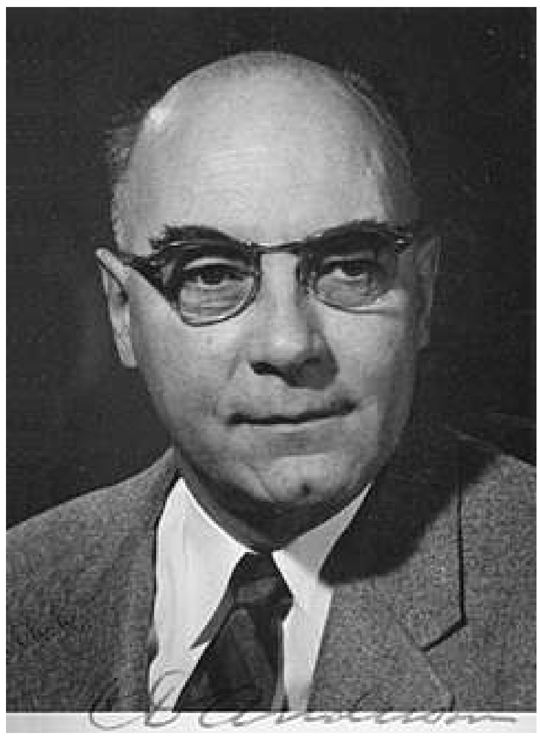

Figure 18.2: **Carl David Anderson. He discovered experimentally the antiparticles whose existence Dirac had predicted.**

18.2 Some equations

For readers with some mathematical background, a few equations are included here.

The relativistic relationship between energy and momentum

$$E^2 - p^2c^2 = m^2c^4 \tag{18.1}$$

Here E stands for energy, p for momentum, m for mass, and c for the velocity of light.

The Klein-Gordon equation

$$\left(-\frac{\hbar^2}{c^2}\frac{\partial^2}{\partial^2 t} + \hbar^2\nabla^2\right)\psi = m^2c^2\psi \tag{18.2}$$

The Klein-Gordon equation can be derived from equation 18.1 by making the substitutions

$$\begin{aligned} E &\rightarrow \frac{\hbar}{i}\frac{\partial}{\partial x_4} \qquad x_4 \equiv ict \\ p_j &\rightarrow \frac{\hbar}{i}\frac{\partial}{\partial x_j} \qquad j = 1, 2, 3 \end{aligned} \tag{18.3}$$

where $\hbar$ is Planck's constant.

Schrödinger's non-relativistic wave equation

The non-relativistic relationship between energy and momentum is given by

$$E = c\sqrt{p^2 + m^2c^2} + V \approx \frac{p^2}{2m} + V \qquad m^2c^2 >> p^2 \tag{18.4}$$

Schrödinger's non-relativistic wave equation,

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = E\psi \tag{18.5}$$

can be derived by making the substitutions

$$p_j \rightarrow \frac{\hbar}{i}\frac{\partial}{\partial x_j} \qquad j = 1, 2, 3 \tag{18.6}$$

If the wave function ψ has time-dependence of the form

$$\psi(\mathbf{x}, t) = \psi(\mathbf{x})e^{iEt/\hbar} \tag{18.7}$$

then we can write

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi \tag{18.8}$$

where

$$H \equiv \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right) \tag{18.9}$$

18.3 Lorentz invariance and 4-vectors

Albert Einstein's special theory of relativity was built on the negative result of the Michelson-Morley experiment, an experiment that attempted to measure the absolute velocity of the earth through space. Einstein boldly postulated that no experiment whatever can measure absolute motion, that is to say, according to his postulate it is impossible for an observer to know whether he is in a state of rest or in a state of uniform motion. All inertial frames are equivalent. Einstein's postulate has been amply confirmed by experiment, and today it is one of the basic principles of modern physics.

The equivalence of all inertial frames can be expressed in another way: Every fundamental physical law must exhibit symmetry between the space and time coordinates in such a way that ict enters on the same footing as the Cartesian coordinates x, y and z. (Here $i \equiv \sqrt{-1}$, while c is the velocity of light, and t is the time.) In relativistic theory, space and time combine to form a pseudo-Euclidean space-time continuum (Minkowski space). A transformation from one inertial frame to another (a Lorentz transformation) corresponds to a rotation in this space, and such a transformation must leave all fundamental physical laws invariant in form.

Every physical quantity that is represented by a 3-component vector in non-relativistic theory has a 4th component in the relativistic 4-dimensional space-time continuum. Thus, for example, the position vector $\mathbf{x} = (x, y, z)$ in 3-dimensional space has a 4th component in relativistic theory:

$$x_\lambda = (x, y, z, ict) = (\mathbf{x}, ict) \tag{18.10}$$

while the vector potential $\mathbf{A} = (A_x, A_y, A_z)$ in electromagnetic theory is the space component of a 4-vector, whose 4th component is i multiplied by the electrostatic potential ϕ:

$$A_\lambda = (A_x, A_y, A_z, i\phi) = (\mathbf{A}, i\phi) \tag{18.11}$$

Similarly, the current density vector $\mathbf{j} = (j_x, j_y, j_z)$ is the space-component of a 4-vector

$$j_\lambda = (j_x, j_y, j_z, ic\rho) = (\mathbf{j}, ic\rho) \tag{18.12}$$

whose time-component is ic multiplied by the charge density ρ. (Throughout this chapter we will represent 3-vectors by writing them in bold-face letters. Thus $j_\lambda = (\mathbf{j}, ic\rho)$ means that the first three components of the 4-vector j_λ are given by $\mathbf{j} = (j_x, j_y, j_z)$, while the

4th component is $ic\rho$.) The gradient operator $\boldsymbol{\partial}$ also becomes the space-component of a 4-vector in relativistic theory:

$$\partial_\lambda \equiv \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}, \frac{\partial}{\partial x_4}\right) = \left(\boldsymbol{\partial}, -\frac{i}{c}\frac{\partial}{\partial t}\right) \tag{18.13}$$

while the Laplacian operator is replaced by the d'Alembertian operator:

$$\Box \equiv \sum_{\lambda=1}^{4} \partial_\lambda^2 \equiv \sum_{\lambda=1}^{4} \frac{\partial^2}{\partial x_\lambda} \tag{18.14}$$

an operator which exhibits the required space-time symmetry, so that its form is the same in all inertial frames. In relativistic electrodynamics, the electric field vector $\boldsymbol{\mathcal{E}}$ and the magnetic field vector $\boldsymbol{\mathcal{H}}$ are components of an antisymmetric tensor $F_{\lambda',\lambda}$, which is related to A_λ by

$$F_{\lambda',\lambda} \equiv \partial_{\lambda'} A_\lambda - \partial_\lambda A_{\lambda'} = \begin{pmatrix} 0 & \mathcal{H}_z & -\mathcal{H}_y & -i\mathcal{E}_x \\ -\mathcal{H}_z & 0 & \mathcal{H}_x & -i\mathcal{E}_y \\ \mathcal{H}_y & -\mathcal{H}_x & 0 & -i\mathcal{E}_z \\ i\mathcal{E}_x & i\mathcal{E}_y & i\mathcal{E}_z & 0 \end{pmatrix} \tag{18.15}$$

The 4-vector A_λ, which represents the electromagnetic potential, is related to the 4-vector representing current density by

$$\Box A_\lambda = -\frac{4\pi}{c} j_\lambda \tag{18.16}$$

When both the current density j_λ and the electromagnetic potential 4-vector A_λ are independent of time, equation (18.16) reduces to:

$$\nabla_1^2 A_\lambda(\mathbf{x}_1) = -\frac{4\pi}{c} j_\lambda(\mathbf{x}_1) \tag{18.17}$$

which has the Green's function solution

$$A_\lambda(\mathbf{x}_1) = \frac{1}{c}\int d^3x_2 \, \frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|} \, j_\lambda(\mathbf{x}_2) \tag{18.18}$$

We can see that (18.18) is a solution to (18.17) because

$$\nabla_1^2 \frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|} = -4\pi\delta^3(\mathbf{x}_1 - \mathbf{x}_2) \equiv -4\pi\delta(x_1 - x_2)\delta(y_1 - y_2)\delta(z_1 - z_2) \tag{18.19}$$

and therefore

$$\begin{aligned} \nabla_1^2 A_\lambda(\mathbf{x}_1) &= \frac{1}{c}\int d^3x_2 \, \nabla_1^2 \frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|} \, j_\lambda(\mathbf{x}_2) \\ &= -\frac{4\pi}{c}\int d^3x_2 \;\; \delta^3(\mathbf{x}_1 - \mathbf{x}_2) \, j_\lambda(\mathbf{x}_2) \\ &= -\frac{4\pi}{c} j_\lambda(\mathbf{x}_1) \end{aligned} \tag{18.20}$$

The subscript 1 on the Laplacian operator means that the operator is acting on the coordinates of the field-point $\mathbf{x}_1$ rather than on the source-point, $\mathbf{x}_2$.

Because of charge conservation, the current density 4-vector obeys the condition

$$\sum_{\lambda=1}^{4} \partial_\lambda j_\lambda = 0 \tag{18.21}$$

Since the current density is related to the electromagnetic potential 4-vector through (18.16), it is natural to work in the Lorentz gauge, where a similar condition is imposed on A_λ:

$$\sum_{\lambda=1}^{4} \partial_\lambda A_\lambda = 0 \tag{18.22}$$

Equations (18.16) and (18.22) are Maxwell's equations in a vacuum, written in a form that makes the space-time symmetry apparent.

18.4 The Dirac equation for an electron in an external electromagnetic potential

P.A.M. Dirac's relativistic wave equation for an electron moving in an external potential A_λ can be written in the form:

$$\left[\sum_{\lambda=1}^{4} \gamma_\lambda \left(\partial_\lambda - \frac{i}{c} A_\lambda\right) + c\right] \chi_\mu = 0 \tag{18.23}$$

where atomic units are used and where the γ_λ's are 4×4 matrices:

$$\gamma_1 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \qquad \gamma_2 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \tag{18.24}$$

$$\gamma_3 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix} \qquad \gamma_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{18.25}$$

In atomic units, the electron rest-mass is equal to 1, and Planck's constant divided by 2π is also equal to 1, while the velocity of light has a value equal to the reciprocal of the fine structure constant:

$$m_0 = 1 \qquad \hbar = 1 \qquad c = 137.036 \tag{18.26}$$

From the definitions of the γ_λ's, it follows that they anticommute:

$$\gamma_{\lambda'}\gamma_\lambda + \gamma_\lambda\gamma_{\lambda'} = 2I\delta_{\lambda',\lambda} \tag{18.27}$$

In equation (18.27), I is a 4×4 unit matrix. Solutions to the 1-electron Dirac equation are 4-component spinors.

18.5 Time-independent problems

In the special case where the external electromagnetic potential 4-vector A_λ is independent of time, it is convenient to write the Dirac equation (18.23) in a different form, where we introduce the notation

$$\boldsymbol{\alpha} = i\gamma_0\boldsymbol{\gamma} \qquad \gamma_0 \equiv \gamma_4 \tag{18.28}$$

From equations (18.24), (18.25) and (18.28) it follows that the components of the 3-vector $\boldsymbol{\alpha}$ can be written in block form as

$$\alpha_j = \left(\begin{array}{c|c} 0 & \sigma_j \\ \hline \sigma_j & 0 \end{array}\right) \qquad j = 1,2,3 \tag{18.29}$$

where, in the off-diagonal blocks, σ_j, $j = 1,2,3$ are the 2×2 Pauli spin matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{18.30}$$

For time-independent problems, the Dirac equation for a single electron can then be written in the form:

$$[H - \epsilon_\mu]\,\chi_\mu(\mathbf{x}) = 0 \tag{18.31}$$

where

$$H = -ic\boldsymbol{\alpha}\cdot\left(\boldsymbol{\partial} - \frac{i}{c}\mathbf{A}(\mathbf{x})\right) + I\phi(\mathbf{x}) + \gamma_0 c^2 \tag{18.32}$$

is the Dirac Hamiltonian of an electron moving in a constant external electromagnetic potential, ϵ_μ is the 1-electron energy, and $\chi_\mu(\mathbf{x})$ is the 4-component time-independent spinor of the electron. The kinetic energy term in the Dirac Hamilton is given by

$$-ic\boldsymbol{\alpha}\cdot\boldsymbol{\partial} = -ic\begin{pmatrix} 0 & 0 & \partial_3 & \partial_- \\ 0 & 0 & \partial_+ & -\partial_3 \\ \partial_3 & \partial_- & 0 & 0 \\ \partial_+ & -\partial_3 & 0 & 0 \end{pmatrix} \tag{18.33}$$

where

$$\partial_\pm \equiv \partial_1 \pm i\partial_2 \tag{18.34}$$

Similarly, the part of the Dirac Hamiltonian involving potentials is

$$-\boldsymbol{\alpha}\cdot\mathbf{A} + I\phi = \begin{pmatrix} \phi & 0 & -A_3 & -A_- \\ 0 & \phi & -A_+ & A_3 \\ -A_3 & -A_- & \phi & 0 \\ -A_+ & A_3 & 0 & \phi \end{pmatrix} \tag{18.35}$$

where

$$A_\pm \equiv A_1 \pm iA_2 \tag{18.36}$$

18.6 The Dirac equation for an electron in the field of a nucleus

When $\mathbf{A}(\mathbf{x}) = 0$, and $\phi(\mathbf{x}) = -Z/r$, equation (18.31) reduces to

$$\left[-ic\boldsymbol{\alpha}\cdot\boldsymbol{\partial} - \frac{Z}{r} + \gamma_0 c^2 - \epsilon_\mu\right]\chi_\mu(\mathbf{x}) = 0 \tag{18.37}$$

which is the Dirac equation for an electron moving in the attractive electrostatic potential of a nucleus with charge Z. Equation (18.37) can be solved exactly, and the solutions have the form

$$\chi_\mu(\mathbf{x}) = \chi_{njlM}(\mathbf{x}) = \begin{pmatrix} ig_{njl}(r)\Omega_{j,l,M}(\theta,\varphi) \\ \\ -f_{njl}(r)\Omega_{j,2j-l,M}(\theta,\varphi) \end{pmatrix} \tag{18.38}$$

Examples are shown in equations (**??**) and (**??**). In equation (18.38), the angular function $\Omega_{j,l,M}(\theta,\varphi)$ is a two-component "spherical spinor", which is an eigenfunction of orbital angular momentum corresponding to the quantum number l, total angular momentum (orbital plus spin) with quantum number j, and the z-component of total angular momentum, with quantum number M. The spherical spinors are built up from spherical harmonics and 2-component spinors by combining them with the appropriate Clebsch-Gordan coefficients in such a way as to produce eigenfunctions of total angular momentum. The Clebsch-Gordan coefficients that enter are different, depending on whether $j = l + \frac{1}{2}$ or $j = l - \frac{1}{2}$. When $j = l + \frac{1}{2}$,

$$\Omega_{j,l,M}(\theta,\varphi) = \begin{pmatrix} \sqrt{\dfrac{l+M+\frac{1}{2}}{2l+1}}\;Y_{l,M-\frac{1}{2}}(\theta,\varphi) \\ \\ \sqrt{\dfrac{l-M+\frac{1}{2}}{2l+1}}\;Y_{l,M+\frac{1}{2}}(\theta,\varphi) \end{pmatrix} \tag{18.39}$$

while when $j = l - \frac{1}{2}$,

$$\Omega_{j,l,M}(\theta,\varphi) = \begin{pmatrix} -\sqrt{\dfrac{l-M+\frac{1}{2}}{2l+1}}\;Y_{l,M-\frac{1}{2}}(\theta,\varphi) \\ \\ \sqrt{\dfrac{l+M+\frac{1}{2}}{2l+1}}\;Y_{l,M+\frac{1}{2}}(\theta,\varphi) \end{pmatrix} \tag{18.40}$$

The radial function $g_{njl}(r)$ is much larger than $f_{njl}(r)$. The large and small radial functions are defined respectively by

$$g_{njl}(r) = \mathcal{N} r^{\gamma-1} e^{-Zr/\bar{n}} \left(W_1(r) - W_2(r)\right) \tag{18.41}$$

and

$$f_{njl}(r) = \mathcal{N} \sqrt{\frac{c^2 - \epsilon_{nj}}{c^2 + \epsilon_{nj}}}\, r^{\gamma-1} e^{-Zr/\bar{n}} \left(W_1(r) + W_2(r)\right) \tag{18.42}$$

where

$$\begin{aligned} W_1(r) &\equiv n_r F\left(j + \frac{1}{2} - n + 1 \middle| 2\gamma + 1 \middle| \frac{2Zr}{\bar{n}}\right) \\ W_2(r) &\equiv (\bar{n} - \kappa) F\left(j + \frac{1}{2} - n \middle| 2\gamma + 1 \middle| \frac{2Zr}{\bar{n}}\right) \end{aligned} \tag{18.43}$$

with

$$\kappa \equiv \begin{cases} -(j + \frac{1}{2}) & j = l + \frac{1}{2} \\ j + \frac{1}{2} & j = l - \frac{1}{2} \end{cases} \tag{18.44}$$

$$\gamma \equiv \sqrt{\left(j + \frac{1}{2}\right)^2 - \left(\frac{Z}{c}\right)^2} \tag{18.45}$$

$$n_r \equiv n - j - \frac{1}{2} \tag{18.46}$$

and

$$\bar{n} \equiv \sqrt{n^2 - 2n_r(j + \frac{1}{2} - \gamma)} \tag{18.47}$$

Just as in the definition of the non-relativistic hydrogenlike orbitals, $F\left(a|b|\zeta\right)$ is a confluent hypergeometric function:

$$F\left(a|b|\zeta\right) \equiv 1 + \frac{a}{b}\zeta + \frac{a(a+1)}{b(b+1)2!}\zeta^2 + \cdots \tag{18.48}$$

When $Z \ll 137$, the 1-electron energies

$$\epsilon_{nj} = \frac{c^2}{\sqrt{1 + \left(\frac{Z}{c(\gamma + n_r)}\right)^2}} \tag{18.49}$$

Suggestions for further reading

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Chapter 19

SHANNON

19.1 Maxwell's demon

In England, the brilliant Scottish theoretical physicist, James Clerk Maxwell (1831-1879) invented a thought experiment which demonstrated that the second law of thermodynamics is statistical in nature and that there is a relationship between entropy and information. It should be mentioned that at the time when Clausius and Maxwell were living, not all scientists agreed about the nature of heat, but Maxwell, like Kelvin, believed heat to be due to the rapid motions of atoms or molecules. The more rapid the motion, the greater the temperature.

In a discussion of the ideas of Carnot and Clausius, Maxwell introduced a model system consisting of a gas-filled box divided into two parts by a wall; and in this wall, Maxwell imagined a small weightless door operated by a "demon". Initially, Maxwell let the temperature and pressure in both parts of the box be equal. However, he made his demon operate the door in such a way as to sort the gas particles: Whenever a rapidly-moving particle approaches from the left, Maxwell's demon opens the door; but when a slowly moving particle approaches from the left, the demon closes it. The demon has the opposite policy for particles approaching from the right, allowing the slow particles to pass, but turning back the fast ones. At the end of Maxwell's thought experiment, the particles are sorted, with the slow ones to the left of the barrier, and the fast ones to the right. Although initially, the temperature was uniform throughout the box, at the end a temperature difference has been established, the entropy of the total system is *decreased* and the second law of thermodynamics is violated.

In 1871, Maxwell expressed these ideas in the following words: "If we conceive of a being whose faculties are so sharpened that he can follow every molecule in its course, such a being, whose attributes are still finite as our own, would be able to do what is at present impossible to us. For we have seen that the molecules in a vessel full of air are moving at velocities by no means uniform... Now let us suppose that such a vessel full of air at a uniform temperature is divided into two portions, A and B, by a division in which there is a small hole, and that a being who can see individual molecules, opens and closes

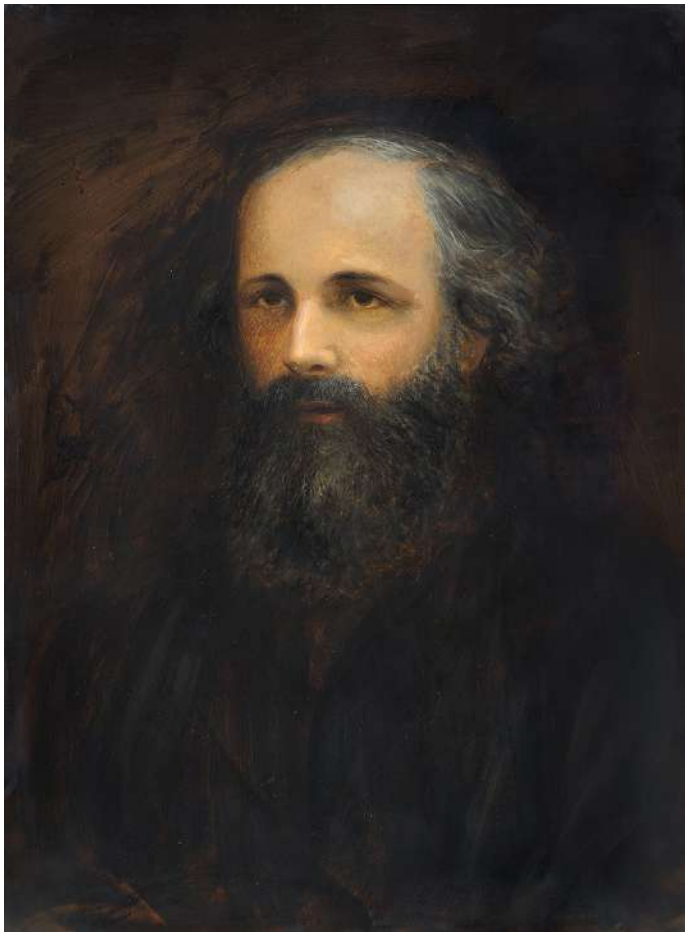

Figure 19.1: **James Clark Maxwell by Jemima Blackburn.**

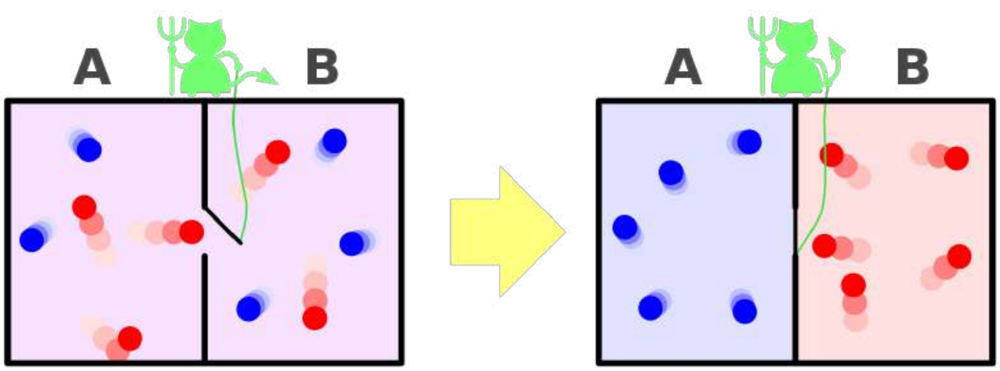

Figure 19.2: **Maxwell's demon, a thought experiment where entropy decreases.**

swifter molecules to pass from A to B, and only slower ones to pass from B to A. He will thus, without the expenditure of work, raise the temperature of B and lower that of A, in contradiction to the second law of thermodynamics." Of course Maxwell admitted that demons and weightless doors do not exist. However, he pointed out, one could certainly imagine a small hole in the partition between the two halves of the box. The sorting could happen by chance (although the probability of its happening decreases rapidly as the number of gas particles becomes large). By this argument, Maxwell demonstrated that the second law of thermodynamics is a statistical law.

An extremely interesting aspect of Maxwell's thought experiment is that his demon uses information to perform the sorting. The demon needs information about whether an approaching particle is fast or slow in order to know whether or not to open the door.

Finally, after the particles have been sorted, we can imagine that the partition is taken away so that the hot gas is mixed with the cold gas. During this mixing, the entropy of the system will increase, and information (about where to find fast particles and where to find slow ones) will be lost. Entropy is thus seen to be a measure of disorder or lack of information. To decrease the entropy of a system, and to increase its order, Maxwell's demon needs information. In the opposite process, the mixing process, where entropy increases and where disorder increases, information is lost.

19.2 Statistical mechanics

Besides inventing an interesting demon (and besides his monumental contributions to electromagnetic theory), Maxwell also helped to lay the foundations of statistical mechanics. In this enterprise, he was joined by the Austrian physicist Ludwig Boltzmann (1844-1906) and by an American, Josiah Willard Gibbs, whom we will discuss later. Maxwell and Boltzmann worked independently and reached similar conclusions, for which they share the credit. Like Maxwell, Boltzmann also interpreted an increase in entropy as an increase in disorder; and like Maxwell he was a firm believer in atomism at a time when this belief was by no means universal. For example, Ostwald and Mach, both important figure in German science at that time, refused to believe in the existence of atoms, in spite of the fact that Dalton's atomic ideas had proved to be so useful in chemistry. Towards the end of his life, Boltzmann suffered from periods of severe depression, perhaps because of attacks on his scientific work by Ostwald and others. In 1906, while on vacation near Trieste, he committed suicide - ironically, just a year before the French physicist J.B. Perrin produced irrefutable evidence of the existence of atoms.

Maxwell and Boltzmann made use of the concept of "phase space", a $6N$-dimensional space whose coordinates are the position and momentum coordinates of each of N particles. However, in discussing statistical mechanics we will use a more modern point of view, the point of view of quantum theory, according to which a system may be in one or another of a set of discrete states, $i = 1,2,3,...$ with energies ϵ_i. Let us consider a set of N identical, weakly-interacting systems; and let us denote the number of the systems which occupy a particular state by n_j, as shown in equation

$$\begin{array}{llllllll} \text{State number} & 1 & 2 & 3 & ... & i & ... \\ \text{Energy} & \epsilon_1, & \epsilon_2, & \epsilon_3, & ... & \epsilon_i, & ... \\ \text{Occupation number} & n_1, & n_2, & n_3, & ... & n_i, & ... \end{array} \tag{19.1}$$

the energy levels and their occupation numbers. This macrostate can be constructed in many ways, and each of these ways is called a "microstate": For example, the first of the N identical systems may be in state 1 and the second in state 2; or the reverse may be the case; and the two situations correspond to different microstates. From combinatorial analysis it is possible to show that the number of microstates corresponding to a given macrostate is given by:

$$W = \frac{N!}{n_1!n_2!n_3!...n_i!...} \tag{19.2}$$

Boltzmann was able to show that the entropy S_N of the N identical systems is related to the quantity W by the equation

$$S_N = k \ln W \tag{19.3}$$

where k is the constant which appears in the empirical law relating the pressure, volume and absolute temperature of an ideal gas;

$$PV = NkT \tag{19.4}$$

This constant,

$$k = 1.38062 \times 10^{-23} \ \frac{\text{joule}}{\text{kelvin}} \tag{19.5}$$

is called Boltzmann's constant in his honor. Boltzmann's famous equation relating entropy to missing information, equation (4.6), is engraved on his tombstone. A more detailed discussion of Boltzmann's statistical mechanics is given in Appendix 1.

19.3 Information theory; Shannon's formula

We have seen that Maxwell's demon needed information to sort gas particles and thus decrease entropy; and we have seen that when fast and slow particles are mixed so that entropy increases, information is lost. The relationship between entropy and lost or missing information was made quantitative by the Hungarian-American physicist Leo Szilard (1898-1964) and by the American mathematician Claude Shannon (1916-2001). In 1929, Szilard published an important article in Zeitschrift für Physik in which he analyzed Maxwell's demon. In this famous article, Szilard emphasized the connection between entropy and missing information. He was able to show that the entropy associated with a unit of

Figure 19.3: **The Hungarian physicist Leo Szilard, whose famous 1929 paper first made the connection between entropy and information using the formula $k \ln 2$, where k is Boltzmann's constant.**

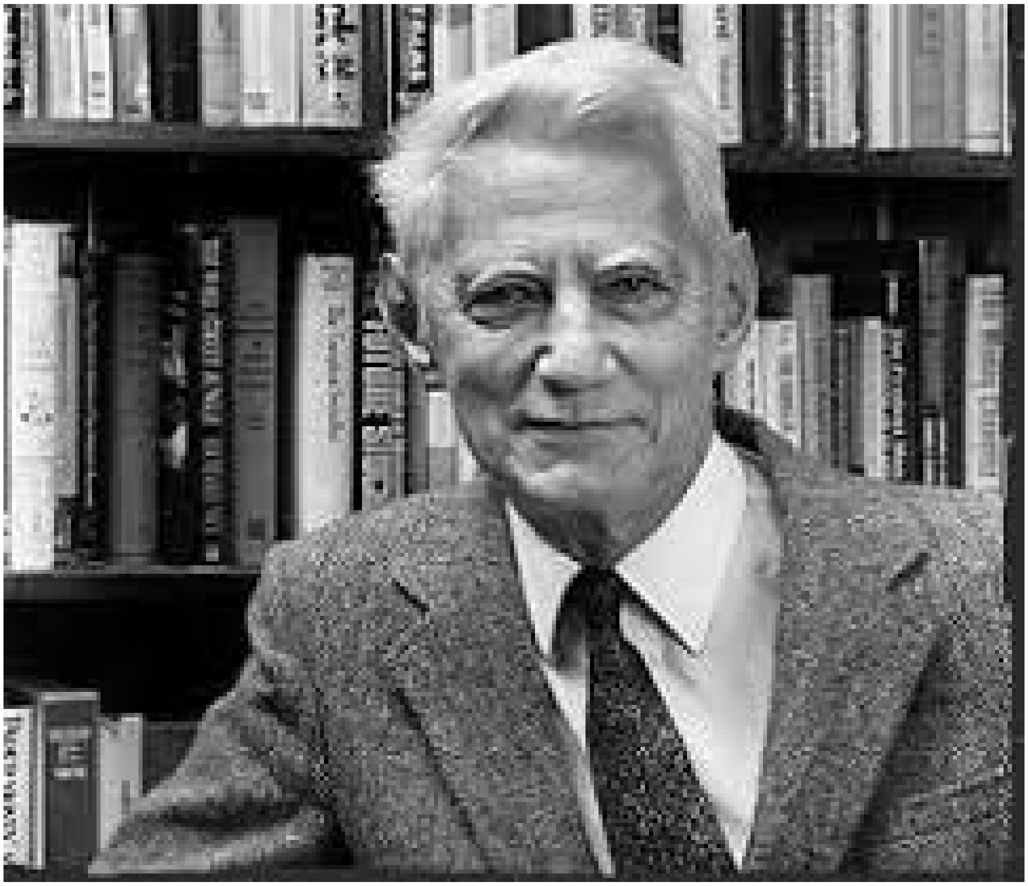

Figure 19.4: **A photograph of Claude Shannon.**

Figure 19.5: **John von Neumann, who advised Shannon to call missing information "entropy".**

information is $k \ln 2$, where k is Boltzmann's constant. We will discuss this relationship in more detail below.

Claude Shannon is usually considered to be the "father of information theory". Shannon graduated from the University of Michigan in 1936, and he later obtained a Ph.D. in mathematics from the Massachusetts Institute of Technology. He worked at the Bell Telephone Laboratories, and later became a professor at MIT. In 1949, motivated by the need of AT&T to quantify the amount of information that could be transmitted over a given line, Shannon published a pioneering study of information as applied to communication and computers. Shannon first examined the question of how many binary digits are needed to express a given integer Ω. In the decimal system we express an integer by telling how many 1's it contains, how many 10's, how many 100's, how many 1000's, and so on. Thus, for example, in the decimal system,

$$105 = 1 \times 10^2 + 0 \times 10^1 + 1 \times 10^0 \tag{19.6}$$

Any integer greater than or equal to 100 but less than 1000 can be expressed with 3 decimal digits; any number greater than or equal to 1000 but less than 10,000 requires 4, and so on.

The natural language of computers is the binary system; and therefore Shannon asked himself how many binary digits are needed to express an integer of a given size. In the binary system, a number is specified by telling how many of the various powers of 2 it contains. Thus, the decimal integer 105, expressed in the binary system, is

$$1101001 \equiv 1 \times 2^6 + 1 \times 2^5 + 0 \times 2^4 + 1 \times 2^3 + 0 \times 2^2 + 0 \times 2^1 + 1 \times 2^0 \tag{19.7}$$

In the many early computers, numbers and commands were read in on punched paper tape, which could either have a hole in a given position, or else no hole. Shannon wished to know how long a strip of punched tape is needed to express a number of a given size - how many binary digits are needed? If the number happens to be an exact power of 2, then the answer is easy: To express the integer

$$\Omega = 2^n \tag{19.8}$$

one needs $n + 1$ binary digits. The first binary digit, which is 1, gives the highest power of 2, and the subsequent digits, all of them 0, specify that the lower powers of 2 are absent. Shannon introduced the word "bit" as an abbreviation of "binary digit". He generalized this result to integers which are not equal to exact powers of 2: Any integer greater than or equal to 2^{n-l}, but less than 2^n, requires n binary digits or "bits". In Shannon's theory, the bit became the unit of information. He defined the quantity of information needed to express an arbitrary integer Ω as

$$I = \log_2 \Omega \text{bits} = \frac{\ln \Omega}{\ln 2} \text{ bits} = 1.442695 \;\; \ln \Omega \text{ bits} \tag{19.9}$$

or

$$I = K \ln \Omega \qquad\qquad K = 1.442695 \text{ bits} \tag{19.10}$$

Of course the information function I, as defined by equation (4.13), is in general not an integer, but if one wishes to find the exact number of binary digits required to express a given integer Ω, one can calculate I and round upwards[1].

Shannon went on to consider quantitatively the amount of information which is missing before we perform an experiment, the result of which we are unable to predict with certainty. (For example, the "experiment" might be flipping a coin or throwing a pair of dice.) Shannon first calculated the missing information, I_N, not for a single performance of the experiment but for N independent performances. Suppose that in a single performance, the probability that a particular result i will occur is given by P_i. If the experiment is performed N times, then as N becomes very large, the fraction of times that the result i occurs becomes more and more exactly equal to P_i. For example, if a coin is flipped N times, then as N becomes extremely large, the fraction of "heads" among the results becomes more and more nearly equal to 1/2. However, some information is still missing because we still do not know the sequence of the results. Shannon was able to show from combinatorial analysis, that this missing information about the sequence of the results is given by

$$I_N = K \ln \Omega \tag{19.11}$$

where

$$\Omega = \frac{N!}{n_1! n_2! n_3! ... n_i! ...} \qquad\qquad n_i \equiv N P_i \tag{19.12}$$

or

$$I_N = K \ln \Omega = K \left[\ln(N!) - \sum_i \ln(n_i) \right] \tag{19.13}$$

Shannon then used Sterling's approximation, $\ln(n_i!) \approx n_i(\ln n_i - 1)$, to rewrite (4.16) in the form

$$I_N = -KN \sum_i P_i \ln P_i \tag{19.14}$$

Finally, dividing by N, he obtained the missing information prior to the performance of a single experiment:

$$I = -K \sum_i P_i \ln P_i \tag{19.15}$$

For example, in the case of flipping a coin, Shannon's equation, (4.18), tells us that the missing information is

$$I = -K \left[\frac{1}{2} \ln \left(\frac{1}{2} \right) + \frac{1}{2} \ln \left(\frac{1}{2} \right) \right] = 1 \text{ bit} \tag{19.16}$$

As a second example, we might think of an "experiment" where we write the letters of the English alphabet on 26 small pieces of paper. We then place them in a hat and draw out one at random. In this second example,

$$P_a = P_b = ... = P_z = \frac{1}{26} \tag{19.17}$$

[1] Similar considerations can also be found in the work of the statistician R.A. Fisher.

and from Shannon's equation we can calculate that before the experiment is performed, the missing information is

$$I = -K\left[\frac{1}{26}\ln\left(\frac{1}{26}\right) + \frac{1}{26}\ln\left(\frac{1}{26}\right) + ...\right] = 4.70 \text{ bits} \tag{19.18}$$

If we had instead picked a letter at random out of an English book, the letters would not occur with equal probability. From a statistical analysis of the frequency of the letters, we would know in advance that

$$P_a = 0.078, \qquad P_b = 0.013, \qquad ... \qquad P_z = 0.001 \tag{19.19}$$

Shannon's equation would then give us a slightly reduced value for the missing information:

$$I = -K\left[0.078\ln 0.078 + 0.013\ln 0.013 + ...\right] = 4.15 \text{ bits} \tag{19.20}$$

Less information is missing when we know the frequencies of the letters, and Shannon's formula tells us exactly how much less information is missing.

When Shannon had been working on his equations for some time, he happened to visit the mathematician John von Neumann, who asked him how he was getting on with his theory of missing information. Shannon replied that the theory was in excellent shape, except that he needed a good name for "missing information". "Why don't you call it entropy?", von Neumann suggested. "In the first place, a mathematical development very much like yours already exists in Boltzmann's statistical mechanics, and in the second place, no one understands entropy very well, so in any discussion you will be in a position of advantage!" Like Leo Szilard, von Neumann was a Hungarian-American, and the two scientists were close friends. Thus von Neumann was very much aware of Szilard's paper on Maxwell's demon, with its analysis of the relationship between entropy and missing information. Shannon took von Neumann's advice, and used the word "entropy" in his pioneering paper on information theory. Missing information in general cases has come to be known as "Shannon entropy". But Shannon's ideas can also be applied to thermodynamics.

19.4 Entropy expressed as missing information

From the standpoint of information theory, the thermodynamic entropy S_N of an ensemble of N identical weakly-interacting systems in a given macrostate can be interpreted as the missing information which we would need in order to specify the state of each system, i.e. the microstate of the ensemble. Thus, thermodynamic information is defined to be the negative of thermodynamic entropy, i.e. the information that would be needed to specify the microstate of an ensemble in a given macrostate. Shannon's formula allows this missing information to be measured quantitatively. Applying Shannon's formula, equation (4.13), to the missing information in Boltzmann's problem we can identify W with Ω, S_N with I_N, and k with K:

$$W \to \Omega \qquad S_N \to I_N \qquad k \to K = \frac{1}{\ln 2} \text{ bits} \tag{19.21}$$

so that

$$k \ln 2 = 1 \text{ bit} = 0.95697 \times 10^{-23} \, \frac{\text{joule}}{\text{kelvin}} \tag{19.22}$$

and

$$k = 1.442695 \text{ bits} \tag{19.23}$$

This implies that temperature has the dimension energy/bit:

$$1 \text{ degree Kelvin} = 0.95697 \times 10^{-23} \, \frac{\text{joule}}{\text{bit}} \tag{19.24}$$

From this it follows that

$$1 \, \frac{\text{joule}}{\text{kelvin}} = 1.04496 \times 10^{23} \text{ bits} \tag{19.25}$$

If we divide equation (4.28) by Avogadro's number we have

$$1 \, \frac{\text{joule}}{\text{kelvin mol}} = \frac{1.04496 \times 10^{23} \text{ bits/molecule}}{6.02217 \times 10^{23} \text{ molecules/mol}} = 0.17352 \, \frac{\text{bits}}{\text{molecule}} \tag{19.26}$$

Figure 4.1 shows the experimentally-determined entropy of ammonia, NH_3, as a function of the temperature, measured in kelvins. It is usual to express entropy in joule/kelvin-mol; but it follows from equation (4.29) that entropy can also be expressed in bits/molecule, as is shown in the figure. Since

$$1 \text{ electron volt} = 1.6023 \times 10^{-19} \text{ joule} \tag{19.27}$$

it also follows from equation (4.29) that

$$1 \, \frac{\text{electron volt}}{\text{kelvin}} = 1.6743 \times 10^{4} \text{ bits} \tag{19.28}$$

Thus, one electron-volt of energy, converted into heat at room temperature, T =298.15 kelvin, will produce an entropy change (or thermodynamic information change) of

$$\frac{1 \text{ electron volt}}{298.15 \text{ kelvin}} = 56.157 \text{ bits} \tag{19.29}$$

When a system is in thermodynamic equilibrium, its entropy has reached a maximum; but if it is not in equilibrium, its entropy has a lower value. For example, let us think of the case which was studied by Clausius when he introduced the concept of entropy: Clausius imagined an isolated system, divided into two parts, one of which has a temperature T_i, and the other a lower temperature, T_2. When heat is transferred from the hot part to the cold part, the entropy of the system increases; and when equilibrium is finally established at some uniform intermediate temperature, the entropy has reached a maximum. The difference in entropy between the initial state of Clausius' system and its final state is a measure of how far away from thermodynamic equilibrium it was initially. From the discussion given above, we can see that it is also possible to interpret this entropy difference as the system's initial content of thermodynamic information.

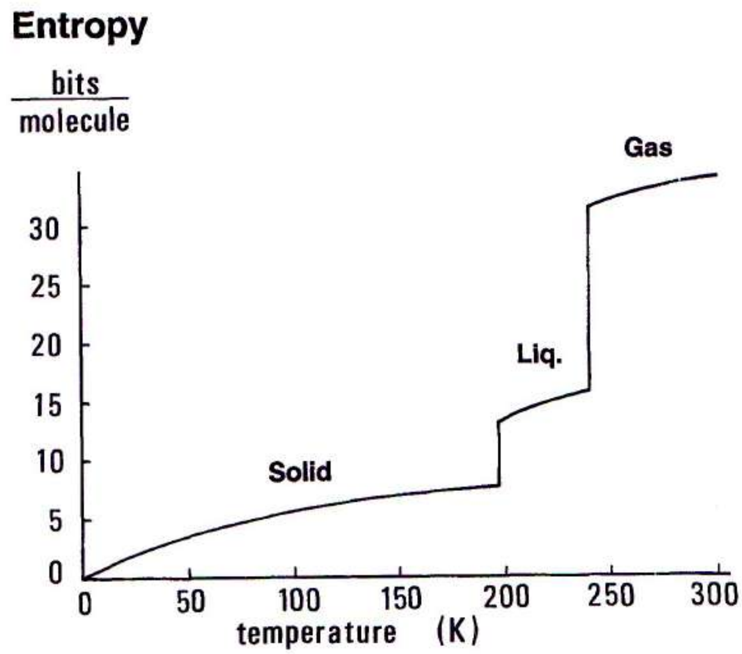

Figure 19.6: This figure shows the entropy of ammonia as a function of temperature. It is usual to express entropy in joule/kelvin-mol, but it can also be expressed in bits/molecule.

Similarly, when a photon from the sun reaches (for example) a drop of water on the earth, the initial entropy of the system consisting of the photon plus the drop of water is smaller than at a later stage, when the photon's energy has been absorbed and shared among the water molecules, with a resulting very slight increase in the temperature of the water. This entropy difference can be interpreted as the quantity of thermodynamic information which was initially contained in the photon-drop system, but which was lost when the photon's free energy was degraded into heat. Equation (4.32) allows us to express this entropy difference in terms of bits. For example, if the photon energy is 2 electron-volts, and if the water drop is at a temperature of 298.15 degrees Kelvin, then $\Delta S = 112.31$ bits; and this amount of thermodynamic information is available in the initial state of the system. In our example, the information is lost; but if the photon had instead reached the leaf of a plant, part of its energy, instead of being immediately degraded, might have been stabilized in the form of high-energy chemical bonds. When a part of the photon energy is thus stabilized, not all of the thermodynamic information which it contains is lost; a part is conserved and can be converted into other forms of information.

19.5 Cybernetic information compared with thermodynamic information

From the discussion given above we can see that there is a close analogy between Shannon entropy and thermodynamic entropy, as well as a close analogy between cybernetic information and thermodynamic information. However, despite the close analogies, there are important differences between Shannon's quantities and those of Boltzmann. Cybernetic information (also called semiotic information) is an abstract quantity related to messages, regardless of the physical form through which the messages are expressed, whether it is through electrical impulses, words written on paper, or sequences of amino acids. Thermodynamic information, by contrast, is a temperature-dependent and size-dependent physical quantity. Doubling the size of the system changes its thermodynamic information content; but neither doubling the size of a message written on paper, nor warming the message will change its cybernetic information content. Furthermore, many exact copies of a message do not contain more cybernetic information than the original message.

The evolutionary process consists in making many copies of a molecule or a larger system. The multiple copies then undergo random mutations; and after further copying, natural selection preserves those mutations that are favorable. It is thermodynamic information that drives the copying process, while the selected favorable mutations may be said to contain cybernetic information.

19.6 The information content of Gibbs free energy

At the beginning of this chapter, we mentioned that the American physicist Josiah Willard Gibbs (1839-1903) made many contributions to thermodynamics and statistical mechanics. In 1863, Gibbs received from Yale the first Ph.D. in engineering granted in America, and after a period of further study in Prance and Germany, he became a professor of mathematical physics at Yale in 1871, a position which he held as long as he lived. During the period between 1876 and 1878, he published a series of papers in the *Transactions of the Connecticut Academy of Sciences*. In these papers, about 400 pages in all, Gibbs applied thermodynamics to chemical reactions. (The editors of the *Transactions of the Connecticut Academy of Sciences* did not really understand Gibbs' work, but, as they said later, "We knew Gibbs, and we took his papers on faith".)

Because the journal was an obscure one, and because Gibbs' work was so highly mathematical, it remained almost unknown to European scientists for a long period. However, in 1892 Gibbs' papers were translated into German by Ostwald, and in 1899 they were translated into French by Le Chatelier; and then the magnitude of Gibbs' contribution was finally recognized. One of his most important innovations was the definition of a quantity which we now call "Gibbs free energy". This quantity allows one to determine whether or not a chemical reaction will take place spontaneously.

Chemical reactions usually take place at constant pressure and constant temperature. If a reaction produces a gas as one of its products, the gas must push against the pressure of the earth's atmosphere to make a place for itself. In order to take into account the work done against external pressure in energy relationships, the German physiologist and physicist Hermann von Helmholtz introduced a quantity (which we now call heat content or enthalpy) defined by

$$H = U + PV \tag{19.30}$$

where U is the internal energy of a system, P is the pressure, and V is the system's volume.

Gibbs went one step further than Helmholtz, and defined a quantity which would also take into account the fact that when a chemical reaction takes place, heat is exchanged with the surroundings. Gibbs defined his free energy by the relation

$$G = U + PV - TS \tag{19.31}$$

or

$$G = H - TS \tag{19.32}$$

where S is the entropy of a system, H is its enthalpy, and T is its temperature.

Gibbs' reason for introducing the quantity G is as follows: The second law of thermodynamics states that in any spontaneous process, the entropy of the universe increases. Gibbs invented a simple model of the universe, consisting of the system (which might, for example, be a beaker within which a chemical reaction takes place) in contact with a large thermal reservoir at constant temperature. The thermal reservoir could, for example, be a water bath so large that whatever happens in the chemical reaction, the temperature of the bath will remain essentially unaltered. In Gibbs' simplified model, the entropy change of the universe produced by the chemical reaction can be split into two components:

$$\Delta S_{universe} = \Delta S_{system} + \Delta S_{bath} \tag{19.33}$$

Now suppose that the reaction is endothermic (i.e. it absorbs heat). Then the reaction beaker will absorb an amount of heat ΔH_{system} from the bath, and the entropy change of the bath will be

$$\Delta S_{bath} = -\frac{\Delta H_{system}}{T} \tag{19.34}$$

Combining (4.36) and (4.37) with the condition requiring the entropy of the universe to increase, Gibbs obtained the relationship

$$\Delta S_{universe} = \Delta S_{system} - \frac{\Delta H_{system}}{T} > 0 \tag{19.35}$$

The same relationship also holds for exothermic reactions, where heat is transferred in the opposite direction. Combining equations (4.38) and (4.35) yields

$$\Delta G_{system} = -T\Delta S_{universe} < 0 \tag{19.36}$$

Thus, the Gibbs free energy for a system must decrease in any spontaneous chemical reaction or process which takes place at constant temperature and pressure. We can also see from equation (4.39) that Gibbs free energy is a measure of a system's content of thermodynamic information. If the available free energy is converted into heat, the quantity of thermodynamic information $\Delta S_{universe} = -\Delta G_{system}/T$ is lost, and we can deduce that in the initial state of the system, this quantity of information was available. Under some circumstances the available thermodynamic information can be partially conserved. In living organisms, chemical reactions are coupled together, and Gibbs free energy, with its content of thermodynamic information, can be transferred from one compound to another, and ultimately converted into other forms of information.

Measured values of the "Gibbs free energy of formation", ΔG_f°, are available for many molecules. To construct tables of these values, the change in Gibbs free energy is measured when the molecules are formed from their constituent elements. The most stable states of the elements at room temperature and atmospheric pressure are taken as zero points. For example, water in the gas phase has a Gibbs free energy of formation

$$\Delta G_f^\circ(H_2O) = -228.59 \ \frac{\text{kJ}}{\text{mol}} \tag{19.37}$$

This means that when the reaction

$$H_2(g) + \frac{1}{2}O_2(g) \to H_2O(g) \tag{19.38}$$

takes place under standard conditions, there is a change in Gibbs free energy of $\Delta G^\circ =$ –228.59 kJ/mol [2]. The elements hydrogen and oxygen in their most stable states at room temperature and atmospheric pressure are taken as the zero points for Gibbs free energy of formation. Since ΔG° is negative for the reaction shown in equation (4.41), the reaction is spontaneous. In general, the change in Gibbs free energy in a chemical reaction is given by

$$\Delta G^\circ = \sum_{products} \Delta G_f^\circ - \sum_{reactants} \Delta G_f^\circ \tag{19.39}$$

where ΔG_f° denotes the Gibbs free energy of formation.

As a second example, we can consider the reaction in which glucose is burned:

$$C_6H_{12}O_6(s) + 6O_2(g) \to 6CO_2(g) + 6H_2O(g) \qquad \Delta G^\circ = -2870 \ \frac{\text{kJ}}{\text{mol}} \tag{19.40}$$

From equation (4.29) it follows that in this reaction,

$$-\frac{\Delta G^\circ}{T} = 1670 \ \frac{\text{bits}}{\text{molecule}} \tag{19.41}$$

If the glucose is simply burned, this amount of information is lost; but in a living organism, the oxidation of glucose is usually coupled with other reactions in which a part of the

[2] The superscript $^\circ$ means "under standard conditions", while kJ is an abbreviation for joule$\times 10^3$.

available thermodynamic information is stored, or utilized to do work, or perhaps converted into other forms of information.

The oxidation of glucose illustrates the importance of enzymes and specific coupling mechanisms in biology. A lump of glucose can sit for years on a laboratory table, fully exposed to the air. Nothing will happen. Even though the oxidation of glucose is a spontaneous process - even though the change in Gibbs free energy produced by the reaction would be negative - even though the state of the universe after the reaction would be much more probable than the initial state, the reaction does not take place, or at least we would have to wait an enormously long time to see the glucose oxidized, because the reaction pathway is blocked by potential barriers.

Suggestions for further reading

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Appendix A

TABLES OF DIFFERENTIALS, INTEGRALS AND SERIES

In the tables shown below, f and g are functions of t, while a and C are constants. The tables include

- Some fundemental differentials
- Some fundemental indefinite integrals
- A few important definite integrals
- Series expansions of functions

Table A.1: **Some fundemental differentials**

$\frac{d}{dt}\left[t^p\right]$	$=$	pt^{p-1}
$\frac{d}{dt}\left[f+g\right]$	$=$	$\frac{df}{dt}+\frac{dg}{dt}$
$\frac{d}{dt}\left[fg\right]$	$=$	$f\frac{dg}{dt}+g\frac{df}{dt}$
$\frac{d}{dt}\left[\frac{f}{g}\right]$	$=$	$\frac{1}{g^2}\left[g\frac{df}{dt}-f\frac{dg}{dt}\right]$
$\frac{d}{dt}\left[e^{at}\right]$	$=$	ae^{at}
$\frac{d}{dt}\left[ln(t)\right]$	$=$	$\frac{1}{t}$
$\frac{d}{dt}\left[f(g)\right]$	$=$	$\frac{df}{dg}\frac{dg}{dt}$
$\frac{d}{dt}\left[\sin(at)\right]$	$=$	$a\cos(at)$

Table A.2: **Some fundemental differentials (continued)**

$\dfrac{d}{dt}\left[\cos(at)\right]$	$=$	$-a\sin(at)$
$\dfrac{d}{dt}\left[\sinh(at)\right]$	$=$	$a\cosh(at)$
$\dfrac{d}{dt}\left[\cosh(at)\right]$	$=$	$a\sinh(at)$
$\dfrac{d}{dt}\left[\sin^{-1}(t)\right]$	$=$	$\dfrac{1}{\sqrt{1-t^2}}$
$\dfrac{d}{dt}\left[\cos^{-1}(t)\right]$	$=$	$\dfrac{-1}{\sqrt{1-t^2}}$
$\dfrac{d}{dt}\left[\tan^{-1}(t)\right]$	$=$	$\dfrac{1}{1+t^2}$
$\dfrac{d}{dt}\left[\cot^{-1}(t)\right]$	$=$	$\dfrac{-1}{1+t^2}$

Table A.3: **Some fundemental indefinite integrals**

$\int dt\ t^p$	$=$	$\dfrac{t^{p+1}}{p+1} + C$	$p \neq -1$
$\int dt\ t^{-1}$	$=$	$\ln(t) + C$	
$\int dt\ e^{at}$	$=$	$\dfrac{e^{at}}{a} + C$	
$\int dt\ \cos(at)$	$=$	$\dfrac{\sin(at)}{a} + C$	
$\int dt\ \sin(at)$	$=$	$-\dfrac{\cos(at)}{a} + C$	
$\int dt\ \sinh(at)$	$=$	$\dfrac{\cosh(at)}{a} + C$	
$\int dt\ \cosh(at)$	$=$	$\dfrac{\sinh(at)}{a} + C$	

Table A.4: **A few important definite integrals**

$\int_0^\infty dt\ t^n e^{-at}$	$=$	$\frac{n!}{a^{n+1}}$	$n =$ positive integer
$\int_0^\infty dt\ t^{2n} e^{-at^2}$	$=$	$\frac{(2n-1)!!}{2^{n+1}a^n}\sqrt{\frac{\pi}{a}}$	$n =$ integer
$\int_0^\infty dt\ t^p e^{-t}$	$\equiv$	$\Gamma(p+1)$	
$\int_0^\infty dt\ \frac{a}{a^2+t^2}$	$=$	$\pm\frac{\pi}{2}$	$\pm\, a > 0,\ a$ real
$\int_0^\infty dt\ \frac{t^{p-1}}{1+t}$	$=$	$\frac{\pi}{\sin(p\pi)}$	$1 > p > 0,\ p$ real
$\int_0^\infty dt\ \frac{\sin^2(t)}{t^2}$	$=$	$\frac{\pi}{2}$	
$\int_0^\infty dt\ \frac{\sin(at)}{t}$	$=$	$\frac{\pi}{2}$	$a > 0$
$\int_0^\pi dt\ \sin^2(nt)$	$=$	$\frac{\pi}{2}$	$n =$ integer
$\int_0^\pi dt\ \cos^2(nt)$	$=$	$\frac{\pi}{2}$	$n =$ integer
$\int_0^\pi dt\ \sin(nt)\sin(mt)$	$=$		$n,\ m =$ integers $n \neq m$
$\int_0^\pi dt\ \cos(nt)\cos(mt)$	$=$		$n,\ m =$ integers $n \neq m$

Table A.5: **Series expansions of functions**

e	$=$	$1+\frac{1}{1!}+\frac{1}{2!}+\frac{1}{3!}+\frac{1}{4!}+\frac{1}{5!}+\cdots$	
e^t	$=$	$1+\frac{t}{1!}+\frac{t^2}{2!}+\frac{t^3}{3!}+\frac{t^4}{4!}+\frac{t^5}{5!}+\cdots$	
a^t	$=$	$1+\frac{t\ln(a)}{1!}+\frac{[t\ln(a)]^2}{2!}+\frac{[t\ln(a)]^3}{3!}+\cdots$	
e^t	$=$	$1+\frac{t}{1!}+\frac{t^2}{2!}+\frac{t^3}{3!}+\frac{t^4}{4!}+\frac{t^5}{5!}+\cdots$	
$\ln(1+t)$	$=$	$\frac{t}{1!}-\frac{t^2}{2!}+\frac{t^3}{3!}-\frac{t^4}{4!}+\frac{t^5}{5!}+\cdots$	$-1<t\leq 1$
$\cos(t)$	$=$	$1-\frac{t^2}{2!}+\frac{t^4}{4!}-\frac{t^6}{6!}+\cdots$	
$\sin(t)$	$=$	$\frac{t}{1!}-\frac{t^3}{3!}+\frac{t^5}{5!}-\frac{t^7}{7!}+\cdots$	
$\cosh(t)$	$=$	$1+\frac{t^2}{2!}+\frac{t^4}{4!}+\frac{t^6}{6!}+\cdots$	
$\sinh(t)$	$=$	$t+\frac{t^3}{3!}+\frac{t^5}{5!}+\frac{t^7}{7!}+\cdots$	

Appendix B

THE HISTORY OF COMPUTERS

B.1 Pascal and Leibniz

If civilization survives, historians in the distant future will undoubtedly regard the invention of computers as one of the most important steps in human cultural evolution - as important as the invention of writing or the invention of printing. The possibilities of artificial intelligence have barely begun to be explored, but already the impact of computers on society is enormous.

The invention of transisters was a crucial step in the history of computers, and this invention in turn depended on the development of quantum theory. Thus quantum theory, despite its highly abstract nature, has had an enormous impact on the modern world.

The first programmable universal computers were completed in the mid-1940's; but they had their roots in the much earlier ideas of Blaise Pascal (1623-1662), Gottfried Wilhelm Leibniz (1646-1716), Joseph Marie Jacquard (1752-1834) and Charles Babbage (1791-1871).

In 1642, the distinguished French mathematician and philosopher Blaise Pascal completed a working model of a machine for adding and subtracting. According to tradition, the idea for his "calculating box" came to Pascal when, as a young man of 17, he sat thinking of ways to help his father (who was a tax collector). In describing his machine, Pascal wrote: "I submit to the public a small machine of my own invention, by means of which you alone may, without any effort, perform all the operations of arithmetic, and may be relieved of the work which has often times fatigued your spirit when you have worked with the counters or with the pen."

Pascal's machine worked by means of toothed wheels. It was much improved by Leibniz, who constructed a mechanical calculator which, besides adding and subtracting, could also multiply and divide. His first machine was completed in 1671; and Leibniz' description of it, written in Latin, is preserved in the Royal Library at Hanover: "There are two parts of the machine, one designed for addition (and subtraction), and the other designed for multiplication (and division); and they should fit together. The adding (and subtracting) machine coincides completely with the calculating box of Pascal. Something, however,

Figure B.1: **Blaise Pascal (1623-1662) was a French mathematician, physicist, writer, inventor and theologian. Pascal, a child prodigy, was educated by his father, who was a tax-collector. He invented his calculating box to make his father's work less tedious.**

Figure B.2: **The German mathematician, philosopher and universal genius Gottfried Wilhelm von Leibniz (1646-1716) was a contemporary of Isaac Newton. He invented differential and integral calculus independently, just as Newton had done many years earlier. However, Newton had not published his work on calculus, and thus a bitter controversy over priority was precipitated. When his patron, the Elector of Hanover moved to England to become George I, Leibniz was left behind because the Elector feared that the controversy would alienate the English. Leibniz extended Pascal's calculating box so that it could perform multiplication and division. Calculators of his design were still being used in the 1960's.**

must be added for the sake of multiplication..."

"The wheels which represent the multiplicand are all of the same size, equal to that of the wheels of addition, and are also provided with ten teeth which, however, are movable so that at one time there should protrude 5, at another 6 teeth, etc., according to whether the multiplicand is to be represented five times or six times, etc."

"For example, the multiplicand 365 consists of three digits, 3, 6, and 5. Hence the same number of wheels is to be used. On these wheels, the multiplicand will be set if from the right wheel there protrude 5 teeth, from the middle wheel 6, and from the left wheel 3."

B.2 Jacquard and Babbage

By 1810, calculating machines based on Leibniz' design were being manufactured commercially; and mechanical calculators of a similar (if much improved) design could be found in laboratories and offices until the 1960's. The idea of a programmable universal computer is due to the English mathematician, Charles Babbage, who was the Lucasian Professor of

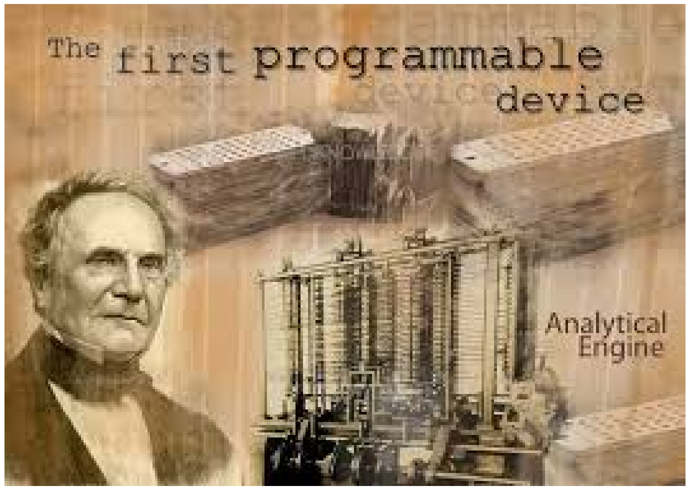

Figure B.3: **Charles Babbage (1791-1871) and his analytical engine.**

Mathematics at Cambridge University. (In the 17th century, Isaac Newton held this post, and in the 20th century, P.A.M. Dirac and Stephen Hawking also held it.)

In 1812, Babbage conceived the idea of constructing a machine which could automatically produce tables of functions, provided that the functions could be approximated by polynomials. He constructed a small machine, which was able to calculate tables of quadratic functions to eight decimal places, and in 1832 he demonstrated this machine to the Royal Society and to representatives of the British government.

The demonstration was so successful that Babbage secured financial support for the construction of a large machine which would tabulate sixth-order polynomials to twenty decimal places. The large machine was never completed, and twenty years later, after having spent seventeen thousand pounds on the project, the British government withdrew its support. The reason why Babbage's large machine was never finished can be understood from the following account by Lord Moulton of a visit to the mathematician's laboratory:

"One of the sad memories of my life is a visit to the celebrated mathematician and inventor, Mr. Babbage. He was far advanced in age, but his mind was still as vigorous as ever. He took me through his workrooms."

"In the first room I saw the parts of the original Calculating Machine, which had been shown in an incomplete state many years before, and had even been put to some use. I asked him about its present form. 'I have not finished it, because in working at it, I came on the idea of my Analytical Machine, which would do all that it was capable of doing, and much more. Indeed, the idea was so much simpler that it would have taken more work to complete the Calculating Machine than to design and construct the other in its entirety; so I turned my attention to the Analytical Machine.'"

"After a few minutes talk, we went into the next workroom, where he showed me the working of the elements of the Analytical Machine. I asked if I could see it. 'I have never completed it,' he said, 'because I hit upon the idea of doing the same thing by a different and far more effective method, and this rendered it useless to proceed on the old lines.'"

Figure B.4: **Joseph Marie Jacquard (1752-1834) invented a loom which could be programed to produce any design by means of punched cards. News of his invention inspired Babbage to invent a universal programmable computing machine.**

"Then we went into a third room. There lay scattered bits of mechanism, but I saw no trace of any working machine. Very cautiously I approached the subject, and received the dreaded answer: 'It is not constructed yet, but I am working at it, and will take less time to construct it altogether than it would have taken to complete the Analytical Machine from the stage in which I left it.' I took leave of the old man with a heavy heart."

Babbage's first calculating machine was a special-purpose mechanical computer, designed to tabulate polynomial functions; and he abandoned this design because he had hit on the idea of a universal programmable computer. Several years earlier, the French inventor Joseph Marie Jacquard had constructed an automatic loom in which large wooden "punched cards" were used to control the warp threads. Inspired by Jacquard's invention, Babbage planned to use punched cards to program his universal computer. (Jacquard's looms could be programmed to weave extremely complex patterns: A portrait of the inventor, woven on one of his looms in Lyon, hung in Babbage's drawing room.)

One of Babbage's frequent visitors was Augusta Ada[1], Countess of Lovelace (1815-1852), the daughter of Lord and Lady Byron. She was a mathematician of considerable ability, and it is through her lucid descriptions that we know how Babbage's never-completed Analytical Machine was to have worked.

[1] The programming language ADA is named after her.

Figure B.5: **Jacquard's loom.**

Figure B.6: **Lord Byron's daughter, Augusta Ada, Countess of Lovelace (1815-1852) was an accomplished mathematician and a frequent visitor to Babbage's workshop. It is through her lucid description of his ideas that we know how Babbage's universal calculating machine was to have worked. The programming language ADA is named after her.**

B.3 Harvard's sequence-controlled calculator

The next step towards modern computers was taken by Herman Hollerith, a statistician working for the United States Bureau of the Census. He invented electromechanical machines for reading and sorting data punched onto cards. Hollerith's machines were used to analyze the data from the 1890 United States Census. Because the Census Bureau was a very limited market, Hollerith branched out and began to manufacture similar machines for use in business and administration. His company was later bought out by Thomas J. Watson, who changed its name to International Business Machines.

In 1937, Howard Aiken, of Harvard University, became interested in combining Babbage's ideas with some of the techniques which had developed from Hollerith's punched card machines. He approached the International Business Machine Corporation, the largest manufacturer of punched card equipment, with a proposal for the construction of a large, automatic, programmable calculating machine.

Aiken's machine, the Automatic Sequence Controlled Calculator (ASCC), was completed in 1944 and presented to Harvard University. Based on geared wheels, in the Pascal-Leibniz-Babbage tradition, ASCC had more than three quarters of a million parts and used 500 miles of wire. ASCC was unbelievably slow by modern standards - it took three-tenths of a second to perform an addition - but it was one of the first programmable general-purpose digital computers ever completed. It remained in continuous use, day and night, for fifteen years.

Figure B.7: **The Automatic Sequence-Controlled Calculator ASCC can still be seen by visitors at Harvard's science building and cafeteria.**

B.4 The first electronic computers

In the ASCC, binary numbers were represented by relays, which could be either on or off. The on position represented 1, while the off position represented 0, these being the only two digits required to represent numbers in the binary (base 2) system. Electromechanical calculators similar to ASCC were developed independently by Konrad Zuse in Germany and by George R. Stibitz at the Bell Telephone Laboratory.

Electronic digital computers

In 1937, the English mathematician A.M. Turing published an important article in the Proceedings of the London Mathematical Society in which envisioned a type of calculating machine consisting of a long row of cells (the "tape"), a reading and writing head, and a set of instructions specifying the way in which the head should move the tape and modify the state and "color" of the cells on the tape. According to a hypothesis which came to be known as the "Church-Turing hypothesis", the type of computer proposed by Turing was capable of performing every possible type of calculation. In other words, the Turing machine could function as a universal computer.

In 1943, a group of English engineers, inspired by the ideas of Alan Turing and those of the mathematician M.H.A. Newman, completed the electronic digital computer Colossus. Colossus was the first large-scale electronic computer. It was used to break the German Enigma code; and it thus affected the course of World War II.

In 1946, ENIAC (Electronic Numerical Integrator and Calculator) became operational. This general-purpose computer, designed by J.P. Eckert and J.W. Mauchley of the University of Pennsylvania, contained 18,000 vacuum tubes, one or another of which was often out of order. However, during the periods when all its vacuum tubes were working, an electronic computer like Colossus or ENIAC could shoot ahead of an electromechanical machine (such as ASCC) like a hare outdistancing a tortoise.

During the summer of 1946, a course on "The Theory and Techniques of Electronic Digital Computers" was given at the University of Pennsylvania. The ideas put forward in this course had been worked out by a group of mathematicians and engineers headed by J.P. Eckert, J.W. Mauchley and John von Neumann, and these ideas very much influenced all subsequent computer design.

Cybernetics

The word "Cybernetics", was coined by the American mathematician Norbert Wiener (1894-1964) and his colleagues, who defined it as "the entire field of control and communication theory, whether in the machine or in the animal". Wiener derived the word from the Greek term for "steersman".

Norbert Wiener began life as a child prodigy: He entered Tufts University at the age of 11 and received his Ph.D. from Harvard at 19. He later became a professor of mathematics at the Massachusetts Institute of Technology. In 1940, with war on the horizon,

Figure B.8: **Alan Turing (1912-1954). He is considered to be the father of theoretical computer science. During World War II, Turing's work allowed the allies to crack the German's code. This appreciably shortened the length of the war in Europe, and saved many lives.**

Figure B.9: **John von Neumann (1903-1957, right) with J. Robert Oppenheimer. In the background is an electronic digital computer.**

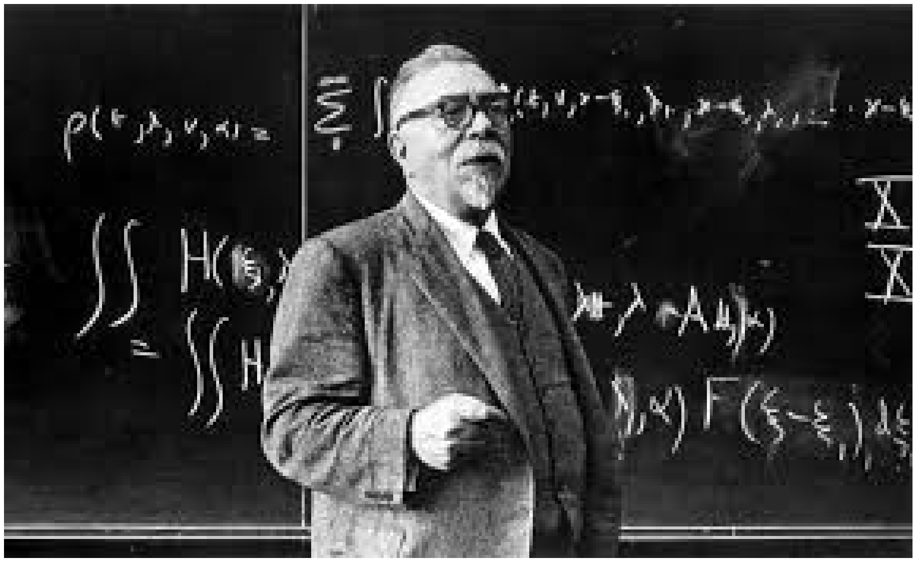

Figure B.10: **MIT's Norbert Wiener (1894-1964) coined the word "Cybernetics", derived from a Greek word meaning "steersman". Wiener was one of the principle organizers of the Macy Conferences.**

Wiener sent a memorandum to Vannevar Bush, another MIT professor who had done pioneering work with analogue computers, and had afterwards become the chairman of the U.S. National Defense Research Committee. Wiener's memorandum urged the American government to support the design and construction of electronic digital computers, which would make use of binary numbers, vacuum tubes, and rapid memories. In such machines, the memorandum emphasized, no human intervention should be required except when data was to be read into or out of the machine.

Like Leo Szilard, John von Neumann, Claude Shannon and Erwin Schrödinger, Norbert Wiener was aware of the relation between information and entropy. In his 1948 book Cybernetics he wrote: "...we had to develop a statistical theory of the amount of information, in which the unit amount of information was that transmitted by a single decision between equally probable alternatives. This idea occurred at about the same time to several writers, among them the statistician R.A. Fisher, Dr. Shannon of Bell Telephone Laboratories, and the author. Fisher's motive in studying this subject is to be found in classical statistical theory; that of Shannon in the problem of coding information; and that of the author in the problem of noise and message in electrical filters... The notion of the amount of information attaches itself very naturally to a classical notion in statistical mechanics: that of entropy. Just as the amount of information in a system is a measure of its degree of organization, so the entropy of a system is a measure of its degree of disorganization; and the one is simply the negative of the other."

During World War II, Norbert Wiener developed automatic systems for control of anti-aircraft guns. His systems made use of feedback loops closely analogous to those with which animals coordinate their movements. In the early 1940's, he was invited to attend a

Figure B.11: **Margaret Mead (1901-1978) and Gregory Bateson (1904-1980). They used the feedback loops studied by Wiener to explain many aspects of human behavior. Bateson is considered to be one of the main founders of the discipline Biosemiotics, which considers information to be the central feature of living organisms.**

series of monthly dinner parties organized by Arturo Rosenbluth, a professor of physiology at Harvard University. The purpose of these dinners was to promote discussions and collaborations between scientists belonging to different disciplines. The discussions which took place at these dinners made both Wiener and Rosenbluth aware of the relatedness of a set of problems that included homeostasis and feedback in biology, communication and control mechanisms in neurophysiology, social communication among animals (or humans), and control and communication involving machines.

Wiener and Rosenbluth therefore tried to bring together workers in the relevant fields to try to develop common terminology and methods. Among the many people whom they contacted were the anthropologists Gregory Bateson and Margaret Mead, Howard Aiken (the designer of the Automatic Sequence Controlled Calculator), and the mathematician John von Neumann. The Josiah Macy Jr. Foundation sponsored a series of ten yearly meetings, which continued until 1949 and which established cybernetics as a new research discipline. It united areas of mathematics, engineering, biology, and sociology which had previously been considered unrelated. Among the most important participants (in addition to Wiener, Rosenbluth, Bateson, Mead, and von Neumann) were Heinz von Foerster, Kurt Lewin, Warren McCulloch and Walter Pitts. The Macy conferences were small and informal, with an emphasis on discussion as opposed to the presentation of formal papers. A stenographic record of the last five conferences has been published, edited by von Foerster. Transcripts of the discussions give a vivid picture of the enthusiastic and creative atmosphere of the meetings. The participants at the Macy Conferences perceived Cybernetics as a much-needed bridge between the natural sciences and the humanities. Hence their enthusiasm. Weiner's feedback loops and von Neumann's theory of games were used by anthropologists Mead and Bateson to explain many aspects of human behavior.

B.5 Biosemiotics

The Oxford Dictionary of Biochemistry and Molecular Biology (Oxford University Press, 1997) defines Biosemiotics as "the study of signs, of communication, and of information in living organisms". The biologists Claus Emmeche and K. Kull offer another definition of Biosemiotics: "biology that interprets living systems as sign systems".

The American philosopher Charles Sanders Peirce (1839-1914) is considered to be one of the founders of Semiotics (and hence also of Biosemiotics). Peirce studied philosophy and chemistry at Harvard, where his father was a professor of mathematics and astronomy. He wrote extensively on philosophical subjects, and developed a theory of signs and meaning which anticipated many of the principles of modern Semiotics. Peirce built his theory on a triad: (1) the sign, which represents (2) something to (3) somebody. For example, the sign might be a broken stick, which represents a trail to a hunter, it might be the arched back of a cat, which represents an aggressive attitude to another cat, it might be the waggle-dance of a honey bee, which represents the coordinates of a source of food to her hive-mates, or it might be a molecule of trans-10-cis-hexadecadienol, which represents irresistible sexual temptation to a male moth of the species Bombyx mori. The sign might be a sequence of nucleotide bases which represents an amino acid to the ribosome-transfer-RNA system, or it might be a cell-surface antigen which represents self or non-self to the immune system. In information technology, the sign might be the presence or absence of a pulse of voltage, which represents a binary digit to a computer. Semiotics draws our attention to the sign and to its function, and places much less emphasis on the physical object which forms the sign. This characteristic of the semiotic viewpoint has been expressed by the Danish biologist Jesper Hoffmeyer in the following words: "The sign, rather than the molecule, is the basic unit for studying life."

A second important founder of Biosemiotics was Jakob von Uexküll (1864-1944). He was born in Estonia, and studied zoology at the University of Tartu. After graduation, he worked at the Institute of Physiology at the University of Heidelberg, and later at the Zoological Station in Naples. In 1907, he was given an honorary doctorate by Heidelberg

Figure B.12: **Charles Sanders Pearce (1839-1914).**

Figure B.13: **Jakob Johann Baron von Uexküll (1964-1944). Together with Pearce and Bateson, he is one of the principle founders of Biosemiotics.**

for his studies of the physiology of muscles. Among his discoveries in this field was the first recognized instance of negative feedback in an organism. Von Uexküll's later work was concerned with the way in which animals experience the world around them. To describe the animal's subjective perception of its environment he introduced the word Umwelt; and in 1926 he founded the Institut fur Umweltforschung at the University of Heidelberg. Von Uexküll visualized an animal - for example a mouse - as being surrounded by a world of its own - the world conveyed by its own special senses organs, and processed by its own interpretative systems. Obviously, the Umwelt will differ greatly depending on the organism. For example, bees are able to see polarized light and ultraviolet light; electric eels are able to sense their environment through their electric organs; many insects are extraordinarily sensitive to pheromones; and a dog's Umwelt far richer in smells than that of most other animals. The Umwelt of a jellyfish is very simple, but nevertheless it exists.[2] Von Uexküll's Umwelt concept can even extend to one-celled organisms, which receive chemical and tactile signals from their environment, and which are often sensitive to light. The ideas and research of Jakob von Uexküll inspired the later work of the Nobel Laureate ethologist Konrad Lorenz, and thus von Uexküll can be thought of as one of the founders of ethology as well as of Biosemiotics. Indeed, ethology and Biosemiotics are closely related.

Biosemiotics also values the ideas of the American anthropologist Gregory Bateson (1904-1980), who was mentioned in Chapter 7 in connection with cybernetics and with the Macy Conferences. He was married to another celebrated anthropologist, Margaret Mead, and together they applied Norbert Wiener's insights concerning feedback mechanisms to sociology, psychology and anthropology. Bateson was the originator of a famous epigrammatic definition of information: "..a difference which makes a difference" . This definition occurs in Chapter 3 of Bateson's book, Mind and Nature: A Necessary Unity, Bantam, (1980), and its context is as follows: "To produce news of a difference, i.e. information", Bateson wrote, "there must be two entities... such that news of their difference can be represented as a difference inside some information-processing entity, such as a brain or, perhaps, a computer. There is a profound and unanswerable question about the nature of these two entities that between them generate the difference which becomes information by making a difference. Clearly each alone is - for the mind and perception - a non-entity, a non-being... the sound of one hand clapping. The stuff of sensation, then, is a pair of values of some variable, presented over time to a sense organ, whose response depends on the ratio between the members of the pair."

Microelectronics

The problem of unreliable vacuum tubes was solved in 1948 by John Bardeen, William Shockley and Walter Brattain of the Bell Telephone Laboratories. Application of quantum theory to solids had lead to an understanding of the electrical properties of crystals. Like atoms, crystals were found to have allowed and forbidden energy levels.

[2] It is interesting to ask to what extent the concept of Umwelt can be equated to that of consciousness. To the extent that these two concepts can be equated, von Uexküll's Umweltforschung offers us the opportunity to explore the phylogenetic evolution of the phenomenon of consciousness.

The allowed energy levels for an electron in a crystal were known to form bands, i.e., some energy ranges with many allowed states (allowed bands), and other energy ranges with none (forbidden bands). The lowest allowed bands were occupied by electrons, while higher bands were empty. The highest filled band was called the "valence band", and the lowest empty band was called the "conduction band".

According to quantum theory, whenever the valence band of a crystal is only partly filled, the crystal is a conductor of electricity; but if the valence band is completely filled with electrons, the crystal is an electrical insulator. (A completely filled band is analogous to a room so packed with people that none of them can move.)

In addition to conductors and insulators, quantum theory predicted the existence of "semiconductors" - crystals where the valence band is completely filled with electrons, but where the energy gap between the conduction band and the valence band is very small. For example, crystals of the elements silicon and germanium are semiconductors. For such a crystal, thermal energy is sometimes enough to lift an electron from the valence band to the conduction band.

Bardeen, Shockley and Brattain found ways to control the conductivity of germanium crystals by injecting electrons into the conduction band, or alternatively by removing electrons from the valence band. They could do this by "doping" the crystals with appropriate impurities, or by injecting electrons with a special electrode. The semiconducting crystals whose conductivity was controlled in this way could be used as electronic valves, in place of vacuum tubes.

By the 1960's, replacement of vacuum tubes by transistors in electronic computers had led not only to an enormous increase in reliability and a great reduction in cost, but also to an enormous increase in speed. It was found that the limiting factor in computer speed was the time needed for an electrical signal to propagate from one part of the central processing unit to another. Since electrical impulses propagate with the speed of light, this time is extremely small; but nevertheless, it is the limiting factor in the speed of electronic computers.

B.6 The Traitorous Eight

According to the Wikipedia article on Shockley,

"In 1956 Shockley moved from New Jersey to Mountain View, California to start Shockley Semiconductor Laboratory to live closer to his ailing mother in Palo Alto, California. The company, a division of Beckman Instruments, Inc., was the first establishment working on silicon semiconductor devices in what came to be known as Silicon Valley.

"His way [of leading the group] could generally be summed up as domineering and increasingly paranoid. In one well-known incident, he claimed that a secretary's cut thumb was the result of a malicious act and he demanded lie detector tests to find the culprit, when in reality, the secretary had simply grabbed at a door handle that happened to have an exposed tack on it for the purpose of hanging paper notes on. After he received the Nobel Prize in 1956 his demeanor changed, as evidenced in his increasingly autocratic, erratic and

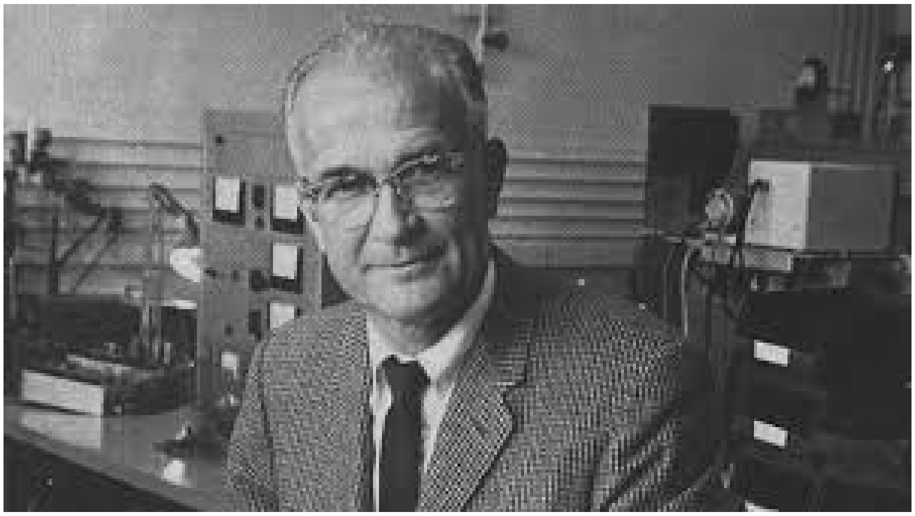

Figure B.14: **William Shockley (1910-1989) shared the 1956 Nobel Prize in Physics with John Bardeen and Walter Brattain.**

hard-to-please management style. In late 1957, eight of Shockley's researchers, who would come to be known as the 'traitorous eight, resigned after Shockley decided not to continue research into silicon-based semiconductors. They went on to form Fairchild Semiconductor, a loss from which Shockley Semiconductor never recovered. Over the course of the next 20 years, more than 65 new enterprises would end up having employee connections back to Fairchild."

Figure B.15: **The Traitorous Eight: From left to right, Gordon Moore, C. Sheldon Roberts, Eugene Kleiner, Robert Noyce, Victor Grinich, Julius Blank, Jean Hoerni and Jay Last.**

B.7 Integrated circuits

In order to reduce the propagation time, computer designers tried to make the central processing units very small; and the result was the development of integrated circuits and microelectronics. (Another motive for miniaturization of electronics came from the requirements of space exploration.)

Integrated circuits were developed in which single circuit elements were not manufactured separately. Instead, the whole circuit was made at one time. An integrated circuit is a sandwich-like structure, with conducting, resisting and insulating layers interspersed with layers of germanium or silicon, "doped " with appropriate impurities. At the start of the manufacturing process, an engineer makes a large drawing of each layer. For example, the drawing of a conducting layer would contain pathways which fill the role played by wires in a conventional circuit, while the remainder of the layer would consist of areas destined to be etched away by acid.

The next step is to reduce the size of the drawing and to multiply it photographically. The pattern of the layer is thus repeated many times, like the design on a piece of wallpaper. The multiplied and reduced drawing is then focused through a reversed microscope onto the surface to be etched.

Successive layers are built up by evaporating or depositing thin films of the appropriate substances onto the surface of a silicon or germanium wafer. If the layer being made is to be conducting, the surface would consist of an extremely thin layer of copper, covered with a photosensitive layer called a "photoresist". On those portions of the surface receiving light from the pattern, the photoresist becomes insoluble, while on those areas not receiving light, the photoresist can be washed away.

The surface is then etched with acid, which removes the copper from those areas not protected by photoresist. Each successive layer of a wafer is made in this way, and finally the wafer is cut into tiny "chips", each of which corresponds to one unit of the wallpaper-like pattern.

Although the area of a chip may be much smaller than a square centimeter, the chip can contain an extremely complex circuit. A typical programmable minicomputer or "microprocessor", manufactured during the 1970's, could have 30,000 circuit elements, all of which were contained on a single chip. By 1986, more than a million transistors were being placed on a single chip.

As a result of miniaturization, the speed of computers rose steadily. In 1960, the fastest computers could perform a hundred thousand elementary operations in a second. By 1970, the fastest computers took less than a second to perform a million such operations. In 1987, a computer called GF11 was designed to perform 11 billion floating-point operations (flops) per second.

GF11 (Gigaflop 11) is a scientific parallel-processing machine constructed by IBM. Approximately ten floating-point operations are needed for each machine instruction. Thus GF11 runs at the rate of approximately a thousand million instructions per second (1,100 MIPS). The high speed achieved by parallel-processing machines results from dividing a job into many sub-jobs on which a large number of processing units can work simultaneously.

Computer memories have also undergone a remarkable development. In 1987, the magnetic disc memories being produced could store 20 million bits of information per square inch; and even higher densities could be achieved by optical storage devices. (A "bit" is the unit of information. For example, the number 25, written in the binary system, is 11001. To specify this 5-digit binary number requires 5 bits of information. To specify an n-digit binary number requires n bits of information. Eight bits make a "byte".)

In the 1970's and 1980's, computer networks were set up linking machines in various parts of the world. It became possible (for example) for a scientist in Europe to perform a calculation interactively on a computer in the United States just as though the distant machine were in the same room; and two or more computers could be linked for performing large calculations. It also became possible to exchange programs, data, letters and manuscripts very rapidly through the computer networks.

B.8 Moore's law

In 1965, only four years after the first integrated circuits had been produced, Dr. Gordon E. Moore, one of the founders of Intel, made a famous prediction which has come to be known as "Moore's Law". He predicted that the number of transistors per integrated circuit would double every two years, and that this trend would continue through 1975. In fact, the general trend predicted by Moore has continued for a much longer time. Although the number of transistors per unit area has not continued to double every two years, the logic density (bits per unit area) has done so, and thus a modified version of Moore's law still holds today. How much longer the trend can continue remains to be seen. Physical limits to miniaturization of transistors of the present type will soon be reached; but there is hope that further miniaturization can be achieved through "quantum dot" technology, molecular switches, and autoassembly.

A typical programmable minicomputer or "microprocessor", manufactured in the 1970's, could have 30,000 circuit elements, all of which were contained on a single chip. By 1989, more than a million transistors were being placed on a single chip; and by 2000, the number reached 42,000,000.

As a result of miniaturization and parallelization, the speed of computers rose exponentially. In 1960, the fastest computers could perform a hundred thousand elementary operations in a second. By 1970, the fastest computers took less than a second to perform a million such operations. In 1987, a massively parallel computer, with 566 parallel processors, called GFll was designed to perform 11 billion floating-point operations per second (flops). By 2002 the fastest computer performed 40 at teraflops, making use of 5120 parallel CPU's.

Computer disk storage has also undergone a remarkable development. In 1987, the magnetic disk storage being produced could store 20 million bits of information per square inch; and even higher densities could be achieved by optical storage devices. Storage density has until followed a law similar to Moore's law.

In the 1970's and 1980's, computer networks were set up linking machines in various

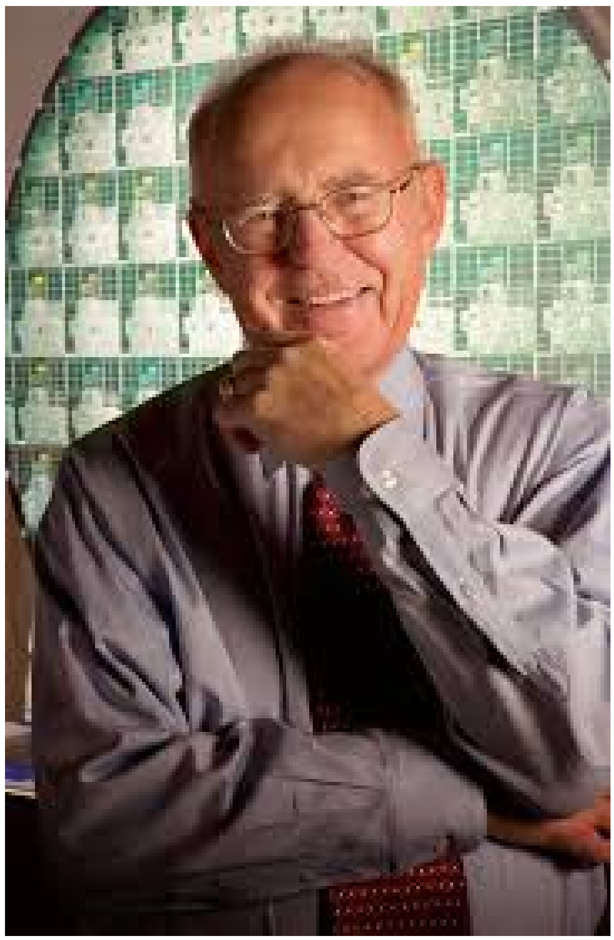

Figure B.16: **Gordon E. Moore (born 1929), a founder of Intel and the author of Moore's Law. In 1965 he predicted that the number of components in integrated circuits would double every year for the next 10 years". In 1975 he predicted the this doubling would continue, but revised the doubling rate to "every two years. Astonishingly, Moore's Law has held much longer than he, or anyone else, anticipated.**

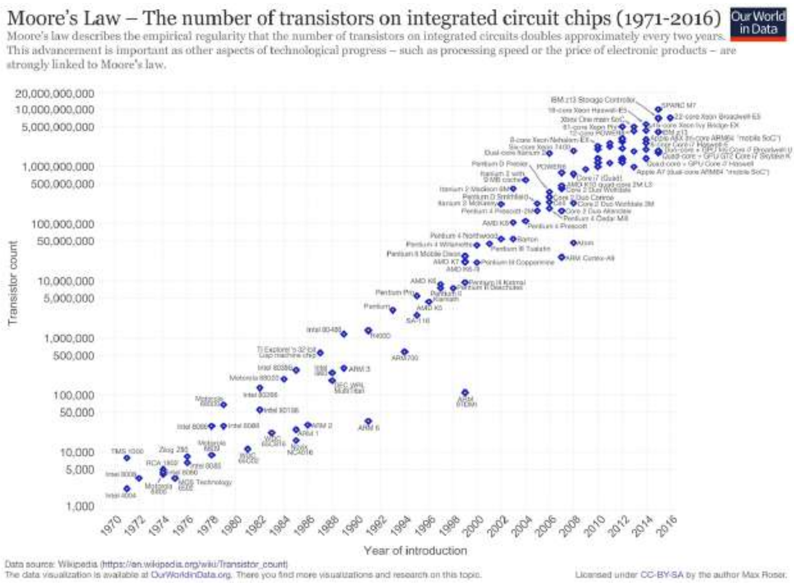

Figure B.17: **Amazingly, Moore's Law has held much longer than he, or anyone else, anticipated. Perhaps quantum dot technologies can extend its validity even longer.**

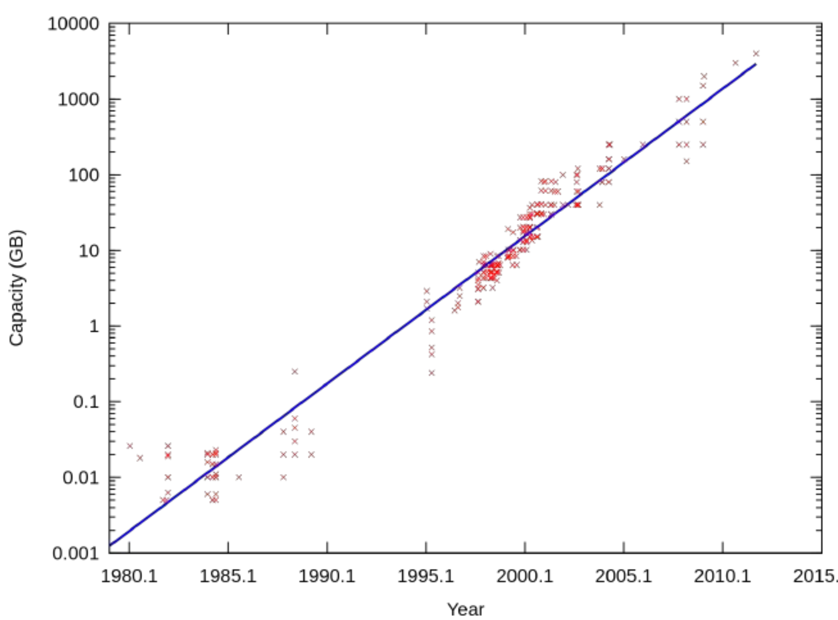

Figure B.18: **A logarithmic plot of the increase in PC hard-drive capacity in gigabytes. An extrapolation of the rate of increase predicts that the individual capacity of a commercially available PC will reach 10,000 gigabytes by 2015, i.e. 10,000,000,000,000 bytes. (After Hankwang and Rentar, Wikimedia Commons)** parts of the world. It became possible (for example) for a scientist in Europe to perform a calculation interactively on a computer in the United States just as though the distant machine were in the same room; and two or more computers could be linked for performing large calculations. It also became possible to exchange programs, data, letters and manuscripts very rapidly through the computer networks.

The exchange of large quantities of information through computer networks was made easier by the introduction of fiber optics cables. By 1986, 250,000 miles of such cables had been installed in the United States. If a ray of light, propagating in a medium with a large refractive index, strikes the surface of the medium at a grazing angle, then the ray undergoes total internal reflection. This phenomenon is utilized in fiber optics: A light signal can propagate through a long, hairlike glass fiber, following the bends of the fiber without losing intensity because of total internal reflection. However, before fiber optics could be used for information transmission over long distances, a technological breakthrough in glass manufacture was needed, since the clearest glass available in 1940 was opaque in lengths more than 10 m. Through studies of the microscopic properties of glasses, the problem of absorption was overcome. By 1987, devices were being manufactured commercially that were capable of transmitting information through fiber-optic cables at the rate of 1.7 billion bits per second.

B.9 Self-reinforcing information accumulation

Humans have been living on the earth for roughly two million years (more or less, depending on where one draws the line between our human and prehuman ancestors, Table 6.1). During almost all of this,time, our ancestors lived by hunting and food-gathering. They were not at all numerous, and did not stand out conspicuously from other animals. Then, suddenly, during the brief space of ten thousand years, our species exploded in numbers from a few million to seven billion, populating all parts of the earth, and even setting foot on the moon. This population explosion, which is still going on, has been the result of dramatic cultural changes. Genetically we are almost identical with our hunter-gatherer ancestors, who lived ten thousand years ago, but cultural evolution has changed our way of life beyond recognition.

Beginning with the development of speech, human cultural evolution began to accelerate. It started to move faster with the agricultural revolution, and faster still with the invention of writing and printing. Finally, modern science has accelerated the rate of social and cultural change to a completely unprecedented speed.

The growth of modern science is accelerating because knowledge feeds on itself. A new idea or a new development may lead to several other innovations, which can in turn start an avalanche of change. For example, the quantum theory of atomic structure led to the invention of transistors, which made high-speed digital computers possible. Computers have not only produced further developments in quantum theory; they have also revolutionized many other fields.

The self-reinforcing accumulation of knowledge - the information explosion - which characterizes modern human society is reflected not only in an explosively-growing global population, but also in the number of scientific articles published, which doubles roughly every ten years. Another example is Moore's law - the doubling of the information density of integrated circuits every two years. Yet another example is the explosive growth of Internet traffic shown in Table 17.1.

The Internet itself is the culmination of a trend towards increasing societal information exchange - the formation of a collective human consciousness. This collective consciousness preserves the observations of millions of eyes, the experiments of millions of hands, the thoughts of millions of brains; and it does not die when the individual dies.

B.10 Automation

During the last three decades, the cost of computing has decreased exponentially by between twenty and thirty percent per year. Meanwhile, the computer industry has grown exponentially by twenty percent per year (faster than any other industry). The astonishing speed of this development has been matched by the speed with which computers have become part of the fabric of science, engineering, industry, commerce, communications, transport, publishing, education and daily life in the industrialized parts of the world.

The speed, power and accuracy of computers has revolutionized many branches of science. For example, before the era of computers, the determination of a simple molecular structure by the analysis of X-ray diffraction data often took years of laborious calculation; and complicated structures were completely out of reach. In 1949, however, Dorothy Crowfoot Hodgkin used an electronic computer to work out the structure of penicillin from X-ray data. This was the first application of a computer to a biochemical problem; and it was followed by the analysis of progressively larger and more complex structures.

Proteins, DNA, and finally even the detailed structures of viruses were studied through the application of computers in crystallography. The enormous amount of data needed for such studies was gathered automatically by computer-controlled diffractometers; and the final results were stored in magnetic-tape data banks, available to users through computer networks.

The application of quantum theory to chemical problems is another field of science which owes its development to computers. When Erwin Schrödinger wrote down his wave equation in 1926, it became possible, in principle, to calculate most of the physical and chemical properties of matter. However, the solutions to the Schrödinger equation for many-particle systems can only be found approximately; and before the advent of computers, even approximate solutions could not be found, except for the simplest systems.

When high-speed electronic digital computers became widely available in the 1960's, it suddenly became possible to obtain solutions to the Schrödinger equation for systems of chemical and even biochemical interest. Quantum chemistry (pioneered by such men as J.C. Slater, R.S. Mullikin, D.R. Hartree, V. Fock, J.H. Van Vleck, L. Pauling, E.B. Wilson, P.O. Löwdin, E. Clementi, C.J. Ballhausen and others) developed into a rapidly-growing field, as did solid state physics. Through the use of computers, it became possible to design new materials with desired chemical, mechanical, electrical or magnetic properties. Applying computers to the analysis of reactive scattering experiments, D. Herschbach, J. Polanyi and Y. Lee were able to achieve an understanding of the dynamics of chemical reactions.

The successes of quantum chemistry led Albert Szent-Györgyi, A. and B. Pullman, H. Scheraga and others to pioneer the fields of quantum biochemistry and molecular dynamics. Computer programs for drug design were developed, as well as molecular-dynamics programs which allowed the conformations of proteins to be calculated from a knowledge of their amino acid sequences. Studies in quantum biochemistry have yielded insights into the mechanisms of enzyme action, photosynthesis, active transport of ions across membranes, and other biochemical processes.

In medicine, computers began to be used for monitoring the vital signs of critically ill patients, for organizing the information flow within hospitals, for storing patients' records, for literature searches, and even for differential diagnosis of diseases.

The University of Pennsylvania has developed a diagnostic program called INTERNIST-1, with a knowledge of 577 diseases and their interrelations, as well as 4,100 signs, symptoms and patient characteristics. This program was shown to perform almost as well as an academic physician in diagnosing difficult cases. QMR (Quick Medical Reference), a microcomputer adaptation of INTERNIST-1, incorporates the diagnostic functions of the earlier program, and also offers an electronic textbook mode.

Beginning in the 1960's, computers played an increasingly important role in engineering and industry. For example, in the 1960's, Rolls Royce Ltd. began to use computers not only to design the optimal shape of turbine blades for aircraft engines, but also to control the precision milling machines which made the blades. In this type of computer-assisted design and manufacture, no drawings were required. Furthermore, it became possible for an industry requiring a part from a subcontractor to send the machine-control instructions for its fabrication through the computer network to the subcontractor, instead of sending drawings of the part.

In addition to computer-controlled machine tools, robots were also introduced. They were often used for hazardous or monotonous jobs, such as spray-painting automobiles; and they could be programmed by going through the job once manually in the programming mode. By 1987, the population of robots in the United States was between 5,000 and 7,000, while in Japan, the Industrial Robot Association reported a robot population of 80,000.

Chemical industries began to use sophisticated computer programs to control and to optimize the operations of their plants. In such control systems, sensors reported current temperatures, pressures, flow rates, etc. to the computer, which then employed a mathematical model of the plant to calculate the adjustments needed to achieve optimum operating conditions.

Not only industry, but also commerce, felt the effects of computerization during the postwar period. Commerce is an information-intensive activity; and in fact some of the crucial steps in the development of information-handling technology developed because of the demands of commerce: The first writing evolved from records of commercial transactions kept on clay tablets in the Middle East; and automatic business machines, using punched cards, paved the way for the development of the first programmable computers.

Computerization has affected wholesaling, warehousing, retailing, banking, stockmarket transactions, transportation of goods - in fact, all aspects of commerce. In wholesaling, electronic data is exchanged between companies by means of computer networks, allowing order-processing to be handled automatically; and similarly, electronic data on prices is transmitted to buyers.

The key to automatic order-processing in wholesaling was standardization. In the United States, the Food Marketing Institute, the Grocery Manufacturers of America, and several other trade organizations, established the Uniform Communications System (UCS) for the grocery industry. This system specifies a standard format for data on products, prices and orders.

Automatic warehouse systems were designed as early as 1958. In such systems, the goods to be stored are placed on pallets (portable platforms), which are stacked automatically in aisles of storage cubicles. A computer records the position of each item for later automatic retrieval.

In retailing, just as in wholesaling, standardization proved to be the key requirement for automation. Items sold in supermarkets in most industrialized countries are now labeled with a standard system of machine-readable thick and thin bars known as the Universal Product Code (UPC). The left-hand digits of the code specify the manufacturer or packer of the item, while the right-hand set of digits specify the nature of the item. A final digit is included as a check, to make sure that the others were read correctly. This last digit (called a modulo check digit) is the smallest number which yields a multiple of ten when added to the sum of the previous digits.

When a customer goes through a check-out line, the clerk passes the purchased items over a laser beam and photocell, thus reading the UPC code into a small embedded computer or microprocessor at the checkout counter, which adds the items to the customer's bill. The microprocessor also sends the information to a central computer and inventory data base. When stocks of an item become low, the central computer generates a replacement order. The financial book-keeping for the retailing operation is also carried out automatically by the central computer.

In many places, a customer passing through the checkout counter of a supermarket is able to pay for his or her purchases by means of a plastic card with a magnetic, machine-readable identification number. The amount of the purchase is then transmitted through a computer network and deducted automatically from the customer's bank account. If the customer pays by check, the supermarket clerk may use a special terminal to determine whether a check written by the customer has ever "bounced".

Most checks are identified by a set of numbers written in the Magnetic-Ink Character Recognition (MICR) system. In 1958, standards for the MICR system were established, and by 1963, 85 percent of all checks written in the United States were identified by MICR numbers. By 1968, almost all banks had adopted this system; and thus the administration of checking accounts was automated, as well as the complicated process by which a check, deposited anywhere in the world, returns to the payers bank.

Container ships were introduced in the late 1950's, and since that time, container systems have increased cargo-handling speeds in ports by at least an order of magnitude. Computer networks contributed greatly to the growth of the container system of transportation by keeping track of the position, ownership and contents of the containers.

In transportation, just as in wholesaling and retailing, standardization proved to be a necessary requirement for automation. Containers of a standard size and shape could be loaded and unloaded at ports by specialized tractors and cranes which required only a very small staff of operators. Standard formats for computerized manifests, control documents, and documents for billing and payment, were instituted by the Transportation Data Coordinating Committee, a non-profit organization supported by dues from shipping firms.

In the industrialized parts of the world, almost every type of work has been made more efficient by computerization and automation. Even artists, musicians, architects and authors find themselves making increasing use of computers: Advanced computing systems, using specialized graphics chips, speed the work of architects and film animators. The author's traditional typewriter has been replaced by a word-processor, the composer's piano by a music synthesizer.

In the Industrial Revolution of the 18th and 19th centuries, muscles were replaced by machines. Computerization represents a Second Industrial Revolution: Machines have begun to perform not only tasks which once required human muscles, but also tasks which formerly required human intelligence.

In industrial societies, the mechanization of agriculture has very much reduced the fraction of the population living on farms. For example, in the United States, between 1820 and 1980, the fraction of workers engaged in agriculture fell from 72 percent to 3.1 percent. There are signs that computerization and automation will similarly reduce the number of workers needed in industry and commerce.

Computerization is so recent that, at present, we can only see the beginnings of its impact; but when the Second Industrial Revolution is complete, how will it affect society? When our children finish their education, will they face technological unemployment?

The initial stages of the First Industrial Revolution produced much suffering, because labor was regarded as a commodity to be bought and sold according to the laws of supply and demand, with almost no consideration for the needs of the workers. Will we repeat this mistake? Or will society learn from its earlier experience, and use the technology of automation to achieve widely-shared human happiness?

The Nobel-laureate economist, Wassily W. Leontief, has made the following comment on the problem of technological unemployment:

"Adam and Eve enjoyed, before they were expelled from Paradise, a high standard of living without working. After their expulsion, they and their successors were condemned to eke out a miserable existence, working from dawn to dusk. The history of technological progress over the last 200 years is essentially the story of the human species working its way slowly and steadily back into Paradise. What would happen, however, if we suddenly found ourselves in it? With all goods and services provided without work, no one would be gainfully employed. Being unemployed means receiving no wages. As a result, until appropriate new income policies were formulated to fit the changed technological conditions, everyone would starve in Paradise."

To say the same thing in a slightly different way: consider what will happen when a factory which now employs a thousand workers introduces microprocessor-controlled industrial robots and reduces its work force to only fifty. What will the nine hundred and fifty redundant workers do? They will not be able to find jobs elsewhere in industry, commerce or agriculture, because all over the economic landscape, the scene will be the same.

There will still be much socially useful work to be done - for example, taking care of elderly people, beautifying the cities, starting youth centers, planting forests, cleaning up pollution, building schools in developing countries, and so on. These socially beneficial goals are not commercially "profitable". They are rather the sort of projects which governments sometimes support if they have the funds for it. However, the money needed to usefully employ the nine hundred and fifty workers will not be in the hands of the government. It will be in the hands of the factory owner who has just automated his production line.

In order to make the economic system function again, either the factory owner will have to be persuaded to support socially beneficial but commercially unprofitable projects, or else an appreciable fraction of his profits will have to be transferred to the government, which will then be able to constructively re-employ the redundant workers.

The future problems of automation and technological unemployment may force us to rethink some of our economic ideas. It is possible that helping young people to make a smooth transition from education to secure jobs will become one of the important responsibilities of governments, even in countries whose economies are based on free enterprise. If such a change does take place in the future, while at the same time socialistic countries are adopting a few of the better features of free enterprise, then one can hope that the world will become less sharply divided by contrasting economic systems.

B.11 Neural networks

Physiologists have begun to make use of insights derived from computer design in their efforts to understand the mechanism of the brain; and computer designers are beginning to construct computers modeled after neural networks. We may soon see the development of computers capable of learning complex ideas, generalization, value judgements, artistic creativity, and much else that was once thought to be uniquely characteristic of the human mind. Efforts to design such computers will undoubtedly give us a better understanding of the way in which the brain performs its astonishing functions.

Much of our understanding of the nervous systems of higher animals is due to the Spanish microscopist, Ramón y Cajal, and to the English physiologists, Alan Hodgkin and Andrew Huxley. Cajal's work, which has been confirmed and elaborated by modern electron microscopy, showed that the central nervous system is a network of nerve cells (neurons) and threadlike fibers growing from them. Each neuron has many input fibers (dendrites), and one output fiber (the axon), which may have several branches.

S It is possible the computers of the future will have pattern-recognition and learning abilities derived from architecture inspired by our understanding of the synapse, by Young's model, or by other biological models. However, pattern recognition and learning can also be achieved by programming, using computers of conventional architecture. Programs already exist which allow computers to understand both handwriting and human speech; and a recent chess-playing program was able to learn by studying a large number of championship games. Having optimized its parameters by means of this learning experience, the chess-playing program was able to win against grand masters!

Like nuclear physics and genesplicing, artificial intelligence presents a challenge: Will society use its new powers wisely and humanely? The computer technology of the future can liberate us from dull and repetitive work, and allow us to use our energies creatively; or it can produce unemployment and misery, depending on how we organize our society. Which will we choose?

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Appendix C

GROUP THEORY

C.1 The definition of a finite group

A finite group is defined by the following conditions:

1. If any two elements belonging to the group are multiplied together, the product is another element belonging to the group.

2. There is an identity element.

3. Each element has an inverse.

4. Multiplication of the elements is associative[1], but necessarily commutative.

5. The group contains g elements, where g is a finite positive integer called the *order* of the group.

As a simple example, we might think of a molecule which is symmetric with respect to rotations through an angle of $2\pi/3$ about some axis but which has no other symmetry. Then the set of geometrical operations that leave the molecule invariant form a group containing 3 elements: the identity element; a rotation through an angle $2\pi/3$ about the axis of symmetry, and a rotation through an angle $4\pi/3$ about the same axis. Let us denote these operations respectively by E, C_3, and C_3^{-1}. We can easily construct a multiplication table for the group. If we do so, *each element of the group will appear once and only once in any row or column of the multiplication table.* This follows from the fact that $AX = B$ has one and only one solution among the group elements. Since A^{-1} and B belong to the group, and since the product of any two elements belongs to the group, $X = A^{-1}B$ is also a uniquely-defined element. Now suppose that the element B appears more than once in the Ath row of the multiplication table. Then $AX = B$ will have more than one solution which is impossible. Since no element can appear more than once, each element must appear once because there are g elements and g places in the row, all of which have to be filled.

[1] A(BC)=(AB)C

C.2 Representations of geometrical symmetry groups

The elements of a geometrical symmetry group are linear coordinate transformations. Such transformations have the form

$$X^i = \sum_{j=1}^{d} \frac{\partial X^i}{\partial x^j} x^j + b^i \tag{C.1}$$

where $\partial X^i/\partial x^j$ and b^i are constants.

Now consider a set of functions Φ_1, Φ_2, ..., Φ_M. We can use equation (C.1) to express $\Phi_1(\mathbf{x})$ as a function of $\mathbf{X}$. If we then expand the resulting function of $\mathbf{X}$ in terms of the other $|\Phi_n\rangle$'s, we shall obtain a relation of the form

$$\Phi_n(\mathbf{x}) = \sum_{n'} \Phi_{n'}(\mathbf{X}) D_{n',n} \tag{C.2}$$

If we denote the coordinate transformation in equation (C.1) by the symbol G, we can rewrite equations (C.1) and (C.2) in the form:

$$\begin{aligned} \mathbf{X} &= G_j \mathbf{x} \\ \Phi_n(\mathbf{x}) &\equiv \Phi_n(G_j^{-1}\mathbf{X}) \equiv G_j \Phi_n(\mathbf{X}) \\ &= \sum_{n'} \Phi_{n'}(\mathbf{X}) D_{n',n}(G) \end{aligned} \tag{C.3}$$

In this sense, the coordinate transformation defines an operator G_j, and $D_{n',n}(G_j)$ is a matrix representing G_j. Is can easily be shown that the matrices representing a set of operators G_1, G_2,...,G_g in a given basis, obey the same multiplication table as the operators themselves. For example, if we know that

$$C_3 C_3^{-1} = E \tag{C.4}$$

and that

$$\begin{aligned} C_3 \Phi_n &= \sum_{n'} \Phi_{n'} D_{n',n}(C_3) \\ C_3^{-1} \Phi_n &= \sum_{n'} \Phi_{n'} D_{n',n}(C_3^{-1}) \\ E \Phi_n &= \sum_{n'} \Phi_{n'} D_{n',n}(E) \end{aligned} \tag{C.5}$$

then it follows that:

$$\begin{aligned} C_3 C_3^{-1} \Phi_n &= \sum_{n'} C_3 \Phi_{n'} D_{n',n}(C_3^{-1}) \\ &= \sum_{n''} \Phi_{n''} \left\{ \sum_{n'} D_{n'',n'}(C_3) D_{n',n}(C_3^{-1}) \right\} \\ &= E\Phi_n = \sum_{n''} \Phi_{n''} D_{n'',n}(E) \end{aligned} \tag{C.6}$$

so that we must have

$$D_{n'',n}(E) = \sum_{n'} D_{n'',n'}(C_3) D_{n',n}(C_3^{-1}) \tag{C.7}$$

Thus *given any set of basis functions* Φ_1, Φ_2, ..., Φ_M *which mix together under the elements of a group* G_1, G_2,...,G_g, *we can obtain a set of matrices* $D_{n',n}(G_j)$ *defined by the relationships*

$$G_j \Phi_n = \sum_{n'} \Phi_{n'} D_{n',n}(G_j) \qquad j = 1, 2, ..., g \tag{C.8}$$

These matrices will obey the same multiplication table as the operators G_1, G_2,...,G_g, *and they are said to form a matrix representation of the group.*

C.3 Similarity transformations

Now let us consider another representation, $D'_{m',m}(G_j)$, based on a set of functions Φ'_1, Φ'_2, ..., Φ'_M which are related to our original set Φ_1, Φ_2, ..., Φ_M by the transformation:

$$\begin{aligned} \Phi'_m &= \sum_n \Phi_n S_{n,m} \\ \Phi_n &= \sum_m \Phi'_m S^{-1}_{m,n} \end{aligned} \tag{C.9}$$

The primed representation is defined by the relationship

$$G_j \Phi'_m = \sum_{m'} \Phi'_{m'} D'_{m',m}(G_j) \qquad j = 1, 2, ..., g \tag{C.10}$$

Then from equations (C.8)-(C.10) we have

$$\begin{aligned} G_j \Phi'_m &= \sum_{m'} \Phi'_{m'} D'_{m',m}(G_j) \\ &= G_j \sum_n \Phi_n S_{n,m} \\ &= \sum_{n,n'} \Phi_{n'} D_{n',n}(G_j) S_{n,m} \\ &= \sum_{m',n,n'} \Phi'_{m'} S^{-1}_{m',n'} D_{n',n}(G_j) S_{n,m} \end{aligned} \tag{C.11}$$

so that we must have

$$D'_{m',m}(G_j) = \sum_{n,n'} S^{-1}_{m',n'} D_{n',n}(G_j) S_{n,m} \tag{C.12}$$

or

$$D' = S^{-1} D S \tag{C.13}$$

A transformation of this type, where the matrix S *need not be unitary, is called a 'similarity transformation'.*

C.4 Characters and reducibility

The character $\chi(G_j)$ of the matrix $D_{n',n}(G_j)$ is defined as the sum of the diagonal elements:

$$\chi(G_j) \equiv \sum_n D_{n,n}(G_j) \tag{C.14}$$

We would like to show that the character of each element in a representation of a finite group is invariant under a similarity transformation. From equations (C.12) and (C.14) we have:

$$\begin{aligned}
\chi'(G_j) &\equiv \sum_m D'_{m,m}(G_j) \\
&= \sum_{m,n,n'} S^{-1}_{m,n'} D_{n',n}(G_j) S_{n,m} \\
&= \sum_{n,n'} \left(\sum_m S_{n,m} S^{-1}_{m,n'} \right) D_{n',n}(G_j) \\
&= \sum_{n,n'} \delta_{n',n} D_{n',n}(G_j) \\
&= \sum_n D_{n,n}(G_j) = \chi(G_j) \qquad \text{q.e.d.}
\end{aligned} \tag{C.15}$$

If two representations are connected by a similarity transformation, then they are said to be 'equivalent'. From (C.15) it follows that when two representations are equivalent, then $\chi'(G_j) = \chi(G_j)$ for $j = 1, 2, ..., g$.

Sometimes it is possible by means of a similarity transformation to bring all the elements of a representation into a block-diagonal form. In other words it may be possible to bring $D'_{m',m}(G_j)$ into a form where the non-zero elements are confined blocks along the diagonal, the blocks being the same for all the group elements. To express the same idea differently, it is sometimes possible to go over by means of a similarity transformation from the original basis set, Φ_1, Φ_2, ..., Φ_M to a new basis set Φ'_1, Φ'_2, ..., Φ'_M which can be divided into two or more subsets, each of which mixes only with itself under the operations G_1, G_2,...,G_g. *A representation based on two or more subsets of basis functions which mix only with themselves under the operations of the group is said to be 'reduced'. Whenever it is possible to bring a representation into a reduced form by means of a similarity transformation, it is said to be 'reducible'. Whenever this is not possible, the representation is said to be 'irreducible'.*

Table A.1 Multiplication table for the group C_3

	E	C_3	C_3^{-1}
E	E	C_3	C_3^{-1}
C_3	C_3	C_3^{-1}	E
C_3^{-1}	C_3^{-1}	E	C_3

Table A.2 Character table for the group C_3

	E	C_3	C_3^{-1}
A	1	1	1
Γ_c	1	$e^{i(2\pi/3)}$	$e^{-i(2\pi/3)}$
Γ_c^*	1	$e^{-i(2\pi/3)}$	$e^{i(2\pi/3)}$

C.5 The great orthogonality theorem

A unitary matrix is a matrix whose conjugate transpose (Hermitian adjoint) is equal to its inverse. It is always possible, by means of a similarity transformation, to bring the matrix representations of a finite group into unitary form. Now let $D^{\alpha}_{n',n}(G_j)$ and $D^{\beta}_{m',m}(G_j)$ be two unitary irreducible representations of a finite group of order g. The great orthogonality theorem, from which much of the power of group theory is derived, then states that

$$\sum_{j=1}^{g} D^{\alpha *}_{n',n}(G_j) D^{\beta}_{m',m}(G_j) = \frac{g}{d_\alpha} \delta_{\alpha,\beta} \delta_{n',m'} \delta_{n,m} \tag{C.16}$$

where d_α is the dimension of the matrices $D^{\alpha}_{n',n}(G_j)$. The proof of the great orthogonality theorem depends on Schur's lemma, which states that if A is a matrix that commutes with every matrix $D^{\alpha}_{n',n}(G_j)$, $j = 1, 2, ..., g$ in a unitary irreducible representation of a finite group, then A must be a multiple of the unit matrix, i.e., if

$$AD(G_j) - D(G_j)A = 0, \qquad j = 1, 2, ..., g \tag{C.17}$$

then

$$A \sim I \tag{C.18}$$

The proof of Schur's lemma is as follows: If A commutes with $D^{\alpha}_{n',n}(G_j)$, $j = 1, 2, ..., g$, then so does its conjugate transpose $A^{\dagger}$. Therefore we can let A be Hermitian without loss of generality, and we can diagonalize A by means of a unitary transformation:

$$UAU^{-1} = A^{(d)} \tag{C.19}$$

where $A^{(d)}$ is diagonal. Then

$$U^{-1}A^{(d)}UD(G_j) - D(G_j)U^{-1}A^{(d)}U = 0, \qquad j = 1, 2, ..., g \tag{C.20}$$

Multiplying on the left by U and on the right by U^{-1} then yields

$$A^{(d)}UD(G_j)U^{-1} - UD(G_j)U^{-1}A^{(d)} = 0, \qquad j = 1, 2, ..., g \tag{C.21}$$

Thus we can write

$$A^{(d)}D'(G_j) - D'(G_j)A^{(d)} = 0, \qquad j = 1, 2, ..., g \tag{C.22}$$

where

$$D'(G_j) \equiv UD(G_j)U^{-1} \tag{C.23}$$

Since $A^{(d)}$ is diagonal we can write $A^{(d)}_{n',n} = A^{(d)}_{n}\delta_{n',n}$. Thus with the indices written out, (C.22) becomes:

$$\sum_{n'} \left(A^{(d)}_{n'} \delta_{n'',n'} D'^{\alpha}_{n',n}(G_j) - D'^{\alpha}_{n'',n'}(G_j) A^{(d)}_{n} \delta_{n',n} \right) = 0, \qquad j = 1, ..., g \tag{C.24}$$

from which it follows that

$$\left(A_{n'}^{(d)} - A_n^{(d)}\right) D'^{\alpha}_{n',n}(G_j) = 0, \qquad j = 1, 2, ..., g \tag{C.25}$$

Without loss of generality, we can choose U in such a way that repeated eigenvalues of $A^{(d)}$ are grouped together along the diagonal. Then $A_{n''}^{(d)} \neq A_n^{(d)}$ implies that

$$D'^{\alpha}_{n',n}(G_j) = D'^{\dagger\alpha}_{n',n}(G_j) = D'^{\alpha}_{n,n'}(G_j^{-1}) = 0, \quad j = 1, 2, ..., g \tag{C.26}$$

Thus $D'^{\alpha}_{n',n}(G_j)$ can only have non-zero elements in the blocks that correspond to repeated eigenvalues of $A^{(d)}$ and it would therefore be reducible unless all of the eigenvalues are equal, which would contradict the original assumption of irreducibility. This proves Schur's lemma.

Having demonstrated the validity of Schur's lemma, we are now in a position to prove the great orthogonality relation. To do so we define the matrix M by the relationship

$$M \equiv \sum_{j=1}^{g} D^{\alpha}(G_j) X D^{\beta}(G_j^{-1}) \tag{C.27}$$

where X is an arbitrary matrix of appropriate dimensions to make matrix multiplication possible and where $D^{\alpha}(G_j)$ and $D^{\beta}(G_j)$ are unitary irreducible representations of the finite group. Then

$$\begin{aligned} D^{\alpha}(G_i) M D^{\beta}(G_i^{-1}) &= \sum_{j=1}^{g} D^{\alpha}(G_i) D^{\alpha}(G_j) X D^{\beta}(G_j^{-1}) D^{\beta}(G_i^{-1}) \\ &= \sum_{k=1}^{g} D^{\alpha}(G_k) X D^{\beta}(G_k^{-1}) = M \end{aligned} \tag{C.28}$$

where $G_i G_j = G_k$ and where we have used the fact that each group element appears once and only once in every row of the multiplication table to replace the sum over j by a sum over k. Multiplying (C.28) from the right by $D^{\beta}(G_i)$ we obtain:

$$D^{\alpha}(G_i) M = M D^{\beta}(G_i) \qquad i = 1, 2, ..., g \tag{C.29}$$

Then, according to Schur's lemma, M must be a multiple of the unit matrix. It may of course be a square matrix consisting entirely of zeros, since such a matrix is also a multiple of the unit matrix. Multiplying (C.29) from the left by M^{-1} we obtain:

$$M^{-1} D^{\alpha}(G_i) M = D^{\beta}(G_i) \qquad i = 1, 2, ..., g \tag{C.30}$$

from which we can see that if M is not the null matrix, then the irreducible representations $D^{\alpha}(G_i)$ and $D^{\beta}(G_i)$ must be the same, i.e., if M is not the null matrix, $\alpha = \beta$.

Let us first consider the case where M is the null matrix and where $\alpha \neq \beta$. Then putting indices into (C.27) we have:

$$\sum_{j=1}^{g}\sum_{n=1}^{d_\alpha}\sum_{m'=1}^{d_\beta} D^{\alpha}_{n',n}(G_j)X_{n,m'}D^{\beta}_{m',m}(G_j^{-1}) = 0 \tag{C.31}$$

But $X_{n,m'}$ is arbitrary, and therefore (C.31) can only hold for all cases if

$$\sum_{j=1}^{g} D^{\alpha}_{n',n}(G_j)D^{\beta}_{m',m}(G_j^{-1}) = 0 \tag{C.32}$$

Now let us consider the second possibility: Suppose that $\alpha = \beta$. Then

$$\delta_{\alpha,\beta}M = \sum_{j=1}^{g} D^{\beta}(G_j)XD^{\beta}(G_j^{-1}) \tag{C.33}$$

Putting indices into (C.33) we have

$$\delta_{\alpha,\beta}M_{n',m} = \sum_{j=1}^{g}\sum_{n=1}^{d_\beta}\sum_{m'=1}^{d_\beta} D^{\alpha}_{n',n}(G_j)X_{n,m'}D^{\beta}_{m',m}(G_j^{-1}) \tag{C.34}$$

Taking the trace of both sides of (C.34) yields

$$\begin{aligned}\delta_{\alpha,\beta}\mathrm{tr}(M) &= \sum_{j=1}^{g}\sum_{m=1}^{d_\beta}\sum_{n=1}^{d_\beta}\sum_{m'=1}^{d_\beta} D^{\beta}_{m,n}(G_j)X_{n,m'}D^{\beta}_{m',m}(G_j^{-1}) \\ &= \sum_{j=1}^{g}\sum_{n=1}^{d_\beta}\sum_{m'=1}^{d_\beta} \delta_{n,m'}X_{n,m'} = g\mathrm{tr}(X) \end{aligned} \tag{C.35}$$

so that

$$I\delta_{\alpha,\beta}\frac{g}{d_\alpha}\mathrm{trX} = \sum_{j=1}^{g}\sum_{n=1}^{d_\beta}\sum_{m'=1}^{d_\beta} D^{\alpha}_{n',n}(G_j)X_{n,m'}D^{\beta}_{m',m}(G_j^{-1}) \tag{C.36}$$

where I is the identity matrix. Because X is arbitrary, this relationship can only hold in all cases if (C.16) is valid.

The great orthogonality relation is very central, and almost all of the results of group theory depend upon it. For example, combining (C.16) with the definition of characters (C.14), we obtain:

$$\begin{aligned}\sum_{j=1}^{g}\chi^{\alpha *}(G_j)\chi^{\beta}(G_j) &\equiv \sum_{j=1}^{g}\left\{\sum_{n} D^{\alpha *}_{n,n}(G_j)\right\}\left\{\sum_{m} D^{\beta}_{m,m}(G_j)\right\} \\ &= \frac{g}{d_\alpha}\delta_{\alpha,\beta}\sum_{n}\sum_{m}\delta_{n,m}\delta_{n,m} = g\delta_{\alpha,\beta}\end{aligned} \tag{C.37}$$

Equation (C.37) holds only for unitary representations, but every representation is equivalent to a unitary representation since it is always possible to perform a similarity transformation that orthonormalizes the basis functions. Therefore, since characters are invariant under similarity transformations, the orthonormality of characters

$$\frac{1}{g}\sum_{j=1}^{g}\chi^{\alpha*}(G_j)\chi^{\beta}(G_j) = \epsilon_{\alpha,\beta} \equiv \begin{cases} 0 & \text{if the representations are inequivlent} \\ 1 & \text{if the representations are equivlent} \end{cases} \tag{C.38}$$

holds even for non-unitary irreducible representations.

Now consider a representation $D_{n',n}(G_j)$ which may be reducible. If we reduce it by means of a similarity transformation, then in its reduced form it will be block-diagonal, each block being irreducible. Taking the trace, we find that the character of an element in the reduced representation $D'_{n',n}(G_j)$ is the sum of the characters of the irreducible representations of which it is composed. Thus

$$\begin{aligned} \chi(G_j) &\equiv \sum_{n=1}^{d} D'_{n,n}(G_j) \\ &= \chi^1(G_j) + \chi^2(G_j) + ... \\ &= \sum_{\beta} n_\beta \chi^\beta(G_j) \end{aligned} \tag{C.39}$$

where n_β is the number of times that the irreducible representation D^β occurs among the diagonal blocks of D'. Then from (C.38) we have

$$\begin{aligned} \frac{1}{g}\sum_{j=1}^{g}\chi^{\alpha*}(G_j)\chi(G_j) &= \sum_{\beta} n_\beta \sum_{j=1}^{g}\chi^{\alpha*}(G_j)\chi^{\beta}(G_j) \\ &= \sum_{\beta} n_\beta \epsilon_{\alpha,\beta} = n_\alpha \end{aligned} \tag{C.40}$$

This gives us a way to find out how many times a particular irreducible representation D^α occurs in a reducible representation D. According to (C.40), we just have to take the scalar product of the characters and divide by the order of the group. When we say that D^α 'occurs' n_α times in D, we mean that it is possible by means of a similarity transformation to bring D into block-diagonal form where D^α occurs n_α times along the diagonal blocks. The relationship is sometimes written in the form

$$D = n_1 D^1 + n_1 D^2 + ... \tag{C.41}$$

Obviously in this decomposition we do not need to distinguish between different equivalent forms of an irreducible representation D^α, since all of them have the same character, and it is possible to go from one to another by means of a similarity transformation.

C.6 Classes

Two elements of a group G_i and G_j are said to be in the same 'class' if there exists another element G_l in the group such that

$$G_i = G_l^{-1} G_j G_l \tag{C.42}$$

Thus, if we start with a particular element G_j, we can generate the set of elements in the same class by keeping j fixed in (C.42) and letting G_l run through all the elements of the group. It also follows from (C.42) that we can construct an operator M_k which commutes with all the elements of the group by summing the elements of a particular class:

$$M_k \equiv \sum_{\text{class } k} G_j \tag{C.43}$$

Then for an arbitrary group element G_l we have

$$\begin{aligned} G_l^{-1}\left[M_k, G_l\right] &= \sum_{\text{class } k} G_l^{-1}\left[G_j, G_l\right] \\ &= \sum_{\text{class } k} \left(G_l^{-1} G_j G_l - G_j\right) \\ &= \sum_{\text{class } k} \left(G_i - G_j\right) = 0 \end{aligned} \tag{C.44}$$

Equation (C.44) can hold only if $[M_k, G_l] = 0$. An operator, such as M_k, which commutes with every element of the group is called an 'invariant'. If there are r classes in a group, there will be r linearly independent invariants that can be constructed in this way.

For any representation of two elements G_i and G_j in the same class, it follows from (C.42) that

$$D(G_i) = D(G_l^{-1}) D(G_j) D(G_l) = D(G_l)^{-1} D(G_j) D(G_l) \tag{C.45}$$

Thus if $D(G_i)$ and $D(G_i)$ represent two elements in the same class, they are connected by a similarity transformation, and therefore they have the same character. In other words, *all elements in the same class have the same character*. This means that in applying equation (C.40) we do not need to go through quite so much work. Instead of summing over all of the elements in the group, we can take the product of characters for a representative element in each class, multiply by the number of elements in the class, and then sum over the classes. If g_k represents the number of elements in the class k, then the orthogonality relation for characters, equation (C.38), can be written in the form

$$\sum_{k=1}^{r} \sqrt{\frac{g_k}{g}} \chi_k^{\alpha *}(G_j) \sqrt{\frac{g_k}{g}} \chi_k^{\beta}(G_j) = \delta_{\alpha,\beta} \tag{C.46}$$

where χ_k^{α} is the character of a representative element in class k.

C.7 Projection operators

The great orthogonality theorem, equation (C.16), can be used to construct group-theoretical projection operators. Suppose that the sets of functions $(\Phi_1^1, \Phi_2^1, ..., \Phi_{d_1}^1)$, $(\Phi_1^2, \Phi_2^2, ...\Phi_{d_2}^2)$, etc. each form the basis for an irreducible representation of a group, and that there are r' nonequivalent irreducible representations. Then

$$G_j \Phi_n^\beta = \sum_{n'=1}^{d_\beta} \Phi_{n'}^\beta D_{n',n}^\beta(G_j) \tag{C.47}$$

Then from (C.16) we have

$$\begin{aligned}\sum_{j=1}^{g} D_{m,m}^{\alpha *}(G_j) G_j \Phi_n^\beta &= \sum_{n'=1}^{d_\beta} \Phi_{n'}^\beta \sum_{j=1}^{g} D_{m,m}^{\alpha *}(G_j) D_{n',n}^\beta(G_j) \\ &= \delta_{\alpha,\beta} \frac{g}{d_\alpha} \sum_{n'=1}^{d_\beta} \Phi_{n'}^\beta \delta_{m,n'} \delta_{m,n} \\ &= \delta_{\alpha,\beta} \frac{g}{d_\alpha} \Phi_m^\beta \delta_{m,n}\end{aligned} \tag{C.48}$$

From (C.48) it follows that if we let

$$P_m^\alpha \equiv \frac{d_\alpha}{g} \sum_{j=1}^{g} D_{m,m}^{\alpha *}(G_j) G_j \tag{C.49}$$

then

$$P_m^\alpha \Phi_n^\beta = \delta_{\alpha,\beta} \delta_{m,n} \Phi_m^\beta \tag{C.50}$$

In other words, when the operator P_m^α defined by equation (C.49) acts on any function in the set $(\Phi_1^1, \Phi_2^1, ..., \Phi_{d_1}^1)$, $(\Phi_1^2, \Phi_2^2, ...\Phi_{d_2}^2)$,..., the function is given back unchanged, provided that $m = n$ and $\alpha = \beta$. Otherwise the function is annihilated. *Thus, P_m^α is a projection operator corresponding to the mth basis function of the αth irreducible representation of the group in a standard unitary representation.* If P_m^α acts on an arbitrary function, it will annihilate all of it except the component that transforms like the mth basis function of D^α.

A second type of group-theoretical projection operator can be defined by the relationship

$$P^\alpha \equiv \sum_{m=1}^{d_\alpha} P_m^\alpha = \frac{d_\alpha}{g} \sum_{j=1}^{g} \sum_{m=1}^{d_\alpha} D_{m,m}^{\alpha *}(G_j) G_j \tag{C.51}$$

which can be rewritten as

$$P^\alpha \equiv \frac{d_\alpha}{g} \sum_{j=1}^{g} \chi^{\alpha *}(G_j) G_j \tag{C.52}$$

From (C.50) it follows that

$$P^\alpha \Phi_n^\beta = \sum_{m=1}^{d_\alpha} P_m^\alpha \Phi_n^\beta = \delta_{\alpha,\beta} \sum_{m=1}^{d_\alpha} \delta_{m,n} \Phi_m^\beta = \delta_{\alpha,\beta} \Phi_n^\beta \tag{C.53}$$

When P^α acts on an arbitrary function, it annihilates everything except the component which can be expressed as a linear combination of basis functions of the irreducible representation D^α. If we sum (C.53) over all of the irreducible representations of the group, we obtain

$$\sum_{\alpha=1}^{r'} P^\alpha \Phi_n^\beta = \sum_{\alpha=1}^{r'} \delta_{\alpha,\beta} \Phi_n^\beta = \Phi_n^\beta \tag{C.54}$$

Therefore the sum acts like the identity operator and we can write

$$\sum_{\alpha=1}^{r'} P^\alpha = E \tag{C.55}$$

Combining (C.55) with (C.52), we obtain

$$\sum_{j=1}^{g} \sum_{\alpha=1}^{r'} \frac{d_\alpha}{g} \chi^{\alpha *}(G_j) G_j = E \equiv G_1 \tag{C.56}$$

Since the group elements $G_1, ..., G_g$ are linearly independent, equation (C.55) implies that

$$\sum_{\alpha=1}^{r'} \frac{d_\alpha}{g} \chi^{\alpha *}(G_j) = \delta_{j,1} \tag{C.57}$$

The character of the identity element in any representation is equal to the dimension of that representation:

$$\chi^{\alpha *}(E) = \chi^\alpha(E) = d_\alpha \tag{C.58}$$

Therefore, when $j = 1$, we obtain from (C.57) the relationship

$$\sum_{\alpha=1}^{r'} d_\alpha^2 = g \tag{C.59}$$

i.e., *the sum of the squares of the dimensions of the irreducible representations is equal to the order of the group.*

C.8 The regular representation

The 'regular representation' of a finite group is a reducible representation D^{reg} in which the basis consists of the group elements themselves:

$$G_j G_n = \sum_{n'=1}^{g} G_{n'} D^{\text{reg}}_{n',n}(G_j) \tag{C.60}$$

D^{reg} must thus be a set of g $g \times g$ matrices. If we know the multiplication table for a finite group, we can construct the regular representation. For example, the multiplication table for the group C_3 is shown above. It can easily be verified that if we let

$$\begin{aligned}
D^{\text{reg}}(E) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\
D^{\text{reg}}(C_3) &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \\
D^{\text{reg}}(C_3^{-1}) &= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}
\end{aligned} \tag{C.61}$$

then the matrices will be the regular representation of the group C_3 according to the definition shown in (C.60) and the multiplication table (A.1). Since $G_i G_j \neq G_j$ for $G_i \neq E$, it follows that the character of every group element except the identity element vanishes in the regular representation. (We can notice that this holds in the example given above.) Therefore in the case of the regular representation, equation (C.40) becomes:

$$n_\alpha = \frac{1}{g} \sum_{j=1}^{g} \chi^{\alpha *}(G_j) \chi^{\text{reg}}(G_j) = \frac{1}{g} \chi^{\alpha *}(E) \chi^{\text{reg}}(E) = d_\alpha \tag{C.62}$$

Thus each irreducible representation of a finite group appears d_α times in the regular representation.

When each element of a group commutes with every other one, a group is said to be Abelian. Then from the definition of classes, (C.42), it follows that in an Abelian group, every element is in a class by itself, so that an Abelian group contains g classes, i.e. $r = g$. We can next ask how many non-equivalent irreducible representations an Abelian group contains. To answer this question, we remember from Schur's lemma that the only matrix that commutes with every matrix in an irreducible representation of a group must be a multiple of the unit matrix. But in an Abelian group, all of the elements commute with each other, and therefore their irreducible representations must all be multiples of the unit matrix. This can happen only if all the irreducible representations are 1-dimensional. Thus for an Abelian group, $d_\alpha = 1, \quad \alpha = 1, 2, ..., r'$ and $r' = g$. It can be seen from the multiplication table of the group C_3 that it is Abelian. In the example of C_3, (C.59) becomes $1 + 1 + 1 = 3$.

C.9 Classification of basis functions

We can us the group-theoretical projection operators to classify basis sets into basis functions for the various irreducible representations of a group. For example, we can construct the projection operators of the group C_3 from the character table:

$$\begin{aligned} P^1 &= \frac{1}{3}\left(E + C_3 + C_3^{-1}\right) \\ P^2 &= \frac{1}{3}\left(E + e^{-i2\pi/3}C_3 + e^{i2\pi/3}C_3^{-1}\right) \\ P^3 &= \frac{1}{3}\left(E + e^{i2\pi/3}C_3 + e^{-i2\pi/3}C_3^{-1}\right) \end{aligned} \tag{C.63}$$

Since the group C_3 is Abelian, all of its irreducible representations are 1-dimensional, and hence there is no difference between projection operators of the type P^α and those of the type P_n^α. Notice that $P^1 + P^2 + P^3 = E$ in accordance with (C.55), and that the projection operators are idempotent, i.e., $P^\alpha P^\beta = \delta_{\alpha,\beta} P^\alpha$. All projection operators must be idempotent, since projecting out a subspace of a Hilbert space twice has the same effect as doing it once, and acting in succession with projection operators corresponding to different subspaces must yield zero.

Now consider the set of functions $\Phi_m = e^{im\varphi}$ where m is an integer. We can use the projection operators of (C.63) to split the Hilbert space spanned by this set of functions into three subspaces. Using the relationships

$$\begin{aligned} Ee^{im\varphi} &= e^{im\varphi} \\ C_3 e^{im\varphi} &= e^{im(\varphi - 2\pi/3)} \\ C_3^{-1} e^{im\varphi} &= e^{im(\varphi + 2\pi/3)} \end{aligned} \tag{C.64}$$

we obtain

$$\begin{aligned} P^1 e^{im\varphi} &= \frac{1}{3} e^{im\varphi}\left(1 + e^{-im2\pi/3} + e^{im2\pi/3}\right) \\ &= \begin{cases} 0 & \text{if } m = \pm1, \pm2, \pm4, \pm5, ... \\ e^{im\varphi} & \text{if } m = 0, \pm3, \pm6, \pm9, ... \end{cases} \end{aligned} \tag{C.65}$$

and similarly

$$\begin{aligned} P^2 e^{im\varphi} &= \begin{cases} 0 & \text{if } m+1 = \pm1, \pm2, \pm4, \pm5, ... \\ e^{im\varphi} & \text{if } m+1 = 0, \pm3, \pm6, \pm9, ... \end{cases} \\ P^3 e^{im\varphi} &= \begin{cases} 0 & \text{if } m-1 = \pm1, \pm2, \pm4, \pm5, ... \\ e^{im\varphi} & \text{if } m-1 = 0, \pm3, \pm6, \pm9, ... \end{cases} \end{aligned} \tag{C.66}$$

Thus the Hilbert space spanned by the functions $\Phi_m = e^{im\varphi}$ is divided into three subspaces each of which consists of basis functions for one of the irreducible representations of C_3. For non-Abelian groups the Hilbert space spanned by a set of basis functions can be divided into still smaller subspaces through the use of projection operators of the type P_n^α defined in equation (C.49). If we wish to have names for the the two types of projection operators, we might call P_m^α 'strong' and P^α 'weak', since P_n^α has a stronger effect than P^α.

Now suppose that we have divided the Hilbert space spanned by a set of basis functions into small subspaces by means of the strong projection operators P_n^α, so that

$$P_n^\alpha \Phi_j = p_j \Phi_j \qquad p_j = 0 \text{ or } 1 \tag{C.67}$$

We will now show that if an operator T commutes with every element of the group, then the matrix elements of T linking functions belonging to different subspaces must necessarily vanish. The proof is as follows: Since T commutes with every element of the group, and since the projection operators are constructed from group elements, we have

$$[P_n^\alpha, T] = 0 \tag{C.68}$$

Then

$$\langle \Phi_j | \, [P_n^\alpha, T] \, | \Phi_k \rangle = (p_j - p_k) \langle \Phi_j | T | \Phi_k \rangle = 0 \tag{C.69}$$

Thus if Φ_j and Φ_k belong to different subspaces when the basis set is classified by the action of the projection operators P_n^α, i.e., if $p_j \neq p_k$, then $\langle \Phi_j | T | \Phi_k \rangle = 0$. *It follows that a matrix representation of the operator T will be block-diagonal if it is based on functions that have been classified by means of the projection operators P_n^α, i.e. if it is based on a set of functions that satisfy (C.67). Such a basis set is said to be 'symmetry-adapted'.*

We can introduce a special notation to represent fully symmetry-adapted basis functions. Let $|\eta_j^{\alpha,n}\rangle$ be such a function.[2] By this we indicate that the function transforms under the action of the group elements like nth basis function of the αth standard irreducible representation of the group, while the index j distinguishes between the various linearly independent functions that have this property. With this notation we can write:

$$P_n^\alpha |\eta_j^{\beta,m}\rangle = \delta_{\alpha,\beta} \delta_{n,m} |\eta_j^{\beta,m}\rangle \tag{C.70}$$

Using this notation, the statement that a matrix representation of the operator T based on symmetry-adapted functions will be block-diagonal can be written in the form:

$$\langle \eta_i^{\alpha,n} | T | \eta_j^{\beta,m} \rangle = \delta_{\alpha,\beta} \delta_{n,m} \langle \eta_i^{\alpha,n} | T | \eta_j^{\beta,m} \rangle \tag{C.71}$$

The eigenvalues and eigenfunctions of T can also be expressed in this notation:

$$T | \Psi_\kappa^{\alpha,m} \rangle = \lambda_\kappa^{\alpha,m} | \Psi_\kappa^{\alpha,m} \rangle \tag{C.72}$$

where

$$| \Psi_\kappa^{\alpha,m} \rangle = \sum_j | \eta_j^{\alpha,m} \rangle C_{j,\kappa} \tag{C.73}$$

[2] We also introduce the Dirac notation here, since it is useful in the discussion of matrix elements.

In other words, *a set of functions all of which transform like the* n*th basis function of the* α*th irreducible representation of a group combine to form an eigenfunction of an operator* T *that commutes with all of the group elements.*

We will now try to find a relationship between the degeneracy of the root $\lambda_\kappa^{\alpha,n}$ and the dimension d_α of the irreducible representation D^α. To do this, we introduce the 'shift operator'

$$P^\alpha_{m',m} \equiv \frac{d_\alpha}{g}\sum_{j=1}^{g} D^{\alpha*}_{m',m}(G_j)G_j \qquad m' \neq m \tag{C.74}$$

Then by an argument similar to (C.48) we have

$$\begin{aligned}
P^\alpha_{m',m}|\eta_j^{\alpha,m}\rangle &= \frac{d_\alpha}{g}\sum_{j=1}^{g} D^{\alpha*}_{m',m}(G_j)G_j|\eta_j^{\alpha,m}\rangle \\
&= \sum_{m''=1}^{d_\alpha}|\eta_j^{\alpha,m''}\rangle\frac{d_\alpha}{g}\sum_{j=1}^{g} D^{\alpha*}_{m',m}(G_j)D^{\alpha}_{m'',m}(G_j) \\
&= \sum_{m''=1}^{d_\alpha}|\eta_j^{\alpha,m''}\rangle\delta_{m'',m'} = |\eta_j^{\alpha,m'}\rangle
\end{aligned} \tag{C.75}$$

where we have made use of the great orthogonality relation (C.16). Since $P^\alpha_{m',m}$ is a linear combination of group elements, it must commute with T:

$$\left[P^\alpha_{m',m}, T\right] = 0 \tag{C.76}$$

Therefore

$$\begin{aligned}
\langle\Psi_\kappa^{\alpha,m'}|\left[P^\alpha_{m',m}, T\right]|\Psi_\kappa^{\alpha,m}\rangle &= \left(\lambda_\kappa^{\alpha,m'} - \lambda_\kappa^{\alpha,m}\right)\langle\Psi_\kappa^{\alpha,m'}|P^\alpha_{m',m}|\Psi_\kappa^{\alpha,m}\rangle \\
&= \left(\lambda_\kappa^{\alpha,m'} - \lambda_\kappa^{\alpha,m}\right) = 0
\end{aligned} \tag{C.77}$$

so that the roots corresponding to the d_α eigenfunctions $|\Psi_\kappa^{\alpha,1}\rangle, ..., |\Psi_\kappa^{\alpha,d_\alpha}\rangle$ must be degenerate. Such a degeneracy is called a 'due degeneracy' because it is due to the symmetry properties of the system. If there are other degeneracies, they are termed 'accidental'.

Appendix D

Sturmian basis sets

D.1 One-electron Coulomb Sturmians

Because of their completeness properties, one-electron Sturmian basis sets have long been used in theoretical atomic physics. Their form is identical with that of the familiar hydrogenlike atomic orbitals, except that the factor Z/n is replaced by a constant k. The one-electron Coulomb Sturmians can be written as

$$\chi_{nlm}(\mathbf{x}) = R_{nl}(r) Y_{lm}(\theta, \phi) \tag{D.1}$$

where Y_{lm} is a spherical harmonic, and where the radial function has the form

$$R_{nl}(r) = \mathcal{N}_{nl}(2kr)^l e^{-kr} F\left(l+1-n|2l+2|2kr\right) \tag{D.2}$$

Here

$$\mathcal{N}_{nl} = \frac{2k^{3/2}}{(2l+1)!}\sqrt{\frac{(l+n)!}{n(n-l-1)!}} \tag{D.3}$$

is a normalizing constant, while

$$F\left(a|b|x\right) \equiv \sum_{t=0}^{\infty} \frac{a^{\bar{t}}}{t! b^{\bar{t}}} x^t = 1 + \frac{a}{b}x + \frac{a(a+1)}{2b(b+1)}x^2 + \cdots \tag{D.4}$$

is a confluent hypergeometric function. Coulomb Sturmian basis functions obey the following one-electron Schrödinger equation (in atomic units):

$$\left[-\frac{1}{2}\nabla^2 - \frac{nk}{r} + \frac{1}{2}k^2\right] \chi_{nlm}(\mathbf{x}) = 0 \tag{D.5}$$

which is just the Schrödinger equation for an electron in a hydrogenlike atom with the replacement $Z/n \to k$. All of the functions in a such a basis set correspond to the same energy,

$$\epsilon = -\frac{1}{2}k^2 \tag{D.6}$$

Table B.1: One-electron Coulomb Sturmian radial functions. If k is replaced by Z/n they are identical to the familiar hydrogenlike radial wave functions.

n	l	$R_{n,l}(r)$
1	0	$2k^{3/2}e^{-kr}$
2	0	$2k^{3/2}(1-kr)e^{-kr}$
2	1	$\frac{2k^{3/2}}{\sqrt{3}}\ kr\ e^{-kr}$
3	0	$2k^{3/2}\left(1-2kr+\frac{2(kr)^2}{3}\right)e^{-kr}$
3	1	$2k^{3/2}\frac{2\sqrt{2}}{3}\ kr\ \left(1-\frac{kr}{2}\right)e^{-kr}$
3	2	$2k^{3/2}\frac{\sqrt{2}}{3\sqrt{5}}\ (kr)^2\ e^{-kr}$

In other words the basis set is isoenergetic. In the wave equation obeyed by the Sturmians, (D.5), the potential is weighted differently for members of the basis set corresponding to different values of n. Equation (D.5) can be written in the form:

$$\left[-\frac{1}{2}\nabla^2 - \beta_n \frac{Z}{r} + \frac{1}{2}k^2\right]\chi_{nlm}(\mathbf{x}) = 0 \qquad \beta_n = \frac{kn}{Z} \tag{D.7}$$

The weighting factors β_n are chosen in such a way as to make all of the solutions isoenergetic. All solutions correspond to the energy $\epsilon = -k^2/2$. In the Hamiltonian formulation of physics, the eigenvalues of the wave equation are a spectrum of allowed energies, but here all of the solutions of the wave equation correspond to the same energy, and the weighting factors play the role of eigenvalues. The functions in a Coulomb Sturmian basis set can be shown to obey and obey a potential-weighted orthonormality relation: To see this, we consider two solutions, $\chi_{nlm}(\mathbf{x})$ and $\chi_{n'l'm'}(\mathbf{x})$, obeying the equations:

$$\begin{aligned}\left[-\frac{1}{2}\nabla^2 + \frac{1}{2}k^2\right]\chi_{nlm}(\mathbf{x}) &= \frac{nk}{r}\chi_{nlm}(\mathbf{x}) \\ \left[-\frac{1}{2}\nabla^2 + \frac{1}{2}k^2\right]\chi^*_{n'l'm'}(\mathbf{x}) &= \frac{n'k}{r}\chi^*_{n'l'm'}(\mathbf{x})\end{aligned} \tag{D.8}$$

Multiplying the two equations from the left respectively by $\chi^*_{n'l'm'}(\mathbf{x})$ and $\chi_{nlm}(\mathbf{x})$, integrating over the coordinates, and subtracting the two equations, we obtain:

$$(n-n')\int d^3x\ \chi^*_{n'l'm'}(\mathbf{x})\frac{1}{r}\chi_{nlm}(\mathbf{x}) = 0 \tag{D.9}$$

where we have also made use of the fact that (from Hermiticity)

$$\begin{aligned}&\int d^3x\ \chi^*_{n'l'm'}(\mathbf{x})\left[-\frac{1}{2}\nabla^2 + \frac{1}{2}k^2\right]\chi_{nlm}(\mathbf{x}) \\ -&\int d^3x\ \chi_{nlm}(\mathbf{x})\left[-\frac{1}{2}\nabla^2 + \frac{1}{2}k^2\right]\chi^*_{n'l'm'}(\mathbf{x}) = 0\end{aligned} \tag{D.10}$$

Thus for $n \neq n'$, the potential-weighted scalar product vanishes, and it vanishes also when $l' \neq l$ or $m' \neq m$ because of the orthogonality of the spherical harmonics. The Coulomb Sturmians are normalized in such a way that the orthonormality relation is:

$$\int d^3x\ \chi^*_{n'l'm'}(\mathbf{x})\frac{1}{r}\chi_{nlm}(\mathbf{x}) = \frac{k}{n}\delta_{n'n}\delta_{l'l}\delta_{m'm} \tag{D.11}$$

Because of their completeness and their close relationship with Coulomb potentials, Coulomb Sturmians are widely used in atomic physics.

D.2 Löwdin-orthogonalized Coulomb Sturmians

The Coulomb Sturmians form a complete set in the sense that any square-integrable function of $\mathbf{x}$ can be expanded in terms of them. For this reason, they are useful as basis functions in many applications. Sometimes it may be convenient to use Coulomb Sturmian basis functions in a form that is orthonormalized in the conventional way. Let us denote the orthogonalized Coulomb Sturmians by $\tilde{\chi}_\mu(\mathbf{x})$, where $\mu \equiv (n, l, m)$. This new basis set is related to the original set of Coulomb Sturmians discussed above by

$$\tilde{\chi}_\mu(\mathbf{x}) = \sum_{\mu'} \chi_\mu(\mathbf{x}) W_{\mu',\mu} \tag{D.12}$$

where $W_{\mu',\mu}$ is a transformation matrix. We wish the transformation to be such that

$$\int d^3x\ \tilde{\chi}^*_{\mu'}(\mathbf{x})\tilde{\chi}_\mu(\mathbf{x}) \equiv \tilde{S}_{\mu',\mu} = \delta_{\mu',\mu} \tag{D.13}$$

Suppose that

$$\int d^3x\ \chi^*_{\mu'}(\mathbf{x})\chi_\mu(\mathbf{x}) = S_{\mu',\mu} \tag{D.14}$$

Then, in matrix notation, the condition that the transformation matrix W must satisfy is

$$W^\dagger S W = I \tag{D.15}$$

where the dagger denotes the Hermitian adjoint, i.e., the conjugate transpose. Following Löwdin and Wannier, we can choose from all the possible solutions to the matrix equation (D.15) the one for which

$$W^\dagger = W \tag{D.16}$$

(This is sometimes called *symmetrical orthogonalization*.) Then (D.15) will be satisfied if

$$W = S^{-1/2} \tag{D.17}$$

In order to find the square root of the overlap matrix S, we diagonalize it, take the inverse square root in the diagonal representation, and then transform back to the original representation. This gives us $W = S^{-1/2}$, which we then use to perform the transformation shown in equation (D.12).

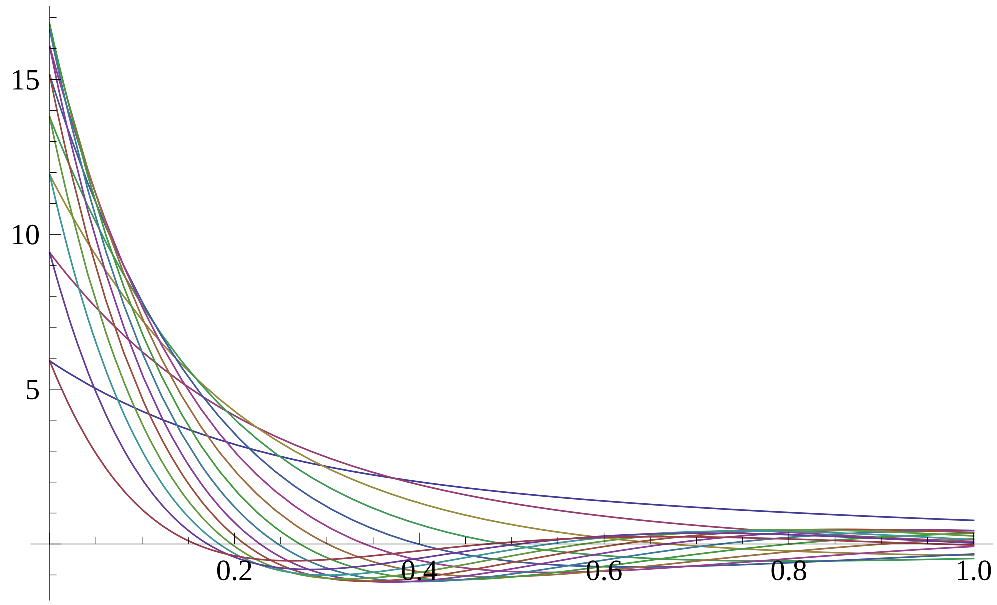

Figure D.1: *A set of 15 Löwdin-orthogonalized Coulomb Sturmians corresponding to $l = 0$ and $k = 1$. The radial parts are shown as functions of r. If an arbitrary radial function is to be expanded in terms of this set, the value of k for the set can be adjusted in such a way as to give maximum accuracy. Löwdin-orthogonalized Coulomb Sturmians are used in the Hartree-Fock calculations of Chapter 2.*

D.3 The Fock projection

Coulomb Sturmian basis functions and their Fourier transforms are related by

$$\chi_{nlm}(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^3}} \int d^3x \; e^{i\mathbf{p}\cdot\mathbf{x}} \chi^t_{nlm}(\mathbf{p}) \tag{D.18}$$

and by the inverse transform

$$\chi^t_{nlm}(\mathbf{p}) = \frac{1}{\sqrt{(2\pi)^3}} \int d^3x \; e^{-i\mathbf{p}\cdot\mathbf{x}} \chi_{nlm}(\mathbf{x}) \tag{D.19}$$

By projecting momentum-space onto the surface of a 4-dimensional hypersphere, V. Fock [**?**], [**?**] was able to show that the Fourier-transformed Coulomb Sturmians can be very simply expressed in terms of 4-dimensional hyperspherical harmonics through the relationship

$$\chi^t_{n,l,m}(\mathbf{p}) = M(p) Y_{n-1,l,m}(\hat{\mathbf{u}}) \tag{D.20}$$

where

$$M(p) \equiv \frac{4k^{5/2}}{(k^2 + p^2)^2} \tag{D.21}$$

and

$$\begin{aligned} u_1 &= \frac{2kp_1}{k^2+p^2} \\ u_2 &= \frac{2kp_2}{k^2+p^2} \\ u_3 &= \frac{2kp_3}{k^2+p^2} \\ u_4 &= \frac{k^2-p^2}{k^2+p^2} \end{aligned} \tag{D.22}$$

The 4-dimensional hyperspherical harmonics are given by [?], [?], [?], [?]

$$Y_{\lambda,l,m}(\hat{\mathbf{u}}) = \mathcal{N}_{\lambda,l} C_{\lambda-l}^{1+l}(u_4) Y_{l,m}(u_1,u_2,u_3) \tag{D.23}$$

where $Y_{l,m}$ is a spherical harmonic of of the familiar type, while

$$\mathcal{N}_{\lambda,l} = (-1)^\lambda i^l (2l)!! \sqrt{\frac{2(\lambda+1)(\lambda-l)!}{\pi(\lambda+l+1)!}} \tag{D.24}$$

is a normalizing constant, and

$$C_j^\alpha(u_4) = \sum_{t=0}^{[j/2]} \frac{(-1)^t \Gamma(j+\alpha-t)}{t!(j-2t)!\Gamma(\alpha)} (2u_4)^{j-2t} \tag{D.25}$$

is a Gegenbauer polynomial. The first few The relationships between hyperspherical harmonics, harmonic polynomials, and harmonic projection will be discussed in Appendix C. Table 5.1 in Chapter 5 shows the first few hyperspherical harmonics.

D.4 Generalized Sturmians and many-particle problems

In 1968, Osvaldo Goscinski [[?]] generalized the concept of Sturmian basis sets by considering isoenergetic sets of solutions to a many-particle Schrödinger equation with a weighted potential:

$$\left[-\frac{1}{2}\Delta + \beta_\nu V_0(\mathbf{x}) - E_\kappa\right] |\Phi_\nu\rangle = 0 \tag{D.26}$$

The weighting factors β_ν are chosen in such a way as to make all of the functions in the set correspond to the same energy, E_κ, and this energy is usually chosen to be that of the quantum mechanical state which is to be represented by a superposition of generalized

Sturmian basis functions. If the basis set is used to treat N-particle systems where the particles have different masses, the operator Δ in the kinetic energy term is given by

$$\Delta \equiv \sum_{j=1}^{N} \frac{1}{m_j} \nabla_j^2 \tag{D.27}$$

while if the masses are all equal, it is given by the generalized Laplacian operator:

$$\Delta \equiv \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2} \tag{D.28}$$

with $d = 3N$ and

$$\mathbf{x} = (x_1, x_2, ..., x_d) \tag{D.29}$$

Like the one-electron Coulomb Sturmians, the functions in generalized Sturmian basis sets can be shown to obey a potential-weighted orthonormality relation [**?**]:

$$\langle \Phi_{\nu'} | V_0(\mathbf{x}) | \Phi_\nu \rangle = \delta_{\nu',\nu} \frac{2E_\kappa}{\beta_\nu} \tag{D.30}$$

D.5 Use of generalized Sturmian basis sets to solve the many-particle Schrödinger equation

If we wish to solve a many-particle Schrödinger equation of the form

$$\left[-\frac{1}{2}\Delta + V(\mathbf{x}) - E_\kappa \right] |\Psi_\kappa\rangle = 0 \tag{D.31}$$

we can approximate a solution as a superposition of generalized Sturmian basis functions

$$|\Psi_\kappa\rangle \approx \sum_\nu |\Phi_\nu\rangle B_{\nu,\kappa} \tag{D.32}$$

Substituting this superposition into the Schrödinger equation and remembering that each of the basis functions satisfies eq.(D.26), we obtain:

$$\begin{aligned} &\sum_\nu \left[-\frac{1}{2}\Delta + V(\mathbf{x}) - E_\kappa \right] |\Phi_\nu\rangle B_{\nu,\kappa} \\ = \;&\sum_\nu \left[V(\mathbf{x}) - \beta_\nu V_0(\mathbf{x}) \right] |\Phi_\nu\rangle B_{\nu,\kappa} \approx 0 \end{aligned} \tag{D.33}$$

If we multiply from the left by a conjugate function from our generalized Sturmian basis set and integrate over all coordinates, we obtain a set of secular equations from which the kinetic energy term has disappeared:

$$\sum_\nu \langle \Phi^*_{\nu'} | \left[V(\mathbf{x}) - \beta_\nu V_0(\mathbf{x}) \right] \Phi_\nu \rangle B_{\nu,\kappa} = 0 \tag{D.34}$$

If we introduce the definition

$$T_{\nu',\nu} \equiv -\frac{1}{p_\kappa}\langle \Phi^*_{\nu'}|V(\mathbf{x})|\Phi_\nu\rangle \tag{D.35}$$

where

$$p_\kappa \equiv \sqrt{-2E_\kappa} \tag{D.36}$$

and make use of the potential-weighted orthonormality relations (D.30), we can rewrite the secular equations in the form:

$$\sum_\nu \left[T_{\nu',\nu} - p_\kappa \delta_{\nu',\nu}\right] B_{\nu,\kappa} = 0 \tag{D.37}$$

The generalized Sturmian secular equations are strikingly different from conventional Hamiltonian secular equations in several ways:

- The kinetic energy term has disappeared.
- The matrix representing the approximate potential $V_0(\mathbf{x})$ is diagonal.
- The roots of the secular equations are not energies, but values of the scaling parameter p_κ, from which the energy can be obtained through the relationship $E_\kappa = -p_\kappa^2/2$.
- For Coulomb potentials, the matrix $T_{\nu',\nu}$ is energy-independent.

D.6 Momentum-space orthonormality relations for Sturmian basis sets

By arguments similar to those used in equations (D.8)-(D.11), a set of generalized Sturmian basis functions can be shown to obey a potential-weighted orthonormality relation in direct space

$$\int dx\ \Phi^*_{\nu'}(\mathbf{x})V_0(\mathbf{x})\Phi_\nu(\mathbf{x}) = \delta_{\nu',\nu}\frac{2E_\kappa}{\beta_\nu} = -\delta_{\nu',\nu}\frac{p_\kappa^2}{\beta_\nu} \tag{D.38}$$

where

$$p_\kappa^2 \equiv -2E_\kappa \tag{D.39}$$

(In equation (D.38) and in the remainder of this appendix, we abandon the Dirac bra and ket notation in order to distinguish between functions of $\mathbf{x} \equiv (\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N)$ and functions of $\mathbf{p} \equiv (\mathbf{p}_1, \mathbf{p}_2, ..., \mathbf{p}_N)$). We would now like to find the momentum-space orthonormality relations obeyed by Fourier transforms of the generalized Sturmian basis set. Because the Fourier transform is unitary, the inner product of any two functions in L_2 is preserved under the operation of taking their Fourier transforms, i.e.

$$\int dx\ f^*(\mathbf{x})g(\mathbf{x}) = \int dp\ f^{t*}(\mathbf{p})g^t(\mathbf{p}) \tag{D.40}$$

Using this well-known relationship with $f^*(\mathbf{x}) = \Phi^*_{\nu'}(\mathbf{x})$ and $g(\mathbf{x}) = V_0(\mathbf{x})\Phi_\nu(\mathbf{x})$, we have

$$\int dx\ \Phi^*_{\nu'}(\mathbf{x})V_0(\mathbf{x})\Phi_\nu(\mathbf{x}) = \int dp\ \Phi^{t*}_{\nu'}(\mathbf{p})\left[V_0\Phi_\nu\right]^t(\mathbf{p}) \tag{D.41}$$

In order to evaluate $\left[V_0\Phi_\nu\right]^t(\mathbf{p})$, we remember the Fourier convolution theorem, which states that the Fourier transform of the product of two functions is the convolution of their Fourier transforms. Thus if a and b are any two functions in L_2,

$$[ab]^t(\mathbf{p}') \equiv \frac{1}{(2\pi)^{d/2}}\int dx\ \ e^{-i\mathbf{p}'\cdot\mathbf{x}}a(\mathbf{x})b(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}}\int dp\ a^t(\mathbf{p}'-\mathbf{p})b^t(\mathbf{p}) \tag{D.42}$$

Letting $a(\mathbf{x}) = V_0(\mathbf{x})$ and $b(\mathbf{x}) = \Phi_\nu(\mathbf{x})$ we have

$$\left[V_0\Phi_\nu\right]^t(\mathbf{p}') = \frac{1}{(2\pi)^{d/2}}\int dp\ V_0^t(\mathbf{p}'-\mathbf{p})\Phi^t_\nu(\mathbf{p}) \tag{D.43}$$

Since the momentum-space integral equation corresponding to (D.26) has the form

$$(p'^2 + p_\kappa^2)\Phi^t_\nu(\mathbf{p}') = -\frac{2\beta_\nu}{(2\pi)^{d/2}}\int dp\ V_0^t(\mathbf{p}'-\mathbf{p})\Phi^t_\nu(\mathbf{p}) \tag{D.44}$$

it follows that

$$\left[V_0\Phi_\nu\right]^t(\mathbf{p}) = -\frac{(p^2+p_\kappa^2)}{2\beta_\nu}\Phi^t_\nu(\mathbf{p}) \tag{D.45}$$

Finally, substituting (D.45) into (D.41), we obtain the momentum-space orthonormality relations for a set of generalized Sturmian basis functions:

$$\int dp\ \Phi^{t*}_{\nu'}(\mathbf{p})\left(\frac{p^2+p_\kappa^2}{2p_\kappa^2}\right)\Phi^t_\nu(\mathbf{p}) = \delta_{\nu',\nu} \tag{D.46}$$

Because all of the functions $\Phi_\nu(\mathbf{x})$ in the generalized Sturmian basis set obey equation (D.26), the potential-weighted direct space orthonormality relations shown in equation (D.38) can be rewritten in the form

$$\int dx\ \Phi^*_{\nu'}(\mathbf{x})\left(\frac{-\Delta+p_\kappa^2}{2p_\kappa^2}\right)\Phi_\nu(\mathbf{x}) = \delta_{\nu',\nu} \tag{D.47}$$

so that the momentum-space and direct-space orthonormality relations can be seen to be related to each other in a symmetrical way. These weighted orthonormality relations in $L_2(\mathbb{R}^d)$ are the usual orthonormality relations in the Sobolev space $W_2^{(1)}(\mathbb{R}^d)$ (see [**?**]). For the case of unequal masses, where

$$\Delta \equiv \sum_{j=1}^{d}\frac{1}{m_j}\frac{\partial^2}{\partial x_j^2} \tag{D.48}$$

the momentum-space orthonormality relations for generalized Sturmians (D.46) takes on the slightly modified form

$$\int dp\ \Phi^{t*}_{\nu'}(\mathbf{p})\left(\frac{\sum_j p_j^2/m_j + p_\kappa^2}{2p_\kappa^2}\right)\Phi^t_\nu(\mathbf{p}) = \delta_{\nu',\nu} \tag{D.49}$$

D.7 Sturmian expansions of d-dimensional plane waves

If the set of generalized Sturmian basis functions is complete in the sense of spanning the Sobolev space $W_2^{(1)}(\mathbb{R}^d)$, we can use it to construct a weakly convergent expansion of a d-dimensional plane wave (valid only in the sense of distributions). Suppose that we let

$$e^{i\mathbf{p}\cdot\mathbf{x}} = \left(\frac{p_\kappa^2 + p^2}{2p_\kappa^2}\right) \sum_\nu \Phi_\nu^{t*}(\mathbf{p}) a_\nu(\mathbf{x}) \tag{D.50}$$

We can then determine the unknown functions $a_\nu(\mathbf{x})$ by means of the orthonormality relations (D.46). Multiplying (D.50) on the left by $\Phi_{\nu'}^{t*}(\mathbf{p})$ and integrating over dp making use of (D.46), we obtain

$$\int dp\ e^{i\mathbf{p}\cdot\mathbf{x}} \Phi_{\nu'}^{t*}(\mathbf{p}) = \sum_\nu \delta_{\nu',\nu} a_\nu(\mathbf{x}) = a_{\nu'}(\mathbf{x}) \tag{D.51}$$

so that

$$a_\nu(\mathbf{x}) = \int dp\ e^{i\mathbf{p}\cdot\mathbf{x}} \Phi_\nu^t(\mathbf{p}) = (2\pi)^{d/2} \Phi_\nu(\mathbf{x}) \tag{D.52}$$

Thus finally we obtain an expansion of the form

$$e^{i\mathbf{p}\cdot\mathbf{x}} = (2\pi)^{d/2} \left(\frac{p_\kappa^2 + p^2}{2p_\kappa^2}\right) \sum_\nu \Phi_\nu^{t*}(\mathbf{p}) \Phi_\nu(\mathbf{x}) \tag{D.53}$$

If the set of generalized Sturmians $\Phi_\nu(\mathbf{x})$ does not span $W_2^{(1)}(\mathbb{R}^d)$, equation (D.53) becomes

$$P\left[e^{i\mathbf{p}\cdot\mathbf{x}}\right] = (2\pi)^{d/2} \left(\frac{p_\kappa^2 + p^2}{2p_\kappa^2}\right) \sum_\nu \Phi_\nu^{t*}(\mathbf{p}) \Phi_\nu(\mathbf{x}) \tag{D.54}$$

where $P\left[e^{i\mathbf{p}\cdot\mathbf{x}}\right]$ is the projection of the d-dimensional plane wave onto the subspace spanned by the set $\{\Phi_\nu(\mathbf{x})\}$. For example, if we are considering a system of N electrons, with $d = 3N$, the generalized Sturmian basis set might be antisymmetric with respect to exchange of the N electron coordinates but otherwise complete. In that case, $P\left[e^{i\mathbf{p}\cdot\mathbf{x}}\right]$ would represent the projection of the plane wave onto that part of Hilbert space corresponding to functions of $\mathbf{x}$ that are antisymmetric with respect to exchange of the N electron coordinates. Neither the expansion shown in equation (D.53) nor that shown in equation (D.54) is point-wise convergent. In other words, we cannot perform the sums shown on the right-hand sides of these equations and expect them to give point-wise convergent representations of the plane wave or its projection. However, the expansions are valid in the sense of distributions. For the case of unequal masses, the generalized Sturmian plane wave expansion takes on the slightly modified form

$$e^{i\mathbf{p}\cdot\mathbf{x}} = (2\pi)^{d/2} \left(\frac{p_\kappa^2 + \sum_j p_j^2/m_j}{2p_\kappa^2}\right) \sum_\nu \Phi_\nu^{t*}(\mathbf{p}) \Phi_\nu(\mathbf{x}) \tag{D.55}$$

D.8 An alternative expansion of a d-dimensional plane wave

In the Hamiltonian formulation of physics, one typically obtains sets of functions whose orthonormality relation has the form

$$\int dx\ \Phi_{\nu'}^*(\mathbf{x})\Phi_\nu(\mathbf{x}) = \delta_{\nu',\nu} \tag{D.56}$$

Such a set of basis functions might, for example be the configurations resulting from the solution of the N-electron approximate Schrödinger equation

$$\left[-\frac{1}{2}\Delta + V_0(\mathbf{x}) - E_\nu\right]\Phi_\nu(\mathbf{x}) = 0 \tag{D.57}$$

with $\mathbf{x} \equiv (x_1, x_2, ..., x_d)$ and $d = 3N$. It is interesting to notice that a d-dimensional plane wave can also be expanded in terms of a basis set with orthonormality relations of the form shown in equation (D.56). To see this we write

$$e^{-i\mathbf{p}\cdot\mathbf{x}} = \sum_\nu a_\nu(\mathbf{p})\Phi_\nu^*(\mathbf{x}) \tag{D.58}$$

Multiplying from the left by $\Phi_{\nu'}(\mathbf{x})$ and integrating over the coordinates, we obtain the relation

$$\begin{aligned}\int dx\ e^{-i\mathbf{p}\cdot\mathbf{x}}\Phi_{\nu'}(\mathbf{x}) &= \sum_\nu a_\nu(\mathbf{p})\int dx\ \Phi_\nu^*(\mathbf{x})\Phi_{\nu'}(\mathbf{x}) \\ &= \sum_\nu a_\nu(\mathbf{p})\delta_{\nu',\nu} = a_{\nu'}(\mathbf{p}) = (2\pi)^{d/2}\Phi_{\nu'}^t(\mathbf{p})\end{aligned} \tag{D.59}$$

Thus we obtain the alternative expansion

$$e^{-i\mathbf{p}\cdot\mathbf{x}} = (2\pi)^{d/2}\sum_\nu \Phi_{\nu'}^t(\mathbf{p})\Phi_\nu^*(\mathbf{x}) \tag{D.60}$$

or

$$e^{i\mathbf{p}\cdot\mathbf{x}} = (2\pi)^{d/2}\sum_\nu \Phi_{\nu'}^{t*}(\mathbf{p})\Phi_\nu(\mathbf{x}) \tag{D.61}$$

The expansion (D.53) was a consequence of the weighted orthonormality relations obeyed by generalized Sturmian basis sets, while the expansion (D.61) resulted from the more conventional orthonormality relations (D.56). Both forms of the expansion are used in Chapter 8.

Appendix E

Angular and hyperangular integrations

The physical importance of the properties of homogeneous and harmonic polynomials comes from their close relationship to spherical and hyperspherical harmonics, and from their relationship to angular and hyperangular integrations. We will see that these properties lead to useful results in both atomic and molecular physics.

E.1 Monomials, homogeneous polynomials, and harmonic polynomials

A *monomial of degree* n in d coordinates is a product of the form

$$m_n = x_1^{n_1} x_2^{n_2} x_3^{n_3} \cdots x_d^{n_d} \tag{E.1}$$

where the n_j's are positive integers or zero and where their sum is equal to n.

$$n_1 + n_2 + \cdots + n_d = n \tag{E.2}$$

For example, x_1^3, $x_1^2 x_2$ and $x_1 x_2 x_3$ are all monomials of degree 3. Since

$$\frac{\partial m_n}{\partial x_j} = n_j x_j^{-1} m_n \tag{E.3}$$

it follows that

$$\sum_{j=1}^{d} x_j \frac{\partial m_n}{\partial x_j} = n m_n \tag{E.4}$$

A homogeneous polynomial of degree n (which we will denote by the symbol f_n) is a series consisting of one or more monomials, all of which have degree n. For example,

$f_3 = x_1^3 + x_1^2 x_2 - x_1 x_2 x_3$ is a homogeneous polynomial of degree 3. Since each of the monomials in such a series obeys (E.4), it follows that

$$\sum_{j=1}^{d} x_j \frac{\partial f_n}{\partial x_j} = n f_n \tag{E.5}$$

This simple relationship has very far-reaching consequences: If we now introduce the generalized Laplacian operator

$$\Delta \equiv \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2} \tag{E.6}$$

and the hyperradius defined by

$$r^2 \equiv \sum_{j=1}^{d} x_j^2 \tag{E.7}$$

we can show (with a certain amount of effort!) that

$$\Delta\left(r^\beta f_\alpha\right) = \beta(\beta + d + 2\alpha - 2) r^{\beta-2} f_\alpha + r^\beta \Delta f_\alpha \tag{E.8}$$

where α and β are positive integers or zero, β being even. We next define a *harmonic polynomial of degree* n to be a homogeneous polynomial of degree n which also satisfies the generalized Laplace equation:

$$\Delta h_n = 0 \tag{E.9}$$

For example, $h_3 = x_1^2 x_2 - x_3^2 x_2 + x_1 x_2 x_3$ is a harmonic polynomial of degree 3. Combining (E.8) and (E.9) we obtain

$$\Delta\left(r^\beta h_\alpha\right) = \beta(\beta + d + 2\alpha - 2) r^{\beta-2} h_\alpha \tag{E.10}$$

E.2 The canonical decomposition of a homogeneous polynomial

Every homogeneous polynomial f_n can be decomposed into a sum of harmonic polynomials multiplied by powers of the hyperradius. This decomposition, which is called *the canonical decomposition of a homogeneous polynomial*, has the form [?]:

$$f_n = h_n + r^2 h_{n-2} + r^4 h_{n-4} + \cdots \tag{E.11}$$

To see how the decomposition may be performed, we can act on both sides of equation (E.11) with the generalized Laplacian operator Δ. If we do this several times, making use of (E.10), we obtain [?], [?], [?]:

$$\begin{aligned}
\Delta f_n &= 2(d + 2n - 4) h_{n-2} + 4(d + 2n - 6) r^2 h_{n-4} + \cdots \\
\Delta^2 f_n &= 8(d + 2n - 6)(d + 2n - 8) h_{n-4} + \cdots \\
\Delta^3 f_n &= 48(d - 2n - 8)(d - 2n - 10)(d - 2n - 12) h_{n-6} + \cdots
\end{aligned} \tag{E.12}$$

and in general

$$\Delta^\nu f_n = \sum_{k=\nu}^{\lfloor \frac{n}{2} \rfloor} \frac{(2k)!!}{(2k-2\nu)!!} \frac{(d+2n-2k-2)!!}{(d+2n-2k-2\nu-2)!!} r^{2k-2\nu} h_{n-2k} \tag{E.13}$$

where

$$\begin{aligned} j!! &\equiv \begin{cases} j(j-2)(j-4)\cdots 4\times 2 & j = \text{even} \\ \\ j(j-2)(j-4)\cdots 3\times 1 & j = \text{odd} \end{cases} \\ 0!! &\equiv 1 \\ (-1)!! &\equiv 1 \end{aligned} \tag{E.14}$$

An important special case occurs when $\nu = n/2$. In that case, (E.13) becomes

$$\Delta^{n/2} f_n = \frac{n!!(d+n-2)!!}{(d-2)!!} h_0 \tag{E.15}$$

or

$$h_0 = \frac{(d-2)!!}{n!!(d+n-2)!!} \Delta^{n/2} f_n \tag{E.16}$$

We will see below that this result leads to powerful angular and hyperangular integration theorems.

E.3 Harmonic projection

Equations (E.12) or (E.13) form a set of simultaneous equations that can be solved to yield expressions for the various harmonic polynomials that occur in the canonical decomposition of a homogeneous polynomial f_n. In this way we obtain the general result:

$$\begin{aligned} h_{n-2\nu} &= \frac{(d+2n-4\nu-2)!!}{(2\nu)!!(d+2n-2\nu-2)!!} \\ &\times \sum_{j=0}^{\lfloor \frac{n}{2}-\nu \rfloor} \frac{(-1)^j (d+2n-4\nu-2j-4)!!}{(2j)!!(d+2n-4\nu-4)!!} r^{2j} \Delta^{j+\nu} f_n \end{aligned} \tag{E.17}$$

If we let $n - 2\nu = \lambda$, this becomes

$$\begin{aligned} O_\lambda[f_n] = h_\lambda &= \frac{(d+2\lambda-2)!!}{(n-\lambda)!!(d+n+\lambda-2)!!} \\ &\times \sum_{j=0}^{\lfloor \lambda/2 \rfloor} \frac{(-1)^j (d+2\lambda-2j-4)!!}{(2j)!!(d+2\lambda-4)!!} r^{2j} \Delta^{j+\frac{1}{2}(n-\lambda)} f_n \end{aligned} \tag{E.18}$$

Here O_λ can be thought of as a projection operator that projects out the harmonic polynomial of degree λ from the canonical decomposition of the homogeneous polynomial f_n. The projection is of course taken to be zero if λ and n have different parities or if $\lambda > n$.

E.4 Generalized angular momentum

The generalized angular momentum operator Λ^2 is defined as

$$\Lambda^2 \equiv -\sum_{i>j}^{d} \left(x_i \frac{\partial}{\partial x_j} - x_j \frac{\partial}{\partial x_i} \right)^2 \tag{E.19}$$

When $d = 3$ it reduces to the familiar orbital angular momentum operator

$$L^2 = L_1^2 + L_2^2 + L_3^2 \tag{E.20}$$

where

$$L_1 = \frac{1}{i} \left(x_2 \frac{\partial}{\partial x_3} - x_3 \frac{\partial}{\partial x_2} \right) \tag{E.21}$$

and where L_2 and L_3 given by similar expressions with cyclic permutations of the coordinates. If we expand the expression in (E.19), we obtain:

$$\Lambda^2 = -r^2 \Delta + \sum_{i,j=1}^{d} x_i x_j \frac{\partial^2}{\partial x_i \partial x_j} + (d-1) \sum_{i=1}^{d} x_i \frac{\partial}{\partial x_i} \tag{E.22}$$

We next allow Λ^2 to act on a homogeneous polynomial f_n, and make use of (E.5). This give us:

$$\Lambda^2 f_n = -r^2 \Delta f_n + n(d-1) f_n + \sum_{i,j=1}^{d} x_i x_j \frac{\partial^2 f_n}{\partial x_i \partial x_j} \tag{E.23}$$

The relationship

$$\sum_{i,j=1}^{d} x_i x_j \frac{\partial^2 f_n}{\partial x_i \partial x_j} = n(n-1) f_n \tag{E.24}$$

can be derived in a manner similar to the derivation of (E.5). Substituting this into (E.24) we have:

$$\Lambda^2 f_n = -r^2 \Delta f_n + n(n+d-2) f_n \tag{E.25}$$

From (E.25) it follows that a harmonic polynomial of degree n is an eigenfunction of the generalized angular momentum operator with the eigenvalue $n(n+d-2)$, i.e.,

$$\Lambda^2 h_n = n(n+d-2) h_n \tag{E.26}$$

It is conventional to use the symbol λ for the degree of a harmonic polynomial. Written in this notation, we have

$$\Lambda^2 h_\lambda = \lambda(\lambda+d-2) h_\lambda \tag{E.27}$$

When $d = 3$ this reduces to

$$L^2 h_l = l(l+1) h_l \tag{E.28}$$

We can conclude from this discussion that the canonical decomposition of a homogeneous polynomial can be viewed as a decomposition into eigenfunctions of generalized angular momentum.

E.5 Angular and hyperangular integration

In a 3-dimensional space the volume element is given by $dx_1dx_2dx_3$ in Cartesian coordinates or by $r^2dr\ d\Omega$ in spherical polar coordinates. Thus we can write

$$dx_1dx_2dx_3 = r^2dr\ d\Omega \tag{E.29}$$

where $d\Omega$ is the element of solid angle. Similarly, in a d-dimensional space we can write

$$dx_1dx_2\cdots dx_d = r^{d-1}dr\ d\Omega \tag{E.30}$$

where r is the hyperradius and where $d\Omega$ is the element of generalized solid angle. From the Hermiticity of the generalized angular momentum operator Λ^2, one can show that its eigenfunctions corresponding to different eigenvalues are orthogonal with respect to hyperangular integration. Thus from (E.27) it follows that

$$\int d\Omega\ h^*_{\lambda'}h_\lambda = 0 \quad \text{if} \ \ \lambda' \neq \lambda \tag{E.31}$$

In the particular case where $\lambda' = 0$, this becomes

$$\int d\Omega\ h^*_0 h_\lambda = h^*_0 \int d\Omega\ h_\lambda = 0 \quad \text{if} \ \ \lambda \neq 0 \tag{E.32}$$

since the constant, h^*_0 can be factored out of the integration over generalized solid angle. Thus we obtain the important result:

$$\int d\Omega\ h_\lambda = 0 \quad \text{if} \ \ \lambda \neq 0 \tag{E.33}$$

Let us now combine this result with equation (E.11), which shows the form of the canonical decomposition of a homogeneous polynomial f_n. From (E.11) and (E.33) it follows that if a homogeneous polynomial is integrated over generalized solid angle, the only term that will survive is the constant term in the canonical decomposition, i.e., h_0. But this term, together with the power of the hyperradius multiplying it, can be factored out of the integration. Thus we obtain the powerful angular and hyperangular integration theorem:

$$\int d\Omega\ f_n = \begin{cases} r^n h_0 \int d\Omega & n = \text{even} \\ \\ 0 & n = \text{odd} \end{cases} \tag{E.34}$$

where we have used the fact that when n is odd, the constant term h_0 does not occur in the canonical decomposition. We already have an explicit expression for h_0, namely equation (E.16). The only task remaining is to evaluate the total generalized solid angle, $\int d\Omega$. We can do this by comparing the integral of e^{-r^2} over the whole d-dimensional space when performed in Cartesian coordinates with the same integral performed in generalized spherical polar coordinates. Since the result must be the same, independent of the coordinate system used, we have:

$$\int_0^\infty dr\ r^{d-1} e^{-r^2} \int d\Omega = \prod_{j=1}^{d} \int_{-\infty}^{\infty} dx_j\ e^{-x_j^2} \tag{E.35}$$

The hyperradial integral can be expressed in terms of the gamma function:

$$\int_0^\infty dr\ r^{d-1} e^{-r^2} = \frac{\Gamma(d/2)}{2} \tag{E.36}$$

as can the integral over each of the Cartesian coordinates:

$$\int_{-\infty}^{\infty} dx_j\ e^{-x_j^2} = \Gamma(1/2) = \pi^{\frac{1}{2}} \tag{E.37}$$

Inserting these results into (E.35) and solving for $\int d\Omega$, we obtain:

$$\int d\Omega = \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} \tag{E.38}$$

Finally, combining (E.11), (E.34) and (E.38), we have an explicit expression for the integral over generalized solid angle of any homogeneous polynomial of degree n:

$$\int d\Omega\ f_n = \begin{cases} \dfrac{2\pi^{d/2} r^n (d-2)!!}{\Gamma(d/2) n!!(d+n-2)!!} \Delta^{\frac{1}{2}n} f_n & n = \text{even} \\ 0 & n = \text{odd} \end{cases} \tag{E.39}$$

Now suppose that $F(\mathbf{x})$ is any function whatever that can be expanded in a convergent series of homogeneous polynomials. If the series has the form:

$$F(\mathbf{x}) = \sum_{n=0}^{\infty} f_n(\mathbf{x}) \tag{E.40}$$

then it follows from (E.39) that

$$\int d\Omega\ F(\mathbf{x}) = \frac{(d-2)!!2\pi^{d/2}}{\Gamma\left(\frac{d}{2}\right)} \sum_{n=0,2,..}^{\infty} \frac{r^n}{n!!(n+d-2)!!} \Delta^{n/2} f_n(\mathbf{x}) \tag{E.41}$$

We can notice that at the point $\mathbf{x} = 0$, all terms in a polynomial vanish, except the constant term. Thus we have

$$\left\lfloor \Delta^{n/2} F(\mathbf{x}) \right\rfloor_{\mathbf{x}=0} = \Delta^{n/2} f_n(\mathbf{x}) \tag{E.42}$$

This allows us to rewrite (E.41) in the form

$$\int d\Omega\ F(\mathbf{x}) = \frac{(d-2)!!2\pi^{d/2}}{\Gamma\left(\frac{d}{2}\right)} \sum_{\nu=0}^{\infty} \frac{r^{2\nu}}{(2\nu)!!(d+2\nu-2)!!} \left\lfloor \Delta^{\nu} F(\mathbf{x}) \right\rfloor_{\mathbf{x}=0} \tag{E.43}$$

where we have made the substitution $n = 2\nu$. In the case where $d = 3$, this reduces to

$$\int d\Omega\ F(\mathbf{x}) = 4\pi \sum_{\nu=0}^{\infty} \frac{r^{2\nu}}{(2\nu+1)!} \left\lfloor \Delta^{\nu} F(\mathbf{x}) \right\rfloor_{\mathbf{x}=0} \tag{E.44}$$

E.6 An alternative method for angular and hyperangular integrations

Theorem:
Let

$$I(\mathbf{n}) \equiv \int d\Omega \left(\frac{x_1}{r}\right)^{n_1} \left(\frac{x_2}{r}\right)^{n_2} \ldots\ldots\ldots \left(\frac{x_d}{r}\right)^{n_d} \tag{E.45}$$

where $x_1, x_2, \ldots.., x_d$ are the Cartesian coordinates of a d-dimensional space, $d\Omega$ is the generalized solid angle, r is the hyperradius, defined by

$$r^2 \equiv \sum_{j=1}^{d} x_j^2 \tag{E.46}$$

and where the n_j's are positive integers or zero. Then

$$I(\mathbf{n}) = \begin{cases} \dfrac{\pi^{d/2}}{2^{(n/2-1)}\Gamma\left(\frac{d+n}{2}\right)} \displaystyle\prod_{j=1}^{d} (n_j-1)!! & \text{if all the } n_j{}'\text{s are even} \\ \\ 0 \qquad \text{otherwise} \end{cases} \tag{E.47}$$

where

$$n \equiv \sum_{j=1}^{d} n_j \tag{E.48}$$

Proof:
We consider the integral

$$\int_0^{\infty} dr\ r^{d-1} e^{-r^2} \int d\Omega\ x_1^{n_1} x_2^{n_2} \ldots\ldots.. x_d^{n_d} = \prod_{j=1}^{d} \int_{-\infty}^{\infty} dx_j\ x_j^{n_j} e^{-x_j^2} \tag{E.49}$$

If n_j is zero or a positive integer, then

$$\int_{-\infty}^{\infty} dx_j\ x_j^{n_j} e^{-x_j^2} = \begin{cases} \dfrac{(n_j-1)!!\sqrt{\pi}}{2^{n_j/2}} & \text{if } n_j \text{ is even} \\ \\ 0 \qquad \text{if } n_j \text{ is odd} \end{cases} \tag{E.50}$$

so that the right-hand side of (E.49) becomes

$$\prod_{j=1}^{d}\int_{-\infty}^{\infty} dx_j\ x_j^{n_j} e^{-x_j^2} = \begin{cases} \dfrac{\pi^{d/2}}{2^{n/2}} \displaystyle\prod_{j=1}^{d}(n_j-1)!! & \text{if all the } n_j\text{'s are even} \\ 0 \qquad \text{otherwise} \end{cases} \tag{E.51}$$

The left-hand side of (5) can be written in the form

$$\int_0^{\infty} dr\ r^{d+n-1} e^{-r^2} \int d\Omega\ \left(\frac{x_1}{r}\right)^{n_1}\left(\frac{x_2}{r}\right)^{n_2} \cdots\cdots\cdot \left(\frac{x_d}{r}\right)^{n_d} = \frac{I(\mathbf{n})}{2}\Gamma\left(\frac{d+n}{2}\right) \tag{E.52}$$

Substituting (E.51) and (E.52) into (E.49), we obtain:

$$I(\mathbf{n}) = \begin{cases} \dfrac{\pi^{d/2}}{2^{(n/2-1)}\Gamma\left(\frac{d+n}{2}\right)} \displaystyle\prod_{j=1}^{d}(n_j-1)!! & \text{if all the } n_j\text{'s are even} \\ 0 \qquad \text{otherwise} \end{cases} \tag{E.53}$$

Q.E.D.

Comments:
In the special case where d=3, equation (E.47) becomes

$$\int d\Omega \left(\frac{x_1}{r}\right)^{n_1}\left(\frac{x_2}{r}\right)^{n_2}\left(\frac{x_d}{r}\right)^{n_3} = \begin{cases} \dfrac{4\pi}{(n+1)!!} \displaystyle\prod_{j=1}^{3}(n_j-1)!! & \text{all } n_j\text{'s even} \\ 0 \qquad \text{otherwise} \end{cases} \tag{E.54}$$

Let us now consider a general polynomial (not necessarily homogeneous) of the form:

$$P(\mathbf{x}) = \sum_{\mathbf{n}} c_{\mathbf{n}}\ x_1^{n_1} x_2^{n_2} \cdots\cdots\cdot x_d^{n_d} \tag{E.55}$$

Then we have

$$\int d\Omega\ P(\mathbf{x}) = \sum_{\mathbf{n}} c_{\mathbf{n}} \int d\Omega\ x_1^{n_1} x_2^{n_2} \cdots\cdots\cdot x_d^{n_d} = \sum_{\mathbf{n}} c_{\mathbf{n}}\ r^n I(\mathbf{n}) \tag{E.56}$$

It can be seen that equation (E.47) can be used to evaluate the generalized angular integral of any polynomial whatever, regardless of whether or not it is homogeneous.

It is interesting to ask what happens if the n_j's are not required to be zero or positive integers. If all the n_j's are real numbers greater than -1, then the right-hand side of (E.49) can still be evaluated and it has the form

$$\prod_{j=1}^{d}\int_{-\infty}^{\infty} dx_j \; x_j^{n_j} e^{-x_j^2} = \prod_{j=1}^{d} \frac{1}{2}\left(1+e^{i\pi n_j}\right)\Gamma\left(\frac{n_j+1}{2}\right) \tag{E.57}$$

Thus (E.47) becomes

$$I(\mathbf{n}) = \frac{2}{\Gamma\left(\frac{d+n}{2}\right)} \prod_{j=1}^{d} \frac{1}{2}\left(1+e^{i\pi n_j}\right)\Gamma\left(\frac{n_j+1}{2}\right) \qquad n_j > -1, \qquad j = 1,...,d \tag{E.58}$$

This more general equation reduces to (E.47) in the special case where the n_j's are required to be either zero or positive integers.

E.7 Angular integrations by a vector-pairing method

Let us consider the following integral in a 3-dimensional space:

$$I = \frac{1}{4\pi}\int d\Omega \; (\hat{\mathbf{x}}\cdot\hat{\mathbf{A}})(\hat{\mathbf{x}}\cdot\hat{\mathbf{B}}) \tag{E.59}$$

where $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ are unit vectors. Since the integral I must be independent of $\mathbf{x}$ and invariant under rotations, it must be proportional to the scalar product, $\hat{\mathbf{A}}\cdot\hat{\mathbf{B}}$, which is the only scalar that can be made out of two vectors. The constant of proportionality can be found by considering the case where $\hat{\mathbf{A}} = \hat{\mathbf{B}}$, and in this way, one finds that

$$\frac{1}{4\pi}\int d\Omega \; (\hat{\mathbf{x}}\cdot\hat{\mathbf{A}})(\hat{\mathbf{x}}\cdot\hat{\mathbf{B}}) = \frac{1}{3}(\hat{\mathbf{A}}\cdot\hat{\mathbf{B}}) \tag{E.60}$$

Building on this approach to angular integration, Avery, Ørmen and Michels [?], [?] were able to show that

$$\frac{1}{4\pi}\int d\Omega \; \prod_{j=1}^{N}(\hat{\mathbf{x}}\cdot\hat{\mathbf{A}}_j)^{n_j}$$
$$= \begin{cases} \dfrac{1}{(n+1)!!}\displaystyle\sum_{\lambda^*}\left(\prod_{k=1}^{N}\frac{n_k!}{(2\lambda_{kk})!!}\right)\prod_{i=1}^{j-1}\prod_{j=1}^{N}\frac{1}{\lambda_{ij}!}(\hat{\mathbf{A}}_i\cdot\hat{\mathbf{A}}_j)^{\lambda_{ij}} & n \text{ even} \\ \\ 0 & n \text{ odd} \end{cases} \tag{E.61}$$

where

$$n \equiv n_1 + n_2 + n_3 + ... + n_N \tag{E.62}$$

In (E.61) the sum $\sum_{\lambda^*}$ denotes a sum over all sets of λ_{ij} values which are positive integers or zero and which fulfil the criteria

$$2\lambda_{jj} + \sum_{i=1}^{j-1} \lambda_{ij} + \sum_{i=j+1}^{N} \lambda_{ji} = n_j \qquad\qquad j = 1, 2, ..., N \tag{E.63}$$

For example, when $N = 2$, $n_1 = 3$ and $n_2 = 3$, the set of λ_{ij} values

$$\lambda_{11} = 1 \qquad \lambda_{22} = 1 \qquad \lambda_{12} = 1 \tag{E.64}$$

fulfils (E.63), and likewise

$$\lambda_{11} = 0 \qquad \lambda_{22} = 0 \qquad \lambda_{12} = 3 \tag{E.65}$$

satisfies (E.63). These are the only possibilities, and thus the sum in (E.61) contains two terms.

It is easy to extend these methods to spaces of higher dimension, and the relevant formulae can be found in references [**?**] and [**?**]. It is also possible to use (E.61) to evaluate integrals of the type

$$W_{l,l',l''} \equiv \frac{1}{4\pi} \int d\Omega \ P_l(\hat{\mathbf{x}} \cdot \hat{\mathbf{A}}) P_{l'}(\hat{\mathbf{x}} \cdot \hat{\mathbf{B}}) P_{l''}(\hat{\mathbf{x}} \cdot \hat{\mathbf{C}}) \tag{E.66}$$

where P_l is a Legendre polynomial, and some examples are shown in the following table, where only non-zero values are shown. In order for $W_{l,l',l''}$ to be nonzero, $l + l' + l''$ must be even and $|l - l'| \leq l'' \leq l + l'$.

Table C.1 Integrals of products of Legendre polynomials, evaluated by the vector pairing method

(l, l', l'')	$W_{l,l',l''} \equiv \frac{1}{4\pi} \int d\Omega \; P_l(\hat{\mathbf{x}} \cdot \hat{\mathbf{A}}) P_{l'}(\hat{\mathbf{x}} \cdot \hat{\mathbf{B}}) P_{l''}(\hat{\mathbf{x}} \cdot \hat{\mathbf{C}})$
$(0, 0, 0)$	1
$(1, 1, 0)$	$\frac{1}{3}(\hat{\mathbf{A}} \cdot \hat{\mathbf{B}})$
$(1, 1, 2)$	$\frac{1}{15}\left[-(\hat{\mathbf{A}} \cdot \hat{\mathbf{B}}) + 3(\hat{\mathbf{A}} \cdot \hat{\mathbf{C}})(\hat{\mathbf{B}} \cdot \hat{\mathbf{C}})\right]$
$(2, 2, 0)$	$\frac{1}{10}\left[-1 + 3(\hat{\mathbf{A}} \cdot \hat{\mathbf{B}})^2\right]$
$(2, 2, 2)$	$\frac{1}{35}\left[2 - 3(\hat{\mathbf{A}} \cdot \hat{\mathbf{B}})^2 - 3(\hat{\mathbf{A}} \cdot \hat{\mathbf{B}})^2 - 3(\hat{\mathbf{A}} \cdot \hat{\mathbf{B}})^2 + 9(\hat{\mathbf{A}} \cdot \hat{\mathbf{B}})(\hat{\mathbf{A}} \cdot \hat{\mathbf{C}})(\hat{\mathbf{B}} \cdot \hat{\mathbf{C}})\right]$
$(1, 2, 3)$	$\frac{3}{70}\left[-(\hat{\mathbf{A}} \cdot \hat{\mathbf{C}}) - 2(\hat{\mathbf{A}} \cdot \hat{\mathbf{B}})(\hat{\mathbf{B}} \cdot \hat{\mathbf{C}}) + 5(\hat{\mathbf{A}} \cdot \hat{\mathbf{C}})(\hat{\mathbf{B}} \cdot \hat{\mathbf{C}})^2\right]$
$(3, 3, 0)$	$\frac{1}{14}\left[-3(\hat{\mathbf{A}} \cdot \hat{\mathbf{B}}) + 5(\hat{\mathbf{A}} \cdot \hat{\mathbf{B}})^3\right]$

Appendix F

Harmonic functions

F.1 Harmonic functions for d=3

Harmonic functions in a 3-dimensional space are solutions to the Laplace equation

$$\nabla^2\phi(\mathbf{x}) = 0 \tag{F.1}$$

Let us begin by listing some of these solutions. The regular solid harmonics

$$\mathsf{R}_{l,m}(\mathbf{x}) \equiv \sqrt{\frac{4\pi}{2l+1}}\, r^l Y_{l,m}(\hat{\mathbf{x}}) \tag{F.2}$$

satisfy the Laplace equation everywhere in space, while the irregular solid harmonics

$$\mathsf{I}_{l,m}(\mathbf{x}) \equiv \sqrt{\frac{4\pi}{2l+1}}\, r^{-(l+1)} Y_{l,m}(\hat{\mathbf{x}}) \tag{F.3}$$

satisfy it everywhere except at the point $r = |\mathbf{x}| = 0$. Here $Y_{l,m}(\hat{\mathbf{x}})$ is a spherical harmonic. From the sum-rule for spherical harmonics,

$$\sum_{m=-l}^{l} Y^*_{l,m}(\hat{\mathbf{a}})Y_{l,m}(\hat{\mathbf{x}}) = \frac{2l+1}{4\pi} P_l(\hat{\mathbf{a}}\cdot\hat{\mathbf{x}}) \tag{F.4}$$

we can see that for any constant vector $\mathbf{a}$, the function

$$\begin{aligned} r^l P_l'(\hat{\mathbf{a}}\cdot\hat{\mathbf{x}}) &\equiv r^l \sum_{m=-l}^{l} \frac{4\pi}{2l+1} Y^*_{l,m}(\hat{\mathbf{a}})Y_{l,m}(\hat{\mathbf{x}}) \\ &= \sum_{t=0}^{[n/2]} \frac{(-1)^t\Gamma(1+1/2-t)(x^2+y^2+z^2)^t(2\hat{\mathbf{a}}\cdot\mathbf{x})^{l-2t}}{t!(1-2t)!\Gamma(1/2)} \end{aligned} \tag{F.5}$$

is harmonic, i.e. it is a solution to the Laplace equation. The function $P_l'(\hat{\mathbf{a}} \cdot \hat{\mathbf{x}})$ might be called a "harmonic Legendre polynomial". Harmonic polynomials are, by definition, homogeneous polynomials that are solutions to the Laplace equation. The functions $r^l Y_{l,m}(\hat{\mathbf{x}})$ satisfy this definition, and they are thus harmonic polynomials.

The spherical harmonics corresponding to a given value of l form an irreducible representation of SO(3). The point groups of chemistry are subgroups of SO(3), and therefore the spherical harmonics corresponding to a given value of l are closed under the operations of the point groups. Thus if $\mathcal{G}$ is such a point group, each $(2l+1)$-dimensional set of spherical harmonics, $Y_{l,m}(\hat{\mathbf{x}})$ can be thought of as invariant subset with respect to $\mathcal{G}$ in the sense discussed elsewhere in this book. Similar considerations hold for the hyperspherical harmonics which will be discussed below.

An alternative set of harmonic polynomials, spanning the same part of Hilbert space as the solid harmonics, can be generated by starting with monomials of the form

$$f_{\mathbf{n}}(\mathbf{x}) = x^{n_1} y^{n_2} z^{n_3} \qquad n_j = 0, 1, 2, 3, ... \tag{F.6}$$

and acting on them several times with the Laplacian operator with appropriate coefficients, as is discussed in Appendix C. We then obtain harmonic polynomials of the form:

$$h_{\mathbf{n}}(\mathbf{x}) = \sum_{j=0}^{\lfloor n/2 \rfloor} \frac{(-1)^j (2n-2j-1)!!}{(2j)!!(2n-1)!!} r^{2j} (\nabla^2)^j f_{\mathbf{n}}(\mathbf{x}) \tag{F.7}$$

where n is the degree of the monomial, and also the degree of the harmonic polynomial:

$$n \equiv n_1 + n_2 + n_3 \tag{F.8}$$

Finally it should be mentioned that the functions

$$g_{\mathbf{n}}(\mathbf{x}) = r^{-(2n+1)} h_{\mathbf{n}}(\mathbf{x}) \tag{F.9}$$

also satisfy the Laplace equation except at the point $r = |\mathbf{x}| = 0$. For some purposes the harmonic functions $h_{\mathbf{n}}(\mathbf{x})$ and $g_{\mathbf{n}}(\mathbf{x})$ may be more convenient than $a_{l,m}(\mathbf{x})$ and $b_{l,m}(\mathbf{x})$.

F.2 Spaces of higher dimension

In a d-dimensional space, the generalized Laplace equation has the form

$$\Delta \phi(\mathbf{x}) = 0 \tag{F.10}$$

where

$$\Delta \equiv \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j} \tag{F.11}$$

and where

$$\mathbf{x} \equiv (x_1, x_2, x_3, ..., x_d) \tag{F.12}$$

is a vector whose components are the Cartesian coordinates for the space. We can introduce the hyperradius r defined by

$$r^2 \equiv \sum_{j=1}^{d} x_j^2 \tag{F.13}$$

and a generalized angular momentum operator

$$\Lambda^2 \equiv -\sum_{i>j}^{d} \sum_{j=1}^{d} \left(x_i \frac{\partial}{\partial x_j} - x_j \frac{\partial}{\partial x_i} \right)^2 \tag{F.14}$$

Written in terms of the hyperradius and the generalized angular momentum operator, the generalized Laplace operator takes the form

$$\Delta = \frac{1}{r^{d-1}} \frac{\partial}{\partial r} r^{d-1} \frac{\partial}{\partial r} - \frac{\Lambda^2}{r^2} \tag{F.15}$$

Hyperspherical harmonics $Y_{\lambda,\mu}(\hat{\mathbf{x}})$, are the d-dimensional analogues of spherical harmonics. They are defined as eigenfunctions of the generalized angular momentum operator such that

$$\Lambda^2 Y_{\lambda,\mu}(\hat{\mathbf{x}}) = \lambda(\lambda + d - 2) Y_{\lambda,\mu}(\hat{\mathbf{x}}) \tag{F.16}$$

and such that $r^\lambda Y_{\lambda,\mu}(\hat{\mathbf{x}})$ is a homogeneous polynomial. Then

$$\begin{aligned} \Delta r^\lambda Y_{\lambda,\mu}(\hat{\mathbf{x}}) &= \left(\frac{1}{r^{d-1}} \frac{\partial}{\partial r} r^{d-1} \frac{\partial}{\partial r} - \frac{\Lambda^2}{r^2} \right) r^\lambda Y_{\lambda,\mu}(\hat{\mathbf{x}}) \\ &= \left(\frac{1}{r^{d-1}} \frac{\partial}{\partial r} r^{d-1} \frac{\partial r^\lambda}{\partial r} - \frac{\lambda(\lambda + d - 2)}{r^2} r^\lambda \right) Y_{\lambda,\mu}(\hat{\mathbf{x}}) = 0 \end{aligned} \tag{F.17}$$

Thus it can be seen that hyperspherical harmonics are defined in such a way that $r^\lambda Y_{\lambda,\mu}(\hat{\mathbf{x}})$ is a harmonic polynomial in the d-dimensional space. The index μ is actually a set of d-2 indices. For hyperspherical harmonics of the standard type, these indices are organized by means of a chain of subgroups:

$$SO(d) \supset SO(d-1) \supset SO(d-2) \supset \cdots \supset SO(2) \tag{F.18}$$

However, when we use hyperspherical harmonics in physical problems, it may be convenient to organize the minor indices μ according to a different chain of subgroups. Tables H.1 and

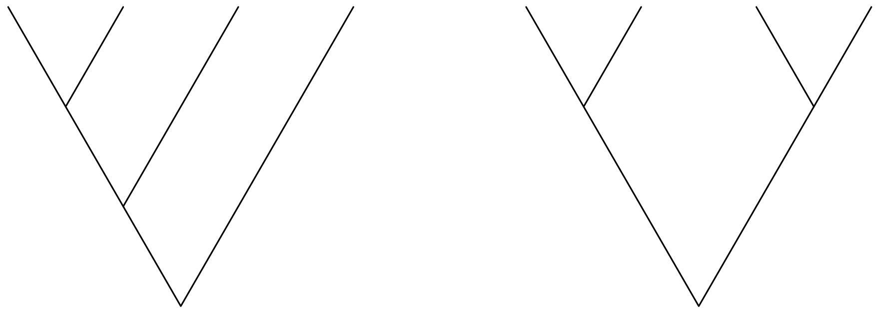

Figure F.1: The standard tree (left) and an alternative tree (right) for 4-dimensional hyperspherical harmonics. The standard tree on the left corresponds to the ordering of subgroups shown in equation (F.18), in which a harmonic polynomials are first found in the space spanned by the coordinates x_1 and x_2. These are then multiplied by x_3 to form homogeneous polynomials of degree 3, from which the harmonic parts are projected out. Finally these are coupled to x_4. The right-hand tree symbolizes the alternative scheme of equation (F.19), where harmonic polynomials are first constructed within the subspaces (x_1, x_2) and (x_3, x_4). Finally these are coupled together, and polynomials that are harmonic in the entire 4-dimensional space are obtained. 4-dimensional hyperspherical harmonics corresponding to the standard tree are shown in Table 5.1, while those corresponding to the alternative tree are shown in Tables H.1 and H.2.

H.2 show an alternative set of 4-dimensional hyperspherical harmonics where the minor indices are organized according to the chain

$$SO(4) \supset SO(2) \times SO(2) \tag{F.19}$$

This alternative way of organizing the minor indices is symbolized by the right-hand tree in Figure H.1. An excellent discussion of the method of trees in hyperspherical harmonic theory can be found in [**?**].

The hyperspherical harmonics corresponding to a given value of the principal quantum number λ form an invariant subspace with respect to all groups $\mathcal{G}$ that are subgroups of SO(d). In the case where $d = 3$ there are $2l + 1$ linearly independent functions in this subspace. In the general case, the corresponding number of linearly independent functions in the invariant subspace can be shown to be [**?**]

$$m_\lambda = \frac{(d + 2\lambda - 2)(d + \lambda - 3)!}{\lambda!(d-2)!} \tag{F.20}$$

The reader can verify that for $d = 3$ and $\lambda = l$, this reduces to the familiar result that there are $2l+1$ linearly independent functions. When $d = 4$, the dimension of the invariant subspace is $(\lambda + 1)^2$. Thus for $\lambda = 0, 1, 2, 3, ...$ there are respectively 1,4,9,16,... linearly independent solutions, as is illustrated in Tables H.1, H.2 and 5.1. These dimensions correspond, through Fock's projection (Appendix B), to the number of degenerate hydrogenlike orbitals with principal quantum numbers $n = 1, 2, 3, 4, ...$ Thus Fock's projection casts light on the puzzling n^2-fold degeneracy of the hydrogenlike orbitals.

Functions of the form

$$\mathcal{H}_{\lambda,\mu}(\mathbf{x}) = r^{\lambda} Y_{\lambda,\mu}(\hat{\mathbf{x}}) \tag{F.21}$$

satisfy the generalized Laplace equation everywhere in our d-dimensional space, while functions of the form

$$\mathcal{I}_{\lambda,\mu}(\mathbf{x}) = r^{-\lambda-d+2} Y_{\lambda,\mu}(\hat{\mathbf{x}}) \tag{F.22}$$

satisfy it at all points except the origin. Equations (F.6)-(F.9) also have d-dimensional analogues:

$$f_{\mathbf{n}}(\mathbf{x}) = \prod_{j=1}^{d} x_j^{n_j} \qquad n_j = 0, 1, 2, 3, ... \tag{F.23}$$

$$h_{\mathbf{n}}(\mathbf{x}) = \sum_{j=0}^{\lfloor n/2 \rfloor} \frac{(-1)^j (d + 2n - 2j - 4)!!}{(2j)!!(d + 2n - 4)!!} r^{2j} \Delta^j f_{\mathbf{n}}(\mathbf{x}) \tag{F.24}$$

$$n = \sum_{j=1}^{d} n_j \tag{F.25}$$

and

$$g_{\mathbf{n}}(\mathbf{x}) = r^{-2n-d+2} h_{\mathbf{n}}(\mathbf{x}) \tag{F.26}$$

The function $h_{\mathbf{n}}(\mathbf{x})$ satisfies the generalized Laplace equation everywhere in space, while $g_{\mathbf{n}}(\mathbf{x})$ is a solution everywhere except at the origin.

The harmonic functions discussed above by no means exhaust the forms that solutions to the generalized Laplace equation in a d-dimensional space can take. Examples of other forms include

$$e^{i\mathbf{k}\cdot\mathbf{x}} \tag{F.27}$$

where $\mathbf{k}$ is a d-dimensional vector of zero length. We can see that this will be a harmonic function because

$$\Delta e^{i\mathbf{k}\cdot\mathbf{x}} = -\mathbf{k}\cdot\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{x}} = 0 \tag{F.28}$$

As an example of a d-dimensional vector of zero length we can think of

$$\begin{aligned} \mathbf{k} &= (k_1, k_2, k_3, ..., k_{d-1}, \pm i k_d) \\ k_d &= \left(k_1^2 + k_2^2 + ... + k_{d-1}^2\right)^{1/2} \\ \mathbf{k}\cdot\mathbf{k} &= k_d^2 - k_d^2 = 0 \end{aligned} \tag{F.29}$$

In fact, if $\mathbf{k}$ is a d-dimensional vector of zero length, any well-behaved function of $\zeta \equiv \mathbf{k} \cdot \mathbf{x}$ will be a solution to the generalized Laplace equation, because

$$\frac{\partial}{\partial x_j} F(\mathbf{k} \cdot \mathbf{x}) = \frac{\partial}{\partial x_j} F(\zeta) = \frac{\partial \zeta}{\partial x_j} \frac{dF}{d\zeta} = k_j \frac{dF}{d\zeta} \tag{F.30}$$

and

$$\frac{\partial^2}{\partial x_j^2} F(\mathbf{k} \cdot \mathbf{x}) = k_j \frac{\partial}{\partial x_j} \frac{dF}{d\zeta} = k_j \frac{\partial \zeta}{\partial x_j} \frac{d^2 F}{d\zeta^2} = k_j^2 \frac{d^2 F}{d\zeta^2} \tag{F.31}$$

Thus

$$\Delta F(\mathbf{k} \cdot \mathbf{x}) = \mathbf{k} \cdot \mathbf{k} \ \frac{d^2 F}{d\zeta^2} = 0 \tag{F.32}$$

In a d-dimensional space, it is possible to define a "harmonic Gegenbauer polynomial"

$$r^\lambda C_\lambda^{\prime\alpha}(\hat{\mathbf{a}} \cdot \hat{\mathbf{x}}) \ \equiv \ \sum_{t=0}^{[\lambda/2]} \frac{(-1)^t \Gamma(\lambda + \alpha - t)(x_1^2 + x_2^2 + ... + x_d^2)^t (2\hat{\mathbf{a}} \cdot \mathbf{x})^{l-2t}}{t!(\lambda - 2t)! \Gamma(\alpha)} \tag{F.33}$$

where $\alpha = d/2 - 1$. The harmonic Gegenbauer polynomial is the d-dimensional generalization of the harmonic Legendre polynomial, and it satisfies the generalized Laplace equation for any constant d-dimensional vector $\mathbf{a}$.

Table H.1 Alternative 4-dimensional hyperspherical harmonics corresponding to the right-hand tree in Figure H.1. The indices m_1 and m_2 are rotational quantum numbers in the subspaces spanned respectively by (x_1, x_2) and (x_3, x_4).

λ	m_1	m_2	$\sqrt{2}\pi\ Y_{\lambda,m_1,m_2}(\mathbf{u})$
0	0	0	1
1	1	0	$\sqrt{2}(u_1 + iu_2)$
1	-1	0	$\sqrt{2}(u_1 - iu_2)$
1	0	1	$\sqrt{2}(u_3 + iu_4)$
1	0	-1	$\sqrt{2}(u_3 - iu_4)$

Table H.2 Alternative 4-dimensional hyperspherical harmonics (continued).

λ	m_1	m_2	$\sqrt{2}\pi\ Y_{\lambda,m_1,m_2}(\mathbf{u})$
2	2	0	$\sqrt{3}(u_1+iu_2)^2$
2	-2	0	$\sqrt{3}(u_1-iu_2)^2$
2	0	2	$\sqrt{3}(u_3+iu_4)^2$
2	0	-2	$\sqrt{3}(u_3-iu_4)^2$
2	1	1	$\sqrt{6}(u_1+iu_2)(u_3+iu_4)$
2	1	-1	$\sqrt{6}(u_1+iu_2)(u_3-iu_4)$
2	-1	1	$\sqrt{6}(u_1-iu_2)(u_3+iu_4)$
2	-1	-1	$\sqrt{6}(u_1-iu_2)(u_3-iu_4)$
2	0	0	$\sqrt{3}(u_1^2+u_2^2-u3^2-u4^2)$

Appendix G

GENERALIZED STURMIANS APPLIED TO ATOMS

G.1 Goscinskian configurations

The Generalized Sturmian Method (Appendix B) is a newly-developed direct method for performing Configuration Interaction calculations on bound states. It avoids the initial Hartree-Fock-Roothaan SCF calculation, and it is especially suitable for calculating large numbers of excited states of few-electron atoms or ions.

When the Generalized Sturmian Method is applied to atoms or atomic ions, it is convenient to use basis functions that are Slater determinants:

$$|\Phi_\nu\rangle = |\chi_\mu \chi_{\mu'} \chi_{\mu''} ...| \equiv \frac{1}{\sqrt{N!}} \begin{vmatrix} \chi_\mu(\mathbf{x}_1) & \chi_{\mu'}(\mathbf{x}_1) & \chi_{\mu''}(\mathbf{x}_1) & ... \\ \chi_\mu(\mathbf{x}_2) & \chi_{\mu'}(\mathbf{x}_2) & \chi_{\mu''}(\mathbf{x}_2) & ... \\ \chi_\mu(\mathbf{x}_3) & \chi_{\mu'}(\mathbf{x}_3) & \chi_{\mu''}(\mathbf{x}_3) & ... \\ \vdots & \vdots & \vdots & \end{vmatrix} \tag{G.1}$$

built from hydrogenlike atomic spin-orbitals of the form

$$\chi_\mu(\mathbf{x}_i) \equiv \chi_{n,l,m,m_s}(\mathbf{x}_i) \equiv R_{n,l}(r_i) Y_{l,m}(\theta_i, \phi_i) \begin{cases} \alpha_i & m_s = 1/2 \\ \beta_i & m_s = -1/2 \end{cases} \tag{G.2}$$

with weighted nuclear charges Q_ν. In other words, the atomic spin-orbitals have the form shown in equation (**??**), with radial functions given by

$$\begin{aligned} R_{1,0}(r) &= 2Q_\nu^{3/2} e^{-Q_\nu r} \\ R_{2,0}(r) &= \frac{Q_\nu^{3/2}}{\sqrt{2}} \left(1 - \frac{Q_\nu r}{2}\right) e^{-Q_\nu r/2} \\ R_{2,1}(r) &= \frac{Q_\nu^{5/2}}{2\sqrt{6}}\, r\, e^{-Q_\nu r/2} \\ R_{3,0}(r) &= \frac{2Q_\nu^{3/2}}{3\sqrt{3}} \left(1 - \frac{2Q_\nu r}{3} + \frac{2Q_\nu^2 r^2}{27}\right) e^{-Q_\nu r/3} \end{aligned}$$

$$\vdots \qquad \vdots \qquad \vdots \tag{G.3}$$

The reader will recognize these as the familiar hydrogenlike radial functions with the nuclear charge Z replaced by Q_ν. If the effective charges Q_ν characterizing the configurations $|\Phi_\nu\rangle$ are chosen in such a way that

$$Q_\nu = \beta_\nu Z = \left(\frac{-2E_\kappa}{\frac{1}{n^2} + \frac{1}{n'^2} + \frac{1}{n''^2} + \cdots} \right)^{1/2} \tag{G.4}$$

so that

$$E_\kappa = -\frac{Q_\nu^2}{2} \left(\frac{1}{n^2} + \frac{1}{n'^2} + \frac{1}{n'^2} + \cdots \right) \tag{G.5}$$

the configurations will obey the approximate N-electron Schrödinger equation:

$$\left[-\frac{1}{2} \sum_{j=1}^{N} \nabla_j^2 + \beta_\nu V_0(\mathbf{x}) - E_\kappa \right] |\Phi_\nu\rangle = 0 \tag{G.6}$$

where

$$V_0(\mathbf{x}) = -\sum_{j=1}^{N} \frac{Z}{r_j} \tag{G.7}$$

is the nuclear attraction potential. In equation (G.6), the energy E_κ is kept constant for the whole basis set, while the weighting factors β_ν are adjusted to make the basis set isoenergetic. Thus the weighting factors β_ν play the role of eigenvalues in equation (G.6). This type of problem has been called the *conjugate eigenvalue problem* by Coulson, Josephs, Goscinski and others, and it is characteristic for the equations defining generalized Sturmian basis sets (Appendix B).

To see that with the special choice of weighted charges shown in equation (G.4) $|\Phi_\nu\rangle$ will satisfy (G.6), we first notice that the hydrogenlike atomic orbitals with weighted nuclear charges obey the 1-electron Schrödinger equation:

$$\left[-\frac{1}{2} \nabla_j^2 + \frac{Q_\nu^2}{2n^2} - \frac{Q_\nu}{r_j} \right] \chi_\mu(\mathbf{x_j}) = 0 \tag{G.8}$$

Since the Slater determinant $|\Phi_\nu\rangle$ is an antisymmetrized product of atomic orbitals, all of which obey (G.8), it follows that

$$\begin{aligned} \left[-\frac{1}{2} \sum_{j=1}^{N} \nabla_j^2 \right] |\Phi_\nu\rangle &= \left[-\left(\frac{Q_\nu^2}{2n^2} + \frac{Q_\nu^2}{2n'^2} + \cdots \right) + \left(\frac{Q_\nu}{r_1} + \frac{Q_\nu}{r_2} + \cdots \right) \right] |\Phi_\nu\rangle \\ &= [E_\kappa - \beta_\nu V_0(\mathbf{x})] \, |\Phi_\nu\rangle \end{aligned} \tag{G.9}$$

and thus equation (G.6) is satisfied. Each configuration $|\Phi_\nu\rangle$ has its own effective nuclear charge Q_ν. Within a particular configuration, the hydrogenlike atomic orbitals are orthonormal

$$\int d\tau_j \; \chi^*_{\mu'}(\mathbf{x}_j)\chi_\mu(\mathbf{x}_j) = \delta_{\mu',\mu} \tag{G.10}$$

and they also obey the virial relationship

$$-\int d\tau_j \; |\chi_\mu(\mathbf{x}_j)|^2 \frac{Q_\nu}{r_j} = -\frac{Q_\nu^2}{n^2} \tag{G.11}$$

From equations (G.6), (G.10) and (G.11), it can be shown [?],[?] that the generalized Sturmian configurations $|\Phi_\nu\rangle$ obey the potential-weighted orthonormality relation

$$\langle \Phi^*_{\nu'}|V_0|\Phi_\nu\rangle = \delta_{\nu',\nu}\frac{2E_\kappa}{\beta_\nu} \tag{G.12}$$

We next introduce the definitions

$$p_\kappa \equiv \sqrt{-2E_\kappa} \tag{G.13}$$

and

$$\mathcal{R}_\nu \equiv \sqrt{\frac{1}{n^2} + \frac{1}{n'^2} + \cdots} \tag{G.14}$$

With the help of these definitions, equation (G.4) can be written in the form

$$Q_\nu = \beta_\nu Z = \frac{p_\kappa}{\mathcal{R}_\nu} \tag{G.15}$$

The set of Sturmian configurations form a set of isoenergetic solutions of the approximate Schrödinger equation (G.6), where the potential is weighted, and the weighting factors β_ν are chosen in such a way as to insure that all the solutions correspond to a common energy. From (G.13) we can see that their common energy E_κ is related to p_κ by

$$E_\kappa = -\frac{p_\kappa^2}{2} \tag{G.16}$$

In previous publications we have called such atomic configurations *Goscinskian configurations* to recognize Prof. Osvaldo Goscinski's pioneering work in generalizing the concept of Sturmian basis sets [?]. The non-relativistic Schrödinger equation of an N-electron atom has the form:

$$\left[-\frac{1}{2}\sum_{j=1}^{N}\nabla_j^2 + V(\mathbf{x}) - E_\kappa\right]|\Psi_\kappa\rangle = 0 \tag{G.17}$$

where

$$V(\mathbf{x}) = V_0(\mathbf{x}) + V'(\mathbf{x}) \tag{G.18}$$

Here $V_0(\mathbf{x})$ is the nuclear attraction potential shown in equation (G.7) while $V'(\mathbf{x})$ is the interelectron repulsion potential

$$V'(\mathbf{x}) = \sum_{i>j}^{N} \frac{1}{r_{ij}} \tag{G.19}$$

We can try to build up the wave function from a superposition of Goscinskian configurations, i.e. from a superposition of isoenergetic solutions of the approximate wave equation (G.6), where V_0 is the nuclear attraction potential of the atom. Thus we write:

$$|\Psi_\kappa\rangle \approx \sum_\nu |\Phi_\nu\rangle C_{\nu,\kappa} \tag{G.20}$$

Inserting this superposition into (G.17) we have

$$\sum_\nu \left[-\frac{1}{2}\Delta + V(\mathbf{x}) - E_\kappa\right] |\Phi_\nu\rangle C_{\nu,\kappa} \approx 0 \tag{G.21}$$

However, each of the basis functions obeys (G.6), and therefore we can rewrite (G.21) in the form

$$\sum_\nu \left[V(\mathbf{x}) - \beta_\nu V_0(\mathbf{x})\right] |\Phi_\nu\rangle C_{\nu,\kappa} \approx 0 \tag{G.22}$$

The energy term E_κ is now nowhere to be seen, and a remark is perhaps needed here to explain what has happened to it: The configurations in our Generalized Sturmian basis set are isoenergetic. They all correspond to the same energy, E_κ, since the weighting factors β_ν are chosen especially to make them do so. What we have done in going from (G.21) to (G.22) is to choose this energy to be the same as that which appears in (G.21). In other words, the energy to which all the members of our basis set correspond is chosen to be equal to the energy of the state that we are trying to approximate.

If we take the scalar product of (G.22) with a conjugate function from our basis set, we obtain the set of secular equations:

$$\sum_\nu \langle\Phi_{\nu'}| \left[V(\mathbf{x}) - \beta_\nu V_0(\mathbf{x})\right] |\Phi_\nu\rangle C_{\nu,\kappa} = 0 \tag{G.23}$$

We now introduce the definitions:

$$T^0_{\nu',\nu} \equiv -\frac{1}{p_\kappa}\langle\Phi^*_{\nu'}|V_0|\Phi_\nu\rangle \tag{G.24}$$

and

$$T'_{\nu',\nu} \equiv -\frac{1}{p_\kappa}\langle\Phi^*_{\nu'}|V'|\Phi_\nu\rangle \tag{G.25}$$

From the potential-weighted orthonormality relations (G.12) we can see that

$$T^0_{\nu',\nu} = \delta_{\nu'\nu} Z\mathcal{R}_\nu \tag{G.26}$$

Notice that the nuclear attraction matrix $T^0_{\nu',\nu}$ is both diagonal and energy-independent. The interelectron repulsion matrix $T'_{\nu',\nu}$ can be evaluated using methods discussed in Appendix D, and it is also energy-independent. In order to see that $T'_{\nu',\nu}$ really is energy-independent, we notice that it is built up from terms of the form

$$\frac{1}{p_\kappa} J_{\mu_1,\mu_2,\mu_3,\mu_4} = \frac{1}{p_\kappa} \int d^3x \int d^3x' \ \rho_{\mu_1,\mu_2}(\mathbf{x}) \frac{1}{|\mathbf{x}-\mathbf{x}'|} \rho_{\mu_3,\mu_4}(\mathbf{x}') \tag{G.27}$$

where densities are defined by

$$\begin{aligned} \rho_{\mu_1,\mu_2}(\mathbf{x}) &\equiv \chi^*_{\mu_1}(\mathbf{x})\chi_{\mu_2}(\mathbf{x}) \\ \rho_{\mu_3,\mu_4}(\mathbf{x}') &\equiv \chi^*_{\mu_3}(\mathbf{x}')\chi_{\mu_4}(\mathbf{x}') \end{aligned} \tag{G.28}$$

and where the orbitals are the hydrogenlike orbitals with weighted nuclear charge shown in equations (G.2) and (G.3). We now let

$$\begin{aligned} \mathbf{s} &\equiv p_\kappa \mathbf{x} \\ \mathbf{s}' &\equiv p_\kappa \mathbf{x}' \end{aligned} \tag{G.29}$$

Then, making the substitution $Q_\nu \to p_\kappa / R_\nu$ in (G.3) we have

$$\begin{aligned} \rho_{\mu_1,\mu_2}(\mathbf{x}) &= p_\kappa^3 \tilde{\rho}_{\mu_1,\mu_2}(\mathbf{s}) \\ \rho_{\mu_3,\mu_4}(\mathbf{x}') &= p_\kappa^3 \tilde{\rho}_{\mu_3,\mu_4}(\mathbf{s}') \end{aligned} \tag{G.30}$$

where $\tilde{\rho}_{\mu_1,\mu_2}(\mathbf{s})$ and $\tilde{\rho}_{\mu_3,\mu_4}(\mathbf{s}')$ are pure functions of $\mathbf{s}$ and $\mathbf{s}'$ respectively. Finally, noticing that

$$\frac{1}{p_\kappa |\mathbf{x}-\mathbf{x}'|} = \frac{1}{|\mathbf{s}-\mathbf{s}'|} \tag{G.31}$$

we can write

$$\frac{1}{p_\kappa} J_{\mu_1,\mu_2,\mu_3,\mu_4} = \int d^3s \int d^3s' \ \tilde{\rho}_{\mu_1,\mu_2}(\mathbf{s}) \frac{1}{|\mathbf{s}-\mathbf{s}'|} \tilde{\rho}_{\mu_3,\mu_4}(\mathbf{s}') \tag{G.32}$$

Since the building-blocks from which it composed are independent of p_κ, the interelectron repulsion matrix $T'_{\nu',\nu}$ is also independent of p_κ and hence independent of energy. The energy-independent interelectron repulsion matrix $T'_{\nu',\nu}$ consists of pure numbers (in atomic units) which can be evaluated once and for all and stored.

With the help of equations (G.24)-(G.26), the secular equation (G.23) can be rewritten in the form:

$$\sum_\nu \left[-p_\kappa \delta_{\nu',\nu} Z\mathcal{R}_\nu - p_\kappa T'_{\nu',\nu} + \beta_\nu p_\kappa \delta_{\nu',\nu} Z\mathcal{R}_\nu \right] C_{\nu,\kappa} = 0 \tag{G.33}$$

Finally, using the relationship

$$\beta_\nu Z\mathcal{R}_\nu = p_\kappa \tag{G.34}$$

and dividing by p_κ, and reversing the signs, we obtain

$$\sum_{\nu} \left[\delta_{\nu',\nu} Z\mathcal{R}_\nu + T'_{\nu',\nu} - p_\kappa \delta_{\nu',\nu}\right] C_{\nu,\kappa} = 0 \tag{G.35}$$

The Generalized Sturmian secular equation for atoms and atomics ions (G.35) differs in several remarkable ways from the secular equations that would be obtained using a Hamiltonian method:

1. The kinetic energy term has disappeared.

2. The nuclear attraction term, $\delta_{\nu',\nu} Z\mathcal{R}_\nu$, is diagonal.

3. The interelectron repulsion matrix $T'_{\nu',\nu}$ is energy-independent. It consists of dimensionless pure numbers.

4. Finally, the roots of the secular equations are not energies but values of the parameter p_κ, which is related to the energy spectrum through equation (G.16). The parameter $p_\kappa = \beta_\nu Z\mathcal{R}_\nu = Q_\nu \mathcal{R}_\nu$ can be thought of as a scaling parameter, since the effective nuclear charges associated with the Goscinskian configurations are proportional to it.

5. The configurations $|\Phi_\nu\rangle$ in the basis set are not fully determined until the secular equations have been solved. Only the form of the basis functions is known in advance, but not the scale. When the secular equation is solved, the resulting spectrum of p_κ values yields not only a spectrum of energies but a nearly optimum set of basis functions for the representation of each state. The basis set for the representation of highly excited states is diffuse, while the set for representation of tightly-bound states is contracted. The step of optimizing Slater exponents for each problem is thus not needed.

6. Once the energy-independent interelectron repulsion matrix $T'_{\nu',\nu}$ has been constructed, the properties of an entire isoelectronic series can be calculated with almost no additional effort.

G.2 Relativistic corrections

If the number of electrons N is kept constant while Z is allowed to increase, the energies calculated from the Generalized Sturmian secular equation approach those found by solution of the non-relativistic Schrödinger equation, but a relativistic correction must be added in order for the energies to approach experimental values. A crude relativistic correction can be found for a multiconfigurational state $\Psi_\kappa(\mathbf{x}) = \sum_\nu \Phi_\nu(\mathbf{x}) C_{\nu\kappa}$ by calculating the ratio of the relativistic energy of the with interelectron repulsion entirely neglected to the non-relativistic energy, again with interelectron repulsion entirely neglected. The ratio can be written in the form

$$f_\kappa(Z) = \frac{E_{\kappa,\text{rel}}}{E_{\kappa,\text{nonrel}}} = \frac{\sum_\nu C_{\nu\kappa}^2 \langle\Phi_\nu|H_0|\Phi_\nu\rangle_{\text{rel}}}{-\frac{1}{2}Z^2 \sum_\nu C_{\nu\kappa}^2 \mathcal{R}_\nu^2} \tag{G.36}$$

Here

$$\langle\Phi_\nu|H_0|\Phi_\nu\rangle_{\text{rel}} = \sum_{\mu\in\nu} \epsilon_{\mu,\text{rel}} \qquad \mu = (n,l,m,m_s) \tag{G.37}$$

is the relativistic energy of the configuration $\Phi_\nu(\mathbf{x})$ with interelectron repulsion entirely neglected, while

$$-\sum_{\mu\in\nu} \frac{1}{2}\frac{Z^2}{n^2} = -\frac{1}{2}Z^2 R_\nu^2 \qquad \mu = (n,l,m,m_s) \tag{G.38}$$

is the nonrelativistic energy of $\Phi_\nu(\mathbf{x})$. The quantity $\epsilon_{\mu,\text{rel}}$ represents the relativistic energy of a single electron moving in the attractive Coulomb potential of a nucleus with charge Z. This energy is easy to calculate exactly [**?**], if effects such as vacuum polarization and the Lamb shift are neglected. It is given by:

$$\epsilon_{\mu,\text{rel}} = \frac{c^2}{\left[1 + \left(\frac{Z}{c(\gamma+n-|j+1/2|)}\right)^2\right]^{1/2}} - c^2 \tag{G.39}$$

$$\gamma \equiv \sqrt{\left(j+\frac{1}{2}\right)^2 - \left(\frac{Z}{c}\right)^2} \qquad c = 137.036 \tag{G.40}$$

where j is the total angular momentum (orbital plus spin) of a single electron, i.e. $l \pm \frac{1}{2}$. The corrected energy, $f_\kappa(Z)E_{\kappa,\text{nonrel}}$, agrees closely with the experimental values of energies, especially when Z is large compared with N.

The approximate relativistic correction discussed here is by no means confined to the Generalized Sturmian Method. It can be used in quantum calculations of every kind, performed on atoms and molecules. The assumption behind the correction is that relativistic effects are due mainly to the nuclear attraction part of the Hamiltonian, and only to a lesser extent to interelectron repulsion terms.

Table G.1: This table shows the relativistic correction for a single electron moving in the field of a nucleus with charge Z, i.e. the relativistic energy without the rest energy, divided by the non-relativistic energy. It is interesting to notice that the correction affects the 4th significant figure of the energy for values of Z as low as 10. In all cases the effect of the relativistic correction is to increase the binding energy.

n	j	Z=1	Z=10	Z=20	Z=30
1	$\frac{1}{2}$	1.00001	1.00133	1.00538	1.01228
2	$\frac{1}{2}$	1.00002	1.00167	1.00673	1.01537
2	$\frac{3}{2}$	1.00000	1.00033	1.00133	1.00301
3	$\frac{1}{2}$	1.00001	1.00133	1.00538	1.01226
3	$\frac{3}{2}$	1.00000	1.00044	1.00178	1.00402
3	$\frac{5}{2}$	1.00000	1.00015	1.00059	1.00133

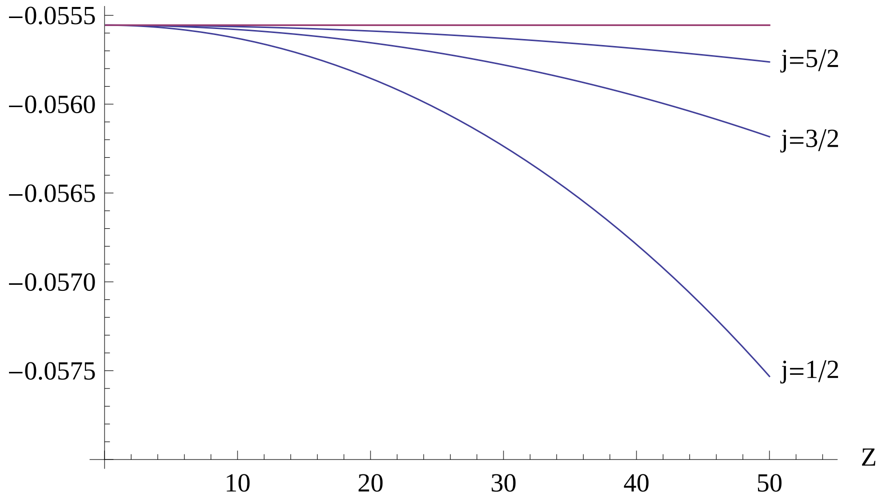

Figure G.1: *This figure shows ϵ_μ/Z^2 for n=3. The non-relativistic energy is the horizontal line $\epsilon_{nonrel} = -1/18$, while the relativistic energies are shown by curves.*

G.3 The large-Z approximation: Restriction of the basis set to an $\mathcal{R}$-block

If interelectron repulsion is entirely neglected, i.e. when disregarding the second term in Eq. (G.35), the calculated energies E_κ become those of a set of N completely independent electrons moving in the field of the bare nucleus:

$$E_\kappa = -\frac{p_\kappa^2}{2} \to -\frac{1}{2}Z^2{\mathcal{R}_\nu}^2 = -\frac{Z^2}{2n_1^2} - \frac{Z^2}{2n_2^2} - \cdots - \frac{Z^2}{2n_N^2} \tag{G.41}$$

In the large-Z approximation, we do not neglect interelectron repulsion, but we restrict the basis set to those Goscinskian configurations that would be degenerate if interelectron repulsion were entirely neglected, i.e., we restrict the basis to a set of configurations all of which correspond to the same value of $\mathcal{R}_\nu$. In that case, the first term in (G.35) is a multiple of the identity matrix, and the eigenvectors $C_{\nu\kappa}$ are the same as those that would be obtained by diagonalizing the energy-independent interelectron repulsion matrix $T'_{\nu'\nu}$, since the eigenfunctions of any matrix are unchanged by adding a multiple of the unit matrix. The simplified secular equation then becomes:

$$\sum_\nu \left[T'_{\nu'\nu} - \lambda_\kappa \delta_{\nu'\nu}\right] C_{\nu\kappa} = 0 \tag{G.42}$$

The roots are shifted by an amount equal to the constant by which the identity matrix is multiplied:

$$p_\kappa = Z\mathcal{R}_\nu + \lambda_\kappa = Z\mathcal{R}_\nu - |\lambda_\kappa| \tag{G.43}$$

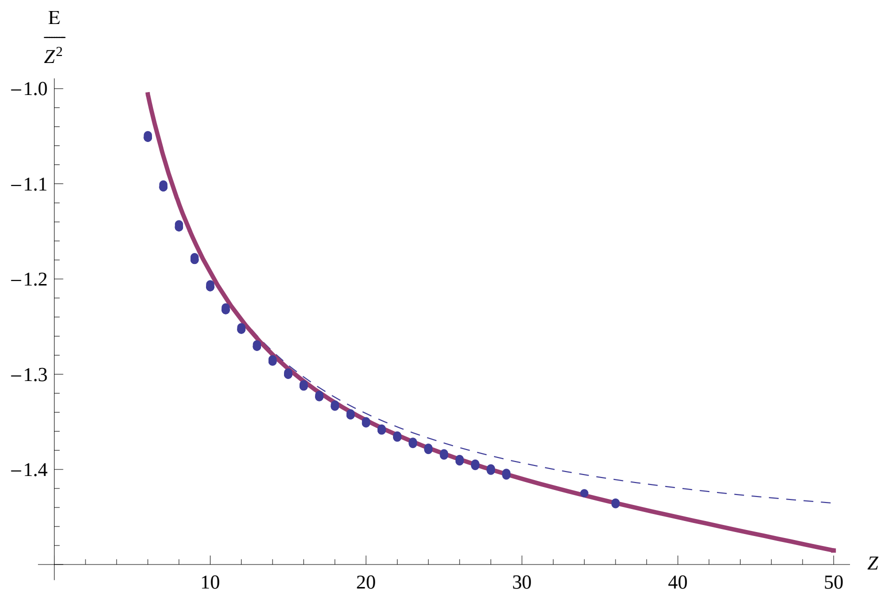

Figure G.2: The ground state of the carbon-like isoelectronic series, calculated in the large-Z approximation. The energies divided by Z^2 are shown as functions of Z. Experimental values are indicates by dots, while the energies calculated from equation (G.44) are shown as curves. The lower (solid) curve, which approaches the experimental values with increasing Z, has been corrected for relativistic effects. The upper (dashed) curve is uncorrected.

and the energies become

$$E_\kappa = -\frac{1}{2}(Z\mathcal{R}_\nu - |\lambda_\kappa|)^2 \tag{G.44}$$

With the relativistic correction of equation (G.36), this becomes

$$E_\kappa = -f(Z)\frac{1}{2}(Z\mathcal{R}_\nu - |\lambda_\kappa|)^2 \tag{G.45}$$

Since the roots λ_κ are always negative, we may use the form $-|\lambda_\kappa|$ in place of λ_κ to make explicit the fact that interelectron repulsion reduces the binding energies, as of course it must. The roots λ_κ are pure numbers that can be calculated once and for all and stored. From these roots, a great deal of information about atomic states can be found with very little effort.

G.4 Electronic potential at the nucleus in the large-Z approximation

The electronic potential $\varphi(\mathbf{x}_1)$ is related to the electronic density distribution by

$$\varphi(\mathbf{x}_1) = \int d^3x'_1 \frac{\rho(\mathbf{x}'_1)}{|\mathbf{x}_1 - \mathbf{x}'_1|} \tag{G.46}$$

If the coordinate system is centered on the nucleus, the electronic potential at the nucleus is then given by

$$\varphi(0) = \int d^3x_1' \frac{\rho(\mathbf{x}_1')}{|\mathbf{x}_1'|} \tag{G.47}$$

But the electron density corresponding to the state Ψ_κ is defined as

$$\rho(\mathbf{x}_1) = N \int ds_1 \int d^3x_2 \int ds_2 ... \int d^3x_N \int ds_N \Psi_\kappa^*(\mathbf{x})\Psi_\kappa(\mathbf{x}) \tag{G.48}$$

where the integral is taken over the spin coordinate of the first electron and over the space and spin coordinates of all the other electrons. The wave function $\Psi_\kappa(\mathbf{x}) = \sum_\nu \Phi_\kappa(\mathbf{x}) B_{\nu\kappa}$ is a linear combination of Goscinskian configurations. Thus the density is given by

$$\rho(\mathbf{x}_1) = \sum_{\nu',\nu} \rho_{\nu'\nu}(\mathbf{x}_1) B_{\nu\kappa}^* B_{\nu\kappa} \tag{G.49}$$

where

$$\begin{aligned} \rho_{\nu'\nu}(\mathbf{x}_1) &= N \int ds_1 \int d^3x_2 \int ds_2 ... \int d^3x_N \int ds_N \Phi_{\nu'}^*(\mathbf{x})\Phi_\nu(\mathbf{x}) \\ &= \begin{cases} 0 & \text{if } \nu' \text{ and } \nu \text{ differ by 2 or more orbitals} \\ \chi_{\mu'}^*(\mathbf{x}_1)\chi_\mu(\mathbf{x}_1) & \text{if } \nu' \text{ and } \nu \text{ differ only by } \mu \to \mu' \\ \sum_{i=1}^N |\chi_{\mu_i}(\mathbf{x}_1)|^2 & \text{if } \nu' = \nu \end{cases} \end{aligned} \tag{G.50}$$

In Equation (G.50) we have made use of the fact that within an $\mathcal{R}$-block, the atomic spin-orbitals are orthonormal.

Within the framework of the large-Z approximation we have

$$\begin{aligned} \int dx \; \Psi_\kappa^*(\mathbf{x}) V_0(\mathbf{x}) \Psi_\kappa(\mathbf{x}) &= \sum_{\nu'} \sum_{\nu} B_{\nu'\kappa}^* B_{\nu\kappa} \int dx \; \Phi_{\nu'}^*(\mathbf{x}) V_0(\mathbf{x}) \Phi_\nu(\mathbf{x}) \\ &= -\frac{p_\kappa^2}{\beta_\nu} \sum_\nu |B_{\nu\kappa}|^2 \end{aligned} \tag{G.51}$$

In the second step above, we make use of the potential weighted orthonormality relation (G.12). Further, since $\sum_\nu |B_{\nu\kappa}|^2 = 1$, Equation (G.51) reduces to

$$\int d\tau \; \Psi_\kappa^*(\mathbf{x}) V_0(\mathbf{x}) \Psi_\kappa(\mathbf{x}) = -\frac{p_\kappa^2}{\beta_\nu} = -p_\kappa Z \mathcal{R}_\nu \tag{G.52}$$

This result can be used to express the electronic potential at the nucleus in a very simple form. Combining (G.47) and (G.48), we obtain

$$\varphi(0) = N \int dx \frac{1}{|\mathbf{x}_1|} \Psi_\kappa^*(\mathbf{x}) \Psi_\kappa(\mathbf{x}) \tag{G.53}$$

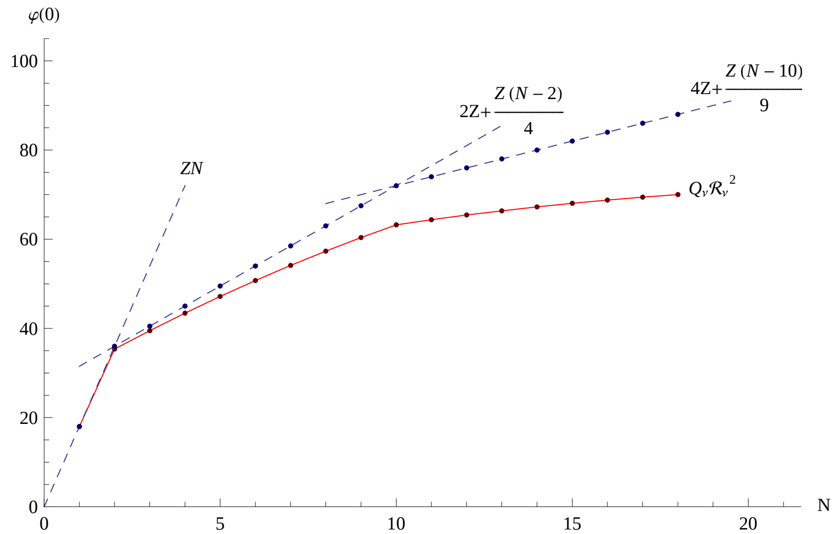

Figure G.3: When interelectron repulsion is entirely neglected, the electronic potential at the nucleus is given by $Z\mathcal{R}_\nu{}^2$, which is exactly piecewise linear in N. The effect of interelectron repulsion is to decrease $\varphi(0)$ and to make the dependence only approximately piecewise linear. The figure shows $\varphi(0)$ neglecting interelectron repulsion (upper values) and including it (lower values). The dots are calculated from the electronic densities of the ground state wave functions, whereas the lines are the closed form expressions found in Equations (G.58) and (G.56).

From the definition of V_0, equation (G.7), and from the fact that each term in the sum in (G.7) gives the same contribution, we have

$$\varphi(0) = -\frac{1}{Z}\int dx \Psi_\kappa^*(\mathbf{x}) V_0(\mathbf{x}) \Psi_\kappa(\mathbf{x}) \tag{G.54}$$

Combining Equations (G.54) and (G.52) we obtain the extremely simple result:

$$\varphi(0) = p_\kappa \mathcal{R}_\nu \tag{G.55}$$

which can alternatively be written in the form:

$$\varphi(0) = Z\mathcal{R}_\nu{}^2 - |\lambda_\kappa|\mathcal{R}_\nu \tag{G.56}$$

or in a third form:

$$\varphi(0) = Q_\nu \mathcal{R}_\nu{}^2 \tag{G.57}$$

since $Q_\nu = Z - |\lambda_\kappa|/\mathcal{R}_\nu$. From Equations (G.55)-(G.57) it follows that for an isonuclear series, the electronic potential at the nucleus depends on N in an approximately piecewise linear way. For example, let us consider the isonuclear series where $Z = 18$. Keeping the nuclear charge Z constant at this value, we begin to add electrons. For the ground state we have:

$$\mathcal{R}_\nu{}^2 \equiv \frac{1}{n_1^2} + \frac{1}{n_2^2} + \cdots + \frac{1}{n_N^2} = \begin{cases} \frac{N}{1} & N \leq 2 \\ \frac{2}{1} + \frac{N-2}{4} & 2 \leq N \leq 10 \\ \frac{2}{1} + \frac{8}{4} + \frac{N-10}{9} & 10 \leq N \leq 18 \end{cases} \tag{G.58}$$

G.5 Core ionization energies

The large-Z approximation can be used to calculate core-ionization energies, i.e., the energies required to remove an electron from the inner shell of an atom. From (G.44) we can see that this energy will be given by

$$\Delta E = \frac{1}{2}\left[(Z\mathcal{R}_\nu - |\lambda_\kappa|)^2 - (Z\mathcal{R}_\nu{}' - |\lambda'_\kappa|)^2\right] \tag{G.59}$$

where the unprimed quantities refer to the original ground state, while the primed quantities refer to the core-ionized states. Since

$$\mathcal{R}_\nu{}^2 - \mathcal{R}_\nu{}'^2 = 1 \tag{G.60}$$

Equation (G.59) can be written in the form

$$\Delta E - \frac{Z^2}{2} = Z\left[\mathcal{R}_\nu{}'|\lambda'_\kappa| - \mathcal{R}_\nu|\lambda_\kappa|\right] + \frac{|\lambda_\kappa|^2 - |\lambda'_\kappa|^2}{2} \tag{G.61}$$

Thus we can see that within the framework of the large-Z approximation, the quantity $\Delta E - Z^2/2$ is linear in Z for an isoelectronic series. This quantity represents the contribution of interelectron repulsion to the core ionization energy, since if interelectron repulsion is completely neglected, the core ionization energy is given by $\Delta E = Z^2/2$. Core ionization energies calculated from Equations (G.59)-(G.61) are shown in Figures G.4 through G.6.

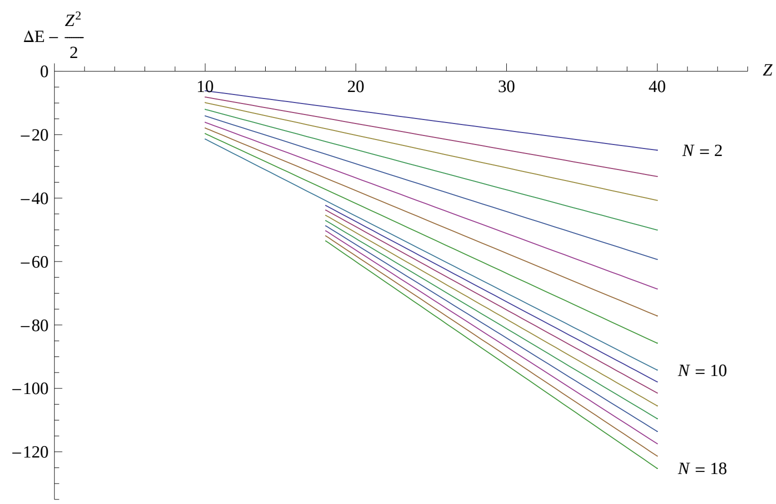

Figure G.4: For isoelectronic series, Equation (G.61) indicates that within the large-Z approximation, the quantity $\Delta E - Z^2/2$ is exactly linear in Z, as is illustrated above. ΔE is the core ionization energy.

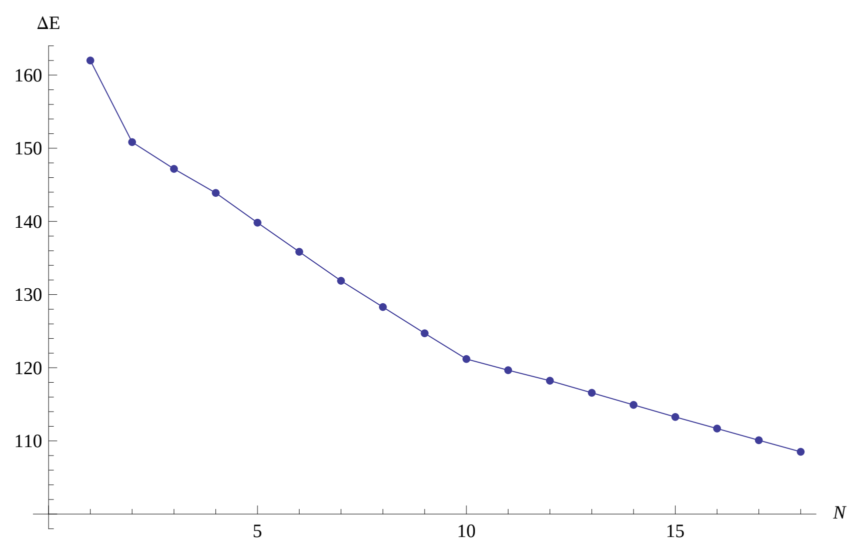

Figure G.5: For isonuclear series, the dependence of the core ionization energy on N is approximately piecewise linear. Whenever a new shell starts to fill, the slope of the line changes. The dots in the figure were calculated using Equation (G.61), where it is not obvious that the dependence ought to be approximately piecewise linear. However, Equations (G.58) and (G.56) can give us some insight into the approximately piecewise linear relationship.

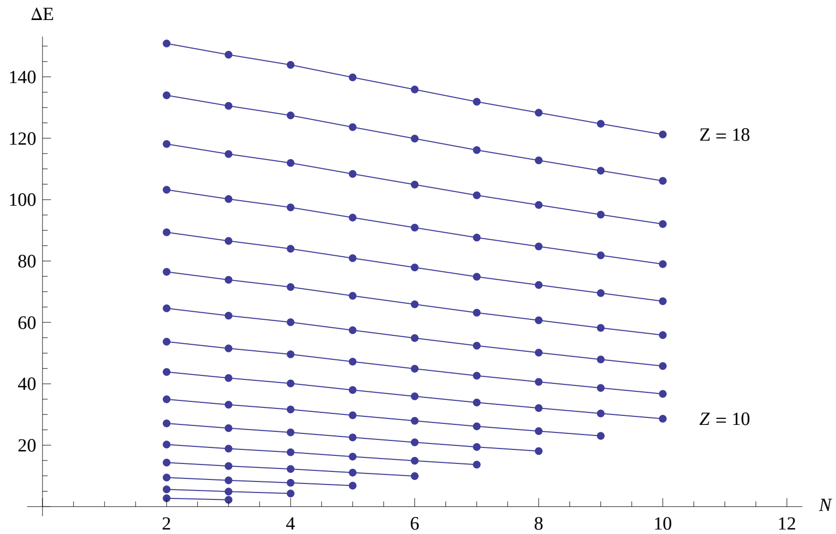

Figure G.6: This figure shows the dependence of the core-ionization energy on both N and Z for the filling of the $n = 2$ shell. Points with $N > Z$ are omitted because the large-Z approximation cannot be used for these points. The energies are in Hartrees.

G.6 Advantages and disadvantages of Goscinskian configurations

We seen that when $V_0(\mathbf{x})$ is chosen to be the the Coulomb attraction of the bare nucleus, the approximate Schrödinger equation

$$\left[-\frac{1}{2}\sum_{j=1}^{N}\nabla_j^2 + \beta_\nu V_0(\mathbf{x}) - E_\kappa\right]|\Phi_\nu\rangle = 0 \qquad \beta_\nu V_0(\mathbf{x}) = -\sum_{j=1}^{N}\frac{Q_\nu}{r_j} \tag{G.62}$$

can be solved exactly using configurations composed of hydrogenlike spin-orbitals with the especially chosen weighted charges Q_ν shown in equation (G.4). There is no need to calculate the weighting factors β_ν. These are obtained automatically when the secular equation is solved. Nor is there a need to normalize the configurations. This is also achieved automatically. Thus the choice of $V_0(\mathbf{x})$ as the potential of the bare nucleus has many advantages; but it also has disadvantages. Just as is the case in perturbation theory, convergence is most rapid if $V_0(\mathbf{x})$ is chosen to be as close as possible to the actual potential. By choosing $V_0(\mathbf{x})$ to be the Coulomb attraction of the bare nucleus, we have neglected interelectron repulsion. This is why the Generalized Sturmian Method with Goscinskian configurations works best when the number of electrons in an atom or ion is small, and why it works especially well when $Z >> N$, i.e., when the Coulomb attraction of the nucleus dominates over the effects of interelectron repulsion.

To extend the range of applicability of the method to atoms and ions with large values of N, we would need to choose a $V_0(\mathbf{x})$ which included some of the effects of interelectron repulsion. For example, we could let it be the Hartree potential. The approximate

Schrödinger equation (G.6) can always be solved provided that it is separable, and it is separable whenever the approximate potential has the form

$$V_0(\mathbf{x}) = \sum_{j=1}^{N} v(\mathbf{x}_j) \tag{G.63}$$

The separated form of (G.6) becomes:

$$\left[-\frac{1}{2}\nabla_j^2 + \beta_\nu v(\mathbf{x}_j) - \epsilon_\zeta\right]\varphi_\zeta(\mathbf{x}_j) = 0 \tag{G.64}$$

where the weighting factors β_ν must be chosen in such a way that

$$\sum_{\zeta\in\nu} \epsilon_\zeta = E_\kappa \tag{G.65}$$

If the spin-orbitals $\varphi_\zeta(\mathbf{x}_j)$ satisfy (G.64), then configurations of the form

$$|\Phi_\nu\rangle = |\varphi_\zeta\varphi_{\zeta'}\varphi_{\zeta''}...| \equiv \frac{1}{\sqrt{N!}}\begin{vmatrix} \varphi_\zeta(\mathbf{x}_1) & \varphi_{\zeta'}(\mathbf{x}_1) & \varphi_{\zeta''}(\mathbf{x}_1) & ... \\ \varphi_\zeta(\mathbf{x}_2) & \varphi_{\zeta'}(\mathbf{x}_2) & \varphi_{\zeta''}(\mathbf{x}_2) & ... \\ \varphi_\zeta(\mathbf{x}_3) & \varphi_{\zeta'}(\mathbf{x}_3) & \varphi_{\zeta''}(\mathbf{x}_3) & ... \\ \vdots & \vdots & \vdots & \end{vmatrix} \tag{G.66}$$

will satisfy the approximate Schrödinger equation (G.6). Some of the neatness of the Generalized Sturmian Method with Goscinskian configurations is certainly lost by choosing a $V_0(\mathbf{x})$ that includes effects of interelectron repulsion, but it could be worth paying this price in order to extend the method to atoms and atomic ions with larger values of N. We are at present exploring these possibilities, and some work in this direction is also being done by Prof. Gustavo Gasaneo and his group in Argentina.

G.7 $\mathcal{R}$-blocks, invariant subsets and invariant blocks

To tie the discussion of this chapter in with the general principles discussed in Chapter 1, we identify T with the operator whose roots and eigenfunctions we wish to study. The group of symmetry operations $\mathcal{G}$ that leave the nuclear attraction and interelectron repulsion matrix of an atom invariant consists of rotations of the entire system about the nucleus, together with reflections and inversions that do not affect the interelectron distances. These operations do not affect the radial parts of the atomic orbitals from which the Goscinskian configurations are constructed, nor do they affect the spin. Thus the set of configurations, all of which are characterized by the same value of

$$\mathcal{R}_\nu \equiv \sqrt{\frac{1}{n^2} + \frac{1}{n'^2} + \frac{1}{n''^2} + \cdots} \tag{G.67}$$

i.e. configurations all of which are built from hydrogenlike atomic spin-orbitals with a particular set of principal quantum numbers $(n, n', n'', ...)$, is closed under $\mathcal{G}$, and it corresponds to an invariant subset as discussed in Chapter 1. The block of T' based on it corresponds to an invariant block. As expected, the eigenfunctions of interelectron repulsion matrix for the $\mathcal{R}$-blocks are the symmetry-adapted basis functions that we desire. In Chapter 1, we mentioned that when the roots of an invariant block are degenerate, then in order to take full advantage of the symmetry of the problem, we need to add an extremely small perturbation which will slightly remove the degeneracy. In the present case, this slight perturbation is given by

$$T_p = aL_z + bS_zF \tag{G.68}$$

where a and b are two very small irrational numbers. (They are chosen to be irrational in order to avoid accidental degeneracies). When this small perturbation is added to T', the degeneracy is slightly removed. The eigenfunctions of $T' + T_p$ for an $\mathcal{R}$-block are then Russell-Saunders states, i.e. they are simultaneous eigenfunctions of the total angular momentum operator L^2, its z-component L_z, the total spin operator S^2, and its z-component S_z. We can ask how many linearly independent configurations there are in a ground-state $\mathcal{R}$-block. The answer is that when the Pauli principle is taken into account, the number of configurations m_k in an $\mathcal{R}$-block is given by the binomial coefficient

Table G.2: Eigenvalues of the 2-electron interelectron repulsion matrix $T'_{\nu',\nu}$ for S=1, M_S=1, $n = 2$ and n'=3, 4, 5.

n'=3 $\lvert\lambda_\kappa\rvert$	term	$n' = 4$ $\lvert\lambda_\kappa\rvert$	term	n'=5 $\lvert\lambda_\kappa\rvert$	term
.108252	^{3}S	.077484	^{3}S	.056075	^{3}S
.134734	^{3}P	.087582	^{3}P	.065019	^{3}P
.135408	^{3}D	.090845	^{3}D	.061128	^{3}P
.138421	^{3}P	.093401	^{3}P	.063370	^{3}D
.155155	^{3}F	.099235	^{3}F	.067758	^{3}F
.160439	^{3}P	.099991	^{3}P	.067934	^{3}P
.165613	^{3}D	.104253	^{3}D	.070494	^{3}D
.168814	^{3}S	.106271	^{3}D	.071269	^{3}D
.173917	^{3}D	.107976	^{3}S	.072413	^{3}F
.186893	^{3}P	.108188	^{3}F	.072857	^{3}S
		.111210	^{3}G	.073295	^{3}G
		.111264	^{3}F	.073588	^{3}G
		.113313	^{3}P	.073920	^{3}F
		.114381	^{3}D	.074306	^{3}G
				.074578	^{3}H
				.074963	^{3}F
				.075173	^{3}P
				.075545	^{3}D

Table G.3: Roots of the ground state $\mathcal{R}$-block of the interelectron repulsion matrix for the Li-like, Be-like, B-like and C-like isoelectronic series.

Li-like $\lvert\lambda_\kappa\rvert$	term	Be-like $\lvert\lambda_\kappa\rvert$	term	B-like $\lvert\lambda_\kappa\rvert$	term	C-like $\lvert\lambda_\kappa\rvert$	term
0.681870	^{2}S	0.986172	^{1}S	1.40355	^{2}P	1.88151	^{3}P
0.729017	^{2}P	1.02720	^{3}P	1.44095	^{4}P	1.89369	^{1}D
		1.06426	^{1}P	1.47134	^{2}D	1.90681	^{1}S
		1.09169	^{3}P	1.49042	^{2}S	1.91623	^{5}S
		1.10503	^{1}D	1.49395	^{2}P	1.995141	^{3}D
		1.13246	^{1}S	1.52129	^{4}S	1.96359	^{3}P
				1.54037	^{2}D	1.98389	^{3}S
				1.55726	^{2}P	1.98524	^{1}D
						1.99742	^{1}P
						2.04342	^{3}P
						2.05560	^{1}D
						2.07900	^{1}S

Table G.4: Roots of the ground state $\mathcal{R}$-block of the interelectron repulsion matrix $T'_{\nu'\nu}$ for the N-like, O-like, F-like and Ne-like isoelectronic series.

N-like $\lvert\lambda_\kappa\rvert$	term	O-like $\lvert\lambda_\kappa\rvert$	term	F-like $\lvert\lambda_\kappa\rvert$	term	Ne-like $\lvert\lambda_\kappa\rvert$	term
2.41491	^{4}S	3.02641	^{3}P	3.68415	^{2}P	4.38541	^{1}S
2.43246	^{2}D	3.03769	^{1}D	3.78926	^{2}S		
2.44111	^{2}P	3.05065	^{1}S				
2.49314	^{4}P	3.11850	^{3}P				
2.52109	^{2}D	3.14982	^{1}P				
2.53864	^{2}S	3.24065	^{1}S				
2.54189	^{2}P						
2.61775	^{2}P						

Table G.5: Eigenvalues of $T'_{\nu',\nu}$ for the carbon-like $\mathcal{R}_\nu = \sqrt{3}$ block.

$\lvert\lambda_\kappa\rvert$	term	degen.	configuration
1.88151	^{3}P	9	$.994467(1s)^2(2s)^2(2p)^2 + .105047(1s)^2(2p)^4$
1.89369	^{1}D	5	$.994467(1s)^2(2s)^2(2p)^2 - .105047(1s)^2(2p)^4$
1.90681	^{1}S	1	$.979686(1s)^2(2s)^2(2p)^2 + .200537(1s)^2(2p)^4$
1.91623	^{5}S	5	$(1s)^2(2s)(2p)^3$
1.95141	^{3}D	15	$(1s)^2(2s)(2p)^3$
1.96359	^{3}P	9	$(1s)^2(2s)(2p)^3$
1.98389	^{3}S	3	$(1s)^2(2s)(2p)^3$
1.98524	^{1}D	5	$(1s)^2(2s)(2p)^3$
1.99742	^{1}P	3	$(1s)^2(2s)(2p)^3$
2.04342	^{3}P	9	$.105047(1s)^2(2s)^2(2p)^2 - .994467(1s)^2(2p)^4$
2.05560	^{1}D	5	$.105047(1s)^2(2s)^2(2p)^2 + .994467(1s)^2(2p)^4$
2.07900	^{1}S	1	$.200537(1s)^2(2s)^2(2p)^2 - .979686(1s)^2(2p)^4$

Appendix H

THE D-DIMENSIONAL HARMONIC OSCILLATOR

H.1 Harmonic oscillators in one dimension

We begin by reviewing the theory of the simple harmonic oscillator in one dimension. We wish to find solutions to the equation

$$\left[-\frac{1}{2}\frac{d^2}{dq^2}+\frac{1}{2}\omega^2 q^2-\epsilon_n\right]\psi_n(q)=0 \tag{H.1}$$

where ω^2 is the force constant, and q is the mass-weighted coordinate. It is convenient to introduce the dimensionless parameter $\zeta = \sqrt{\omega}q$. Then the solutions to equation (H-1) have the form

$$\psi_n(\zeta) = N_n e^{-\zeta^2/2} H_n(\zeta) \tag{H.2}$$

Here, $H_n(\zeta)$ is a Hermite polynomial, named after the French mathematician Charles Hermite (1822-1901), whose name is also associated with self-adjointness. The first few Hermite polynomials are

$$\begin{array}{rcl} H_0(\zeta) &=& 1 \\ H_1(\zeta) &=& 2\zeta \\ H_2(\zeta) &=& 4\zeta^2-2 \\ H_3(\zeta) &=& 8\zeta^3-12\zeta \\ \vdots & \vdots & \vdots \end{array} \tag{H.3}$$

If the solutions are normalized in such a way that

$$\int_{-\infty}^{\infty} dq\ \psi_{n'}(\sqrt{\omega}q)\psi_n(\sqrt{\omega}q) = \delta_{n',n} \tag{H.4}$$

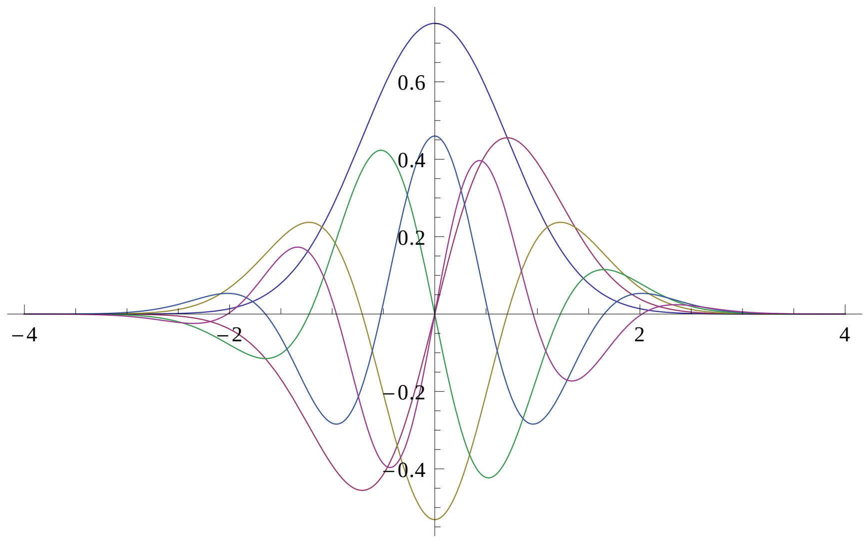

Figure H.1: This figure shows the first few wave functions for a 1-dimensional harmonic oscillator. The functions with quantum numbers n have n nodes. When n is even the functions are symmetric with respect to inversion, while when n is odd, they are odd.

then the normalization constant is

$$N_n = \sqrt{\frac{\sqrt{m\omega}}{2^n n! \sqrt{\pi}}} \tag{H.5}$$

In atomic units, where $\hbar = 1$, the corresponding energies are

$$\epsilon_n = \omega \left(n + \frac{1}{2} \right) \tag{H.6}$$

H.2 Creation and annihilation operators for harmonic oscillators

Equation (H.1) can be rewritten in the form

$$H|n\rangle = \epsilon_n |n\rangle \tag{H.7}$$

where

$$H = \frac{1}{2} \left(-\frac{\partial^2}{\partial q^2} + \omega^2 q^2 \right) \tag{H.8}$$

If we let

$$p \equiv \frac{1}{i} \frac{\partial}{\partial q} \tag{H.9}$$

then

$$H = \frac{1}{2}\left(p^2 + \omega^2 q^2\right) \tag{H.10}$$

Also we can see the p and q obey the commutation relations

$$[p, q] = -i \qquad [p, p] = 0 \qquad [q, q] = 0 \tag{H.11}$$

From these commutations relations it follows that

$$\begin{aligned} [H, p] &= \frac{1}{2}\omega^2 [q^2, p] \\ &= \frac{1}{2}\omega^2 (q[q, p] + [q, p]q) \\ &= i\omega^2 q \end{aligned} \tag{H.12}$$

and

$$\begin{aligned} [H, q] &= \frac{1}{2}[p^2, q] \\ &= \frac{1}{2}(p[p, q] + [p, q]p) \\ &= -ip \end{aligned} \tag{H.13}$$

Now suppose that we have found an eigenfunction of H, so that

$$H|n\rangle = \epsilon_n |n\rangle \tag{H.14}$$

We can show by means of the commutation relations (H.13) and (H.14) that when the operator $p \pm i\omega q$ acts on $|n\rangle$, the resulting function is also an eigenfunction of H:

$$\begin{aligned} H(p \pm i\omega q)|n\rangle &= \{[H, p] \pm [H, q] + (p \pm i\omega q)H\} |n\rangle \\ &= \left\{i\omega^2 q \pm i\omega(-ip) + (p \pm i\omega q)\epsilon_n\right\} |n\rangle \\ &= (\epsilon_n \pm \omega)(p \pm i\omega q)|n\rangle \end{aligned} \tag{H.15}$$

Equation (H.15) shows that the function $(p \pm i\omega q)|n\rangle$ is an eigenfunction of H corresponding to the eigenvalue $\epsilon_n \pm \omega$. The operator $p + i\omega q$ is thus a “raising operator”. When it acts on $|n\rangle$, it produces a new eigenfunction, whose eigenvalue is raised by an amount ω. Similarly, $p - i\omega q$ is a lowering operator. When it acts on $|n\rangle$, it produces a new eigenfunction, whose eigenvalue is lowered by an amount ω.

If we continue to act on $|n\rangle$ with the lowering operator $p - i\omega q$, we must eventually come to the ground state of the harmonic oscillator, a state of minimum energy beyond which it is impossible to lower the energy eigenvalue. Let us represent the ground state by the symbol $|0\rangle$. The lowering operator, acting on the ground state, must give zero, since it cannot give an eigenfunction corresponding to a lower energy. Therefore we have the relation:

$$(p - i\omega q)|0\rangle = 0 \tag{H.16}$$

Acting on (H.16) with $p + i\omega q$, we obtain

$$\begin{aligned}(p + i\omega q)(p - i\omega q)|0\rangle &= \left(p^2 + \omega^2 q^2 + i\omega[p, q]\right)|0\rangle \\ &= (2H - \omega)\,|0\rangle \\ &= (2\epsilon_0 - \omega)\,|0\rangle = 0 \end{aligned} \tag{H.17}$$

Thus the energy of the ground state is given by

$$\epsilon_0 = \frac{\omega}{2} \tag{H.18}$$

Combining (H.18) and (H.15), we can see that the energy of a general state $|n\rangle$ is given by

$$\epsilon_n = \omega\left(n + \frac{1}{2}\right) \tag{H.19}$$

It is convenient to define a normalized raising operator, which we will call a "creation operator",

$$a^\dagger \equiv \mathcal{N}(-ip + \omega q) \tag{H.20}$$

and a normalized lowering operator, which we will call an "annihilation operator".

$$a \equiv \mathcal{N}(ip + \omega q) \tag{H.21}$$

The constant of normalization is chosen in such a way that

$$a^\dagger|n\rangle = \sqrt{n+1}\;|n+1\rangle \tag{H.22}$$

and

$$a|n+1\rangle = \sqrt{n+1}\;|n\rangle \tag{H.23}$$

Then

$$\begin{aligned} aa^\dagger|n\rangle &= a\sqrt{n+1}\;|n+1\rangle \\ &= (n+1)|n\rangle \\ &= \mathcal{N}^2(p - i\omega q)(p + i\omega q)|n\rangle \\ &= \mathcal{N}^2\left(2H + i\omega[p, q]\right)|n\rangle \\ &= \mathcal{N}^2 2\omega(n+1)|n\rangle \end{aligned} \tag{H.24}$$

Solving (H.24) for $\mathcal{N}$, we obtain

$$\mathcal{N} = \frac{1}{\sqrt{2\omega}} \tag{H.25}$$

Thus

$$a^\dagger = \frac{1}{\sqrt{2\omega}}(-ip + \omega q) \tag{H.26}$$

and

$$a = \frac{1}{\sqrt{2\omega}}(ip + \omega q) \tag{H.27}$$

We can also solve for p and q in terms of the creation and annihilation operators:

$$p = i\sqrt{\frac{\omega}{2}}(a^\dagger - a) \tag{H.28}$$

while

$$q = i\frac{1}{\sqrt{2\omega}}(a^\dagger + a) \tag{H.29}$$

Then, making use of (H.10) we have

$$H = \omega\left(a^\dagger a + \frac{1}{2}\right) \tag{H.30}$$

From (H.28), (H.29) and (H.11), it follows that $a^\dagger$ and a obey the commutation relations

$$\begin{aligned} [a, a^\dagger] &= 1 \\ \left[a^\dagger, a^\dagger\right] &= 0 \\ [a, a] &= 0 \end{aligned} \tag{H.31}$$

H.3 A collection of harmonic oscillators

Let us now consider a system whose Hamiltonian can be represented by a sum of simple harmonic oscillator Hamiltonians:

$$H = \sum_{k=1}^{d} \omega_k \left(a_k^\dagger a_k + \frac{1}{2}\right) \tag{H.32}$$

Then the commutation relations corresponding to (H.31) will be

$$\begin{aligned} [a_{k'}, a_k^\dagger] &= \delta_{k',k} \\ \left[a_{k'}^\dagger, a_k^\dagger\right] &= 0 \\ [a_{k'}, a_k] &= 0 \end{aligned} \tag{H.33}$$

The eigenfunctions of the Hamiltonian are just products of simple harmonic oscillator eigenfunctions, and they can be labelled by a set of numbers $n_1, n_2, \cdots, n_d$, one quantum number for each normal mode of the system. If we use the symbol $|n_1, n_2, \cdots, n_d\rangle$ to denote such a state, then we have:

$$\begin{aligned} H|n_1, n_2, \cdots, n_d\rangle &= \sum_{k=1}^{d} \omega_k \left(a_k^\dagger a_k + \frac{1}{2} \right) |n_1, n_2, \cdots, n_d\rangle \\ &= \sum_{k=1}^{d} \omega_k \left(n_k + \frac{1}{2} \right) |n_1, n_2, \cdots, n_d\rangle \end{aligned} \tag{H.34}$$

The operator $a_k^\dagger a_k$ is called the "number operator", because its eigenvalues correspond to the quantum number n_k.

H.4 d-dimensional isotropic harmonic oscillators

In terms of the mass-weighted coordinates $\mathbf{q} = \sqrt{m}\ \mathbf{x}$, the Schrödinger equation of a d-dimansional isotropic harmonic oscillator can be written in the form

$$\sum_{i=1}^{d} \frac{1}{2} \left[-\frac{\partial^2}{\partial q_i^2} + \omega^2 q_i^2 \right] \Psi_{\mathbf{n}}(\mathbf{q}) = E_{\mathbf{n}} \Psi_{\mathbf{n}}(\mathbf{q}) \tag{H.35}$$

If we let

$$\begin{aligned} \Psi_{\mathbf{n}}(\mathbf{q}) &= \prod_{i=1}^{d} \psi_{n_i}(q_i) \\ E_{\mathbf{n}} &= \sum_{i=1}^{d} \epsilon_{n_i} \end{aligned} \tag{H.36}$$

Then (H.35) separates into d independent equations of the form

$$\frac{1}{2} \left[-\frac{\partial^2}{\partial q_i^2} + \omega^2 q_i^2 \right] \psi_{n_i}(q_i) = \epsilon_{n_i} \psi_{n_i}(q_i) \tag{H.37}$$

In other words, the isotropic d-dimensional harmonic oscillator can be treated as a system of independent simple harmonic oscillators, all having the same frequency. so that

$$\sum_{i=1}^{d} \epsilon_{n_i} = \omega \sum_{i=1}^{d} \left(n_i + \frac{1}{2} \right) \tag{H.38}$$

Alternatively we can write the Schrödinger equation in the form:

$$\left[-\frac{1}{2m} \Delta + \frac{1}{2} m \omega^2 r^2 - E_{n,\lambda} \right] \chi_{n,\lambda,\mu}(\mathbf{x}) = 0 \tag{H.39}$$

where Δ is the generalized Laplacian operator. We can try to find solutions which are functions of the hyperradius multiplied by hyperspherical harmonics:

$$\chi_{n,\lambda,\mu}(\mathbf{x}) = R_{n,\lambda}(r) Y_{\lambda,\mu}(\mathbf{u}) \tag{H.40}$$

Substitutine this into equation (H.39), we find that the hyperradial part of the solution must obey an ordinary differential equation. If we use units for which $m = 1$ and make use of equations (**??**) and (**??**), we have

$$\begin{aligned}
& \left[-\Delta + \omega^2 r^2 - 2E_{n,\lambda}\right] R_{n,\lambda}(r) \\
= & \left[-\frac{1}{r^{d-1}}\frac{d}{dr}r^{d-1}\frac{d}{dr} - \frac{\Lambda^2}{r^2} + \omega^2 r^2 - 2E_{n,\lambda}\right] R_{n,\lambda}(r) \\
= & \left[-\frac{1}{r^{d-1}}\frac{d}{dr}r^{d-1}\frac{d}{dr} - \frac{\lambda(\lambda+d-2)}{r^2} + \omega^2 r^2 - 2E_{n,\lambda}\right] R_{n,\lambda}(r) = 0
\end{aligned} \tag{H.41}$$

With the substitution $\zeta = \sqrt{\omega} r$, equation (21) becomes

$$\left[\frac{d^2}{d\zeta^2} + \frac{d-1}{\zeta}\frac{d}{d\zeta} + \frac{\lambda(\lambda+d-2)}{\zeta^2} - \zeta^2 + 2E_{n,\lambda}\right] R_{n,\lambda}(\zeta) = 0 \tag{H.42}$$

According to Valliéres et al. ([**?**]), this equation has a solution of the form

$$R_{n,\lambda}(\zeta) = \sqrt{\frac{2n!}{\Gamma(\lambda+n+d/2)}}\ \zeta^\lambda e^{-\zeta^2/2} L_n^{\lambda+(d-2)/2}(\zeta^2) \tag{H.43}$$

where L is an associated Legendre polynomial and

$$E_{n,\lambda} = 2n + \lambda + d/2 \tag{H.44}$$

The normalization is chosen so that

$$\int_0^\infty d\zeta\ \zeta^{d-1} |R_{n,\lambda}(\zeta)|^2 = 1 \tag{H.45}$$

Written in terms of the hyperradius r, rather than $\zeta = \sqrt{\omega} r$, we have

$$R_{n,\lambda}(r) = \sqrt{\frac{2n!\omega^{d/2}}{\Gamma(\lambda+n+d/2)}}\ (\sqrt{\omega} r)^\lambda e^{-\omega r^2/2} L_n^{\lambda+(d-2)/2}(\omega r^2) \tag{H.46}$$

This radial wave function is normalized in such a way that

$$\int_0^\infty dr\ r^{d-1} |R_{n,\lambda}(r)|^2 = 1 \tag{H.47}$$

It satisfies equation (H.42) with

$$E_{n,\lambda} = \omega(2n + \lambda + d/2) \tag{H.48}$$

Comparing this with equation (H.38), we can see that we must make the identification

$$2n + \lambda = \sum_{i=1}^{d} n_i \tag{H.49}$$

For $d = 3$ this becomes

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{l(l+1)}{r^2} - \omega^2 r^2 + 2E\right] R_{n,l}(r) = 0 \tag{H.50}$$

which has solutions of the form

$$R_{n,l}(r) = N_{n,l}\ r^l\ e^{-\omega r^2/2} L_n^{l+1/2}(\omega r^2) \tag{H.51}$$

where

$$N_{n,l} = \sqrt{\sqrt{\frac{\omega^3}{4\pi}} \frac{2^{n+l+3} n! \omega^l}{(2n+2l+1)!!}} \tag{H.52}$$

is a normalizing constant, and $L_n^{l+1/2}$ is an associated Legendre polynomial. Analogous solutions can be found for higher values of d. The 3-dimensional isotropic harmonic oscillator radial wave functions shown in equations (H.51) and (H.52) obey the orthonormality relation:

$$\int_0^\infty dr\ r^2 R_{n',l}(r) R_{n,l}(r) = \delta_{n',n} \tag{H.53}$$

Since they are solutions to the same differential equation (differently expressed) it must be possible to expand these functions in terms of those solutions to (H.35) which correspond to the same energy.

$$R_{n,\lambda}(r) Y_{\lambda,\mu}(\hat{\mathbf{u}}) = \sum_{\mathbf{n}}{}' \Psi_{\mathbf{n}}(\mathbf{q})\ U_{\mathbf{n};n,\lambda,\mu} \tag{H.54}$$

The prime over the sum in (H.54) indicates that it includes only those values of $\mathbf{n}$ that fulfill equation (H.49).

H.5 Fourier transforms of 3-dimensional harmonic oscillator wave functions

Let

$$\chi_{n,l,m}(\mathbf{x}) = R_{n,l}(r) Y_{l,m}(\mathbf{u}) \tag{H.55}$$

be a 3-dimensional harmonic oscillator wave function expressed in spherical polar coordinates. Its Fourier transform is given by

$$\begin{aligned}
\chi^t_{n,l,m}(\mathbf{p}) &= \frac{1}{(2\pi)^{3/2}} \int d\mathbf{x}\ \chi_{n,l,m}(\mathbf{x})\ e^{-i\mathbf{p}\cdot\mathbf{x}} \\
&= \frac{1}{(2\pi)^{3/2}} \int_0^\infty dr\ r^2\ R_{n,l}(r) \int d\Omega_3 Y_{l,m}(\mathbf{u})\ e^{-i\mathbf{p}\cdot\mathbf{x}} \\
&= \frac{4\pi}{(2\pi)^{3/2}} (-i)^l Y_{l,m}(\mathbf{u}_p) \int_0^\infty dr\ r^2\ R_{n,l}(r) j_l(pr) \\
&= (-i)^l Y_{l,m}(\mathbf{u}_p) R^t_{n,l}(p) \qquad \text{(H.56)}
\end{aligned}$$

where we have made use of the expansion

$$e^{-i\mathbf{p}\cdot\mathbf{x}} = 4\pi \sum_{l=0}^\infty (-i)^l\ j_l(pr) \sum_{m'=-l}^{l} Y_{l,m'}(\mathbf{u}_p) Y^*_{l,m'}(\mathbf{u}) \qquad \text{(H.57)}$$

and where

$$R^t_{n,l}(p) = \sqrt{\frac{2}{\pi}} \int dr\ r^2\ R^t_{n,l}(p) j_l(pr) \qquad \text{(H.58)}$$

Using equation (H.51), we can write this transform as

$$R^t_{n,l}(p) = N_{n,l} \sqrt{\frac{2}{\pi}} \int_0^\infty dr\ r^2\ r^l e^{-\omega r^2/2} L_n^{l+1/2}(\omega r^2) j_l(pr) \qquad \text{(H.59)}$$

Mathematica is not able to evaluate this integral for general n or l, but it can do so if we give it particular values of n and l. Looking at sufficiently many particular cases, we can make the generalization:

$$R^t_{n,l}(p) = N_{n,l}\ \frac{(-1)^n}{\omega^{(l+3)/2}}\ e^{-p^2/(2\omega)} (p^2/\omega)^{l/2} L_n^{l+1/2}(p^2/\omega) \qquad \text{(H.60)}$$

The Bessel transformed radial functions obey the orthonormality relation

$$\int_0^\infty dp\ p^2 R^t_{n',l}(p) R^t_{n,l}(p) = \delta_{n',n} \qquad \text{(H.61)}$$

H.6 The hyperspherical Bessel transform of the radial function

By analogy with equations (H.46) and (H.60), we make the guess

$$\begin{aligned}
&R^t_{n,\lambda}(p) \\
&= \sqrt{\frac{2n!}{\Gamma(\lambda+n+d/2)\omega^{d/2}}}\ (-1)^n\ e^{-p^2/(2\omega)} (p^2/\omega)^{\lambda/2} L_n^{\lambda+(d-2)/2}(p^2/\omega)
\end{aligned}$$

(H.62)

We can check that $R^t_{n,\lambda}(p)$ obeys the orthonormality relation

$$\int_0^\infty dp\ p^{d-1} R^t_{n',\lambda}(p) R^t_{n,\lambda}(p) = \delta_{n',n} \tag{H.63}$$

We can also use the expansion of a d-dimensional plane wave in terms of hyperspherical harmonics and hyperspherical Bessel functions

$$e^{-i\mathbf{p}\cdot\mathbf{x}} = (d-2)!!I(0) \sum_{\lambda=0}^{\infty} (-i)^\lambda j^d_\lambda(pr) \sum_{\mu'} Y^*_{\lambda,\mu}(\mathbf{u}) Y_{\lambda,\mu}(\mathbf{u}_p) \tag{H.64}$$

to evaluate the d-dimensional Fourier-Bessel transform:

$$\begin{aligned}
&\frac{1}{(2\pi)^{d/2}} \int_0^\infty dr\ r^{d-1} \int d\Omega_d\ R_{n,\lambda}(r) Y_{\lambda,\mu}(\mathbf{u}) e^{-i\mathbf{p}\cdot\mathbf{x}} \\
=\ & (-i)^\lambda Y_{\lambda,\mu}(\mathbf{u}_p) \frac{(d-2)!!I(0)}{(2\pi)^{d/2}} \int_0^\infty dr\ r^{d-1}\ j^d_\lambda(pr) R_{n,\lambda}(r) \\
=\ & (-i)^\lambda Y_{\lambda,\mu}(\mathbf{u}_p) R^t_{n,\lambda}(p)
\end{aligned} \tag{H.65}$$

where $I(0)$ is the total solid angle in the d-dimensional space. Mathematica is unable to perform the hyperradial integral of equation (H.65) for general values of n and λ, but it can do so for particular values, and thus we can check the hypothesis shown in equation (H.62).

H.7 Coupling coefficients for harmonic oscillator wave functions

The d-dimensional harmonic oscillator wave functions obey the orthonormality relation

$$\int d\mathbf{x}\ \chi^*_{\nu'}(\mathbf{x}) \chi_\nu(\mathbf{x}) = \delta_{\nu',\nu} \tag{H.66}$$

If we double the value of the frequency ω, the relationship is the same:

$$\int d\mathbf{x}\ \chi^*_{\nu'}(2\omega, \mathbf{x}) \chi_\nu(2\omega, \mathbf{x}) = \delta_{\nu',\nu} \tag{H.67}$$

We can use the orthonormality relation (H.67) to express the product of two d-dimensional harmonic oscillator wave functions as a sum of single functions of the same kind, but with double the frequency. Let

$$\chi^*_{\nu_1}(\mathbf{x}) \chi_{\nu_2}(\mathbf{x}) = \sum_{\nu'} \chi_{\nu'}(2\omega, \mathbf{x})\ C^{\nu'}_{\nu_1,\nu_2} \tag{H.68}$$

Then, making use of (H.67), we have

$$\begin{aligned}\int d\mathbf{x}\ \chi^*_\nu(2\omega,\mathbf{x})\chi^*_{\mu_1}(\mathbf{x})\chi_{\mu_2}(\mathbf{x}) &= \sum_{\nu'}\int d\mathbf{x}\ \chi^*_\nu(2\omega,\mathbf{x})\chi_{\nu'}(2\omega,\mathbf{x})\ C^{\nu'}_{\nu_1,\nu_2}\\ &= \sum_{\nu'}\delta_{\nu,\nu'}C^{\nu'}_{\nu_1,\nu_2} = C^{\nu}_{\nu_1,\nu_2}\end{aligned} \tag{H.69}$$

The integral on the left-hand side of (H.69) can be separated into a hyperradial part and a hyperangular part:

$$\begin{aligned}C^{\nu}_{\nu_1,\nu_2} &= \int d\mathbf{x}\ \chi^*_\nu(2\omega,\mathbf{x})\chi^*_{\nu_1}(\mathbf{x})\chi_{\nu_2}(\mathbf{x})\\ &= \int_0^\infty dr\ r^{d-1}R_{n,\lambda_1+\lambda_2}(2\omega,r)R_{n_1,\lambda_1}(r)R_{n_2,\lambda_2}(r)\\ &\times \int d\Omega_d\ Y^*_{\lambda,\mu}(\mathbf{u})Y^*_{\lambda_1,\mu_1}(\mathbf{u})Y_{\lambda_2,\mu_2}(\mathbf{u})\end{aligned} \tag{H.70}$$

The hyperangular integral in equation (H.70) can be evaluated rapidly and exactly by means of our general theorem (**??**)-(**??**). The hyperradial integral can also be evaluated exactly, and the sum in equation (H.68) terminates after a finite number of terms.

H.8 Normal modes

We next consider the small vibrations of a classical system of particles about the equilibrium positions. Suppose that the kinetic energy of the system is given by

$$T = \frac{1}{2}\sum_{i=1}^{d}\sum_{j=1}^{d} m_i\delta_{i,j}\frac{dx^i}{dt}\frac{dx^j}{dt} \tag{H.71}$$

while the leading term in a Taylor series expansion of the potential energy has the form

$$V = \frac{1}{2}\sum_{i=1}^{d}\sum_{j=1}^{d} V_{i,j}x^i x^j \tag{H.72}$$

The coordinates $x^1, x^2\cdots, x^d$, which represent small displacements from the equilibrium positions of the particles, are by no means the most convenient ones for solving the equations of motion of the system. We can bring the kinetic energy into a more convenient form by going over to the mass-weighted coordinates defined by

$$X^i \equiv \sqrt{m_i}\ x^i \qquad\qquad i = 1, 2, \cdots, d \tag{H.73}$$

In terms of these coordinates, the kinetic energy has the form

$$T = \frac{1}{2}\sum_{i=1}^{d}\sum_{j=1}^{d}\delta_{i,j}\frac{dX^i}{dt}\frac{dX^j}{dt} \tag{H.74}$$

while the potential energy becomes

$$V = \frac{1}{2} \sum_{i=1}^{d} \sum_{j=1}^{d} \frac{V_{i,j}}{\sqrt{m_i m_j}} X^i X^j \tag{H.75}$$

The mass-weighted coordinates are still not the most convenient ones that we can find, since the potential energy matrix $V_{i,j}$ may contain off-diagonal terms. and we would like to get rid of these. We can find a unitary transformation which diagonalizes $V_{i,j}/\sqrt{m_i m_j}$ by solving the secular equations

$$\sum_{j=1}^{d} \left(\frac{V_{i,j}}{\sqrt{m_i m_j}} - \mathcal{V}(k)\delta_{i,j} \right) U_{j,k} = 0 \tag{H.76}$$

Having performed the diagonalization, we can express the potential energy and the kinetic energy of the system in terms of the *normal coordinates* defined by

$$q^k = \sum_{i=1}^{d} X^i U_{i,k} = \sum_{i=1}^{d} \sqrt{m_i}\ x^i U_{i,k} \tag{H.77}$$

When we do this, the kinetic energy retains its diagonal form because of the unitarity of $U_{j,k}$:

$$T = \frac{1}{2} \sum_{k=1}^{d} \left(\frac{dq^k}{dt} \right)^2 \tag{H.78}$$

but the off-diagonal terms in the potential energy disappear:

$$V = \frac{1}{2} \sum_{k=1}^{d} \mathcal{V}(k)(q^k)^2 \tag{H.79}$$

From (H.78) and (H.79) we can see that the Lagrangian of the system can be written in the form

$$L = T - V = \sum_{k=1}^{d} L_k \tag{H.80}$$

where

$$L_k = \frac{1}{2} \left[\left(\frac{dq^k}{dt} \right)^2 - \mathcal{V}(k)(q^k)^2 \right] \tag{H.81}$$

The canonically conjugate momentum paired with the coordinate q^k is defined in mechanics to be

$$p_k = \frac{\partial L}{\partial \dot{q}^k} = \frac{dq^k}{dt} \tag{H.82}$$

he Hamiltonian of the system can be written in the form

$$H = T + V = \sum_{k=1}^{d} H_k \tag{H.83}$$

where

$$H_k = \frac{1}{2}\left(p_k^2 + \omega_k^2 q_k^2\right) \tag{H.84}$$

and

$$\omega_k = \sqrt{\mathcal{V}(k)} \tag{H.85}$$

In other words, when the Hamiltonian which represents small vibrations of a classical system is expressed in terms of the normal coordinates (or normal modes), it reduces to a sum of simple harmonic oscillator Hamiltonians. The normal coordinates are found by diagonalizing the mass-weighted potential energy matrix. The harmonic oscillator frequency of each is found by taking the square root of the corresponding eigenvalue of the mass-weighted potential energy matrix.

To illustrate this procedure, we can think of a system, whose Lagrangian is given by

$$L = \frac{1}{2}\sum_{i=1}^{d}\sum_{j=1}^{d}\left(m\ \delta_{i,j}\frac{dx^i}{dt}\frac{dx^j}{dt} - V_{i,j}x^i x^j\right) \tag{H.86}$$

where $V_{i,j} = 2\kappa$ if $i = j$ and $V_{i,j} = -\kappa$ if $i = j \pm 1$, while being zero every where else in the matrix. This Lagrangian corresponds to a linear system of point masses, each joined elastically to the next. Then the secular equations (H.76) have the form

$$-\kappa U_{k-1,k} + \left[2\kappa - \mathcal{V}(k)\right] U_{k,k} - \kappa U_{k+1,k} = 0 \qquad\qquad k = 2, \ldots, d-1 \tag{H.87}$$

The trial solution

$$U_{j,k} = \sqrt{\frac{2}{d+1}}\ \sin(jka) \tag{H.88}$$

makes all of the secular equations redundant, All of them redundantly require that

$$\mathcal{V}(k) = \kappa\left[1 - \cos(ka)\right] \tag{H.89}$$

Imposing homogeneous boundary conditions (i.e clamping the two ends of the line) restricts the allowed values of k, and we must have

$$k = \frac{\pi}{(d+1)a}, \frac{2\pi}{(d+1)a}, \cdots, \frac{\pi d}{(d+1)a} \tag{H.90}$$

where $(d+1)a$ is the length of the chain. The frequency spectrum of the normal modes is given by

$$\omega_k = \sqrt{\frac{\mathcal{V}(k)}{m}} = \sqrt{\frac{2\kappa\,[1-\cos(2ka)]}{m}} \tag{H.91}$$

In terms of the normal mode coordinates and their time derivatives, the Lagrangian of the system becomes

$$L = \frac{1}{2}\sum_k \left[\left(\frac{dq^k}{dt}\right)^2 - (\omega_k q^k)^2\right] \tag{H.92}$$

which can be recognized as a sum of harmonic oscillator Lagrangians.

H.9 Molecular vibrations and rotations

In the simplest possible approximation, we can regard a molecule (or a cluster in a non-melted state) as a collection of point masses held together by springlike bonds. When we calculate the normal modes of such a system, we always find that there are six zero-frequency modes. Three of these correspond to the degrees of freedom associated with translation of the whole system, and three with rotation. Let us use the symbols $\mathbf{R}_s$ to represent the equilibrium position of the atom s, and $\mathbf{x}_s$ to represent the displacement of the atom from its equilibrium position. Then in our simple model, the classical potential energy of the molecule can be written in the form

$$V = \frac{1}{2}\sum_{t>s}^{N}\sum_{s=1}^{N} k_{st}\left(|\mathbf{x}_s + \mathbf{R}_s - \mathbf{x}_t - \mathbf{R}_t| - |\mathbf{R}_s - \mathbf{R}_t|\right)^2 \tag{H.93}$$

Here k_{st} represents the force constant of the "spring" which connects atom s with atom t. Let us also introduce the notation

$$\begin{aligned} \mathbf{R}_{st} &\equiv \mathbf{R}_s - \mathbf{R}_t \\ \mathbf{x}_{st} &\equiv \mathbf{x}_s - \mathbf{x}_t \end{aligned} \tag{H.94}$$

Then, if we assume that $|\mathbf{x}_{st}| << |\mathbf{R}_{st}|$ and expand V in a Taylor series, we obtain the leading term

$$\begin{aligned} V &\approx \sum_{t>s}^{N}\sum_{s=1}^{N} \frac{k_{st}}{|\mathbf{R}_{st}|^2}(\mathbf{R}_{st}\cdot\mathbf{x}_{st})^2 \\ &\equiv \frac{1}{2}\sum_{t>s}^{N}\sum_{s=1}^{N}\sum_{\mu=1}^{3}\sum_{\nu=1}^{3} V_{s,\mu;t,\nu}x_{s,\mu}x_{t,\nu} \end{aligned} \tag{H.95}$$

where

$$\mathbf{x}_s \equiv (x_{s1}, x_{s2}, x_{s3}) \tag{H.96}$$

By diagonalizing the mass-weighted potential energy matrix

$$\frac{V_{s,\mu;t,\nu}}{\sqrt{m_s m_t}} \tag{H.97}$$

we can find the normal modes of the system, and as mentioned, six of them will be zero-frequency modes corresponding to translations and rotations of the entire system.

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