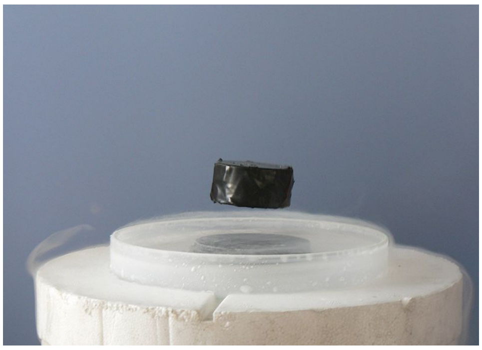
Fundamentals of Physics and Nuclear Physics

Main articles

Physics

Physics (Greek: physis – φύσις meaning "nature") a natural science, is the study of matter[1] and its motion through spacetime and all that derives from these, such as energy and force.[2] More broadly, it is the general analysis of nature, conducted in order to understand how the world and universe behave.[3] [4]



A magnet levitating above a superconductor demonstrates the Meissner effect.

Physics is one of the oldest academic disciplines, perhaps the oldest through its inclusion of astronomy.[5] Over the last two millennia, physics had been considered synonymous with philosophy, chemistry, and certain branches of mathematics and biology, but during the Scientific Revolution in the 16th century, it emerged to become a unique modern science in its own right.[6] However, in some subject areas such as in mathematical physics and quantum chemistry, the boundaries of physics remain difficult to distinguish.

Physics is both significant and influential, in part because advances in its understanding have often translated into new technologies, but also because new ideas in physics often resonate with the other sciences, mathematics and philosophy. For example, advances in the understanding of electromagnetism led directly to the development of new products which have dramatically transformed modern-day society (e.g., television, computers, and domestic appliances); advances in → thermodynamics led to the development of motorized transport; and advances in mechanics inspired the development of calculus.

Scope and Aims

This parabola-shaped lava flow illustrates Galileo's law of falling bodies as well as blackbody radiation – you can tell the temperature from the color of the blackbody.

Physics covers a wide range of phenomena, from the smallest sub-atomic particles, to the largest galaxies. Included in this are the very most basic objects from which all other things are composed of, and therefore physics is sometimes said to be the "fundamental science".[7]

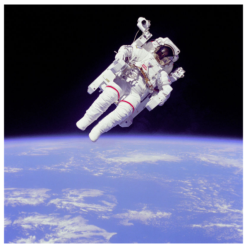
Physics aims to describe the various phenomena that occur in nature in terms of simpler phenomena. Thus, physics aims to both connect the things we see around us to root causes, and then to try to connect these causes together in the hope of finding an ultimate reason for why nature is as it is. For example, the ancient Chinese observed that certain rocks (lodestone) were attracted to one another by some invisible force. This effect was later called magnetism, and was first rigorously studied in the 17th century. A little earlier than the Chinese, the ancient Greeks knew of other objects such as amber, that when rubbed with fur would cause a similar invisible attraction between the two. This was also first studied rigorously in the 17th century, and came to be called electricity. Thus, physics had come to understand two observations of nature in terms of some root cause (electricity and magnetism). However, further work in the 19th century revealed that these two forces were just two different aspects of one force – electromagnetism. This process of "unifying" forces continues today (see section *Current research* for more information).

The Scientific Method

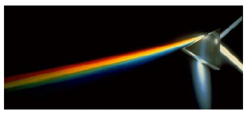
Physics uses the scientific method to test the validity of a physical theory, using a methodical approach to compare the implications of the theory in question with the associated conclusions drawn from experiments and observations conducted to test it. Experiments and observations are to be collected and matched with the predictions and hypotheses made by a theory, thus aiding in the determination or the validity/invalidity of the theory.

Theories which are very well supported by data and have never failed any competent empirical test are often called scientific laws, or natural laws. Of course, all theories, including those called scientific laws, can always be replaced by more accurate, generalized statements if a disagreement of theory with observed data is ever found.[8]

Theory and experiment



The astronaut and Earth are both in free-fall



Dispersion of light by a prism

The culture of physics has a higher degree of separation between theory and experiment than many other sciences. Since the twentieth century, most individual physicists have specialized in either theoretical physics or experimental physics. In contrast, almost all the successful theorists in biology and chemistry (e.g. American quantum chemist and biochemist Linus Pauling) have also been experimentalists, although this is changing as of late.

Theorists seek to develop mathematical models that both agree with existing experiments and successfully predict future results, while experimentalists devise and perform experiments to test theoretical predictions and explore new phenomena. Although theory and experiment are developed separately, they are strongly dependent upon each other. Progress in physics frequently comes about when experimentalists make a discovery that existing theories cannot explain, or when new theories generate experimentally testable predictions, which inspire new experiments. In the absence of experiment, theoretical research can go in the wrong direction; this is one of the criticisms that has been leveled against M-theory, a popular theory in high-energy physics for which no practical experimental test has ever been devised. It is also worth noting there are some physicists who work at the interplay of theory and experiment who are called phenomenologists. Phenomenologists look at the complex phenomena observed in experiment and work to relate them to fundamental theory.


Lightning is electric current

Theoretical physics is closely related to mathematics, which provides the language of physical theories, and large areas of mathematics, such as calculus, have been invented specifically to solve problems in physics. Theorists may also rely on numerical analysis and computer simulations. The fields of mathematical and computational physics are active areas of research. Theoretical physics has historically rested on philosophy and metaphysics; electromagnetism was unified this way.[9] Beyond the known universe, the field of theoretical physics also deals with hypothetical issues,[10] such as parallel universes, a multiverse, and higher dimensions. Physicists speculate on these possibilities, and from them, hypothesize theories.

Experimental physics informs, and is informed by, engineering and technology. Experimental physicists involved in basic research design and perform experiments with equipment such as particle accelerators and lasers, whereas those involved in applied research often work in industry, developing technologies such as magnetic resonance imaging (MRI) and transistors. Feynman has noted that experimentalists may seek areas which are not well explored by theorists.

Relation to mathematics and the other sciences

In the *Assayer* (1622), Galileo noted that mathematics is the language in which Nature expresses its laws.[11] Most of the experimental results in physics are numerical measurements and theories in physics use mathematics to give numerical results to match these measurements. Physics relies on mathematics to provide the logical framework in which physical laws can be precisely formulated and predictions quantified. Whenever analytic solutions of equations are not feasible, numerical analysis and simulations can be utilized. Thus, scientific computation is an integral part of physics, and the field of computational physics is an active area of research.

A key difference between physics and mathematics is that since physics is ultimately concerned with descriptions of the material world, it tests its theories by comparing the predictions of its theories with data procured from observations and experimentation, whereas mathematics is concerned with abstract patterns, not limited by those observed in the real world. The distinction, however, is not always clear-cut. There is a large area of research intermediate between physics and mathematics, known as mathematical physics.

Physics is also intimately related to many other sciences, as well as applied fields like engineering and medicine. The principles of physics find applications throughout the other natural sciences as some phenomena studied in physics, such as the conservation of energy, are common to *all* material systems. Other phenomena, such as superconductivity, stem from these laws, but are not laws themselves because they only appear in some systems. Physics is often said to be the "fundamental science" (chemistry is sometimes included), because each of the other disciplines (biology, chemistry, geology, material science, engineering, medicine etc.) deals with particular types of material systems that obey the laws of physics.[7] For example, chemistry is the science of collections of matter (such as gases and liquids formed of atoms and molecules) and the processes known as chemical reactions that result in the change of chemical substances. The structure, reactivity, and properties of a chemical compound are determined by the properties of the underlying molecules, which can be described by areas of physics such as → quantum mechanics (called in this case quantum chemistry), → thermodynamics, and electromagnetism.

Philosophical implications

Physics in many ways stemmed from ancient Greek philosophy. From Thales' first attempt to characterize matter, to Democritus' deduction that matter ought to reduce to an invariant state, the Ptolemaic astronomy of a crystalline firmament, and Aristotle's book *Physics*, different Greek philosophers advanced their own theories of nature. Well into the 18th century, physics was known as "Natural philosophy".

By the 19th century physics was realized as a positive science and a distinct discipline separate from philosophy and the other sciences. Physics, as with the rest of science, relies on philosophy of science to give an adequate description of the scientific method.[12] The scientific method employs a priori reasoning as well as a posteriori reasoning and the use of Bayesian inference to measure the validity of a given theory.[13]

> “ Truth is ever to be found in the simplicity, and not in the multiplicity and confusion of things. ”
>
> —*Isaac Newton*

The development of physics has answered many questions of early philosophers, but has also raised new questions. Study of the philosophical issues surrounding physics, the philosophy of physics, involves issues such as the nature of space and time, determinism, and metaphysical outlooks such as empiricism, naturalism and realism.[14]

Many physicists have written about the philosophical implications of their work, for instance Laplace, who championed causal determinism,[15] and Erwin Schrödinger, who wrote on Quantum Mechanics.[16] The mathematical physicist Roger Penrose has been called a Platonist by Stephen Hawking,[17] a view Penrose discusses in his book, *The Road to Reality*.[18] Hawking refers to himself as an "unashamed reductionist" and takes issue with Penrose's views.[19]

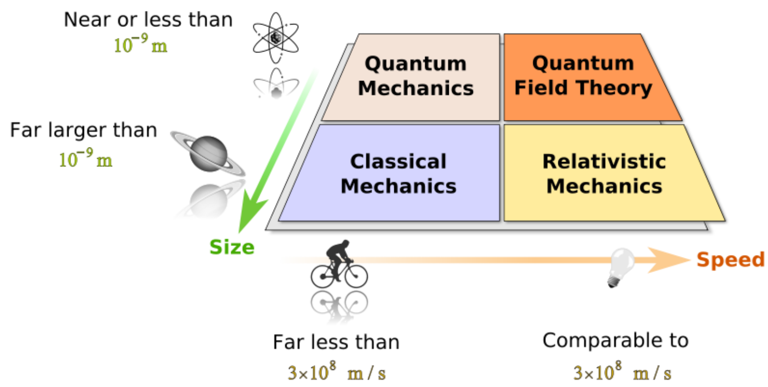
History

Since antiquity, people have tried to understand the behavior of the natural world. One great mystery was the predictable behavior of celestial objects such as the Sun and the Moon. Several theories were proposed, the majority of which were disproved. Early physical theories were largely couched in philosophical terms, and never verified by systematic experimental testing as is popular today. Many of the commonly accepted works of Ptolemy and Aristotle are not always found to match everyday observations. Even so, Indian philosophers and astronomers gave many correct descriptions in atomism and astronomy, and the Greek thinker Archimedes derived many correct quantitative descriptions of mechanics and hydrostatics.

Aristotle

Branches of Physics

While physics deals with a wide variety of systems, there are certain theories that are used by all physicists. Each of these theories were experimentally tested numerous times and found correct as an approximation of Nature (within a certain domain of validity). For instance, the theory of classical mechanics accurately describes the motion of objects, provided they are much larger than atoms and moving at much less than the speed of light. These theories continue to be areas of active research; for instance, a remarkable aspect of classical mechanics known as chaos was discovered in the 20th century, three centuries after the original formulation of classical mechanics by Isaac Newton (1642–1727). These "central theories" are important tools for research into more specialized topics, and any physicist, regardless of his or her specialization, is expected to be literate in them.

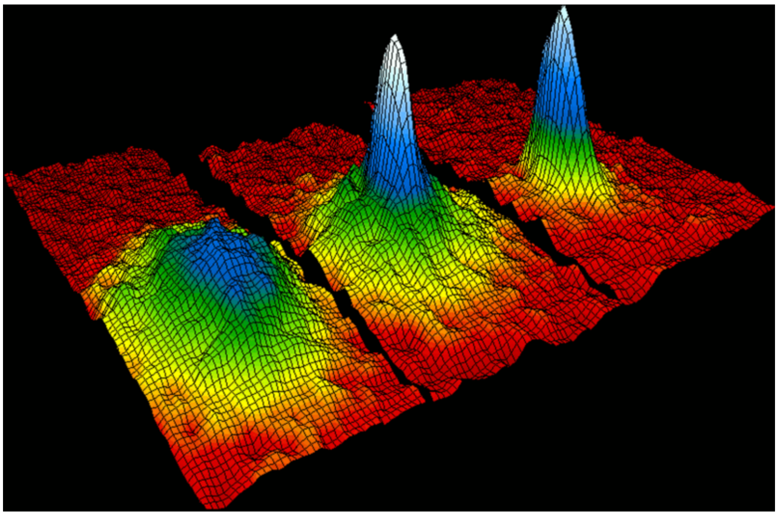


Domains of major fields of physics

Research fields

Contemporary research in physics can be broadly divided into condensed matter physics; → atomic, molecular, and optical physics; → particle physics; astrophysics; geophysics and → biophysics. Some physics departments also support research in Physics education. Since the twentieth century, the individual fields of physics have become increasingly specialized, and today most physicists work in a single field for their entire careers. "Universalists" such as Albert Einstein (1879–1955) and Lev Landau (1908–1968), who worked in multiple fields of physics, are now very rare.[20]

Condensed matter



Velocity-distribution data of a gas of rubidium atoms, confirming the discovery of a new phase of matter, the Bose–Einstein condensate

Condensed matter physics is the field of physics that deals with the macroscopic physical properties of matter. In particular, it is concerned with the "condensed" phases that appear whenever the number of constituents in a system is extremely large and the interactions between the constituents are strong. The most familiar examples of condensed phases are solids and liquids, which arise from the bonding and electromagnetic force between atoms. More exotic condensed phases include the superfluid and the Bose-Einstein condensate found in certain atomic systems at very low temperature, the superconducting phase exhibited by conduction electrons in certain materials, and the ferromagnetic and antiferromagnetic phases of spins on atomic lattices.

Condensed matter physics is by far the largest field of contemporary physics. By one estimate, one third of all American physicists identify themselves as condensed matter physicists. Historically, condensed matter physics grew out of solid-state physics, which is now considered one of its main subfields. The term *condensed matter physics* was apparently coined by Philip Anderson when he renamed his research group — previously *solid-state theory* — in 1967. In 1978, the Division of Solid State Physics at the American Physical Society was renamed as the Division of Condensed Matter Physics.[21] Condensed matter physics has a large overlap with chemistry, materials science, nanotechnology and engineering.

Atomic, molecular, and optical physics

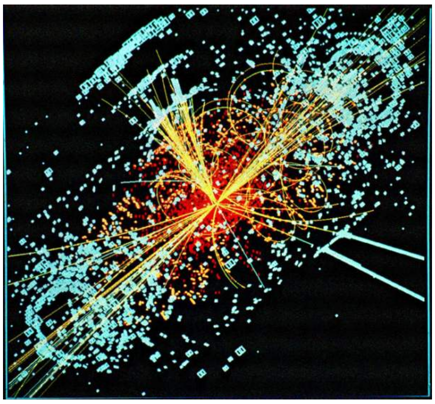
Atomic, molecular, and optical physics (AMO) is the study of matter-matter and light-matter interactions on the scale of single atoms or structures containing a few atoms. The three areas are grouped together because of their interrelationships, the similarity of methods used, and the commonality of the energy scales that are relevant. All three areas include both classical and quantum treatments; they can treat their subject from a microscopic view (in contrast to a macroscopic view).

Atomic physics studies the electron shells of atoms. Current research focuses on activities in quantum control, cooling and trapping of atoms and ions, low-temperature collision dynamics, the collective behavior of atoms in weakly interacting gases (Bose-Einstein Condensates and dilute Fermi degenerate systems), precision measurements of fundamental constants, and the effects of electron correlation on structure and dynamics. Atomic physics is influenced by the nucleus (see, e.g., hyperfine splitting), but intra-nuclear phenomenon such as fission and → fusion are considered part of high energy physics.

Molecular physics focuses on multi-atomic structures and their internal and external interactions with matter and light. Optical physics is distinct from optics in that it tends to focus not on the control of classical light fields by macroscopic objects, but on the fundamental properties of optical fields and their interactions with matter in the microscopic realm.

High energy/particle physics

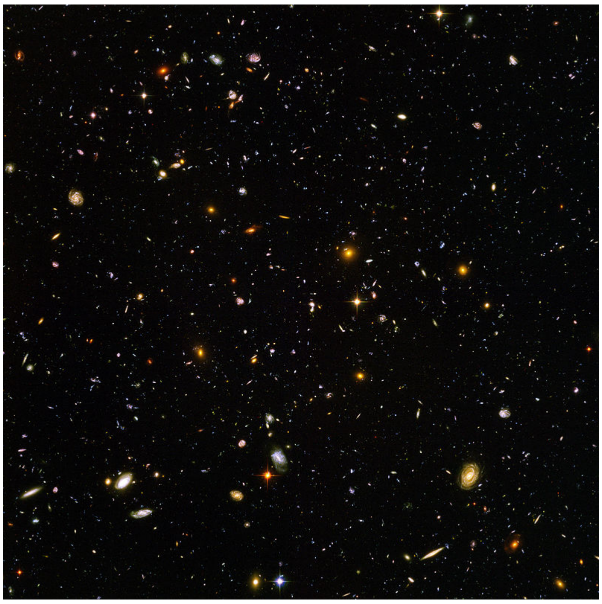
→ Particle physics is the study of the elementary constituents of matter and energy, and the interactions between them. It may also be called "high energy physics", because many elementary particles do not occur naturally, but are created only during high energy collisions of other particles, as can be detected in particle accelerators.



A simulated event in the CMS detector of the Large Hadron Collider, featuring the appearance of the Higgs boson.

Currently, the interactions of elementary particles are described by the Standard Model. The model accounts for the 12 known particles of matter that interact via the strong, weak, and electromagnetic fundamental forces. Dynamics are described in terms of matter particles exchanging messenger particles that carry the forces. These messenger particles are known as gluons; W^- and W^+ and Z bosons; and the photons, respectively. The Standard Model also predicts a particle known as the Higgs boson, the existence of which has not yet been verified.

Astrophysics



The deepest visible-light image of the universe, the Hubble Ultra Deep Field

Astrophysics and astronomy are the application of the theories and methods of physics to the study of stellar structure, stellar evolution, the origin of the solar system, and related problems of cosmology. Because astrophysics is a broad subject, astrophysicists typically apply many disciplines of physics, including mechanics, electromagnetism, statistical mechanics, thermodynamics, quantum mechanics, relativity, nuclear and particle physics, and atomic and molecular physics.

The discovery by Karl Jansky in 1931 that radio signals were emitted by celestial bodies initiated the science of radio astronomy. Most recently, the frontiers of astronomy have been expanded by space exploration. Perturbations and interference from the earth's atmosphere make space-based observations necessary for infrared, ultraviolet, gamma-ray, and X-ray astronomy.

Physical cosmology is the study of the formation and evolution of the universe on its largest scales. Albert Einstein’s theory of relativity plays a central role in all modern cosmological theories. In the early 20th century, Hubble's discovery that the universe was expanding, as shown by the Hubble diagram, prompted rival explanations known as the steady state universe and the Big Bang. The Big Bang was confirmed by the success of Big Bang nucleosynthesis and the discovery of the cosmic microwave background in 1964. The Big Bang model rests on two theoretical pillars: Albert Einstein's general relativity and the cosmological principle. Cosmologists have recently established a precise model of the evolution of the universe, which includes cosmic inflation, dark energy and dark matter.

Application and influence

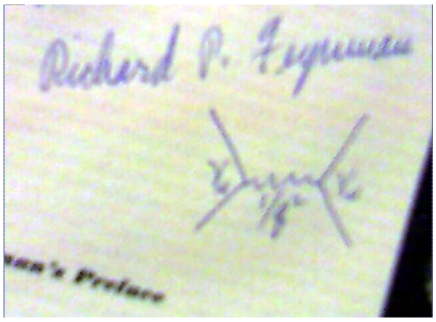
Archimedes' screw uses simple machines to lift water.

Applied physics is a general term for physics research which is intended for a particular use. An applied physics curriculum usually contains a few classes in an applied discipline, like geology or electrical engineering. It usually differs from engineering in that an applied physicist may not be designing something in particular, but rather is using physics or conducting physics research with the aim of developing new technologies or solving a problem. The approach is similar to that of applied mathematics. Applied physicists can also be interested in the use of physics for scientific research. For instance, people working on accelerator physics might seek to build better particle detectors for research in theoretical physics.

Physics is used heavily in engineering. For example, Statics, a subfield of mechanics, is used in the building of bridges and other structures. The understanding and use of acoustics results in better concert halls; similarly, the use of optics creates better optical devices. An understanding of physics makes for more realistic flight simulators, video games, and movies, and is often critical in forensic investigations.

With the standard consensus that the laws of physics are universal and do not change with time, physics can be used to study things that would ordinarily be mired in uncertainty. For example, in the study of the origin of the Earth, one can reasonably model Earth's mass, temperature, and rate of rotation, over time. It also allows for simulations in engineering which drastically speed up the development of a new technology.

Current research



Feynman diagram signed by R. P. Feynman

Research in physics is continually progressing on a large number of fronts.

In condensed matter physics, an important unsolved theoretical problem is that of high-temperature superconductivity. Many condensed matter experiments are aiming to fabricate workable spintronics and quantum computers.

In particle physics, the first pieces of experimental evidence for physics beyond the Standard Model have begun to appear. Foremost among these are indications that neutrinos have non-zero mass. These experimental results appear to have solved the long-standing solar neutrino problem, and the physics of massive neutrinos remains an area of active theoretical and experimental research. In the next several years, particle accelerators will begin probing energy scales in the TeV range, in which experimentalists are hoping to find evidence[22] for the Higgs boson and supersymmetric particles.

Theoretical attempts to unify → quantum mechanics and general relativity into a single theory of quantum gravity, a program ongoing for over half a century, have not yet been decisively resolved. The current leading candidates are M-theory, superstring theory and loop quantum gravity.

Many astronomical and cosmological phenomena have yet to be satisfactorily explained, including the existence of ultra-high energy cosmic rays, the baryon asymmetry, the acceleration of the universe and the anomalous rotation rates of galaxies.

Although much progress has been made in high-energy, quantum, and astronomical physics, many everyday phenomena involving complexity, chaos, or turbulence are still poorly understood. Complex problems that seem like they could be solved by a clever application of dynamics and mechanics remain unsolved; examples include the formation of sandpiles, nodes in trickling water, the shape of water droplets, mechanisms of surface tension catastrophes, and self-sorting in shaken heterogeneous collections. These complex phenomena have received growing attention since the 1970s for several reasons, including the availability of modern mathematical methods and computers, which enabled complex systems to be modeled in new ways. Complex physics has become part of increasingly interdisciplinary research, as exemplified by the study of turbulence in aerodynamics and the observation of pattern formation in biological systems. In 1932, Horace Lamb said:

> “ I am an old man now, and when I die and go to heaven there are two matters on which I hope for enlightenment. One is quantum electrodynamics, and the other is the turbulent motion of fluids. And about the former I am rather optimistic. ”
>
> —*Horace Lamb*[23]

See also

General

- Classical physics
- Glossary of classical physics
- List of basic physics topics
- List of physics topics
- Perfection in physics and chemistry
- Philosophy of physics
- *Physics* (Aristotle) – an early book on physics, which attempted to analyze and define motion from a philosophical point of view
- → Unsolved problems in physics

Related fields

- Astronomy
- Chemistry
- Engineering
- Mathematics
- Science

References

[1] R. P. Feynman, R. B. Leighton, M. Sands (1963), *The Feynman Lectures on Physics*, ISBN 0-201-02116-1 Hard-cover. p.1-1 Feynman begins with the atomic hypothesis, as his most compact statement of all scientific knowledge: "If, in some cataclysm, all of scientific knowledge were to be destroyed, and only one sentence passed on to the next generations ..., what statement would contain the most information in the fewest words? I believe it is ... that *all things are made up of atoms – little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another.* ..." vol. **I** p. I–2

[2] James Clerk Maxwell (1878), *Matter and Motion* (http://books.google.com/books?id=noRgWP0_UZ8C&printsec=titlepage&dq=matter+and+motion&source=gbs_summary_r&cad=0). New York: D. Van Nostrand. p.1: "Nature of Physical Science – Physical science is that department of knowledge which relates to the order of nature." | accessdate=2008-11-04

[3] H.D. Young & R.A. Freedman, *University Physics with Modern Physics*: 11th Edition: International Edition (2004), Addison Wesley. Chapter 1, section 1.1, page 2 has this to say: "Physics is an *experimental* science. Physicists observe the phenomena of nature and try to find patterns and principles that relate these phenomena. These patterns are called physical theories or, when they are very well established and of broad use, physical laws or principles."
Steve Holzner, *Physics for Dummies* (2006), Wiley. Chapter 1, page 7 says: "Physics is the study of your world and the world and universe around you." See Amazon Online Reader: Physics For Dummies (For Dummies(Math & Science)) (http://www.amazon.com/gp/reader/0764554336), retrieved 24 Nov 2006

[4] Note: The term 'universe' is defined as everything that physically exists: the entirety of space and time, all forms of matter, energy and momentum, and the physical laws and constants that govern them. However, the term 'universe' may also be used in slightly different contextual senses, denoting concepts such as the cosmos or the philosophical world.

[5] Evidence exists that the earliest civilizations dating back to beyond 3000BC, such as the Sumerians, Ancient Egyptians, and the Indus Valley Civilization, all had a predictive knowledge and a very basic understanding of the motions of the Sun, Moon, and stars.

[6] Francis Bacon's 1620 *Novum Organum* was critical in the development of scientific method.

[7] *The Feynman Lectures on Physics* Volume I. Feynman, Leighton and Sands. ISBN 0-201-02115-3 See Chapter 3 : "The Relation of Physics to Other Sciences" for a general discussion. For the philosophical issue of whether other sciences can be "reduced" to physics, see reductionism and special sciences).

[8] Some principles, such as Newton's laws of motion, are still generally called "laws" even though they are now known to be limiting cases of newer theories. Thus, for example, in Thomas Brody (1993, Luis de la Peña and Peter Hodgson, eds.) *The Philosophy Behind Physics* ISBN 0-387-55914-0, pp 18–24 (Chapter 2), explains the

'epistemic cycle' in which a student of physics discovers that physics is not a finished product but is instead the process of creating [that product].
[9] See, for example, the influence of Kant and Ritter on Oersted.
[10] Concepts which are denoted *hypothetical* can change with time. For example, the atom of nineteenth century physics was denigrated by some, including Ernst Mach's critique of Ludwig Boltzmann's formulation of statistical mechanics. By the end of World War II, the atom was no longer deemed hypothetical.
[11] "Philosophy is written in that great book which ever lies before our eyes. I mean the universe, but we cannot understand it if we do not first learn the language and grasp the symbols in which it is written. This book is written in the mathematical language, and the symbols are triangles, circles and other geometrical figures, without whose help it is humanly impossible to comprehend a single word of it, and without which one wanders in vain through a dark labyrinth." – Galileo (1623), *The Assayer*, as quoted by G. Toraldo Di Francia (1976), *The Investigation of the Physical World* ISBN 0-521-29925-X p.10
[12] Rosenberg, Alex (2006). *Philosophy of Science*. Routledge. ISBN 0-415-34317-8. See Chapter 1 for a discussion on the necessity of philosophy of science.
[13] Peter Godfrey-Smith (2003), Chapter 14 "Bayesianism and Modern Theories of Evidence" *Theory and Reality: an introduction to the philosophy of science* ISBN 0-226-30063-3
[14] Peter Godfrey-Smith (2003), Chapter 15 "Empiricism, Naturalism, and Scientific Realism?" *Theory and Reality: an introduction to the philosophy of science* ISBN 0-226-30063-3
[15] See Laplace, Pierre Simon, *A Philosophical Essay on Probabilities*, translated from the 6th French edition by Frederick Wilson Truscott and Frederick Lincoln Emory, Dover Publications (New York, 1951)
[16] See "The Interpretation of Quantum Mechanics" Ox Bow Press (1995) ISBN 1881987094. and "My View of the World" Ox Bow Press (1983) ISBN 0918024307.
[17] Stephen Hawking and Roger Penrose (1996), *The Nature of Space and Time* ISBN 0-691-05084-8 p.4 "I think that Roger is a Platonist at heart but he must answer for himself."
[18] Roger Penrose, *The Road to Reality* ISBN 0-679-45443-8
[19] Penrose, Roger; Abner Shimony, Nancy Cartwright, Stephen Hawking (1997). *The Large, the Small and the Human Mind*. Cambridge University Press. ISBN 0-521-78572-3.
[20] Yet, universalism is encouraged in the culture of physics. For example, the World Wide Web, which was innovated at CERN by Tim Berners-Lee, was created in service to the computer infrastructure of CERN, and was/is intended for use by physicists worldwide. The same might be said for arXiv.org
[21] "Division of Condensed Matter Physics Governance History" (http://dcmp.bc.edu/page.php?name=governance_history). . Retrieved on 2007-02-13.
[22] 584 co-authors "Direct observation of the strange 'b' baryon Ξ_b^- " Fermilab-Pub-07/196-E, June 12, 2007 http://arxiv.org/abs/0706.1690v2 finds a mass of 5.774 GeV for the Ξ_b^-
[23] Goldstein, Sydney (1969). "Fluid Mechanics in the First Half of this Century". *Annual Reviews in Fluid Mechanics* **1**: 1–28. doi: 10.1146/annurev.fl.01.010169.000245 (http://dx.doi.org/10.1146/annurev.fl.01.010169.000245).

External links

- A large number of textbooks, popular books, and webpages about physics are available for further reading.
- Important publications in physics

General

- HyperPhysics website (http://hyperphysics.phy-astr.gsu.edu/Hbase/hframe.html) – HyperPhysics, a physics and astronomy mind-map from Georgia State University
- Physics Today (http://www.physicstoday.org) – Your daily physics news and research source
- Physics.org (http://www.physics.org/) – Web portal run by the Institute of Physics (http://www.iop.org/)
- *The Skeptic's Guide to Physics* (http://musr.physics.ubc.ca/~jess/hr/skept/)
- Usenet Physics FAQ (http://math.ucr.edu/home/baez/physics/) – A FAQ compiled by sci.physics and other physics newsgroups
- Website of the Nobel Prize in physics (http://nobelprize.org/nobel_prizes/physics/)

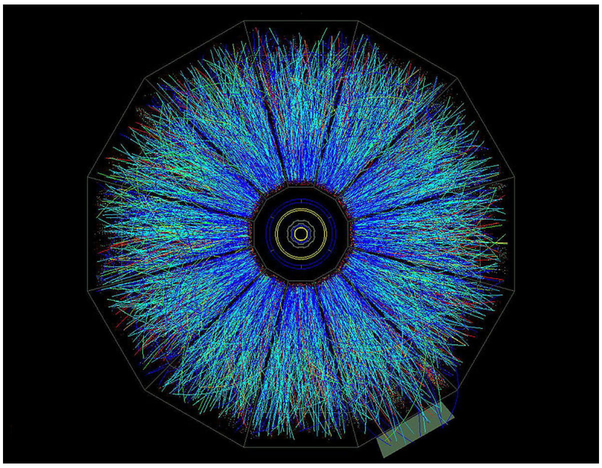
- World of Physics (http://scienceworld.wolfram.com/physics/) – An online encyclopedic dictionary of physics
- PlanetPhysics.org (http://planetphysics.org/)

Organizations

- AIP.org (http://www.aip.org/index.html) – Website of the American Institute of Physics
- APS.org (http://www.aps.org) – Website of the American Physical Society
- IOP.org (http://www.iop.org) – Website of the Institute of Physics
- PlanetPhysics.org (http://planetphysics.org/)
- Physics & Math Forums (http://www.physicsmathforums.com)
- Royal Society (http://www.royalsoc.ac.uk) – Although not exclusively a physics institution, it has a strong history of physics
- SPS National (http://www.spsnational.org) – Website of the Society of Physics Students

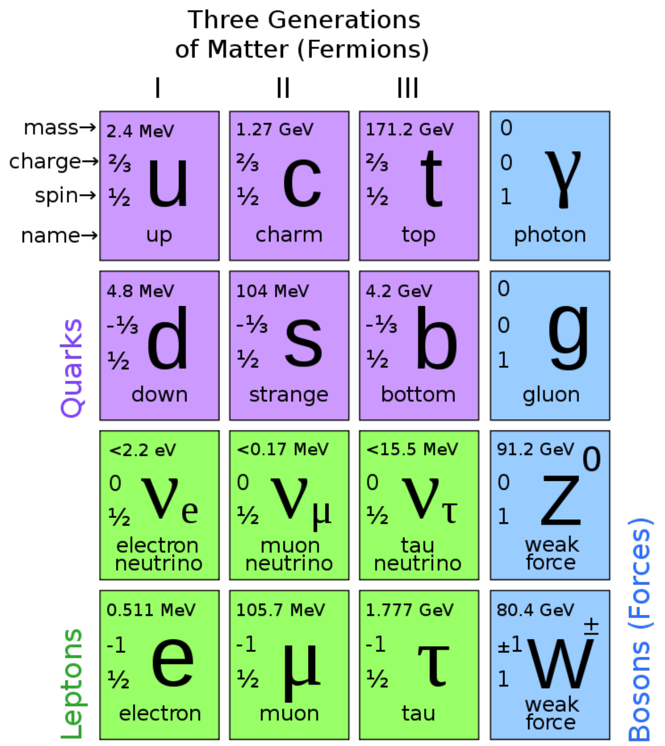
Particle physics

Particle physics is a branch of → physics that studies the elementary constituents of matter and radiation, and the interactions between them. It is also called **high energy physics**, because many elementary particles do not occur under normal circumstances in nature, but can be created and detected during energetic collisions of other particles, as is done in particle accelerators. Research in this area has produced a long list of particles.



Collision of 2 beams of gold atoms recorded by RHIC

Subatomic particles



An image showing 6 quarks, 6 leptons and the interacting particles, according to the Standard Model

Modern particle physics research is focused on subatomic particles, which have less structure than atoms. These include atomic constituents such as electrons, protons, and neutrons (protons and neutrons are actually composite particles, made up of quarks), particles produced by radiative and scattering processes, such as photons, neutrinos, and muons, as well as a wide range of exotic particles.

Strictly speaking, the term *particle* is a misnomer because the dynamics of particle physics are governed by → quantum mechanics. As such, they exhibit wave-particle duality, displaying particle-like behavior under certain experimental conditions and wave-like behavior in others (more technically they are described by state vectors in a Hilbert space; see → quantum field theory). Following the convention of particle physicists, "elementary particles" refer to objects such as electrons and photons, it is well known that these "particles" display wave-like properties as well.

All the particles and their interactions observed to date can almost be described entirely by a → quantum field theory called the Standard Model. The Standard Model has 17 species of elementary particles (12 fermions (24 if you count antiparticles separately), 4 vector bosons (5 if you count antiparticles separately), and 1 scalar bosons), which can combine to form composite particles, accounting for the hundreds of other species of particles discovered since the 1960s. The Standard Model has been found to agree with almost all the experimental tests conducted to date. However, most particle physicists believe that it is an incomplete description of nature, and that a more fundamental theory awaits discovery. In recent years, measurements of neutrino mass have provided the first experimental deviations from the Standard Model.

Particle physics has had a large impact on the philosophy of science. Some particle physicists adhere to reductionism, a point of view that has been criticized and defended by philosophers and scientists. Part of the debate is described below.[1] [2] [3] [4]

History

The idea that all matter is composed of elementary particles dates to at least the 6th century BC. The philosophical doctrine of atomism and the nature of elementary particles were studied by ancient Greek philosophers such as Leucippus, Democritus and Epicurus; ancient Indian philosophers such as Kanada, Dignāga and Dharmakirti; medieval scientists such as Alhazen, Avicenna and Algazel; and early modern European physicists such as Pierre Gassendi, Robert Boyle and Isaac Newton. The particle theory of light was also proposed by Alhazen, Avicenna, Gassendi and Newton. These early ideas were founded in abstract, philosophical reasoning rather than experimentation and empirical observation.

In the 19th century, John Dalton, through his work on stoichiometry, concluded that each element of nature was composed of a single, unique type of particle. Dalton and his contemporaries believed these were the fundamental particles of nature and thus named them atoms, after the Greek word *atomos*, meaning "indivisible". However, near the end of the century, physicists discovered that atoms were not, in fact, the fundamental particles of nature, but conglomerates of even smaller particles. The early 20th century explorations of nuclear physics and quantum physics culminated in proofs of nuclear fission in 1939 by Lise Meitner (based on experiments by Otto Hahn), and → nuclear fusion by Hans Bethe in the same year. These discoveries gave rise to an active industry of generating one atom from another, even rendering possible (although not profitable) the transmutation of lead into gold. They also led to the development of nuclear weapons. Throughout the 1950s and 1960s, a bewildering variety of particles were found in scattering experiments. This was referred to as the "particle zoo". This term was deprecated after the formulation of the Standard Model during the 1970s in which the large number of particles was explained as combinations of a (relatively) small number of fundamental particles.

The Standard Model

The current state of the classification of elementary particles is the Standard Model. It describes the strong, weak, and electromagnetic fundamental forces, using mediating gauge bosons. The species of gauge bosons are the gluons, W^- and W^+ and Z bosons, and the photons. The model also contains 24 fundamental particles, which are the constituents of matter. Finally, it predicts the existence of a type of boson known as the Higgs boson, which has yet to be discovered.

Experimental Laboratories

In particle physics, the major international laboratories are:

- Brookhaven National Laboratory, located on Long Island, USA. Its main facility is the Relativistic Heavy Ion Collider which collides heavy ions such as gold ions and polarized protons. It is the world's first heavy ion collider, and the world's only polarized proton collider.
- Budker Institute of Nuclear Physics (Novosibirsk, Russia)
- CERN, located on the French-Swiss border near Geneva. Its main project is now the Large Hadron Collider (LHC), which had its first beam circulation on 10 September 2008 and will be the world's most energetic collider. Earlier facilities include LEP, the Large Electron Positron collider, which was stopped in 2001 and then dismantled to give way for LHC; and SPS, or the Super Proton Synchrotron, which is being reused as a

pre-accelerator for LHC.
- DESY, located in Hamburg, Germany. Its main facility is HERA, which collides electrons or positrons and protons.
- Fermilab, located near Chicago, USA. Its main facility is the Tevatron, which collides protons and antiprotons and is presently the highest energy particle collider in the world.
- KEK, the High Energy Accelerator Research Organization of Japan, located in Tsukuba, Japan. It is the home of a number of experiments such as K2K, a neutrino oscillation experiment and Belle, an experiment measuring the CP-symmetry violation in the B-meson.
- SLAC, located near Palo Alto, USA. Its main facility is PEP-II, which collides electrons and positrons.

Many other particle accelerators exist.

The techniques required to do modern experimental particle physics are quite varied and complex, constituting a subspecialty nearly completely distinct from the theoretical side of the field. See Category:Experimental particle physics for a partial list of the ideas required for such experiments.

Theory

Theoretical particle physics attempts to develop the models, theoretical framework, and mathematical tools to understand current experiments and make predictions for future experiments. See also theoretical physics. There are several major efforts in theoretical particle physics today and each includes a range of different activities. The efforts in each area are interrelated. There are five most important states in particle theory: one of the major activities in theoretical particle physics is the attempt to better understand the standard model and its tests. By extracting the parameters of the Standard Model from experiments with less uncertainty, this work probes the limits of the Standard Model and therefore expands our understanding of nature. These efforts are made challenging by the difficult nature of calculating many quantities in → quantum chromodynamics. Some theorists making these efforts refer to themselves as **phenomenologists** and may use the tools of → quantum field theory and effective field theory. Others make use of lattice field theory and call themselves **lattice theorists**.

Another major effort is in model building where **model builders** develop ideas for what physics may lie beyond the Standard Model (at higher energies or smaller distances). This work is often motivated by the hierarchy problem and is constrained by existing experimental data. It may involve work on supersymmetry, alternatives to the Higgs mechanism, extra spatial dimensions (such as the Randall-Sundrum models), Preon theory, combinations of these, or other ideas.

A third major effort in theoretical particle physics is string theory. **String theorists** attempt to construct a unified description of → quantum mechanics and general relativity by building a theory based on small strings, and branes rather than particles. If the theory is successful, it may be considered a "Theory of Everything".

There are also other areas of work in theoretical particle physics ranging from particle cosmology to loop quantum gravity.

This division of efforts in particle physics is reflected in the names of categories on the preprint archive [5]: hep-th (theory), hep-ph (phenomenology), hep-ex (experiments), hep-lat (lattice gauge theory).

The future

Particle physicists internationally agree on the most important goals of particle physics research in the near and intermediate future. The overarching goal, which is pursued in several distinct ways, is to find and understand what physics may lie beyond the standard model. There are several powerful experimental reasons to expect new physics, including dark matter and neutrino mass. There are also theoretical hints that this new physics should be found at accessible energy scales. Most importantly, though, there may be unexpected and unpredicted surprises which will give us the most opportunity to learn about nature.

Much of the efforts to find this new physics are focused on new collider experiments. A (relatively) near term goal is the completion of the Large Hadron Collider (LHC) in 2008 which will continue the search for the Higgs boson, supersymmetric particles, and other new physics. An intermediate goal is the construction of the International Linear Collider (ILC) which will complement the LHC by allowing more precise measurements of the properties of newly found particles. A decision for the technology of the ILC has been taken in August 2004, but the site has still to be agreed upon.

Additionally, there are important non-collider experiments which also attempt to find and understand physics beyond the Standard Model. One important non-collider effort is the determination of the neutrino masses since these masses may arise from neutrinos mixing with very heavy particles. In addition, cosmological observations provide many useful constraints on the dark matter, although it may be impossible to determine the exact nature of the dark matter without the colliders. Finally, lower bounds on the very long lifetime of the proton put constraints on Grand Unification Theories at energy scales much higher than collider experiments will be able to probe any time soon.

See also

- Atomic physics
- Beyond the Standard Model
- Introduction to quantum mechanics
- Fundamental particle
- List of accelerators in particle physics
- Standard model (basic details)
- Subatomic particle
- High pressure physics
- Rochester conference
- Stanford Physics Information Retrieval System
- arXiv preprint server

References

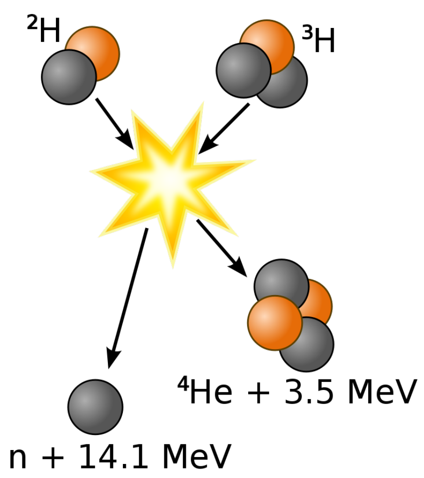
[1] "Review of particle physics" (http://pdg.lbl.gov/). .
[2] "Particle Physics News and Resources" (http://www.interactions.org/). .
[3] "CERN Courier - International Journal of High-Energy Physics" (http://cerncourier.com). .
[4] "Particle physics in 60 seconds" (http://www.symmetrymagazine.org/cms/?pid=1000345). .
[5] http://www.arxiv.org

External links

- The Particle Adventure (http://particleadventure.org/) - educational project sponsored by the Particle Data Group of the Lawrence Berkeley National Laboratory (LBNL)
- *symmetry* magazine (http://www.symmetrymagazine.org)
- *Introduction to Particle Physics* by Matthew Nobes (published on Kuro5hin):
  - Part 1 (http://www.kuro5hin.org/story/2002/5/1/3712/31700), Part 2 (http://www.kuro5hin.org/story/2002/5/14/19363/8142), Part 3a (http://www.kuro5hin.org/story/2002/7/15/173318/784), Part 3b (http://www.kuro5hin.org/story/2002/8/21/195035/576)

Nuclear fusion

In nuclear physics and nuclear chemistry, **nuclear fusion** is the process by which multiple like-charged atomic nuclei join together to form a heavier nucleus. It is accompanied by the release or absorption of energy, which allows matter to enter a plasma state.



Fusion of deuterium with tritium creating helium-4, freeing a neutron, and releasing 17.59 MeV of energy, as an appropriate amount of mass converting to the kinetic energy of the products, in agreement with $E = \Delta m\, c^2$.[1]

The fusion of two nuclei with lower mass than iron (which, along with nickel, has the largest binding energy per nucleon) generally releases energy while the fusion of nuclei heavier than iron absorbs energy; vice-versa for the reverse process, nuclear fission. In the simplest case of hydrogen fusion, two protons have to be brought close enough for their mutual electric repulsion to be overcome by the nuclear force and the subsequent release of energy.

Nuclear fusion occurs naturally in stars. Artificial fusion in human enterprises has also been achieved, although has not yet been completely controlled. Building upon the nuclear transmutation experiments of Ernest Rutherford done a few years earlier, fusion of light nuclei (hydrogen isotopes) was first observed by Mark Oliphant in 1932; the steps of the main cycle of nuclear fusion in stars were subsequently worked out by Hans Bethe throughout the remainder of that decade. Research into fusion for military purposes began in the early 1940s as part of the Manhattan Project, but was not successful until 1952. Research into controlled fusion for civilian purposes began in the 1950s, and continues to this day.

Overview

Fusion reactions power the stars and produce all but the lightest elements in a process called nucleosynthesis. Although the fusion of lighter elements in stars releases energy, production of the heavier elements absorbs energy.

When the fusion reaction is a sustained uncontrolled chain, it can result in a thermonuclear explosion, such as that generated by a hydrogen bomb. Reactions which are not self-sustaining can still release considerable energy, as well as large numbers of neutrons.

Research into controlled fusion, with the aim of producing fusion power for the production of electricity, has been conducted for over 50 years. It has been accompanied by extreme scientific and technological difficulties, but resulted in steady progress. At present, break-even (self-sustaining) controlled fusion reactions have been demonstrated in a few tokamak-type reactors around the world. These have enabled the creation of workable designs for a reactor which will deliver ten times more fusion energy than the amount needed to heat up plasma to required temperatures (see → ITER which is scheduled to be operational in 2018).

It takes considerable energy to force nuclei to fuse, even those of the lightest element, hydrogen. This is because all nuclei have a positive charge (due to their protons), and as like charges repel, nuclei strongly resist being put too close together. Accelerated to high speeds (that is, heated to thermonuclear temperatures), they can overcome this electromagnetic repulsion and get close enough for the attractive nuclear force to be sufficiently strong to achieve fusion. The fusion of lighter nuclei, which creates a heavier nucleus and a free neutron, generally releases more energy than it takes to force the nuclei together; this is an exothermic process that can produce self-sustaining reactions.

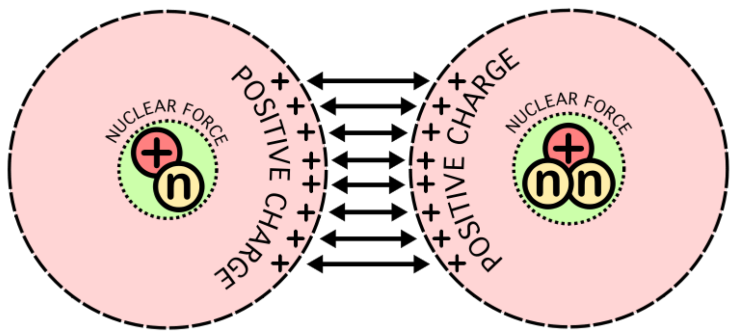
The energy released in most nuclear reactions is much larger than that in chemical reactions, because the binding energy that holds a nucleus together is far greater than the energy that holds electrons to a nucleus. For example, the ionization energy gained by adding an electron to a hydrogen nucleus is 13.6 electron volts—less than one-millionth of the 17 MeV released in the D-T (deuterium-tritium) reaction shown in the diagram to the right. Fusion reactions have an energy density many times greater than nuclear fission; i.e., the reactions produce far greater energies per unit of mass even though *individual* fission reactions are generally much more energetic than *individual* ones, which are themselves millions of times more energetic than chemical reactions. Only the direct conversion of mass into energy, such as that caused by the collision of matter and antimatter, is more energetic per unit of mass than nuclear fusion.

Requirements

A substantial energy barrier of electrostatic forces must be overcome before fusion can occur. At large distances two naked nuclei repel one another because of the repulsive electrostatic force between their positively charged protons. If two nuclei can be brought close enough together, however, the electrostatic repulsion can be overcome by the attractive nuclear force which is stronger at close distances.

When a nucleon such as a proton or neutron is added to a nucleus, the nuclear force attracts it to other nucleons, but primarily to its immediate neighbours due to the short range of the force. The nucleons in the interior of a nucleus have more neighboring nucleons than those on the surface. Since smaller nuclei have a larger surface area-to-volume ratio, the binding energy per nucleon due to the strong force generally increases with the size of the nucleus but approaches a limiting value corresponding to that of nucleus with a diameter of about four nucleons.

The electrostatic force, on the other hand, is an inverse-square force, so a proton added to a nucleus will feel an electrostatic repulsion from *all* the other protons in the nucleus. The electrostatic energy per nucleon due to the electrostatic force thus increases without limit as nuclei get larger.



At short distances the attractive nuclear force is stronger than the repulsive electrostatic force. As such, the main technical difficulty for fusion is getting the nuclei close enough to fuse. Distances not to scale.

The net result of these opposing forces is that the binding energy per nucleon generally increases with increasing size, up to the elements iron and nickel, and then decreases for heavier nuclei. Eventually, the binding energy becomes negative and very heavy nuclei (all with more than 208 nucleons, corresponding to a diameter of about 6 nucleons) are not stable. The four most tightly bound nuclei, in decreasing order of binding energy, are ^{62}Ni, ^{58}Fe, ^{56}Fe, and ^{60}Ni.[2] Even though the nickel isotope ,^{62}Ni, is more stable, the iron isotope ^{56}Fe is an order of magnitude more common. This is due to a greater disintegration rate for ^{62}Ni in the interior of stars driven by photon absorption.

A notable exception to this general trend is the helium-4 nucleus, whose binding energy is higher than that of lithium, the next heaviest element. The Pauli exclusion principle provides an explanation for this exceptional behavior—it says that because protons and neutrons are fermions, they cannot exist in exactly the same state. Each proton or neutron energy state in a nucleus can accommodate both a spin up particle and a spin down particle. Helium-4 has an anomalously large binding energy because its nucleus consists of two protons and two neutrons; so all four of its nucleons can be in the ground state. Any additional nucleons would have to go into higher energy states.

The situation is similar if two nuclei are brought together. As they approach each other, all the protons in one nucleus repel all the protons in the other. Not until the two nuclei actually come in contact can the strong nuclear force take over. Consequently, even when the final energy state is lower, there is a large energy barrier that must first be overcome. It is called the Coulomb barrier.

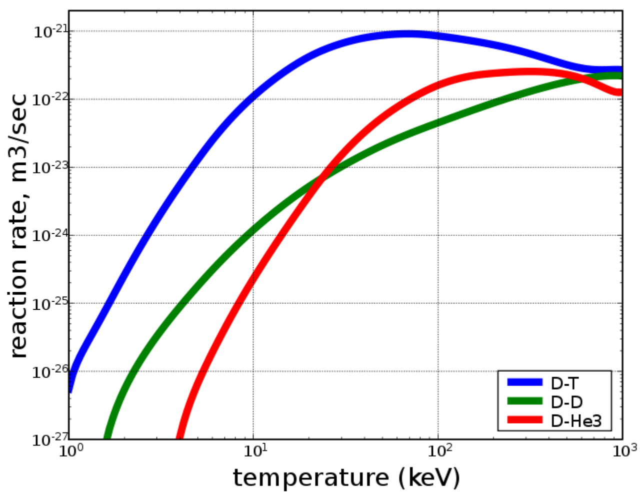
The Coulomb barrier is smallest for isotopes of hydrogen—they contain only a single positive charge in the nucleus. A bi-proton is not stable, so neutrons must also be involved, ideally in such a way that a helium nucleus, with its extremely tight binding, is one of the products.

Using deuterium-tritium fuel, the resulting energy barrier is about 0.01 MeV. In comparison, the energy needed to remove an electron from hydrogen is 13.6 eV, about 750 times less energy. The (intermediate) result of the fusion is an unstable ^{5}He nucleus, which immediately ejects a neutron with 14.1 MeV. The recoil energy of the remaining ^{4}He nucleus is 3.5 MeV, so the total energy liberated is 17.6 MeV. This is many times more than what was needed to overcome the energy barrier.

If the energy to initiate the reaction comes from accelerating one of the nuclei, the process is called *beam-target* fusion; if both nuclei are accelerated, it is *beam-beam* fusion. If the nuclei are part of a plasma near thermal equilibrium, one speaks of *thermonuclear* fusion. Temperature is a measure of the average kinetic energy of particles, so by heating the nuclei they will gain energy and eventually have enough to overcome this 0.01 MeV. Converting the units between electronvolts and kelvins shows that the barrier would be overcome at a temperature in excess of 120 million kelvins, obviously a very high temperature.

There are two effects that lower the actual temperature needed. One is the fact that temperature is the *average* kinetic energy, implying that some nuclei at this temperature would actually have much higher energy than 0.01 MeV, while others would be much lower. It is the nuclei in the high-energy tail of the velocity distribution that account for most of the fusion reactions. The other effect is quantum tunneling. The nuclei do not actually have to have enough energy to overcome the Coulomb barrier completely. If they have nearly enough energy, they can tunnel through the remaining barrier. For this reason fuel at lower temperatures will still undergo fusion events, at a lower rate.

The reaction **cross section** σ is a measure of the probability of a fusion reaction as a function of the relative velocity of the two reactant nuclei. If the reactants have a distribution of velocities, e.g. a thermal distribution with thermonuclear fusion, then it is useful to perform an average over the distributions of the product of cross section and velocity. The reaction rate (fusions per volume per time) is <σv> times the product of the reactant number densities:



The fusion reaction rate increases rapidly with temperature until it maximizes and then gradually drops off. The DT rate peaks at a lower temperature (about 70 keV, or 800 million kelvins) and at a higher value than other reactions commonly considered for fusion energy.

$$f = n_1 n_2 \langle \sigma v \rangle.$$

If a species of nuclei is reacting with itself, such as the DD reaction, then the product $n_1 n_2$ must be replaced by $(1/2)n^2$.

$\langle \sigma v \rangle$ increases from virtually zero at room temperatures up to meaningful magnitudes at temperatures of 10 – 100 keV. At these temperatures, well above typical ionization energies (13.6 eV in the hydrogen case), the fusion reactants exist in a plasma state.

The significance of $\langle \sigma v \rangle$ as a function of temperature in a device with a particular energy confinement time is found by considering the Lawson criterion.

Gravitational confinement

One force capable of confining the fuel well enough to satisfy the Lawson criterion is gravity. The mass needed, however, is so great that gravitational confinement is only found in stars (the smallest of which are brown dwarfs). Even if the more reactive fuel deuterium were used, a mass greater than that of the planet Jupiter would be needed.

Production methods

A variety of methods are known to effect nuclear fusion. Some are "cold" in the strict sense that no part of the material is hot (except for the reaction products), some are "cold" in the limited sense that the bulk of the material is at a relatively low temperature and pressure but the reactants are not, and some are "hot" fusion methods that create macroscopic regions of very high temperature and pressure.

Locally cold fusion

- Muon-catalyzed fusion is a well-established and reproducible fusion process that occurs at ordinary temperatures. It was studied in detail by Steven Jones in the early 1980s. It has not been reported to produce net energy. Net energy production from this reaction is not believed to be possible because of the energy required to create muons, their 2.2 µs half-life, and the chance that a muon will bind to the new alpha particle and thus stop catalyzing fusion.

Magnetic confinement

See Magnetic confinement fusion for more information.

Electrically charged particles (such as fuel ions) will follow magnetic field lines (see Guiding center#Gyration). The fusion fuel can therefore be trapped using a strong magnetic field. A variety of magnetic configurations exist, including the toroidal geometries of tokamaks and stellarators and open-ended mirror confinement systems.

Inertial confinement

See Inertial fusion energy for more information.

A third confinement principle is to apply a rapid pulse of energy to a large part of the surface of a pellet of fusion fuel, causing it to simultaneously "implode" and heat to very high pressure and temperature. If the fuel is dense enough and hot enough, the fusion reaction rate will be high enough to burn a significant fraction of the fuel before it has dissipated. To achieve these extreme conditions, the initially cold fuel must be explosively compressed. Inertial confinement is used in the hydrogen bomb, where the driver is x-rays created by a fission bomb. Inertial confinement is also attempted in "controlled" nuclear fusion, where the driver is a laser, ion, or electron beam, or a Z-pinch. Another method is to use conventional high explosive material to compress a fuel to fusion conditions.[3] [4] The UTIAS explosive-driven-implosion facility was used to produce stable, centered and focused hemispherical implosions[5] to generate neutrons from D-D reactions. The simplest and most direct method proved to be in a predetonated stoichiometric mixture of deuterium-oxygen. The other successful method was using a miniature Voitenko compressor,[6] where a plane diaphragm was driven by the implosion wave into a secondary small spherical cavity that contained pure deuterium gas at one atmosphere.

Some confinement principles have been investigated, such as muon-catalyzed fusion, the Farnsworth-Hirsch fusor and Polywell (inertial electrostatic confinement), and bubble fusion.

Generally cold, locally hot fusion

- Accelerator based light-ion fusion. Using particle accelerators it is possible to achieve particle kinetic energies sufficient to induce many light ion fusion reactions. Accelerating light ions is relatively easy, cheap, and can be done in an efficient manner - all it takes is a vacuum tube, a pair of electrodes, and a high-voltage transformer; fusion can be observed with as little as 10 kilovolt between electrodes. The key problem with accelerator-based fusion (and with cold targets in general) is that fusion cross sections are many orders of magnitude lower than Coulomb interaction cross sections. Therefore vast majority of ions ends up expending their energy on bremsstrahlung and ionization of atoms of the target. Devices referred to as sealed-tube neutron generators are particularly relevant to this discussion. These small devices are miniature particle accelerators filled with deuterium and tritium gas in an arrangement which allows ions of these nuclei to be accelerated against hydride targets, also containing deuterium and tritium, where fusion takes place. Hundreds of neutron generators are produced annually for use in the petroleum industry where they are used in measurement equipment for locating and mapping oil reserves. Despite periodic reports in the popular press by scientists claiming to have invented "table-top" fusion machines, neutron generators have been around for half a century. The sizes of these devices vary but the smallest instruments are often packaged in sizes smaller than a loaf of bread. These devices do not produce a net power output.
- In sonoluminescence, acoustic shock waves create temporary bubbles that collapse shortly after creation, producing very high temperatures and pressures. In 2002, Rusi P. Taleyarkhan reported the possibility that bubble fusion occurs in those collapsing bubbles (aka sonofusion). As of 2005, experiments to determine whether fusion is occurring give conflicting results. If fusion is occurring, it is because the local temperature and pressure are sufficiently high to produce hot fusion.[7] In an episode of Horizon, on BBC television, results were presented showing that, although temperatures were reached which could initiate fusion on a large scale, no fusion was occurring, and inaccuracies in the measuring system were the cause of anomalous results.
- The Farnsworth-Hirsch Fusor is a tabletop device in which fusion occurs. This fusion comes from high effective temperatures produced by electrostatic acceleration of ions. The device can be built inexpensively, but it too is unable to produce a net power output.
- The Polywell is a concept for a tabletop device in which fusion occurs. The device is a non-thermodynamic equilibrium machine which uses electrostatic confinement to accelerate ions into a center where they fuse together.
- Antimatter-initialized fusion uses small amounts of antimatter to trigger a tiny fusion explosion. This has been studied primarily in the context of making nuclear pulse propulsion feasible. This is not near becoming a practical power source, due to the cost of manufacturing antimatter alone.
- Pyroelectric fusion was reported in April 2005 by a team at UCLA. The scientists used a pyroelectric crystal heated from −34 to 7°C (−30 to 45°F), combined with a tungsten needle to produce an electric field of about 25 gigavolts per meter to ionize and

accelerate deuterium nuclei into an erbium deuteride target. Though the energy of the deuterium ions generated by the crystal has not been directly measured, the authors used 100 keV (a temperature of about 10^9 K) as an estimate in their modeling.[8] At these energy levels, two deuterium nuclei can fuse together to produce a helium-3 nucleus, a 2.45 MeV neutron and bremsstrahlung. Although it makes a useful neutron generator, the apparatus is not intended for power generation since it requires far more energy than it produces.[9] [10] [11] [12]

Hot fusion

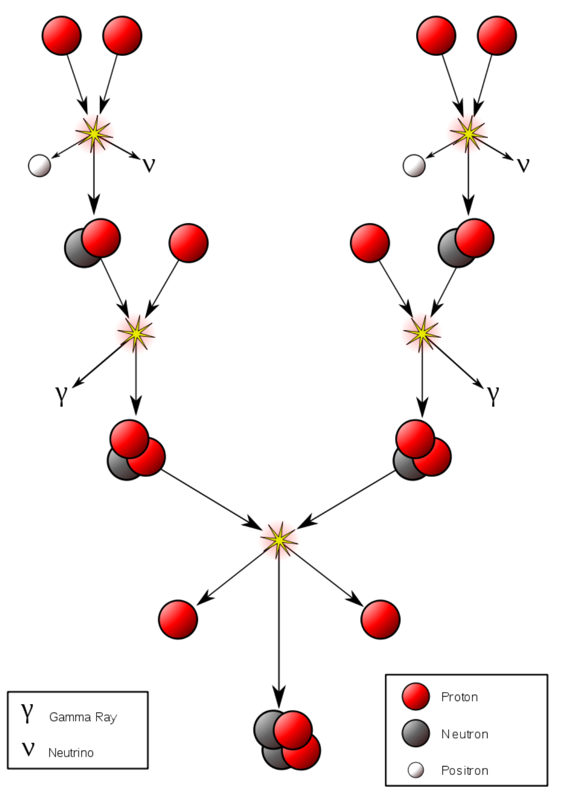
In "standard" "hot" → fusion, the fuel reaches tremendous temperature and pressure inside a fusion reactor or nuclear weapon.

The methods in the second group are examples of non-equilibrium systems, in which very high temperatures and pressures are produced in a relatively small region adjacent to material of much lower temperature. In his doctoral thesis for MIT, Todd Rider did a theoretical study of all quasineutral, isotropic, non-equilibrium fusion systems. He demonstrated that all such systems will leak energy at a rapid rate due to bremsstrahlung produced when electrons in the plasma hit other electrons or ions at a cooler temperature and suddenly decelerate. The problem is not as pronounced in a hot plasma because the range of temperatures, and thus the magnitude of the deceleration, is much lower. Note that Rider's work does not apply to non-neutral and/or anisotropic non-equilibrium plasmas.

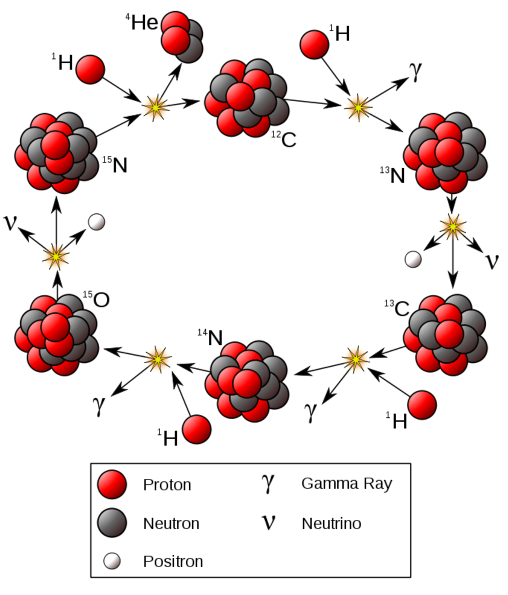
Important reactions

Astrophysical reaction chains

The most important fusion process in nature is that which powers the stars. The net result is the fusion of four protons into one alpha particle, with the release of two positrons, two neutrinos (which changes two of the protons into neutrons), and energy, but several individual reactions are involved, depending on the mass of the star. For stars the size of the sun or smaller, the proton-proton chain dominates. In heavier stars, the CNO cycle is more important. Both types of processes are responsible for the creation of new elements as part of stellar nucleosynthesis.



The proton-proton chain dominates in stars the size of the Sun or smaller.



The CNO cycle dominates in stars heavier than the Sun.

At the temperatures and densities in stellar cores the rates of fusion reactions are notoriously slow. For example, at solar core temperature ($T \approx 15$ MK) and density ($160\ \mathrm{g/cm^3}$), the energy release rate is only $276\ \mu\mathrm{W/cm^3}$—about a quarter of the volumetric rate at which a resting human body generates heat.[13] Thus, reproduction of stellar core conditions in a lab for nuclear fusion power production is completely impractical. Because nuclear reaction rates strongly depend on temperature ($\exp(-E/kT)$), then in order to achieve reasonable rates of energy production in terrestrial fusion reactors 10–100 times higher temperatures (compared to stellar interiors) are required $T \approx 0.1$–1.0 GK.

Criteria and candidates for terrestrial reactions

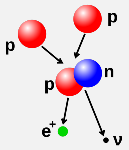
In man-made fusion, the primary fuel is not constrained to be protons and higher temperatures can be used, so reactions with larger cross-sections are chosen. This implies a lower Lawson criterion, and therefore less startup effort. Another concern is the production of neutrons, which activate the reactor structure radiologically, but also have the advantages of allowing volumetric extraction of the fusion energy and tritium breeding. Reactions that release no neutrons are referred to as *aneutronic*.

In order to be useful as a source of energy, a fusion reaction must satisfy several criteria. It must

- **be exothermic**: This may be obvious, but it limits the reactants to the low Z (number of protons) side of the curve of binding energy. It also makes helium ^{4}He the most common product because of its extraordinarily tight binding, although ^{3}He and ^{3}H also show up;
- **involve low *Z* nuclei**: This is because the electrostatic repulsion must be overcome before the nuclei are close enough to fuse;
- **have two reactants**: At anything less than stellar densities, three body collisions are too improbable. It should be noted that in inertial confinement, both stellar densities and temperatures are exceeded to compensate for the shortcomings of the third parameter of the Lawson criterion, ICF's very short confinement time;
- **have two or more products**: This allows simultaneous conservation of energy and momentum without relying on the electromagnetic force;
- **conserve both protons and neutrons**: The cross sections for the weak interaction are too small.

Few reactions meet these criteria. The following are those with the largest cross sections:

(1)	21D	+	31T	→	42He	(	3.5 MeV	)	+	n^0	(	14.1 MeV	)						
(2i)	21D	+	21D	→	31T	(	1.01 MeV	)	+	p^+	(	3.02 MeV	)						50%
(2ii)				→	32He	(	0.82 MeV	)	+	n^0	(	2.45 MeV	)						50%
(3)	21D	+	32He	→	42He	(	3.6 MeV	)	+	p^+	(	14.7 MeV	)						
(4)	31T	+	31T	→	42He				+	2 n^0						+	11.3 MeV		
(5)	32He	+	32He	→	42He				+	2 p^+						+	12.9 MeV		
(6i)	32He	+	31T	→	42He				+	p^+	+	n^0				+	12.1 MeV		51%
(6ii)				→	42He	(	4.8 MeV	)	+	21D	(	9.5 MeV	)						43%
(6iii)				→	42He	(	0.5 MeV	)	+	n^0	(	1.9 MeV	)	+	p^+	(	11.9 MeV	)	6%
(7i)	21D	+	63Li	→	2 42He	+	22.4 MeV												
(7ii)				→	32He	+	42He		+	n^0						+	2.56 MeV		
(7iii)				→	73Li	+	p^+									+	5.0 MeV		
(7iv)				→	74Be	+	n^0									+	3.4 MeV		
(8)	p^+	+	63Li	→	42He	(	1.7 MeV	)	+	32He	(	2.3 MeV	)						
(9)	32He	+	63Li	→	2 42He	+	p^+									+	16.9 MeV		
(10)	p^+	+	115B	→	3 42He											+	8.7 MeV		

Nucleosynthesis
 • Stellar nucleosynthesis • Big Bang nucleosynthesis • Supernova nucleosynthesis • Cosmic ray spallation
Related topics

• Astrophysics
• → Nuclear fusion
  • R-process
  • S-process
• Nuclear fission

edit [14]

For reactions with two products, the energy is divided between them in inverse proportion to their masses, as shown. In most reactions with three products, the distribution of energy varies. For reactions that can result in more than one set of products, the branching ratios are given.

Some reaction candidates can be eliminated at once.[15] The D-^{6}Li reaction has no advantage compared to p^+-115B because it is roughly as difficult to burn but produces substantially more neutrons through 21D-21D side reactions. There is also a p^+-73Li reaction, but the cross section is far too low, except possibly when T_i > 1 MeV, but at such high temperatures an endothermic, direct neutron-producing reaction also becomes very significant. Finally there is also a p^+-94Be reaction, which is not only difficult to burn, but 94Be can be easily induced to split into two alpha particles and a neutron.

In addition to the fusion reactions, the following reactions with neutrons are important in order to "breed" tritium in "dry" fusion bombs and some proposed fusion reactors:

n^0	+	63Li	→	31T	+	42He		
n^0	+	73Li	→	31T	+	42He	+	n^0

To evaluate the usefulness of these reactions, in addition to the reactants, the products, and the energy released, one needs to know something about the cross section. Any given fusion device will have a maximum plasma pressure that it can sustain, and an economical device will always operate near this maximum. Given this pressure, the largest fusion output is obtained when the temperature is chosen so that $\langle\sigma v\rangle/T^2$ is a maximum. This is also the temperature at which the value of the triple product $nT\tau$ required for ignition is a minimum, since that required value is inversely proportional to $\langle\sigma v\rangle/T^2$ (see Lawson criterion). (A plasma is "ignited" if the fusion reactions produce enough power to maintain the temperature without external heating.) This optimum temperature and the value of $\langle\sigma v\rangle/T^2$ at that temperature is given for a few of these reactions in the following table.

fuel	*T* [keV]	$\langle\sigma v\rangle/T^2$ [m³/s/keV²]
21D-31T	13.6	1.24×10^{-24}

21D-21D	15	1.28×10^{-26}
21D-32He	58	2.24×10^{-26}
p^+-63Li	66	1.46×10^{-27}
p^+-115B	123	3.01×10^{-27}

Note that many of the reactions form chains. For instance, a reactor fueled with 31T and 32He will create some 21D, which is then possible to use in the 21D-32He reaction if the energies are "right". An elegant idea is to combine the reactions (8) and (9). The 32He from reaction (8) can react with 63Li in reaction (9) before completely thermalizing. This produces an energetic proton which in turn undergoes reaction (8) before thermalizing. A detailed analysis shows that this idea will not really work well, but it is a good example of a case where the usual assumption of a Maxwellian plasma is not appropriate.

Neutronicity, confinement requirement, and power density

Any of the reactions above can in principle be the basis of → fusion power production. In addition to the temperature and cross section discussed above, we must consider the total energy of the fusion products E_{fus}, the energy of the charged fusion products E_{ch}, and the atomic number Z of the non-hydrogenic reactant.

The only fusion reactions thus far produced by humans to achieve ignition are those which have been created in hydrogen bombs, the first of which, Ivy Mike, is shown here.

Specification of the 21D-21D reaction entails some difficulties, though. To begin with, one must average over the two branches (2) and (3). More difficult is to decide how to treat the 31T and 32He products. 31T burns so well in a deuterium plasma that it is almost impossible to extract from the plasma. The 21D-32He reaction is optimized at a much higher temperature, so the burnup at the optimum 21D-21D temperature may be low, so it seems reasonable to assume the 31T but not the 32He gets burned up and adds its energy to the net reaction. Thus we will count the 21D-21D fusion energy as E_{fus} = (4.03+17.6+3.27)/2 = 12.5 MeV and the energy in charged particles as E_{ch} = (4.03+3.5+0.82)/2 = 4.2 MeV.

Another unique aspect of the 21D-21D reaction is that there is only one reactant, which must be taken into account when calculating the reaction rate.

With this choice, we tabulate parameters for four of the most important reactions.

fuel	Z	E_{fus} [MeV]	E_{ch} [MeV]	neutronicity

21D-31T	1	17.6	3.5	0.80
21D-21D	1	12.5	4.2	0.66
21D-32He	2	18.3	18.3	~0.05
p^+-115B	5	8.7	8.7	~0.001

The last column is the **neutronicity** of the reaction, the fraction of the fusion energy released as neutrons. This is an important indicator of the magnitude of the problems associated with neutrons like radiation damage, biological shielding, remote handling, and safety. For the first two reactions it is calculated as $(E_{fus}-E_{ch})/E_{fus}$. For the last two reactions, where this calculation would give zero, the values quoted are rough estimates based on side reactions that produce neutrons in a plasma in thermal equilibrium.

Of course, the reactants should also be mixed in the optimal proportions. This is the case when each reactant ion plus its associated electrons accounts for half the pressure. Assuming that the total pressure is fixed, this means that density of the non-hydrogenic ion is smaller than that of the hydrogenic ion by a factor $2/(Z+1)$. Therefore the rate for these reactions is reduced by the same factor, on top of any differences in the values of $\langle\sigma v\rangle/T^2$. On the other hand, because the 21D-21D reaction has only one reactant, the rate is twice as high as if the fuel were divided between two hydrogenic species.

Thus there is a "penalty" of (2/(Z+1)) for non-hydrogenic fuels arising from the fact that they require more electrons, which take up pressure without participating in the fusion reaction. (It is usually a good assumption that the electron temperature will be nearly equal to the ion temperature. Some authors, however discuss the possibility that the electrons could be maintained substantially colder than the ions. In such a case, known as a "hot ion mode", the "penalty" would not apply.) There is at the same time a "bonus" of a factor 2 for 21D-21D because each ion can react with any of the other ions, not just a fraction of them.

We can now compare these reactions in the following table.

fuel	**$\langle\sigma v\rangle/T^2$**	**penalty/bonus**	**reactivity**	**Lawson criterion**	**power density ($W/m^3/kPa^2$)**	**relation of power density**
21D-31T	1.24×10^{-24}	1	1	1	34	1
21D-21D	1.28×10^{-26}	2	48	30	0.5	68
21D-32He	2.24×10^{-26}	2/3	83	16	0.43	80
p^+-63Li	1.46×10^{-27}	1/2	1700		0.005	6800
p^+-115B	3.01×10^{-27}	1/3	1240	500	0.014	2500

The maximum value of $\langle\sigma v\rangle/T^2$ is taken from a previous table. The "penalty/bonus" factor is that related to a non-hydrogenic reactant or a single-species reaction. The values in the column "reactivity" are found by dividing 1.24×10^{-24} by the product of the second and third columns. It indicates the factor by which the other reactions occur more slowly than the 21D-31T reaction under comparable conditions. The column "Lawson criterion" weights these results with E_{ch} and gives an indication of how much more difficult it is to achieve ignition with these reactions, relative to the difficulty for the 21D-31T reaction. The last column is labeled "power density" and weights the practical reactivity with E_{fus}. It indicates how much lower the fusion power density of the other reactions is compared to the

21D-31T reaction and can be considered a measure of the economic potential.

Bremsstrahlung losses in quasineutral, isotropic plasmas

The ions undergoing fusion in many systems will essentially never occur alone but will be mixed with electrons that in aggregate neutralize the ions' bulk electrical charge and form a plasma. The electrons will generally have a temperature comparable to or greater than that of the ions, so they will collide with the ions and emit x-ray radiation of 10-30 keV energy (Bremsstrahlung). The Sun and stars are opaque to x-rays, but essentially any terrestrial fusion reactor will be optically thin for x-rays of this energy range. X-rays are difficult to reflect but they are effectively absorbed (and converted into heat) in less than mm thickness of stainless steel (which is part of a reactor's shield). The ratio of fusion power produced to x-ray radiation lost to walls is an important figure of merit. This ratio is generally maximized at a much higher temperature than that which maximizes the power density (see the previous subsection). The following table shows the rough optimum temperature and the power ratio at that temperature for several reactions.[16]

fuel	T_i (keV)	$P_{fusion}/P_{Bremsstrahlung}$
21D-31T	50	140
21D-21D	500	2.9
21D-32He	100	5.3
32He-32He	1000	0.72
p^+-63Li	800	0.21
p^+-115B	300	0.57

The actual ratios of fusion to Bremsstrahlung power will likely be significantly lower for several reasons. For one, the calculation assumes that the energy of the fusion products is transmitted completely to the fuel ions, which then lose energy to the electrons by collisions, which in turn lose energy by Bremsstrahlung. However because the fusion products move much faster than the fuel ions, they will give up a significant fraction of their energy directly to the electrons. Secondly, the plasma is assumed to be composed purely of fuel ions. In practice, there will be a significant proportion of impurity ions, which will lower the ratio. In particular, the fusion products themselves *must* remain in the plasma until they have given up their energy, and *will* remain some time after that in any proposed confinement scheme. Finally, all channels of energy loss other than Bremsstrahlung have been neglected. The last two factors are related. On theoretical and experimental grounds, particle and energy confinement seem to be closely related. In a confinement scheme that does a good job of retaining energy, fusion products will build up. If the fusion products are efficiently ejected, then energy confinement will be poor, too.

The temperatures maximizing the fusion power compared to the Bremsstrahlung are in every case higher than the temperature that maximizes the power density and minimizes the required value of the fusion triple product. This will not change the optimum operating point for 21D-31T very much because the Bremsstrahlung fraction is low, but it will push the other fuels into regimes where the power density relative to 21D-31T is even lower and the required confinement even more difficult to achieve. For 21D-21D and 21D-32He, Bremsstrahlung losses will be a serious, possibly prohibitive problem. For 32He-32He, p^+-63Li and p^+-115B the Bremsstrahlung losses appear to make a fusion reactor using these fuels with a quasineutral, anisotropic plasma impossible. Some ways out of this dilemma are considered—and rejected—in *Fundamental limitations on plasma fusion systems not in thermodynamic equilibrium* by Todd Rider [17].[18] This limitation does not apply to non-neutral and anisotropic plasmas; however, these have their own challenges to contend with.

See also

- → Fusion power
- Pulsed power
- Nuclear physics
- Nuclear fission
- Nuclear reactor
- Nucleosynthesis
- Helium fusion
- Helium-3
- Neutron source
- Neutron generator
- Timeline of nuclear fusion
- Periodic table

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[18] http://fusion.ps.uci.edu/artan/Posters/aps_poster_2.pdf Portable Document Format (PDF)

External links

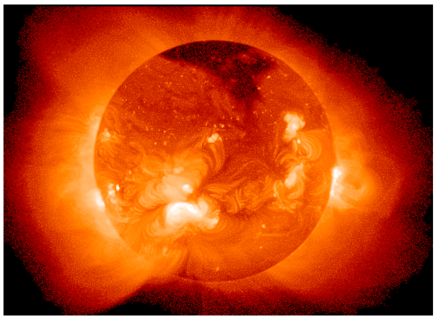
- International Fusion Research and Prototype reactor (http://www.iter.org/)
- IEC Fusion Video Presentation (http://video.google.com/videoplay?docid=1996321846673788606&q=engedu) – Presentation on inertial electrostatic confinement fusion from Dr. Robert Bussard
- Fusion.org.uk (http://www.fusion.org.uk/) – A guide to fusion from the UKAEA
- Fusion as an Energy Source (http://www.iop.org/activity/policy/Publications/file_31695.pdf)– A guide from the Institute of Physics
- Fusion Science and Technology (http://www.ans.org/pubs/journals/fst/)– Technical journal published by the American Nuclear Society.
- JET (http://www.jet.efda.org/)– Nuclear Fusion Research at the Joint European Torus
- Nuclear Files.org (http://www.nuclearfiles.org/menu/key-issues/nuclear-weapons/basics/what-is-fusion.htm) What is Nuclear Fusion?
- Nature: Chaos could keep fusion under control (http://www.nature.com/news/2006/060522/full/060522-2.html)
- Nuclear fusion reactions (http://www.oup.co.uk/pdf/0-19-856264-0.pdf) First chapter of *The Physics of Inertial Fusion, Stefano Atzeni and Jürgen Meyer-ter-Vehn*
- Science or Fiction - Is there a Future for Nuclear? (http://www.ecology.at/ecology/files/pr577_1.pdf) (Nov. 2007) - A publication from the Austrian Ecology Institute about 'Generation IV' and Fusion reactors.

Fusion power

Fusion power is the power generated by → nuclear fusion reactions. In this kind of reaction, two light atomic nuclei fuse together to form a heavier nucleus and in doing so, release a large amount of energy. In a more general sense, the term can also refer to the production of net usable power from a fusion source, similar to the usage of the term "steam power." Most design studies for fusion power plants involve using the fusion reactions to create heat, which is then used to operate a steam turbine, which drives generators to produce electricity. Except for the use of a thermonuclear heat source, this is similar to most coal-fired power stations and fission-driven nuclear power stations.

The largest current experiment is the Joint European Torus (JET). In 1997, JET produced a peak of 16.1 MW of fusion power (65% of input power), with fusion power of over 10 MW sustained for over 0.5 sec. In June 2005, the construction of the experimental reactor → ITER, designed to produce several times more fusion power than the power put into the plasma over many minutes, was announced. They are currently preparing the site (September 2008). The production of net electrical power from fusion is planned for DEMO, the next generation experiment after ITER. Additionally, the High Power laser Energy Research facility (HiPER) is undergoing preliminary design for possible construction in the European Union starting around 2010.

Fuel cycle


The Sun is a natural fusion reactor.

The basic concept behind any fusion reaction is to bring two or more atoms close enough together so that the strong nuclear force in their nuclei will pull them together into one larger atom. If two light nuclei fuse, they will generally form a single nucleus with a slightly smaller mass than the sum of their original masses. The difference in mass is released as energy according to Albert Einstein's mass-energy equivalence formula $E = mc^2$. If the input atoms are sufficiently massive, the resulting fusion product will be heavier than the reactants, in which case the reaction requires an external source of energy. The dividing line between "light" and "heavy" is iron-56. Above this atomic mass, energy will generally be released by nuclear fission reactions; below it, by fusion.

Fusion between the atoms is opposed by their shared electrical charge, specifically the net positive charge of the nuclei. In order to overcome this electrostatic force, or "Coulomb barrier", some external source of energy must be supplied. The easiest way to do this is to heat the atoms, which has the side effect of stripping the electrons from the atoms and leaving them as bare nuclei. In most experiments the nuclei and electrons are left in a fluid known as a plasma. The temperatures required to provide the nuclei with enough energy to overcome their repulsion is a function of the total charge, so hydrogen, which has the smallest nuclear charge therefore reacts at the lowest temperature. Helium has an extremely low mass per nucleon and therefore is energetically favoured as a fusion product. As a consequence, most fusion reactions combine isotopes of hydrogen ("protium", deuterium, or tritium) to form isotopes of helium (^{3}He or ^{4}He).

Perhaps the three most widely considered fuel cycles are based on the D-T, D-D, and p-^{11}B reactions. Other fuel cycles (D-^{3}He and ^{3}He-^{3}He) would require a supply of ^{3}He, either from other nuclear reactions or from extraterrestrial sources, such as the surface of the moon or the atmospheres of the gas giant planets. The details of the calculations comparing these reactions can be found here.

D-T fuel cycle

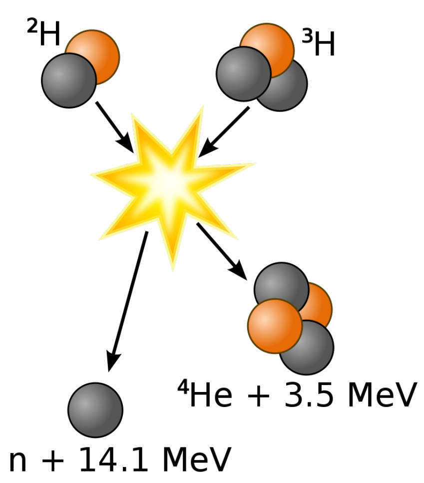


Diagram of the D-T reaction

The easiest (according to the Lawson criterion) and most immediately promising nuclear reaction to be used for fusion power is:

$D + T \rightarrow {}^4He + n$

Deuterium is a naturally occurring isotope of hydrogen and as such is universally available. The large mass ratio of the hydrogen isotopes makes the separation rather easy compared to the difficult uranium enrichment process. Tritium is also an isotope of hydrogen, but it occurs naturally in only negligible amounts due to its radioactive half-life of 12.32 years. Consequently, the deuterium-tritium fuel cycle requires the breeding of tritium from lithium using one of the following reactions:

$n + {}^6Li \rightarrow T + {}^4He$

$n + {}^7Li \rightarrow T + {}^4He + n$

The reactant neutron is supplied by the D-T fusion reaction shown above, the one which also produces the useful energy. The reaction with ^6Li is exothermic, providing a small energy gain for the reactor. The reaction with ^7Li is endothermic but does not consume the neutron. At least some ^7Li reactions are required to replace the neutrons lost by reactions with other elements. Most reactor designs use the naturally occurring mix of lithium isotopes. The supply of lithium is more limited than that of deuterium, but still large enough to supply the world's energy demand for thousands of years.

Several drawbacks are commonly attributed to D-T fusion power:

1. It produces substantial amounts of neutrons that result in induced radioactivity within the reactor structure.
2. Only about 20% of the fusion energy yield appears in the form of charged particles (the rest neutrons), which limits the extent to which direct energy conversion techniques might be applied.
3. The use of D-T fusion power depends on lithium resources, which are less abundant than deuterium resources.
4. It requires the handling of the radioisotope tritium. Similar to hydrogen, tritium is difficult to contain and may leak from reactors in some quantity. Some estimates suggest that this would represent a fairly large environmental release of radioactivity.[1]

The neutron flux expected in a commercial D-T fusion reactor is about 100 times that of current fission power reactors, posing problems for material design. Design of suitable materials is under way but their actual use in a reactor is not proposed until the generation after → ITER. After a single series of D-T tests at JET, the largest fusion reactor yet to use this fuel, the vacuum vessel was sufficiently radioactive that remote handling needed to be used for the year following the tests.

On the other hand, the volumetric deposition of neutron power can also be seen as an advantage. If all the power of a fusion reactor had to be transported by conduction through the surface enclosing the plasma, it would be very difficult to find materials and a construction that would survive, and it would probably entail a relatively poor efficiency.

D-D fuel cycle

Though more difficult to facilitate than the deuterium-tritium reaction, fusion can also be achieved through the reaction of deuterium with itself. This reaction has two branches that occur with nearly equal probability:

D + D	→ T	+ p
	→ ^{3}He	+ n

The optimum temperature for this reaction is 15 keV, only slightly higher than the optimum for the D-T reaction. The first branch does not produce neutrons, but it does produce tritium, so that a D-D reactor will not be completely tritium-free, even though it does not require an input of tritium or lithium. Most of the tritium produced will be burned before leaving the reactor, which reduces the tritium handling required, but also means that more neutrons are produced and that some of these are very energetic. The neutron from the second branch has an energy of only 2.45 MeV, whereas the neutron from the D-T reaction has an energy of 14.1 MeV, resulting in a wider range of isotope production and material damage. Assuming complete tritium burn-up, the reduction in the fraction of fusion energy carried by neutrons is only about 18%, so that the primary advantage of the D-D fuel cycle is that tritium breeding is not required. Other advantages are independence from limitations of lithium resources and a somewhat softer neutron spectrum. The price to pay compared to D-T is that the energy confinement (at a given pressure) must be 30 times better and the power produced (at a given pressure and volume) is 68 times less.

p-^{11}B fuel cycle

If aneutronic fusion is the goal, then the most promising candidate may be the proton-boron reaction:

$$p + {}^{11}B \rightarrow 3\,{}^{4}He$$

Under reasonable assumptions, side reactions will result in about 0.1% of the fusion power being carried by neutrons.[2] At 123 keV, the optimum temperature for this reaction is nearly ten times higher than that for the pure hydrogen reactions, the energy confinement must be 500 times better than that required for the D-T reaction, and the power density will be 2500 times lower than for D-T. Since the confinement properties of conventional approaches to fusion such as the tokamak and laser pellet fusion are marginal, most proposals for aneutronic fusion are based on radically different confinement concepts.

History of research

The idea of using human-initiated fusion reactions was first made practical for military purposes, in nuclear weapons. In a hydrogen bomb, the energy released by a fission weapon is used to compress and heat fusion fuel, beginning a fusion reaction which can release a very large amount of energy. The first fusion-based weapons released some 500 times more energy than early fission weapons.

Civilian applications, in which explosive energy production must be replaced by a controlled production, are still being developed. Although it took less than ten years to go from military applications to civilian fission energy production,[3] it has been very different in the fusion energy field; more than fifty years have already passed[4] without any commercial fusion energy production plant coming into operation.

Magnetic approach

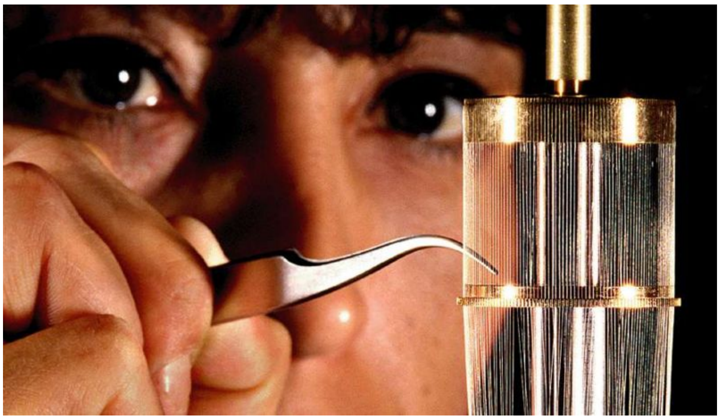
Registration of the first patent related to a fusion reactor[5] by the United Kingdom Atomic Energy Authority, the inventors being Sir George Paget Thomson and Moses Blackman, dates back to 1946. Some basic principles used in the ITER experiment are described in this patent: toroidal vacuum chamber, magnetic confinement, and radio frequency plasma heating.

The U.S. fusion program began in 1951 when Lyman Spitzer began work on a stellarator under the code name Project Matterhorn. His work led to the creation of the Princeton Plasma Physics Laboratory, where magnetically confined plasmas are still studied. The stellarator concept fell out of favor for several decades afterwards, plagued by poor confinement issues, but recent advances in computer technology have led to a significant resurgence in interest in these devices. A wide variety of other magnetic geometries were also experimented with, notably with the magnetic mirror. These systems also suffered from similar problems when higher performance versions were constructed.

A new approach was outlined in the theoretical works fulfilled in 1950–1951 by I.E. Tamm and A.D. Sakharov in the Soviet Union, which first discussed a tokamak like approach. Experimental research on these designs began in 1956 at the Kurchatov Institute in Moscow by a group of Soviet scientists led by Lev Artsimovich. The group constructed the first tokamaks, the most successful being the T-3 and its larger version T-4. T-4 was tested in 1968 in Novosibirsk, producing the first quasistationary thermonuclear fusion reaction ever.[6] The tokamak was dramatically more efficient than the other approaches of that era, and most research after the 1970s has concentrated on variations of this theme.

The same is true today, where very large tokamaks like → ITER are expected to pass several milestones toward commercial power production, including a burning plasma with long burn times, high power output, and online fueling. There are no guarantees that the project will be successful; previous generations of tokomak machines have uncovered new problems many times. But the entire field of high temperature plasmas is much better understood now than formerly, and there is considerable optimism that ITER will meet its goals. If successful, ITER would be followed by a "commercial demonstrator" system, similar in purpose to the very earliest power-producing fission reactors built in the era before wide-scale commercial deployment of larger machines started in the 1960s and 1970s. Even with these goals met, there are a number of major engineering problems remaining, notably finding suitable "low activity" materials for reactor construction, demonstrating secondary systems including practical tritium extraction, and building reactor designs that allow their reactor core to be removed when its materials becomes embrittled due to the neutron flux. Practical commercial generators based on the tokamak concept are far in the future. The public at large has been disappointed, as the initial outlook for practical fusion power plants was much rosier; a pamphlet from the 1970s printed by General Atomic stated that "Several commercial fusion reactors are expected to be online by the year 2000."

Pinch devices


A "wires array" used in Z-pinch confinement, during the building process.

The Z-pinch phenomenon has been known since the end of the 18th century.[7] Its use in the fusion field comes from research made on toroidal devices, initially in the Los Alamos National Laboratory right from 1952 (Perhapsatron), and in the United Kingdom from 1954 (ZETA), but its physical principles remained for a long time poorly understood and controlled. Pinch devices were studied as potential development paths to practical fusion devices through the 1950s, but studies of the data generated by these devices suggested that instabilities in the collapse mechanism would doom any pinch-type device to power levels that were far too low to suggest continuing along these lines would be practical. Most work on pinch-type devices ended by the 1960s. Recent work on the basic concept started as a result of the appearance of the "wires array" concept in the 1980s, which allowed a more efficient use of this technique. The Sandia National Laboratory runs a continuing wire-array research program with the Zpinch machine. In addition, the University of Washington's ZaP Lab [8] have shown quiescent periods of stability hundreds of times longer than expected for plasma in a Z-pinch configuration, giving promise to the confinement technique.

Laser inertial devices

The technique of implosion of a microcapsule irradiated by laser beams, the basis of laser inertial confinement, was first suggested in 1962 by scientists at Lawrence Livermore National Laboratory, shortly after the invention of the laser itself in 1960. Lasers of the era were very low powered, but low-level research using them nevertheless started as early as 1965. More serious research started in the early 1970s when new types of lasers offered a path to dramatically higher power levels, levels that made inertial-confinement fusion devices appear practical for the first time. By the late 1970s great strides had been made in laser power, but with each increase new problems were found in the implosion technique that suggested even more power would be required. By the 1980s these increases were so large that using the concept for generating net energy seemed remote. Most research in this field turned to weapons research, always a second line of research, as the implosion concept is somewhat similar to hydrogen bomb operation. Work on very large versions continued as a result, with the very large National Ignition Facility in the US and Laser Mégajoule in France supporting these research programs.

More recent work had demonstrated that significant savings in the required laser energy are possible using a technique known as "fast ignition". The savings are so dramatic that the concept appears to be a useful technique for energy production again, so much so that it is a serious contender for pre-commercial development. There are proposals to build an experimental facility dedicated to the fast ignition approach, known as HiPER. At the same time, advances in solid state lasers appear to improve the "driver" systems' efficiency by about ten times (to 10- 20%), savings that make even the large "traditional" machines almost practical, and might make the fast ignition concept outpace the magnetic approaches in further development. The laser-based concept has other advantages as well. The reactor core is mostly exposed, as opposed to being wrapped in a huge magnet as in the tokamak. This makes the problem of removing energy from the system somewhat simpler, and should mean that a laser-based device would be much easier to perform maintenance on, such as core replacement. Additionally, the lack of strong magnetic fields allows for a wider variety of low-activation materials, including carbon fiber, which would reduce both the frequency of such neutron activations and the rate of irradiation to the core. In other ways the program has many of the same problems as the tokamak; practical methods of energy removal and tritium recycling need to be demonstrated.

Other systems

Throughout the history of fusion power research there have been a number of devices that have produced fusion at a much smaller level, not being suitable for energy production, but nevertheless starting to fill other roles.

Philo T. Farnsworth, the inventor of the first all-electronic television system in 1927, patented his first Fusor design in 1968, a device which uses inertial electrostatic confinement. Towards the end of the 1960s, Robert Hirsch designed a variant of the Farnsworth Fusor known as the Hirsch-Meeks fusor. This variant is a considerable improvement over the Farnsworth design, and is able to generate neutron flux in the order of one billion neutrons per second. Although the efficiency was very low at first, there were hopes the device could be scaled up, but continued development demonstrated that this approach would be impractical for large machines. Nevertheless, fusion could be achieved using a "lab bench top" type set up for the first time, at minimal cost. This type of fusor found its first application as a portable neutron generator in the late 1990s. An automated sealed reaction chamber version of this device, commercially named Fusionstar was developed by EADS but abandoned in 2001. Its successor is the NSD-Fusion neutron generator.

Robert W. Bussard's Polywell concept is roughly similar to the Fusor design, but replaces the problematic grid with a magnetically contained electron cloud which holds the ions in position and gives an accelerating potential. Bussard claimed that a scaled up version would be capable of generating net power.

In April 2005, a team from UCLA announced [9] it had devised a novel way of producing fusion using a machine that "fits on a lab bench", using lithium tantalate to generate enough voltage to smash deuterium atoms together. However, the process does not generate net power. See Pyroelectric fusion. Such a device would be useful in the same sort of roles as the fusor.

Safety and the environment

Accident potential

The likelihood of *small industrial* accidents including the local release of radioactivity and injury to staff cannot be estimated yet. Nevertheless the likelihood of a *catastrophic* accident in a fusion reactor resulting in major release of radioactivity to the environment or injury to non-staff, is estimated to be much smaller than that in a fission reactor. The primary reason is that the fission products in a fission reactor continue to generate heat through beta-decay for several hours or even days after reactor shut-down, meaning that a meltdown is possible even after the reactor has been stopped. In contrast, fusion requires precisely controlled conditions of temperature, pressure and magnetic field parameters in order to generate net energy. If the reactor were damaged, these parameters would be disrupted and the heat generation in the reactor would rapidly cease.

There is also no risk of a runaway reaction in a fusion reactor, since the plasma is normally burnt at optimal conditions, and any significant change will render it unable to produce excess heat. In fusion reactors the reaction process is so delicate that this level of safety is inherent; no elaborate failsafe mechanism is required. Although the plasma in a fusion power plant will have a volume of 1000 cubic meters or more, the density of the plasma is extremely low, and the total amount of fusion fuel in the vessel is very small, typically a few grams. If the fuel supply is closed, the reaction stops within seconds. In comparison, a fission reactor is typically loaded with enough fuel for one or several years, and no additional fuel is necessary to keep the reaction going.

In the magnetic approach, strong fields are developed in coils that are held in place mechanically by the reactor structure. Failure of this structure could release this tension and allow the magnet to "explode" outward. The severity of this event would be similar to any other industrial accident, and could be effectively stopped with a containment building similar to those used in existing (fission) nuclear generators. The laser-driven inertial approach is generally lower-stress. Although failure of the reaction chamber is possible, simply stopping fuel delivery would prevent any sort of catastrophic failure.

Most reactor designs rely on the use of liquid lithium as both a coolant and a method for converting stray neutrons from the reaction into tritium, which is fed back into the reactor as fuel. Lithium is highly flammable, and in the case of a fire it is possible that the lithium stored on-site could be burned up and escape. In this case the tritium contents of the lithium would be released into the atmosphere, posing a radiation risk. However, calculations suggest that the total amount of tritium and other radioactive gases in a typical power plant would be so small, about 1 kg, that they would have diluted to legally acceptable limits by the time they blew as far as the plant's perimeter fence.[10]

Effluents during normal operation

The natural product of the fusion reaction is a small amount of helium, which is completely harmless to life and does not contribute to global warming. Of more concern is tritium, which, like other isotopes of hydrogen, is difficult to retain completely. During normal operation, some amount of tritium will be continually released. There would be no acute danger, but the cumulative effect on the world's population from a fusion economy could be a matter of concern. The 12 year half-life of tritium would at least prevent unlimited build-up and long-term contamination without appropriate containment techniques. Current ITER designs are investigating total containment facilities for any tritium.

Waste management

The large flux of high-energy neutrons in a reactor will make the structural materials radioactive. The radioactive inventory at shut-down may be comparable to that of a fission reactor, but there are important differences.

The half-life of the radioisotopes produced by fusion tend to be less than those from fission, so that the inventory decreases more rapidly. Unlike fission reactors, whose waste remains radioactive for thousands of years, most of the radioactive material in a fusion reactor would be the reactor core itself, which would be dangerous for about 50 years, and low-level waste another 100. Although this waste will be considerably more radioactive during those 50 years than fission waste, the very short half-life makes the process very attractive, as the waste management is fairly straightforward. By 300 years the material would have the same radioactivity as coal ash.[10]

Additionally, the choice of materials used in a fusion reactor is less constrained than in a fission design, where many materials are required for their specific neutron cross-sections. This allows a fusion reactor to be designed using materials that are selected specifically to be "low activation", materials that do not easily become radioactive. Vanadium, for example, would become much less radioactive than stainless steel. Carbon fibre materials are also low-activation, as well as being strong and light, and are a promising area of study for laser-inertial reactors where a magnetic field is not required.

In general terms, fusion reactors would create far less radioactive material than a fission reactor, the material it would create is less damaging biologically, and the radioactivity "burns off" within a time period that is well within existing engineering capabilities.

Nuclear proliferation

Although fusion power uses nuclear technology, the overlap with nuclear weapons technology is small. Tritium is a component of the trigger of hydrogen bombs, but not a major problem in production. The copious neutrons from a fusion reactor could be used to breed plutonium for an atomic bomb, but not without extensive redesign of the reactor, so that production would be difficult to conceal. The theoretical and computational tools needed for hydrogen bomb design are closely related to those needed for inertial confinement fusion, but have very little in common with the more scientifically developed magnetic confinement fusion.

As a sustainable energy source

Large-scale reactors using neutronic fuels (e.g. → ITER) and thermal power production (turbine based) are most comparable to fission power from an engineering and economics viewpoint. Both fission and fusion power plants involve a relatively compact heat source powering a conventional steam turbine-based power plant, while producing enough neutron radiation to make activation of the plant materials problematic. The main distinction is that fusion power produces no high-level radioactive waste (though activated plant materials still need to be disposed of). There are some power plant ideas which may significantly lower the cost or size of such plants; however, research in these areas is nowhere near as advanced as in tokamaks.

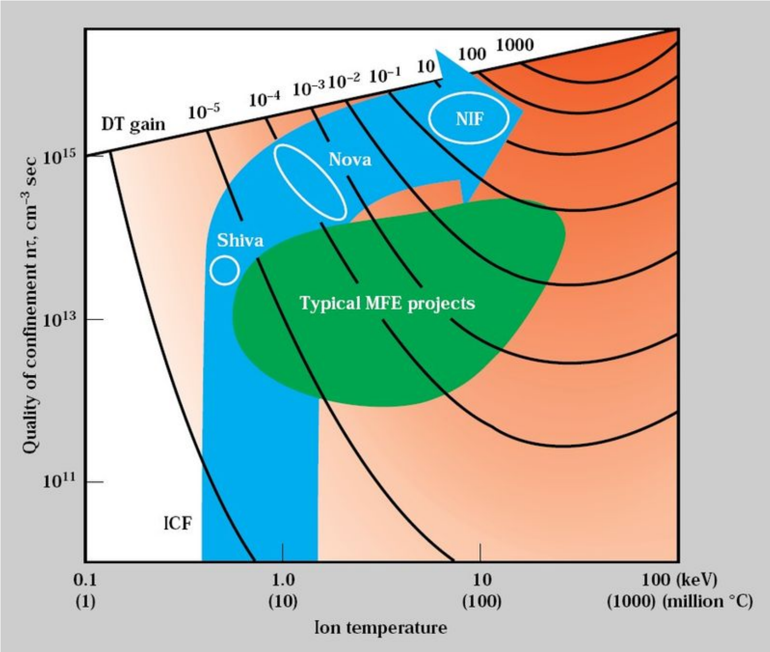
Fusion power commonly proposes the use of deuterium, an isotope of hydrogen, as fuel and in many current designs also use lithium. Assuming a fusion energy output equal to the 1995 global power output of about 100 EJ/yr (= 1 x 10^{20} J/yr) and that this does not increase in the future, then the known current lithium reserves would last 3000 years, lithium from sea water would last 60 million years, and a more complicated fusion process using only deuterium from sea water would have fuel for 150 billion years.[11] To put this in context, 150 billion years is over ten times the currently measured age of the universe, and is close to 30 times the remaining lifespan of the sun.[12]

Theoretical power plant designs

Confinement concepts

Confinement refers to all the conditions necessary to keep a plasma dense and hot long enough to undergo fusion:

- Equilibrium: There must be no net forces on any part of the plasma, otherwise it will rapidly disassemble. The exception, of course, is inertial confinement, where the relevant physics must occur faster than the disassembly time.
- Stability: The plasma must be so constructed that small deviations are restored to the initial state, otherwise some unavoidable disturbance will occur and grow exponentially until the plasma is destroyed.
- Transport: The loss of particles and heat in all channels must be sufficiently slow. The word "confinement" is often used in the restricted sense of "energy confinement".



Parameter space occupied by inertial fusion energy and magnetic fusion energy devices as of the mid 1990s. The regime allowing thermonuclear ignition with high gain lies near the upper right corner of the plot.

The first human-made, large-scale fusion reaction was the test of the hydrogen bomb, Ivy Mike, in 1952. As part of the PACER (fusion) project, it was once proposed to use hydrogen bombs as a source of power by detonating them in underground caverns and then generating electricity from the heat produced, but such a power plant is unlikely ever to be constructed, for a variety of reasons. *Controlled* thermonuclear fusion (CTF) refers to the alternative of continuous power production, or at least the use of explosions that are so small that they do not destroy a significant portion of the machine that produces them.

To produce self-sustaining fusion, the energy released by the reaction (or at least a fraction of it) must be used to heat new reactant nuclei and keep them hot long enough that they also undergo fusion reactions. Retaining the heat is called energy confinement and may be accomplished in a number of ways.

The hydrogen bomb really has no confinement at all. The fuel is simply allowed to fly apart, but it takes a certain length of time to do this, and during this time fusion can occur. This approach is called inertial confinement. If more than milligram quantities of fuel are used (and efficiently fused), the explosion would destroy the machine, so theoretically, controlled thermonuclear fusion using inertial confinement would be done using tiny pellets of fuel which explode several times a second. To induce the explosion, the pellet must be compressed to about 30 times solid density with energetic beams. If the beams are focused directly on the pellet, it is called direct drive, which can in principle be very efficient, but in practice it is difficult to obtain the needed uniformity. An alternative approach is indirect drive, in which the beams heat a shell, and the shell radiates x-rays, which then implode the pellet. The beams are commonly laser beams, but heavy and light ion beams and electron beams have all been investigated.

Inertial confinement produces plasmas with impressively high densities and temperatures, and appears to be best suited to weapons research, X-ray generation, very small reactors, and perhaps in the distant future, spaceflight. They rely on fuel pellets with close to a "perfect" shape in order to generate a symmetrical inward shock wave to produce the high-density plasma, and in practice these have proven difficult to produce. A recent development in the field of laser induced ICF is the use of ultrashort pulse multi-petawatt lasers to heat the plasma of an imploding pellet at exactly the moment of greatest density after it is imploded conventionally using terawatt scale lasers. This research will be carried out on the (currently being built) OMEGA EP petawatt and OMEGA lasers at the University of Rochester and at the GEKKO XII laser at the institute for laser engineering in Osaka Japan, which if fruitful, may have the effect of greatly reducing the cost of a laser fusion based power source.

At the temperatures required for fusion, the fuel is in the form of a plasma with very good electrical conductivity. This opens the possibility to confine the fuel and the energy with magnetic fields, an idea known as magnetic confinement. The Lorenz force works only perpendicular to the magnetic field, so that the first problem is how to prevent the plasma from leaking out the ends of the field lines. There are basically two solutions.

The first is to use the magnetic mirror effect. If particles following a field line encounter a region of higher field strength, then some of the particles will be stopped and reflected. Advantages of a magnetic mirror power plant would be simplified construction and maintenance due to a linear topology and the potential to apply direct conversion in a natural way, but the confinement achieved in the experiments was so poor that this approach has been essentially abandoned.

The second possibility to prevent end losses is to bend the field lines back on themselves, either in circles or more commonly in nested toroidal surfaces. The most highly developed system of this type is the *tokamak*, with the *stellarator* being next most advanced, followed by the Reversed field pinch. Compact toroids, especially the *Field-Reversed Configuration* and the spheromak, attempt to combine the advantages of toroidal magnetic surfaces with those of a simply connected (non-toroidal) machine, resulting in a mechanically simpler and smaller confinement area. Compact toroids still have some enthusiastic supporters but are not backed as readily by the majority of the fusion community.

Finally, there are also *electrostatic confinement fusion* systems, in which ions in the reaction chamber are confined and held at the center of the device by electrostatic forces, as in the Farnsworth-Hirsch Fusor, which is not believed to be able to be developed into a power plant. The Polywell, an advanced variant of the fusor, has shown a degree of research interest as of late; however, the technology is relatively immature, and major scientific and engineering questions remain which researchers under the auspices of the U.S. Office of Naval Research hope to further investigate.

Other approaches

A more subtle technique is to use more unusual particles to catalyse fusion. The best known of these is Muon-catalyzed fusion which uses muons, which behave somewhat like electrons and replace the electrons around the atoms. These muons allow atoms to get much closer and thus reduce the kinetic energy required to initiate fusion. Muons require more energy to produce than can be obtained from muon-catalysed fusion, making this approach impractical for the generation of power.

Some scientists have reported excess heat, neutrons, tritium, helium and other nuclear effects in so-called cold fusion systems. In 2004, a peer review panel was commissioned by the U.S. Department of Energy to study these claims[13]. This identified basic areas of research which were necessary for acceptance of the idea, but did not recommend a federally-funded program.

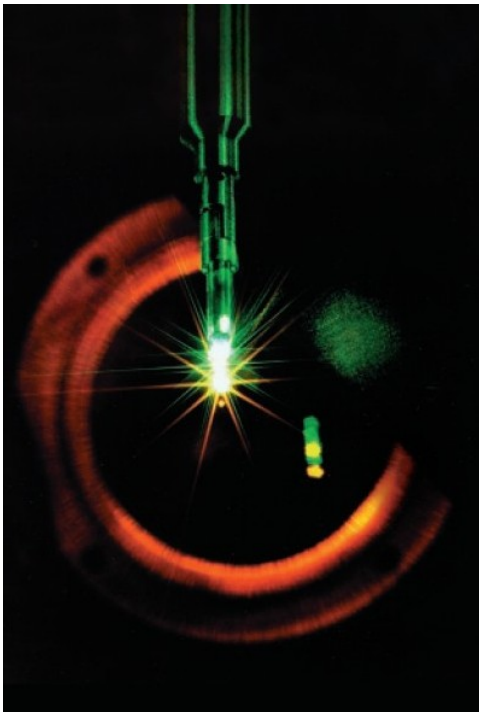
Research into sonoluminescence induced fusion, sometimes known as "*bubble fusion*", also continues, although it is met with as much skepticism as cold fusion is by most of the scientific community.

Subsystems

In fusion research, achieving a fusion energy gain factor $Q = 1$ is called breakeven and is considered a significant although somewhat artificial milestone. Ignition refers to an infinite Q, that is, a self-sustaining plasma where the losses are made up for by fusion power without any external input. In a practical fusion reactor, some external power will always be required for things like current drive, refueling, profile control, and burn control. A value on the order of $Q = 20$ will be required if the plant is to deliver much more energy than it uses internally.

There have been many design studies for fusion power plants. Despite many differences, there are several systems that are common to most. To begin with, a fusion power plant, like a fission power plant, is customarily divided into the nuclear island and the balance of plant. The balance of plant is the conventional part that converts high-temperature heat into electricity via steam turbines. It is much the same in a fusion power plant as in a fission or coal power plant. In a fusion power plant, the nuclear island has a plasma chamber with an associated vacuum system, surrounded by plasma-facing components (first wall and divertor) maintaining the vacuum boundary and absorbing the thermal radiation coming from the plasma, surrounded in turn by a blanket where the neutrons are absorbed to breed tritium and heat a working fluid that transfers the power to the balance of plant. If magnetic confinement is used, a magnet system, using primarily cryogenic superconducting magnets, is needed, and usually systems for heating and refueling the plasma and for driving current. In inertial confinement, a driver (laser or accelerator) and a focusing system are needed, as well as a means for forming and positioning the pellets.

Although the standard solution for electricity production in fusion power plant designs is conventional steam turbines using the heat deposited by neutrons, there are also designs for direct conversion of the energy of the charged particles into electricity. These are of little value with a D-T fuel cycle, where 80% of the power is in the neutrons, but are indispensable with aneutronic fusion, where less than 1% is. Direct conversion has been most commonly proposed for open-ended magnetic configurations like magnetic mirrors or Field-Reversed Configurations, where charged particles are lost along the magnetic field lines, which are then expanded to convert a large fraction of the random energy of the fusion products into directed motion. The particles are then collected on electrodes at various large electrical potentials. Typically the claimed conversion efficiency is in the range of 80%, but the converter may approach the reactor itself in size and expense.



Inertial confinement fusion implosion on the Nova laser creates "microsun" conditions of tremendously high density and temperature.

Materials

Developing materials for fusion reactors has long been recognized as a problem nearly as difficult and important as that of plasma confinement, but it has received only a fraction of the attention. The neutron flux in a fusion reactor is expected to be about 100 times that in existing pressurized water reactors (PWR). Each atom in the blanket of a fusion reactor is expected to be hit by a neutron and displaced about a hundred times before the material is replaced. Furthermore the high-energy neutrons will produce hydrogen and helium in various nuclear reactions that tends to form bubbles at grain boundaries and result in swelling, blistering or embrittlement. One also wishes to choose materials whose primary components and impurities do not result in long-lived radioactive wastes. Finally, the mechanical forces and temperatures are large, and there may be frequent cycling of both.

The problem is exacerbated because realistic material tests must expose samples to neutron fluxes of a similar level for a similar length of time as those expected in a fusion power plant. Such a neutron source is nearly as complicated and expensive as a fusion reactor itself would be. Proper materials testing will not be possible in → ITER, and a proposed materials testing facility, IFMIF, was still at the design stage in 2005.

The material of the plasma facing components (PFC) is a special problem. The PFC do not have to withstand large mechanical loads, so neutron damage is much less of an issue. They do have to withstand extremely large thermal loads, up to 10 MW/m², which is a difficult but solvable problem. Regardless of the material chosen, the heat flux can only be accommodated without melting if the distance from the front surface to the coolant is not more than a centimeter or two. The primary issue is the interaction with the plasma. One can choose either a low-Z material, typified by graphite although for some purposes beryllium might be chosen, or a high-Z material, usually tungsten with molybdenum as a second choice. Use of liquid metals (lithium, gallium, tin) has also been proposed, e.g., by injection of 1-5 mm thick streams flowing at 10 m/s on solid substrates.

If graphite is used, the gross erosion rates due to physical and chemical sputtering would be many meters per year, so one must rely on redeposition of the sputtered material. The location of the redeposition will not exactly coincide with the location of the sputtering, so one is still left with erosion rates that may be prohibitive. An even larger problem is the tritium co-deposited with the redeposited graphite. The tritium inventory in graphite layers and dust in a reactor could quickly build up to many kilograms, representing a waste of resources and a serious radiological hazard in case of an accident. The consensus of the fusion community seems to be that graphite, although a very attractive material for fusion experiments, cannot be the primary PFC material in a commercial reactor.

The sputtering rate of tungsten can be orders of magnitude smaller than that of carbon, and tritium is not so easily incorporated into redeposited tungsten, making this a more attractive choice. On the other hand, tungsten impurities in a plasma are much more damaging than carbon impurities, and self-sputtering of tungsten can be high, so it will be necessary to ensure that the plasma in contact with the tungsten is not too hot (a few tens of eV rather than hundreds of eV). Tungsten also has disadvantages in terms of eddy currents and melting in off-normal events, as well as some radiological issues.

Economics

It is unclear whether nuclear fusion will be economically competitive with other forms of power. The many estimates that have been made of the cost of fusion power cover a wide range, and indirect costs of and subsidies for fusion power and its alternatives make any cost comparison difficult. The low estimates for fusion appear to be competitive with but not drastically lower than other alternatives. The high estimates are several times higher than alternatives.

While fusion power is still in early stages of development, substantial sums have been and continue to be invested in research. In the EU almost € 10 billion was spent on fusion research up to the end of the 1990s, and the new → ITER reactor alone is budgeted at € 10 billion. It is estimated that up to the point of possible implementation of electricity generation by nuclear fusion, R&D will need further promotion totalling around € 60-80 billion over a period of 50 years or so (of which € 20-30 billion within the EU).[14] Nuclear fusion research receives € 750 million (excluding ITER funding), compared with € 810 million for all non-nuclear energy research combined,[15] putting research into fusion power well ahead of that of any single rivaling technology.

Advantages

Fusion power would provide much more energy for a given weight of fuel than any technology currently in use,[16] and the fuel itself (primarily deuterium) exists abundantly in the Earth's ocean: about 1 in 6500 hydrogen atoms in seawater is deuterium.[17] Although this may seem a low proportion (about 0.015%), because nuclear fusion reactions are so much more energetic than chemical combustion and seawater is easier to access and more plentiful than fossil fuels, some experts estimate that fusion could supply the world's energy needs for millions of years.[18] [19]

An important aspect of fusion energy in contrast to many other energy sources is that the cost of production is inelastic. The cost of wind energy, for example, goes up as the optimal locations are developed first, while further generators must be sited in less ideal conditions. With fusion energy, the production cost will not increase much, even if large numbers of plants are built. It has been suggested that even 100 times the current energy consumption of the world is possible.

Some problems which are expected to be an issue in this century such as fresh water shortages can actually be regarded merely as problems of energy supply. For example, in desalination plants, seawater can be purified through distillation or reverse osmosis. However, these processes are energy intensive. Even if the first fusion plants are not competitive with alternative sources, fusion could still become competitive if large scale desalination requires more power than the alternatives are able to provide.

Despite being technically non-renewable, fusion power has many of the benefits of long-term renewable energy sources (such as being a sustainable energy supply compared to presently-utilized sources and emitting no greenhouse gases) as well as some of the benefits of the much more limited energy sources as hydrocarbons and nuclear fission (without reprocessing). Like these currently dominant energy sources, fusion could provide very high power-generation density and uninterrupted power delivery (due to the fact that it is not dependent on the weather, unlike wind and solar power).

Current status

Despite optimism dating back to the 1950s about the wide-scale harnessing of fusion power, there are still significant barriers standing between current scientific understanding and technological capabilities and the practical realization of fusion as an energy source. Research, while making steady progress, has also continually thrown up new difficulties. Therefore it remains unclear that an economically viable fusion plant is possible.[20] An editorial in New Scientist magazine opined that "if commercial fusion is viable, it may well be a century away."[20] Interestingly, a pamphlet printed by General Atomics in 1970s stated that "By the year 2000, several commercial fusion reactors are expected to be on-line."

Several fusion D-T burning tokamak test devices have been built (TFTR, JET), but these were not built to produce more thermal energy than electrical energy consumed. Despite research having started in the 1950s, no commercial fusion reactor is expected before 2050. The → ITER project is currently leading the effort to commercialize fusion power.

A recent paper, published January 2009 and part of the IAEA Fusion Conference Proceedings at Geneva last October, claims that small 50 MW Tokamak style reactors are feasible.[21]

See also

- Inertial confinement fusion
- Magnetic confinement fusion
- Electrostatic confinement fusion
- Polywell
- Dense Plasma Focus
- Cold fusion
- Bubble fusion
- Sonoluminescence
- Low-carbon economy
- List of emerging technologies

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External links

- Fusion as an Energy Source (http://www.iop.org/activity/policy/Publications/file_31695.pdf)– A guide from the Institute of Physics
- U.S. Fusion Energy Science Program (http://www.ofes.fusion.doe.gov/)
- Latest Fusion Energy Research News (http://www.whatsnextnetwork.com/technology/index.php?s=fusion+energy&sentence=AND&submit=Search)
- EURATOM/UKAEA Fusion Association (http://www.fusion.org.uk/)
- ITER (http://www.iter.org)
- FIRE (http://fire.pppl.gov)
- FUSION FAQ (http://fusedweb.llnl.gov/faq.html)
- European Fusion Development Agreement (http://www.efda.org)
- Fusion Power Associates (http://fusionpower.org/) A Washington, DC area lobbying organization; "a non-profit, tax-exempt research and educational foundation, providing timely information on the status of fusion development." Edits the *Journal of Fusion Energy*.
- Plasma/Fusion Glossary (http://fusedweb.pppl.gov/Glossary/glossary.html)
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ITER

ITER (originally the **International Thermonuclear Experimental Reactor**) is an international tokamak (magnetic confinement fusion) research/engineering project that could help to make the transition from today's studies of plasma physics to future electricity-producing → fusion power plants. It builds on research done with devices such as DIII-D, EAST, KSTAR, TFTR, ASDEX Upgrade, Joint European Torus, JT-60, Tore Supra and T-15.

On November 21, 2006, the seven participants formally agreed to fund the creation of a nuclear fusion reactor.[1] The program is anticipated to last for 30 years — 10 for construction, and 20 of operation. ITER was originally expected to cost approximately €10bn (£9bn), but the rising price of raw materials and changes to the initial design may see that amount double.[2] The reactor is expected to take nearly 10 years to build and is scheduled to be switched on in 2018.[2] If completed, ITER would be one of the most expensive modern technoscientific megaprojects. Site preparation has begun in Cadarache, France and procurement of large components has started.[3]

ITER is designed to produce approximately 500 MW (500,000,000 watts) of fusion power sustained for up to 1,000 seconds[4] (compared to JET's peak of 16 MW for less than a second) by the fusion of about 0.5 g of deuterium/tritium mixture in its approximately 840 m^3 reactor chamber. Although ITER is expected to produce (in the form of heat) 5-10 times more energy than the amount consumed to heat up the plasma to fusion temperatures, the generated heat will not be used to generate any electricity.

According to the ITER consortium, fusion power offers the potential of "environmentally benign, widely applicable and essentially inexhaustible"[5] electricity, properties that they believe will be needed as world energy demands increase while simultaneously greenhouse gas emissions must be reduced.[6]

ITER was originally an acronym for ***I****nternational* ***T****hermonuclear* ***E****xperimental* ***R****eactor*, but that title was dropped due to the negative popular connotation of "thermonuclear," especially when in conjunction with "experimental". "Iter" also means "journey", "direction" or "way" in Latin[7] , reflecting ITER's potential role in harnessing → nuclear fusion as a peaceful power source.

Objectives

ITER's mission is to demonstrate feasibility in nuclear power, and prove that it can work without negative impact.[8] Specifically, this includes:

- To momentarily produce ten times more thermal energy from fusion heating than is supplied by auxiliary heating (a *Q* value of 10).
- To produce a steady-state plasma with a *Q* value greater than 5.
- To maintain a fusion pulse for up to eight minutes.
- To ignite a 'burning' (self-sustaining) plasma.
- To develop technologies and processes needed for a fusion power plant — including superconducting magnets and remote handling (maintenance by robot).
- To verify tritium breeding concepts.
- To refine neutron shield/heat conversion technology (most of energy in the D+T fusion reaction is released in the form of fast neutrons).

Reactor overview

See also: → Nuclear fusion

When deuterium and tritium fuse, two nuclei come together to form a helium nucleus (an alpha particle), and a high-energy neutron.

$$^2_1\mathrm{H} + ^3_1\mathrm{H} \rightarrow ^4_2\mathrm{He} + ^1_0\mathrm{n} + 17.6\ \mathrm{MeV}$$

While in fact nearly all stable isotopes lighter on the periodic table than iron will fuse with some other isotope and release energy, deuterium and tritium are by far the most attractive for energy generation as they require the lowest activation energy (thus lowest temperature) to do so.

All proto- and mid-life stars radiate enormous amounts of energy generated by fusion processes. Mass for mass, the deuterium-tritium fusion process releases roughly three times as much energy as uranium 235 fission, and millions of times more energy than a chemical reaction such as the burning of coal. It is the goal of a fusion power plant to harness this energy to produce electricity.

The activation energy for fusion is so high because the protons in each nucleus will tend to strongly repel one another, as they each have the same positive charge. A heuristic for estimating reaction rates is that nuclei must be able to get within 100 femtometer (1×10^{-13} meter) of each other, where the nuclei are increasingly likely to undergo quantum tunnelling past the electrostatic barrier and the turning point where the strong nuclear force and the electrostatic force are equally balanced, allowing them to fuse. In ITER, this distance of approach is made possible by high temperatures and magnetic confinement. High temperatures give the nuclei enough energy to overcome their electrostatic repulsion (see Maxwell-Boltzmann distribution). For deuterium and tritium, the optimal reaction rates occur at temperatures on the order of 100,000,000 K. The plasma is heated to a high temperature by ohmic heating (running a current through the plasma). Additional heating is applied using neutral beam injection (which cross magnetic field lines without a net deflection and will not cause a large electromagnetic disruption) and radio frequency (RF) or microwave heating.

At such high temperatures, particles have a vast kinetic energy, and hence velocity. If unconfined, the particles will rapidly escape, taking the energy with them, cooling the plasma to the point where net energy is no longer produced. A successful reactor would need to contain the particles in a small enough volume for a long enough time for much of the plasma to fuse. In ITER and many other magnetic confinement reactors, the plasma, a gas of charged particles, is confined using magnetic fields. A charged particle moving through a magnetic field experiences a force perpendicular to the direction of travel, resulting in centripetal acceleration, thereby confining it to move in a circle.

A solid confinement vessel is also needed, both to shield the magnets and other equipment from high temperatures and energetic photons and particles, and to maintain a near-vacuum for the plasma to populate. The containment vessel is subjected to a barrage of very energetic particles, where electrons, ions, photons, alpha particles, and neutrons constantly bombard it and degrade the structure. The material must be designed to endure this environment so that a powerplant would be economical. Tests of such materials will be carried out both at ITER and at IFMIF (International Fusion Materials Irradiation Facility).

Once fusion has begun, high energy neutrons will radiate from the reactive regions of the plasma, crossing magnetic field lines easily due to charge neutrality (see neutron flux).

Since it is the neutrons that receive the majority of the energy, they will be ITER's primary source of energy output. Ideally, alpha particles will expend their energy in the plasma, further heating it.

Beyond the inner wall of the containment vessel one of several test blanket modules will be placed. These are designed to slow and absorb neutrons in a reliable and efficient manner, limiting damage to the rest of the structure, and breeding tritium from lithium and the incoming neutrons for fuel. Energy absorbed from the fast neutrons is extracted and passed into the primary coolant. This heat energy would then be used to power an electricity-generating turbine in a real power plant; however, in ITER this heat is not of scientific interest, and will be extracted and disposed.

History

ITER began in 1985 as a collaboration between the European Union (through EURATOM), the USA, the then Soviet Union and Japan. Conceptual and engineering design phases led to an acceptable, detailed design in 2001, underpinned by 650 million USD worth of research and development by the "ITER Parties" to establish its practical feasibility. These parties (with the Russian Federation replacing the Soviet Union and with the USA opting out of the project in 1999 and returning in 2003) were joined in negotiations on the future construction, operation and decommissioning of ITER by Canada (who then terminated their participation at the end of 2003), the People's Republic of China, and the Republic of Korea. India officially became part of ITER on 6 December 2005. The project is expected to cost about 5 billion EUR (7.6 billion USD) over its thirty year life .

On 28 June 2005, it was officially announced that ITER will be built in the European Union in Southern France. The negotiations that led to the decision ended in a compromise between the EU and Japan, in that Japan was promised 20 percent of the research staff on the French location of ITER, as well as the head of the administrative body of ITER. In addition, another research facility for the project will be built in Japan, and the European Union has agreed to contribute about 50% of the costs of this institution.[9]

On November 21 2006, an international consortium signed a formal agreement to build the reactor.[10]

On September 24, 2007, the People's Republic of China became the seventh party who had deposited the ITER Agreement to the IAEA.

On October 24, 2007, the ITER Agreement entered into force and the ITER Organization legally came into existence.

ITER will run in parallel with a materials test facility, the International Fusion Materials Irradiation Facility (IFMIF), which will develop materials suitable for use in the extreme conditions that will be found in future fusion power plants. Both of these will be followed by a demonstration power plant, DEMO, which would generate electricity. DEMO would be the first to produce electric energy for commercial use.

A "fast track" plan to a commercial fusion power plant has been sketched out.[11] This scenario, which assumes that ITER continues to demonstrate that the tokamak line of magnetic confinement is the most promising for power generation, anticipates a full-scale power plant coming on-line in 2050, potentially leading to a large-scale adoption of fusion power over the following thirty years.

Technical design

Selected facts: The central solenoid coil will use superconducting niobium-tin, to carry 46 kA and produce a field of 13.5 teslas. The 18 toroidal field coils will also use niobium-tin. At maximum field of 11.8 T they will store 41 GJ. They have been tested at a record 80 kA. Other lower field ITER magnets (PF and CC) will use niobium-titanium.

Location

Location of Cadarache, France, EU

The process of selecting a location for ITER was long and drawn out. The most likely sites were Cadarache in Provence-Alpes-Côte-d'Azur, France and Rokkasho, Aomori, Japan. Additionally, Canada announced a bid for the site in Clarington in May 2001, but withdrew from the race in 2003. Spain also offered a site at Vandellòs on 17 April 2002, but the EU decided to concentrate its support solely behind the French site in late November 2003. From this point on, the choice was between France and Japan.

On 3 May 2005, the EU and Japan agreed to a process which would settle their dispute by July.

At the final meeting in Moscow on 28 June 2005, the participating parties agreed on the site in Cadarache in Provence-Alpes-Côte-d'Azur, France.

Construction of the ITER complex began in 2008, while assembly of the tokamak itself is scheduled to begin in the year 2011.[12]

Participants

Currently there are seven national and supranational parties participating in the ITER program: the European Union (EU), India, Japan, People's Republic of China, Russia, South Korea, and the USA.[13] Portugal, a member of the EU, aims to include Brazil in the project via an agreement between the governments of both countries.[14]

Canada was previously a full member, but has since pulled out due to a lack of funding from the Federal government. The lack of funding also resulted in Canada withdrawing from its bid for the ITER site in 2003.

It was announced that participants in the ITER will consider Kazakhstan's offer to join the program.[15]

Funding

As it stands now, the proposed costs for ITER are € 5 billion for the construction, maintenance and the research connected with it during its lifetime. At the June 2005 conference in Moscow the participating members of the ITER cooperation agreed on the following division of funding contributions: 50% by the hosting member, the European Union and 10% by each non-hosting member.[16] According to sources at the ITER meeting at Jeju, Korea, the six non-host partners will now contribute 6/11th of the total cost — a little over half — while EU will put in the rest. As for the industrial contribution, China, India, Korea, Russia, and the U.S. will contribute 1/11th each, Japan 2/11th, and EU 4/11th.[17]

Although Japan's financial contribution as a non-hosting member is 1/11th of the total, the EU agreed to grant it a special status so that Japan will provide for 2/11th of the research staff at Cadarache and be awarded 2/11th of the construction contracts, while the European Union's staff and construction components contributions will be cut from 5/11th to 4/11th.

In December 2007, the United States zeroed funding for ITER in fiscal year 2008.[18]

Criticism

Jan Vande Putte of Greenpeace International said that "Governments should not waste our money on a dangerous toy which will never deliver any useful energy". "Instead, they should invest in renewable energy which is abundantly available, not in 2080 but today."[19]

A French association including about 700 anti-nuclear groups, Sortir du nucléaire (Get Out of Nuclear Energy), claimed that ITER was a hazard because scientists did not yet know how to manipulate the high-energy deuterium and tritium hydrogen isotopes used in the fusion process.[20]

The ITER project confronts numerous technically challenging issues. French physicist Sébastien Balibar, director of research at the CNRS said "We say that we will put the sun into a box. The idea is pretty. The problem is, we don't know how to make the box".[21] [22]

A technical concern is that the 14 MeV neutrons produced by the fusion reactions will damage the materials from which the reactor is built.[23] Research is in progress to determine how and/or if reactor walls can be designed to last long enough to make a commercial power plant economically viable in the presence of the intense neutron bombardment. The damage is primarily caused by high energy neutrons knocking atoms out of their normal position in the crystal lattice. A related problem for a future commercial fusion power plant is that the neutron bombardment will induce radioactivity in the reactor itself. Maintaining and decommissioning a commercial reactor may thus be difficult and expensive. Another problem is that superconducting magnets are damaged by neutron fluxes. A new special research facility is planned for this activity, IFMIF.

Rebecca Harms, Green/EFA member of the European Parliament's Committee on Industry, Research and Energy, said: "In the next 50 years nuclear fusion will neither tackle climate change nor guarantee the security of our energy supply." Arguing that the EU's energy research should be focused elsewhere, she said: "The Green/EFA group demands that these funds be spent instead on energy research that is relevant to the future. A major focus should now be put on renewable sources of energy." French Green party lawmaker Noël Mamère claims that more concrete efforts to fight present-day global warming will be neglected as a result of ITER: "This is not good news for the fight against the greenhouse effect because we're going to put ten billion euros towards a project that has a term of 30-50 years when we're not even sure it will be effective."[24]

A number of fusion researchers working on non-tokamak systems, such as Robert Bussard and Eric Lerner, have been critical of ITER for diverting funding that they believe could be used for their potentially more reasonable and/or cost effective fusion power plant designs.[25] [26] Criticisms levied often revolve around claims of the unwillingness by ITER researchers to face up to potential problems (both technical and economic) due to the dependence of their jobs on the continuation of tokamak research.[25] An informal overview of the last decade of work was presented at the 57th International Astronautical Congress in October 2006.[27]

Response to criticism

Proponents believe that much of the ITER criticism is misleading and inaccurate, in particular the allegations of the experiment's "inherent danger." The stated goals for a commercial fusion power station design are that the amount of radioactive waste produced be hundreds of times less than that of a fission reactor, that it produce no long-lived radioactive waste, and that it is impossible for any fusion reactor to undergo a large-scale runaway chain reaction. This is because direct contact with the walls of the reactor would contaminate the plasma, cooling it down immediately and stopping the fusion process. Besides which, the amount of fuel planned to be contained in a fusion reactor chamber (one half gram of deuterium/tritium fuel[28]) is only enough to sustain the reaction for an hour at maximum,[29] whereas a fission reactor usually contains several years' worth of fuel.[30] In case of accident (or intentional act of terrorism) a fusion reactor releases far less radioactive pollution than an ordinary fission nuclear plant. Besides, tritium, being lighter than air, would rise up into the stratosphere and dilute to concentrations whereby the radiation released would be far below the natural background radioactivity of air. Proponents note that large-scale fusion power — if it works — will be able to produce reliable electricity on demand and with virtually zero pollution (no gaseous CO_2 / SO_2 / NO_x by-products are produced).

According to researchers at a demonstration reactor in Japan, a fusion generator should be feasible in the 2030s and no later than the 2050s. Japan is pursuing its own research program with several operational facilities exploring different aspects of practicability.[31]

In the United States alone, electricity accounts for US$210 billion in annual sales.[32] Asia's electricity sector attracted US$93 billion in private investment between 1990 and 1999.[33] These figures take into account only current prices. With petroleum prices widely expected to rise, political pressure on carbon production, and steadily increasing demand, these figures will undoubtedly also rise. Proponents contend that an investment in research now should be viewed as an attempt to earn a far greater future return for the economy. Also, worldwide investment of less than US$1 billion per year into ITER is not incompatible with concurrent research into other methods of power generation.

Contrary to criticism, proponents of ITER assert that there are significant employment benefits associated with the project. ITER will provide employment for hundreds of physicists, engineers, material scientists, construction workers and technicians in the short term, and if successful, will lead to a global industry of fusion-based power generation.

Supporters of ITER emphasize that the only way to convincingly prove ideas for withstanding the intense neutron flux is to experimentally subject materials to that flux — one of the primary missions of ITER and the IFMIF,[34] and both facilities will be of vital importance to the effort due to the differences in neutron power spectra between a real D-T burning plasma and the spectrum to be produced by IFMIF.[35] The purpose of ITER is to explore the scientific and engineering questions surrounding fusion power plants, such that it may be possible to build one intelligently in the future. It is nearly impossible to get satisfactory theoretical results regarding the properties of materials under an intense energetic neutron flux, and burning plasmas are expected to have quite different properties from externally heated plasmas. The point has been reached, according to supporters, where answering these questions about fusion reactors by experiment (via ITER) is an economical research investment, given the monumental potential benefit.

Furthermore the main line of research—the tokamak—has been developed to the point that it is now possible to undertake the penultimate step in magnetic confinement plasma physics research—the investigation of ‘burning’ plasmas in which the vast majority of the heating is provided by the fusion event itself. A detailed engineering design, has been developed for a tokamak experiment which would explore burning plasma physics and integrate reactor relevant technology. In the tokamak research program, recent advances in controlling the internal configuration of the plasma have led to the achievement of substantially improved energy and pressure confinement in tokamaks—the so-called ‘advanced tokamak’ modes—which reduces the projected cost of electricity from tokamak reactors by a factor of two to a value only about 50% more than the projected cost of electricity from advanced light-water reactors. In parallel, progress in the development of advanced, low activation structural materials supports the promise of environmentally benign fusion reactors, and research into alternate confinement concepts is yielding promise of future improvements in confinement.[36]

Finally, supporters point out that other potential replacements to the current use of fossil fuel sources have environmental issues of their own. Solar, wind, and hydroelectric power all have a relatively low power output per square kilometer compared to ITER's successor DEMO which, at 2000 MW,[37] should have an energy density that exceeds even large fission power plants [38]

Assessment of the vacuum vessel

ITER has decided to ask AIB-Vinçotte International (an inspection organisation located in Belgium and accredited by the French Nuclear Authorities ASN) to assess the confinement(vacuum) vessel, heart of the project, following the French Nuclear Regulatory requirements.

The Vacuum Vessel is the central part of the ITER machine: a double walled steel container in which the plasma is contained by means of magnetic fields.

The ITER Vacuum Vessel will be the biggest fusion furnace ever built. It will be twice as large and 16 times as heavy as any previously manufactured fusion vessel: each of the nine torus shaped sectors will weigh between 390 and 430 tonnes.[39] When all the shielding and port structures are included, this adds up to a total of 5,116 tonnes. Its external diameter will measure 19.4 m, the internal 6.5 m. Once assembled, the whole structure will be 11.3 m high.

The primary function of the Vacuum Vessel is to provide a hermetically sealed plasma container. Its main components are the main vessel, the port structures and the supporting system. The main vessel is a double walled structure with poloidal and toroidal stiffening ribs between 60 mm thick shells to reinforce the vessel structure. These ribs also form the flow passages for the cooling water. The space between the double walls will be filled with shield structures made of austenitic stainless steel which is corrosion resistant and does not conduct heat well. The inner surfaces of the vessel will be covered with blanket modules. These modules will provide shielding from the high-energy neutrons produced by the fusion reactions and some will also be used for tritium breeding concepts.

The Vacuum Vessel has 18 upper, 17 equatorial and 9 lower ports that will be used for remote handling operations, diagnostic systems, neutral beam injections and vacuum pumping.

Similar Projects

Other fusion reactor designs could also be potential sources of energy in the future. DEMO,[40] Wendelstein 7-X[41] , NIF[42] , HiPER[43] , the International Fusion Materials Irradiation Facility,[44] and JET[45] are several of them.

See also

- → Fusion power
- Nuclear power in France

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External links

- ITER home page (http://www.iter.org/), includes pictures and diagrams available to use for educational purposes
  - ITER Design (http://www.iter.org/pdfs/ITER_Design_Phase.pdf) Thorough overview of entire project
  - Beyond ITER (http://www.iter.org/Future-beyond.htm) The timescale to a commercial fusion power plant by 2050.
  - ITER Technical Objectives (http://www.iter.org/reduced.htm)
- French Government ITER page (http://www.iter.gouv.fr/index.php)
- ITER website in Belgium (http://www.iterbelgium.be/en/iter-belgium)
- CEA ITER page (http://www-fusion-magnetique.cea.fr/gb/index.html)

- Commission particulière du débat public Projet ITER (French site) (http://www.debatpublic-iter.org/)
- EFDA home page (http://www.efda.org/)
- IFMIF home page (http://www.frascati.enea.it/ifmif/).
- FIRE home page (http://fire.pppl.gov), with current news on ITER and other burning plasma developments
- Princeton Plasma Physics Laboratory (http://www.pppl.gov)
- The Fast Track To Fusion Power (http://vmsstreamer1.fnal.gov/VMS_Site_03/Lectures/Colloquium/050428Smith/index.htm) by Chris Llewellyn Smith of the UK Atomic Energy Authority
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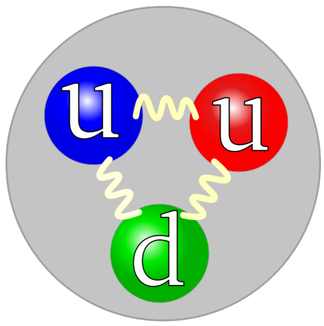
Geographical coordinates: 43°41′15″N 5°45′42″E

Quarks

A **quark** (pronounced /ˈkwɔrk/ or English pronunciation: /ˈkwɑrk/) is an elementary particle and a fundamental constituent of matter. Quarks combine to form composite particles called hadrons, the best-known of which are protons and neutrons. They are the only particles in the Standard Model to experience the strong interaction in addition to the three other fundamental interactions, also known as *fundamental forces*.[1] Due to a phenomenon known as *color confinement*, quarks are never in isolation; they can only be found within hadrons.[2] [3] For this reason, much of what is known about quarks has been drawn from observations of the hadrons themselves.



A proton, composed of two up quarks and one down quark

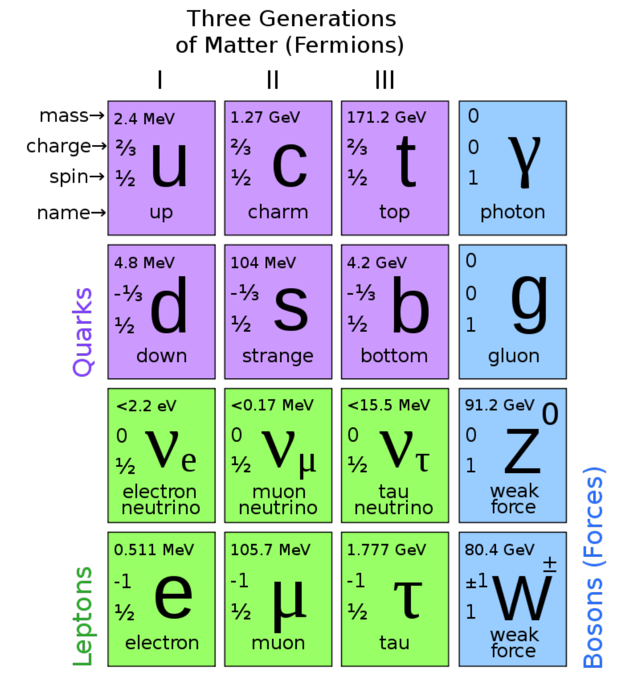
There are six different types of quarks, known as *flavors*: up (symbol: u), down (d), charm (c), strange (s), top (t) and bottom (b).[4] Up and down quarks have the lowest masses of all quarks, and thus are generally stable and very common in the universe. The other quarks are much more massive, and will rapidly decay into the lighter up and down quarks. Because of this, the heavier charm, strange, top and bottom quarks can only be produced in high energy collisions, such as in particle accelerators and in collisions involving cosmic rays.

Quarks have various intrinsic properties, including electric charge, color charge, spin and mass. For every quark flavor there is a corresponding type of antiparticle, called *antiquark*, that differs from the quark only in that some of its properties have the opposite sign. Quarks are the only known elementary particles whose electric charge comes in fractions of the elementary charge.

The quark model was independently proposed by physicists Murray Gell-Mann and George Zweig in 1964.[5] Quarks were originally introduced as part of an ordering scheme for hadrons, and there was little evidence for their actual physical existence until 1968, when electron–proton scattering experiments indicated that the electrons were scattering off three point-like constituents inside the proton.[6] [7] All six flavors of quark have now been observed; the top quark was the last to be detected and was first observed at Fermilab in 1995.[5]

Classification

The Standard Model is the theoretical framework describing all the currently known elementary particles, plus the unobserved Higgs boson.[8] This model contains six flavors of quarks, named *up*, *down*, *charm*, *strange*, *top* and *bottom*.[9] [4] The top and bottom flavors are sometimes known as *truth* and *beauty*, respectively.[10] Antiparticles of quarks are called *antiquarks*, and are denoted by a bar over the symbol for the corresponding quark, such as u for an up antiquark. As with antimatter in general, antiquarks have the same mass, lifetime and spin as their respective quarks, but the electric charge and other charges have the opposite sign.[11]



Six of the particles in the Standard Model are quarks (shown in purple). Each of the first three columns form a *generation* of matter.

Quarks are fermions, meaning that their spin quantum number is a half-integer (more specifically, $^1\!/_2$ for quarks); according to the spin-statistics theorem, this implies that they are subject to the Pauli exclusion principle, which states that no two identical fermion [12] can simultaneously occupy the same quantum state. This is in contrast to bosons (particles with integer spin), of which any number can be in the same state.[13] Quarks, unlike leptons, have a color charge, which allows them to engage in the strong interaction.

Elementary fermions are grouped into three generations, each comprising two leptons and two quarks. The first generation includes up and down quarks, the second charm and strange quarks, and the third top and bottom quarks. All searches for a fourth generation of quarks and other elementary fermions have failed,[14] [15] and there is strong indirect evidence that more than three generations do not exist.[16] [17] [18] [19] Particles in higher generations generally have greater mass and lesser stability, tending to decay into lower-generation, less massive particles by means of weak interactions. Only first-generation up and down quarks occur commonly in nature – heavier can only be created in high-energy collisions (such as in those involving cosmic rays) and decay quickly. These particles were probably more prominent in earlier, hotter phases of cosmic evolution. Most studies conducted on heavier quarks have been performed in artificially created conditions, such as in particle accelerators.[20]

Attractions between different quarks result in the formation of composite particles known as *hadrons*. The color charge in quarks and the resulting strong interaction is integral to this process of *hadronization* (see Strong interaction and color charge below). There are two types of hadrons: baryons, formed of three quarks, and mesons, formed of a quark and an antiquark.[21] The quarks which determine the quantum numbers of hadrons are called *valence quarks*. Apart from these, any hadron may contain an indefinite number of virtual (or "sea") quarks, antiquarks and gluons which do not influence their quantum numbers.[22]

The building blocks of the atomic nucleus—the proton and the neutron—are baryons.[4] [23] A great number of hadrons are known (see List of baryons and List of mesons), most of them differentiated by their quark content and the properties these constituent quarks confer.[10] The existence of "exotic" hadrons with more valence quarks, such as tetraquarks (qqqq) and pentaquarks (qqqqq), has been postulated.[24] [25] Several experiments claimed to have proven the existence of tetraquarks and pentaquarks in the early 2000s;[26] but, while the status of tetraquarks is still a matter of debate,[26] all the reported pentaquark candidates have been established as being non-existent since.[27]

Having electric charge, flavor, color charge and mass, quarks are the only known elementary particles that engage in all four fundamental interactions of contemporary physics: electromagnetism, weak interaction, strong interaction and gravitation.[23] Gravitation, however, is usually irrelevant at subatomic scales, and is not described by the Standard Model.

See the table of properties below for a more complete analysis of the six quark flavors' properties.

History

The quark model was independently postulated by physicists Murray Gell-Mann[28] and George Zweig[29] [30] in 1964,[5] shortly after Gell-Mann's early 1960s formulation of a particle classification system known as the *Eightfold Way* – or in more technical terms, SU(3) flavor symmetry. Israeli physicist Yuval Ne'eman had independently developed a similar theory to the Eightfold Way in 1962, but played no part in the subsequent postulation of the quark theory. At the time of the quark theory's inception, the "particle zoo" consisted of a few leptons and a multitude of hadrons. Partially as a result of Gell-Mann and Ne'eman's model, Gell-Mann and Zweig posited that hadrons were not elementary particles, but were instead composed of combinations of quarks and antiquarks.[31] Their

Murray Gell-Mann in 2007. Gell-Mann and George Zweig proposed the quark model in 1964.

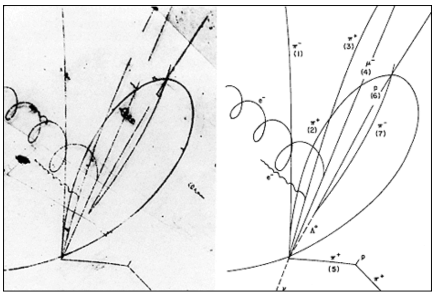
model involved three flavors of quarks—up, down and strange—to which they ascribed properties such as spin and electric charge.[28] [29] [30]

The initial reaction of the physics community to the proposal was mixed. There was particular contention about whether the quark was a physical entity, or an abstraction used to explain certain concepts that were not well understood at the time.[32]

In less than a year, extensions to the Gell-Mann–Zweig model were proposed when another duo of physicists, Sheldon Lee Glashow and James Bjorken, predicted the existence of a fourth flavor of quark, which they referred to as *charm*. The addition was proposed because it allowed a better description of the weak interaction (the mechanism that allows quarks to decay), equalized the number of known quarks with the number of known leptons, and implied a mass formula that correctly reproduced the masses of the known mesons.[33]

In 1968, deep inelastic scattering experiments at the Stanford Linear Accelerator Center (SLAC) showed that the proton was not an elementary particle, but instead contained much smaller, point-like objects.[6] [7] [34] While this proved that hadrons indeed had a substructure, as predicted by the quark model, physicists remained reluctant to identify these smaller objects with quarks. Instead, they became known as partons (a term proposed by Richard Feynman, and also used by some experimental project reports).[35] [36] [37] The objects that were observed at the SLAC would later be identified as up and down quarks as the other flavors began to surface. Their discovery validated the existence of the strange quark, because it was necessary to the model Gell-Mann and Zweig had proposed.[38]

In a 1970 paper, Glashow, John Iliopoulos and Luciano Maiani gave more compelling theoretical arguments for the as-yet undiscovered charm quark.[39] [40] The number of supposed quark flavors grew to the current six in 1973, following extensions to the quark model from Makoto Kobayashi and Toshihide Maskawa; the two had noted that the experimental observation of CP violation[41] could be explained if there were another pair of quarks, which were eventually named *top* and *bottom*.[42] [43]


1974 discovery photograph of a possible charmed baryon, now identified as the Σ++c baryon

It was the observation of the charm quark that finally convinced the physics community of the quark model's validity.[37] Following a decade without empirical evidence supporting their existence, charm quarks were produced and observed almost simultaneously by two teams in November 1974 (see November Revolution)—one at the Stanford Linear Accelerator Center under Burton Richter, and one at Brookhaven National Laboratory under Samuel Ting. The two parties had assigned the discovered particle two different symbols, J and ψ. The particle thus became formally known as the J/ψ meson and was found to be the charm quark–charm antiquark pair that Glashow and Bjorken had predicted.[31]

In 1977, the bottom quark was observed by Leon Lederman and a team at Fermilab.[5] This was a strong indicator of the top quark's existence; without the top quark, the bottom quark would have been without a partner. However, it was not until eighteen years later, in 1995, that the top quark was finally observed,[5] with a mass much greater than had been expected at the time its existence had been postulated[44] —almost as heavy as a gold atom. Reasons for the top quark's extremely large mass remain unclear.[45]

Etymology

Gell-Mann originally named the quark after the sound made by ducks.[46] For some time, he was undecided on an actual spelling for the term he intended to coin, until he found the word *quark* in James Joyce's book *Finnegans Wake*:

> Three quarks for Muster Mark!
> Sure he has not got much of a bark
> And sure any he has it's all beside the mark.
>
> —*James Joyce, Finnegans Wake*[47]

Gell-Mann went into further detail regarding the name of the quark in his book, *The Quark and the Jaguar*:[48]

In 1963, when I assigned the name "quark" to the fundamental constituents of the nucleon, I had the sound first, without the spelling, which could have been "kwork". Then, in one of my occasional perusals of *Finnegans Wake*, by James Joyce, I came across the word "quark" in the phrase "Three quarks for Muster Mark". Since "quark" (meaning, for one thing, the cry of the gull) was clearly intended to rhyme with "Mark", as well as "bark" and other such words, I had to find an excuse to pronounce it as "kwork". But the book represents the dream of a publican named Humphrey Chimpden Earwicker. Words in the text are typically drawn from several sources at once, like the "portmanteau" words in "Through the Looking-Glass". From time to time, phrases occur in the book that are partially determined by calls for drinks at the bar. I argued, therefore, that perhaps one of the multiple sources of the cry "Three quarks for Muster Mark" might be "Three quarts for Mister Mark", in which case the pronunciation "kwork" would not be totally unjustified. In any case, the number three fitted perfectly the way quarks occur in nature.

Zweig preferred the name *ace* for the particle he had theorized, but Gell-Mann's terminology came to prominence once the quark model had been commonly accepted.[49]

Properties

Electric charge

Quarks have fractional electric charge values, either $-\frac{1}{3}$ or $+\frac{2}{3}$ times the elementary charge (e) depending on flavor—up, charm and top quarks (collectively referred to as *up-type quarks*) have a charge of $+\frac{2}{3}$, while down, strange and bottom quarks (*down-type quarks*) have $-\frac{1}{3}$. Antiquarks have the opposite charge to their corresponding quarks: up-type antiquarks have charges of $-\frac{2}{3}$ and down-type antiquarks have charges of $+\frac{1}{3}$. Since the electric charge of a hadron is the sum of the charges of the constituent quarks, the combinations of either three quarks, three anti-quarks, or a quark and an anti-quark always result in integer charge.[50] For example, the hadron constituents of atomic nuclei, neutrons and protons, have charges of 0 and +1 respectively; the neutron is composed of two down quarks and one up quark, and the proton of two up quarks and one down quark.[23]

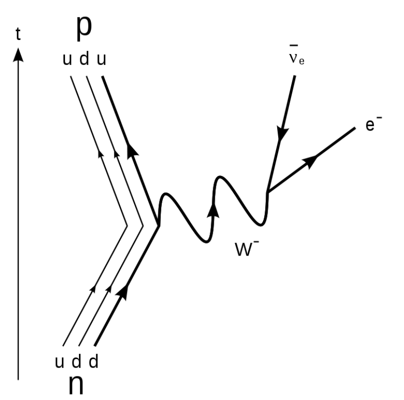
Spin

Spin is an intrinsic property of quantum particles, and its direction is an important degree of freedom. It is sometimes visualized as the rotation of an object around its own axis (hence the name *spin*), but this notion is somewhat misguided at subatomic scales because elementary particles are believed to be point-like.[51]

It can be represented by a vector whose length is measured in units of $h/(2\pi)$, where h is the Planck constant. This value is often denoted by $\hbar$ ("h bar"), and called the "reduced Planck constant". The result of a measurement of the component of the spin of a quark along any axis is always either $\hbar/2$ or $-\hbar/2$; for this reason quarks are classified as spin-$\frac{1}{2}$ particles, or fermions.[52] The component of spin along a given axis—by convention the z axis—is often denoted by an up arrow ↑ for the value $+\frac{1}{2}$ and down arrow ↓ for the value $-\frac{1}{2}$, placed after the symbol for flavor. For example, an up quark with a spin of $+\frac{1}{2}$ along the z axis is denoted by u↑.[53]

Weak interaction

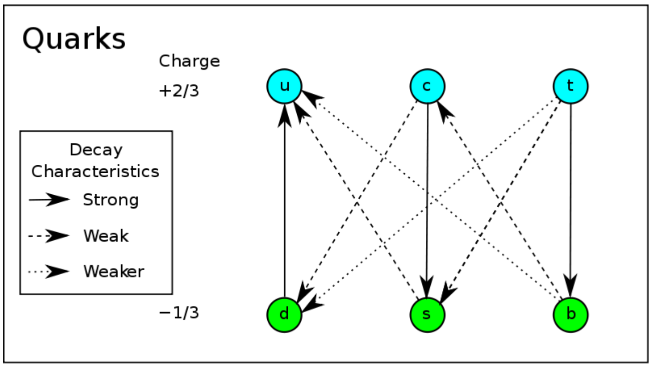
A quark of one flavor can transform into a quark of another flavor only through the weak interaction, one of the four fundamental interactions in particle physics. By absorbing or emitting a W boson, any up-type quark (up, charm, and top quarks) can change into any down-type quark (down, strange, and bottom quarks) and vice versa. This mechanism ultimately causes the radioactive process of beta decay, by which a neutron (n) "splits" into a proton (p), an electron (e^-) and an electron antineutrino (νe) (see picture). This occurs when one of the down quarks in the neutron (udd) decays into an up quark by emitting a virtual W^- boson, transforming the neutron into a proton (uud). The W^- boson then decays into an electron and an electron antineutrino.[54]



Feynman diagram of beta decay with time flowing upwards. The CKM matrix (discussed below) describes what is occurring to the left of the W boson.

n	→	$p + e^- + \nu e$	(Beta decay, hadron notation)
udd	→	$uud + e^- + \nu e$	(Beta decay, quark notation)

There is also a reverse process, called *inverse beta decay*, by which a proton (p) transforms into a neutron (n) by emitting an W^+ boson, which then decays into an antielectron (often called a *positron*) (e^+) and an electron neutrino (νe).[54] Both beta decay and inverse beta decay are routinely used in medical applications such as positron emission tomography (PET) or in high-energy experiments such as neutrino detection.



A pictorial representation of the six quarks' decay modes, with mass increasing from left to right. The "intensity" of the lines are dictated by the CKM matrix.

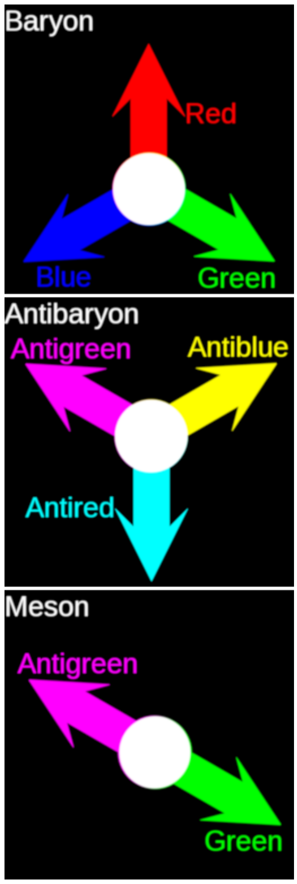
While the process by which quarks transform into one-another is the same for all quarks, each quark has a certain preference to transform into the quark of its own generation. The relative tendencies of the various transformations from quarks of one flavor to quarks of another are described in a comprehensive mathematical table called the Cabibbo–Kobayashi–Maskawa matrix (or CKM matrix). The approximate magnitudes of the entries of the CKM matrix are:[55]

$$\begin{bmatrix} |V_{\mathrm{ud}}| & |V_{\mathrm{us}}| & |V_{\mathrm{ub}}| \\ |V_{\mathrm{cd}}| & |V_{\mathrm{cs}}| & |V_{\mathrm{cb}}| \\ |V_{\mathrm{td}}| & |V_{\mathrm{ts}}| & |V_{\mathrm{tb}}| \end{bmatrix} \approx \begin{bmatrix} 0.974 & 0.226 & 0.004 \\ 0.226 & 0.973 & 0.041 \\ 0.009 & 0.041 & 0.999 \end{bmatrix},$$

where V_{ij} relates to the tendency that a quark of flavor i will change into a quark of flavor j.

There also exists an equivalent weak interaction matrix for the leptons (right side of the W boson on the above beta decay diagram), called the Pontecorvo–Maki–Nakagawa–Sakata matrix (PMNS matrix).[56] Together, the CKM and PMNS matrices keep track of everything related to the weak interaction, but the links between the two are not yet clear.[57] Some have proposed "leptoquark" particles based on the mathematical properties of these matrices,[58] but such particles remain largely theoretical.[55]

Strong interaction and color charge



All types of hadrons always have zero total color charge.

Quarks possess a property called *color charge*. There are three types of color charge, arbitrarily labeled *blue*, *green* and *red*. Each of them is complemented by an anti-color—*antiblue*, *antigreen* and *antired*. Each quark carries a color, while each antiquark carries an anticolor.[59]

The system of attraction and repulsion between quarks charged with different combinations of the three colors is called strong interaction. The area of physics that studies strong interactions is called → quantum chromodynamics (QCD). A quark charged with one color value can be bound with an antiquark carrying the corresponding anticolor, while three quarks all charged with different colors will similarly be bound together. Quarks obtain their color and interact in this way via force-mediating particles known as *gluons*; this is discussed at length below.

The three color types play a role in the process of hadronization. The result of two attracting quarks that form a stable quark–antiquark pair will be color neutrality: a quark with color charge ξ plus an antiquark with color charge $-\xi$ will result in a color charge of 0 (or "white" color) and the formation of a meson. Analogous to the additive color model in basic optics, the combination of three quarks, each with a different color charge, will similarly result in a "white" color charge and the formation of a baryon.[60]

In modern particle physics, gauge symmetries – a type of symmetry group – are used to relate interactions between particles (see gauge theories). Color SU(3) ($SU(3)_c$) is the gauge symmetry that relates the color charge in quarks and is the defining symmetry for quantum chromodynamics.[61] Because the quark colors are not uniquely defined, the designation of which colors are which is arbitrary. The differing states of quarks as represented by the three colors can be compared to the differering states of a spatial co-ordinate system as it is symmetrically rotated; such variations in quark state are related by $SU(3)_c$. Quark color transformations correspond to "rotations" in color space (which, mathematically speaking, is a complex space); these transformations are parts of the $SU(3)_c$ symmetry. $SU(3)_c$ was introduced after the discovery of color charge and the subsequent realisation that there are at least eighteen distinct types of quarks, three subtypes to each flavor.[62] Its basic multiplet is a set of three colored quarks with no defined flavors (qB, qG, qR);[63] the other members of the symmetry are fundamentally associated with this set. The quark interactions prescribed by $SU(3)_c$ require eight gluon types to act as force-carriers for the strong interaction and the color charge.[64] Moreover, the fact that $SU(3)_c$ and the color types themselves vary with conditions – that the symmetry is "local" – can be attributed to the presence of the gluon gauge boson in the symmetry group.

Mass

There are two terms used when referring to a quark's mass; *current quark mass* refers to the mass of a quark by itself, while *constituent quark mass* refers to the current quark mass plus the mass of the gluon particle field surrounding the quark.[65] These values are typically very different in their relative size, for several reasons.

In a hadron, most of the mass comes from the gluons that bind the constituent quarks together, rather than from the quarks themselves. While gluons are inherently massless, they possess energy—or, more specifically, → quantum chromodynamics binding energy (QCBE)—and it is this that contributes so greatly to the overall mass of the hadron (see mass in special relativity). For example, a proton is composed of one d and two u quarks and has an overall mass of approximately 938 MeV/c^2, of which the rest mass of three valence quarks contributes only 11 MeV/c^2; much of the remainder can be attributed to the gluons' QCBE.[] [66] [67]

The masses of most quarks were within predicted ranges at the time of their discovery, with the notable exception of the top quark, which was found to have a mass approximately equal to that of a gold nucleus, significantly heavier than expected.[68] Several theories have been offered to explain this very large mass. The Standard Model posits that elementary particles derive their masses from the Higgs mechanism, which is tied to the unobserved Higgs boson. Physicists hope that, in the next years, the detection of the Higgs boson in particle accelerators (such as the Large Hadron Collider) and the study of the top quark's interaction with the Higgs field might help answer the question.[45]

Table of properties

The following table summarizes the key properties of the six quarks. Flavor quantum numbers (isospin (I_z), strangeness (S, not to be confused with spin), charmness (C), bottomness (B') and topness (T)) are assigned to certain quark flavors, and denote qualities of quark-based systems and hadrons. The baryon number (B) is $+\frac{1}{3}$ for all quarks, as baryons are made of three quarks. For antiquarks, the electric charge (Q) and all flavor quantum numbers (B, I_z, C, S, T, and B') are of opposite sign. Mass and total angular momentum (J) do not change sign for the antiquarks.

Quark flavor properties

Name	Symbol	Mass (MeV/c^2)	J	B	Q	I_z	C	S	T	B'	Antiparticle	Antiparticle symbol
First generation												
Up	u	1.5 to 3.3	$\frac{1}{2}$	$+\frac{1}{3}$	$+\frac{2}{3}$	$+\frac{1}{2}$	0	0	0	0	Antiup	u
Down	d	3.5 to 6.0	$\frac{1}{2}$	$+\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{1}{2}$	0	0	0	0	Antidown	d
Second generation												
Charm	c	1270+70−110	$\frac{1}{2}$	$+\frac{1}{3}$	$+\frac{2}{3}$	0	+1	0	0	0	Anticharm	c
Strange	s	104+26−34	$\frac{1}{2}$	$+\frac{1}{3}$	$-\frac{1}{3}$	0	0	−1	0	0	Antistrange	s
Third generation												
Top	t	171200±2100	$\frac{1}{2}$	$+\frac{1}{3}$	$+\frac{2}{3}$	0	0	0	+1	0	Antitop	t

Bottom	b	4200+170−70	$\frac{1}{2}$	$+\frac{1}{3}$	$-\frac{1}{3}$	0	0	0	0	−1	Antibottom	b

J = spin, *B* = baryon number, *Q* = electric charge, I_z = isospin, *S* = strangeness, *C* = charmness, *B′* = bottomness, *T* = topness.

Notation like 104+26−34 denotes measurement uncertainty.

Gluons, asymptotic freedom, and color confinement

As described by quantum chromodynamics, the strong interaction between quarks is mediated by gluons, zero-rest mass quanta of a vector gauge boson field. Each gluons carries one color charge and one anticolor charge.[69] In the standard picture of particle interactions (part of a more general formulation known as perturbation theory), gluons are constantly exchanged between quarks through a virtual emission and absorption process. When a gluon is transferred between one quark and another, a color change occurs in the receiving and emitting quark;[70] [71] for example, if a red quark emits a red–antigreen gluon, it becomes green, and if a green quark absorbs a red-antigreen gluon, it becomes red.[72] Therefore, while the specific quark colors continuously change, the fact that each quark always carries a single color, and hence interacts via the strong force, is preserved.[73]

One peculiarity of quantum chromodynamics is that, since gluons themselves carry color charges, they themselves can emit and absorb other gluons. This interaction between the force carriers themselves is at the root of a number of very specific properties of the strong force. The first is known as *asymptotic freedom*: As quarks come closer to each other, the chromodynamic binding force between them weakens. That is why the early inelastic scattering experiments were able to detect the proton's three quasi-free parton quarks.

Conversely, as the distance between quarks increases, the chromodynamic binding force between them strenghtens. The color field becomes stressed, much as an elastic band is stressed when stretched, and more gluons of appropriate color are spontaneously created to strengthen the field. Above a certain threshold energy, a new quark-antiquark pair will be created. In this way, any attempt to wrench a quark from a hadron will result in the formation of further hadrons.[74] The direct consequence is known as *color confinement*: quarks cannot appear in isolation. In consequence, almost all of what is known about them has been indirectly inferred from the properties of the hadrons of which they form a part.[75] The top quark is an exception to this rule because its lifetime is so short that it does not have a chance to hadronize before decaying into lighter particles.[76]

The fact that gluons can emit gluons and exchange gluons with other gluons has led to theories regarding the possible existence of glueballs—objects that are purely made of gluons—despite previous observations indicating that gluons cannot exist without attached quarks.[77]

Sea quarks

Along with the *valence quarks* (qv) that contribute to the quantum numbers of hadrons, virtual quark–antiquark (qq) pairs known as *sea quarks* (qs) may also be found within hadrons. Such sea quarks form when a gluon splits within the hadron's color field; this process also works in reverse in that the annihilation of two sea quarks produces a gluon.[78] Sea quarks are much less stable than their valence counterparts, and they typically annihilate each other very quickly within the interior of the hadron. Despite this, sea quarks can hadronize into baryonic or mesonic particles under the right circumstances.[79] A constant flux of sea quarks are born from the vacuum, allowing for a steady cycle of gluon splits and rebirths. This flux is colloquially known as "the sea".[80]

Virtual quark–antiquark pairs have a tendency to form what can be described as a kind of "cloud" or "shield" around the valence quarks in hadrons. This cloud is complemented by another layer of virtual gluons that lies beyond it.[81] These layers adopt color charges based on that of the valence quark they surround. Quantum chromodynamics causes the virtual antiquarks in the cloud, which exhibit the anticolor of the valence quark, to be closer to the inside of the field. In the case of a red quark, for instance, the antired virtual antiquarks would tend to be closer to the red valence quark than their red virtual quark partners. This disparity in proximity and the anticolor barrier it creates has the effect of "de-amplifying" the color charge of the valence quark.[81] However, this anticolor tilt is neutralized by the virtual gluon field beyond, which carries the original color charge and "re-amplifies" the valence quark's color. The canceling of these two influences on the valence quark results in the balanced color charge that valence quarks have been observed to possess.[82]

Other phases of quark matter

Conjectures that, under sufficiently extreme conditions, quarks may become deconfined and exist as free particles, go back more than thirty years.[83] In the course of asymptotic freedom, the strong interaction becomes weaker at higher temperatures. Eventually, color confinement would be lost and an extremely dense plasma of freely moving quarks and gluons would be formed.[84] This conjectured phase of matter is called quark-gluon plasma. The exact conditions needed to give rise to this state are unknown and have been the subject of a great deal of speculation and experimentation; CERN made many attempts to produce such conditions in the 1980s and 1990s. A recent estimate puts the needed temperature at $\sim 1.90 \pm 0.02 \times 10^{12}$ K. While a state of properly free quarks and gluons has never been achieved, recent experiments at the Relativistic Heavy Ion Collider has yielded evidence for liquid-like quark matter exhibiting "nearly perfect" fluid motion.[85]

The quark-gluon plasma would be characterised by a great increase in the volume of heavier quark pairs in relation to the volume of up and down quark pairs. It is believed that in the period prior to 10^{-6} seconds after the Big Bang (the quark epoch), the universe was filled with quark–gluon plasma, as the temperature was too high for hadrons to be stable.[86]

Given sufficiently high baryon densities and relatively low temperatures, quark matter is expected to degenerate into a Fermi surface of weakly-interacting quarks. The nature of QCD and the color SU(3) imply that this surface would be characterized by a condensation of quark Cooper pairs – even though such a condensate would defy the local symmetry of $SU(3)_c$ as it is presently known. Such a phase of quark matter would be color superconductive; that is, color charge would be able to pass through it with no resistance.[87] This color superconductivity is explained by the properties of asymptotic freedom; as quark matter becomes denser, the strong interaction becomes weaker and the average interaction lengths between individual quarks become shorter.

See also

- Eightfold way (physics) – Gell-Mann's original classification of hadrons into octets
- Fundamental interactions – Processes by which elementary particles interact with each other
  - Gravitational force – Attraction between bodies with mass
    - Quantum gravity – The attempt to find a quantum theory for gravity
  - Electromagnetic force – Force that the electromagnetic field exerts on electrically charged particles
    - Quantum electrodynamics – The quantum theory of the electromagnetic force
  - Strong interaction – The interaction responsible for the formation of hadrons
    - → Quantum chromodynamics – The study of the strong interaction
  - Weak interaction – The interaction by which quarks decay into other quarks
    - Electroweak theory – The unified theory of the weak interaction and of electromagnetism
- Gauge boson – Force mediating particles
  - Gluons – Particles mediating the strong interaction
  - Gravitons – The hypothetical particles mediating the gravitational force
  - Photons – Particles mediating the electromagnetic force
  - W and Z bosons – Particles mediating the weak interaction
- Hadrons – Particles made of quarks
  - Mesons – Particles made of a quark and an antiquark
    - Quarkonium – Mesons made of a quark and antiquark of the same flavor
  - Baryons – Particles made of three quarks
    - Diquarks – A hypothetical state of two quarks grouped inside a baryon, treated as a single particle with which the third quark interacts
  - Tetraquarks – Hypothetical exotic mesons, made of two quarks and two anti quarks
  - Pentaquarks – Hypothetical exotic baryons, made of four quarks and one anti quark
- Leptons – The other fundamental particles of matter
- Partons – Model used to analyze high-energy hadron collisions
- Preons – Hypothetical particles which were once postulated to be subcomponents of quarks and leptons
- Quark–lepton complementarity – Possible fundamental relation between quarks and leptons
- Quark star – A hypothetical degenerate neutron star with extreme density

Notes

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External links

- The Top Quark And The Higgs Particle by T.A. Heppenheimer (http://books.nap.edu/books/0309048931/html/236.html) – A description of CERN's experiment to count the families of quarks.
- An elementary popular introduction (http://www.scribd.com/word/view/1025)
- The original English word *quark* and its adaptation to particle physics (http://www.bartleby.com/61/67/Q0016700.html)
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Gluons

Gluon	
Composition:	Elementary particle
Family:	Boson
Group:	Gauge boson
Interaction:	Strong interaction
Theorized:	Murray Gell-Mann (1962)[1]
Discovered:	TASSO collaboration at DESY (1979)[2] [3]
Symbol(s):	g
Types:	8
Mass:	0 MeV/c^2 (Theoretical value)[4] < 20 MeV/c^2 (Experimental limit)[5]
Electric charge:	0 e[4]
Color charge:	octet (8 types)
Spin:	1

Gluons (*glue* and the suffix *-on*) are elementary expressions of quark interaction, and are indirectly involved with the binding of protons and neutrons together in atomic nuclei.

In technical terms, they are vector gauge bosons that mediate strong color charge interactions of quarks in → quantum chromodynamics (QCD). Unlike the electric charge neutral photon of quantum electrodynamics (QED), gluons themselves carry color charge and therefore participate in the strong interaction in addition to mediating it. The gluon has the ability to do this as it carries the color charge and so interacts with itself, making QCD significantly harder to analyze than QED.

Properties

The gluon is a vector boson; like the photon, it has a spin of 1. While massive spin-1 particles have three polarization states, massless gauge bosons like the gluon have only two polarization states because gauge invariance requires the polarization to be transverse. In → quantum field theory, unbroken gauge invariance requires that gauge bosons have zero mass (experiment limits the gluon's mass to less than a few MeV). The gluon has negative intrinsic parity and zero isospin. It is its own antiparticle.

Numerology of gluons

Unlike the single photon of QED or the three W and Z bosons of the weak interaction, there are eight independent types of gluon in QCD.

This may be difficult to understand intuitively. Quarks carry three types of color charge; antiquarks carry three types of anticolor. Gluons may be thought of as carrying both color and anticolor, but to correctly understand how they are combined, it is necessary to consider the mathematics of color charge in more detail.

Color charge and superposition

In → quantum mechanics, the states of particles may be added according to the principle of superposition; that is, they may be in a "combined state" with a *probability*, if some particular quantity is measured, of giving several different outcomes. A relevant illustration in the case at hand would be a gluon with a color state described by:

$$(r\bar{b} + b\bar{r})/\sqrt{2}$$

This is read as "red-antiblue plus blue-antired." (The factor of the square root of two is required for normalization, a detail which is not crucial to understand in this discussion.) If one were somehow able to make a direct measurement of the color of a gluon in this state, there would be a 50% chance of it having red-antiblue color charge and a 50% chance of blue-antired color charge.

Color singlet states

It is often said that the stable strongly-interacting particles observed in nature are "colorless," but more precisely they are in a "color singlet" state, which is mathematically analogous to a *spin* singlet state.[6] Such states allow interaction with other color singlets, but not with other color states; because long-range gluon interactions do not exist, this illustrates that gluons in the singlet state do not exist either.[7]

The color singlet state is[8] :

$$(r\bar{r} + b\bar{b} + g\bar{g})/\sqrt{3}$$

In words, if one could measure the color of the state, there would be equal probabilities of it being red-antired, blue-antiblue, or green-antigreen.

Eight gluon colors

There are eight remaining independent color states, which correspond to the "eight types" or "eight colors" of gluons. Because states can be mixed together as discussed above, there are many ways of presenting these states, which are known as the "color octet." One commonly used list is[8] :

$(r\bar{b} + b\bar{r})/\sqrt{2}$	$-i(r\bar{b} - b\bar{r})/\sqrt{2}$
$(r\bar{g} + g\bar{r})/\sqrt{2}$	$-i(r\bar{g} - g\bar{r})/\sqrt{2}$
$(b\bar{g} + g\bar{b})/\sqrt{2}$	$-i(b\bar{g} - g\bar{b})/\sqrt{2}$
$(r\bar{r} - b\bar{b})/\sqrt{2}$	$(r\bar{r} + b\bar{b} - 2g\bar{g})/\sqrt{6}$

These are equivalent to the Gell-Mann matrices; the translation between the two is that red-antired is the upper-left matrix entry, red-antiblue is the left middle entry, blue-antigreen is the bottom middle entry, and so on. The critical feature of these particular eight states is that they are linearly independent, and also independent of the singlet state; there is no way to add any combination of states to produce any other. (It is also impossible to add them to make $r\bar{r}$, $g\bar{g}$, or $b\bar{b}$ [9] ; otherwise the forbidden singlet state could also be made.) There are many other possible choices, but all are mathematically equivalent, at least equally complex, and give the same physical results.

Group theory details

Technically, QCD is a gauge theory with SU(3) gauge symmetry. Quarks are introduced as spinor fields in N_f flavours, each in the fundamental representation (triplet, denoted **3**) of the color gauge group, SU(3). The gluons are vector fields in the adjoint representation (octets, denoted **8**) of color SU(3). For a general gauge group, the number of force-carriers (like photons or gluons) is always equal to the dimension of the adjoint representation. For the simple case of SU(N), the dimension of this representation is N^2-1.

In terms of group theory, the assertion that there are no color singlet gluons is simply the statement that → quantum chromodynamics has an SU(3) rather than a U(3) symmetry. There is no known *a priori* reason for one group to be preferred over the other, but as discussed above, the experimental evidence supports SU(3).[10]

Confinement

Since gluons themselves carry color charge, they participate in strong interactions. These gluon-gluon interactions constrain color fields to string-like objects called "flux tubes", which exert constant force when stretched. Due to this force, quarks are confined within composite particles called hadrons. This effectively limits the range of the strong interaction to 10^{-15} meters, roughly the size of an atomic nucleus. (Beyond a certain distance, the energy of the flux tube binding two quarks increases linearly. At a large enough distance, it becomes energetically more favorable to pull a quark-antiquark pair out of the vacuum rather than increase the length of the flux tube.)

Gluons also share this property of being confined within hadrons. One consequence is that gluons are not directly involved in the nuclear forces between hadrons. The force mediators for these are other hadrons called mesons.

Although in the normal phase of QCD single gluons may not travel freely, it is predicted that there exist hadrons which are formed entirely of gluons — called **glueballs**. There are also conjectures about other **exotic hadrons** in which real gluons (as opposed to virtual ones found in ordinary hadrons) would be primary constituents. Beyond the normal phase of QCD (at extreme temperatures and pressures), quark gluon plasma forms. In such a plasma there are no hadrons; quarks and gluons become free particles.

Experimental observations

The first direct experimental evidence of gluons was found in 1979 when three-jet events were observed at the electron-positron collider called PETRA at DESY in Hamburg.

Experimentally, confinement is verified by the failure of free quark searches. Free gluons have never been observed, however at Fermilab single production of top quarks has been statistically shown[11] . Although there have been hints of exotic hadrons, no glueball has been observed either. Quark-gluon plasma has been found recently at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratories (BNL).

See also

- Quark
- Hadron
- Meson
- Gauge boson
- Glueball
- Exotic hadrons
- Quark model
- → Quantum chromodynamics
- Standard model
- Three-jet events
- Deep inelastic scattering

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[7] *Griffiths*, 281 (first complete footnote)

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[12] http://pdg.lbl.gov/2004/tables/contents_tables.html

[13] http://www.desy.de/pr-info/desyhome/html/presse/glossary.html#G

[14] http://www.symmetrymag.org/cms/?pid=1000160

[15] http://math.ucr.edu/home/baez/physics/ParticleAndNuclear/gluons.html

Parton

Parton may refer to:

Physics

- Parton (particle physics), is the name for a particle

People

- Dick Parton, (d.2006), Australian rules footballer
- Dolly Parton, an American country singer, songwriter, composer, author, and actress
- James Parton, (1822-1891), American biographer
- Jim Parton, fathers' rights activist
- Julia Parton, American porn star
- Randy Parton, an American country singer and business person
- Stella Parton, an American country singer
- V. R. Parton, (1897-1974), English chessplayer

Places

- Parton, Cumbria, England
  - includes Parton railway station
- Parton, Dumfries and Galloway, Scotland
- Parton, Herefordshire, England

Quantum chromodynamics

Quantum chromodynamics (abbreviated as QCD) is a theory of the strong interaction (color force), a fundamental force describing the interactions of the quarks and gluons making up hadrons (such as the proton, neutron or pion). It is the study of the SU(3) Yang–Mills theory of color-charged fermions (the quarks). QCD is a → quantum field theory of a special kind called a non-abelian gauge theory. It is an important part of the Standard Model of → particle physics. A huge body of experimental evidence for QCD has been gathered over the years.

QCD enjoys two peculiar properties:

- **Asymptotic freedom**, which means that in very high-energy reactions, quarks and gluons interact very weakly. This prediction of QCD was first discovered in the early 1970s by David Politzer and by Frank Wilczek and David Gross. For this work they were awarded the 2004 Nobel Prize in Physics.
- **Confinement**, which means that the force between quarks does not diminish as they are separated. Because of this, it would take an infinite amount of energy to separate two quarks; they are forever bound into hadrons such as the proton and the neutron. Although analytically unproven, confinement is widely believed to be true because it explains the consistent failure of free quark searches, and it is easy to demonstrate in lattice QCD.

Moreover: the above-mentioned two properties are *continuous* all the way, i.e. there is no phase-transition line separating them.

Terminology

The word *quark* was coined by American physicist Murray Gell-Mann (b. 1929) in its present sense, the word having been taken from the phrase "Three quarks for Muster Mark" in *Finnegans Wake* by James Joyce. Gell-Mann wrote in a private letter of June 27, 1978, to the editor of the Oxford English Dictionary that he had been influenced by Joyce's words: "The allusion to three quarks seemed perfect" (originally there were only three subatomic quarks.) Gell-Mann, however, wanted to pronounce the word with (ô) not (ä), as Joyce seemed to indicate by rhyming words in the vicinity such as *Mark*. Gell-Mann got around that "by supposing that one ingredient of the line 'Three quarks for Muster Mark' was a cry of 'Three quarts for Mister . . . ' heard in H.C. Earwicker's pub," a plausible suggestion given the complex punning in Joyce's novel. [1]

The three kinds of charge in QCD (as opposed to two in Quantum electrodynamics or QED) are usually referred to as "color charge" by loose analogy to the three kinds of color (red, green and blue) perceived by humans. Since the theory of electric charge is dubbed "electrodynamics", the Greek word "chroma" Χρώμα (meaning color) is applied to the theory of color charge, "chromodynamics".

Lagrangian

The dynamics of the quarks and gluons are controlled by the quantum chromodynamics Lagrangian. The gauge invariant QCD Lagrangian is

$$\begin{aligned}\mathcal{L}_{\mathrm{QCD}} &= \bar{\psi}_i \left(i\gamma^\mu (D_\mu)_{ij} - m\,\delta_{ij} \right) \psi_j - \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu}_a \\ &= \bar{\psi}_i (i\gamma^\mu \partial_\mu - m)\psi_i - g G^a_\mu \bar{\psi}_i \gamma^\mu T^a_{ij} \psi_j - \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu}_a \,,\end{aligned}$$

where $\psi_i(x)$ is the quark field, a dynamical function of space-time, in the fundamental representation of the SU(3) gauge group, indexed by $i,\, j,\, \ldots$; $G^a_\mu(x)$ are the gluon fields, also a dynamical function of space-time, in the adjoint representation of the SU(3) gauge group, indexed by $a, b, \ldots$; γ^μ are the Dirac matrices, connecting the spinor representation to the vector representation of the Lorentz group; and T^a_{ij} are the generators, connecting the fundamental, antifundamental and adjoint representations of the SU(3) gauge group. The Gell-Mann matrices provide one such representation for the generators.

The symbol $G^a_{\mu\nu}$ represents the gauge invariant gluonic field strength tensor, analogous to the electromagnetic field strength tensor, $F^{\mu\nu}$, in Electrodynamics. It is given by

$$G^a_{\mu\nu} = \partial_\mu G^a_\nu - \partial_\nu G^a_\mu - g f^{abc} G^b_\mu G^c_\nu \,,$$

where f_{abc} are the structure constants of SU(3). Note that the rules to move-up or pull-down the *a*, *b*, or *c* indexes are *trivial*, (+......+), so that $f^{abc} = f_{abc}$, whereas for the *μ* or *ν* indexes one has the non-trivial *relativistic* rules, corresponding e.g. to the signature (+---). Furthermore, for mathematicians, according to this formula the gluon colour field can be represented by a SU(3)-Lie algebra-valued "curvature"-2-form $\mathbf{G} = \mathrm{d}\tilde{\mathbf{G}} - g\,\tilde{\mathbf{G}} \wedge \tilde{\mathbf{G}}$, where $\tilde{\mathbf{G}}$ is a "vector potential"-1-form corresponding to $\mathbf{G}$ and $\wedge$ is the (antisymmetric) "wedge product" of this algebra, producing the "structure constants" f^{abc}.

The constants m and g control the quark mass and coupling constants of the theory, subject to renormalization in the full quantum theory.

An important theoretical notion concerning the final term of the above Lagrangian is the *Wilson loop* variable. This loop variable plays a most-important role in discretized forms of the QCD (see lattice QCD), and more generally, it distinguishes confined and deconfined states of a gauge theory. It was introduced by the Noble-prize winner Kenneth G. Wilson and is treated in a separate article.

History

With the invention of bubble chambers and spark chambers in the 1950s, experimental → particle physics discovered a large and ever-growing number of particles called hadrons. It seemed that such a large number of particles could not all be fundamental. First, the particles were classified by charge and isospin by Eugene Wigner and Werner Heisenberg; then, in 1953, according to strangeness by Murray Gell-Mann and Kazuhiko Nishijima. To gain greater insight, the hadrons were sorted into groups having similar properties and masses using the *eightfold way*, invented in 1961 by Gell-Mann and Yuval Ne'eman. Gell-Mann and George Zweig, correcting an earlier approach of Shoichi Sakata, went on to propose in 1963 that the structure of the groups could be explained by the existence of three flavours of smaller particles inside the hadrons: the quarks.

At this stage, one particle, the Δ^{++} remained mysterious; in the quark model, it is composed of three up quarks with parallel spins. However, since quarks are fermions, this combination is forbidden by the Pauli exclusion principle. In 1965, Moo-Young Han with Yoichiro Nambu and Oscar W. Greenberg independently resolved the problem by proposing that quarks possess an additional SU(3) gauge degree of freedom, later called colour charge. Han and Nambu noted that quarks might interact via an octet of vector gauge bosons: the gluons.

Since free quark searches consistently failed to turn up any evidence for the new particles, and because an elementary particle back then was *defined* as a particle which could be separated and isolated, Gell-Mann often said that quarks were merely convenient mathematical constructs, not real particles. The meaning of this statement was usually clear in context: he meant quarks are confined. But he also was implying that the strong interactions could probably not be fully described by quantum field theory.

Richard Feynman argued that high energy experiments showed quarks are real particles: he called them *partons* (since they were parts of hadrons). By particles, Feynman meant objects which travel along paths, elementary particles in a field theory.

The difference between Feynman's and Gell-Mann's approaches reflected a deep split in the theoretical physics community. Feynman thought the quarks have a distribution of position or momentum, like any other particle, and he (correctly) believed that the diffusion of parton momentum explained diffractive scattering. Although Gell-Mann believed that certain quark charges could be localized, he was open to the possibility that the quarks themselves could not be localized because space and time break down. This was the more radical approach of S-matrix theory.

James Bjorken proposed that pointlike partons would imply certain relations should hold in deep inelastic scattering of electrons and protons, which were spectacularly verified in experiments at SLAC in 1969. This led physicists to abandon the S-matrix approach for the strong interactions.

The discovery of asymptotic freedom in the strong interactions by David Gross, David Politzer and Frank Wilczek allowed physicists to make precise predictions of the results of many high energy experiments using the quantum field theory technique of perturbation theory. Evidence of gluons was discovered in three jet events at PETRA in 1979. These experiments became more and more precise, culminating in the verification of perturbative QCD at the level of a few percent at the LEP in CERN.

The other side of asymptotic freedom is confinement. Since the force between color charges does not decrease with distance, it is believed that quarks and gluons can never be liberated from hadrons. This aspect of the theory is verified within lattice QCD computations, but is not mathematically proven. One of the Millennium Prize Problems announced by the Clay Mathematics Institute requires a claimant to produce such a proof. Other aspects of non-perturbative → QCD are the exploration of phases of quark matter, including the quark-gluon plasma.

The relation between the short-distance particle limit and the confining long-distance limit is one of the topics recently explored using string theory, the modern form of S-matrix theory.[2] [3]

The theory

→ Unsolved problems in physics: *QCD in the non-perturbative regime:*

- **Confinement**: the equations of QCD remain unsolved at energy scales relevant for describing atomic nuclei. How does QCD give rise to the physics of nuclei and nuclear constituents?
- **Quark matter**: the equations of QCD predict that a sea of quarks and gluons should be formed at high temperature and density. What are the properties of this phase of matter?

Some definitions

Every field theory of → particle physics is based on certain symmetries of nature whose existence is deduced from observations. These can be

- local symmetries, that is the symmetry acts independently at each point in space-time. Each such symmetry is the basis of a gauge theory and requires the introduction of its own gauge bosons.
- global symmetries, which are symmetries whose operations must be simultaneously applied to all points of space-time.

QCD is a gauge theory of the SU(3) gauge group obtained by taking the color charge to define a local symmetry.

Since the strong interaction does not discriminate between different flavors of quark, QCD has approximate **flavor symmetry**, which is broken by the differing masses of the quarks.

There are additional global symmetries whose definitions require the notion of chirality, discrimination between left and right-handed. If the spin of a particle has a positive projection on its direction of motion then it is called left-handed; otherwise, it is right-handed. Chirality and handedness are not the same, but become approximately equivalent at high energies.

- **Chiral** symmetries involve independent transformations of these two types of particle.

- **Vector** symmetries (also called diagonal symmetries) mean the same transformation is applied on the two chiralities.
- **Axial** symmetries are those in which one transformation is applied on left-handed particles and the inverse on the right-handed particles.

The symmetry groups

The color group SU(3) corresponds to the local symmetry whose gauging gives rise to QCD. The electric charge labels a representation of the local symmetry group U(1) which is gauged to give QED: this is an abelian group. If one considers a version of QCD with N_f flavors of massless quarks, then there is a global (chiral) flavor symmetry group $SU_L(N_f) \times SU_R(N_f) \times U_B(1) \times U_A(1)$. The chiral symmetry is spontaneously broken by the QCD vacuum to the vector (L+R) $SU_V(N_f)$ with the formation of a chiral condensate. The vector symmetry, $U_B(1)$ corresponds to the baryon number of quarks and is an exact symmetry. The axial symmetry $U_A(1)$ is exact in the classical theory, but broken in the quantum theory, an occurrence called an anomaly. Gluon field configurations called instantons are closely related to this anomaly.

There are two different types of SU(3) symmetry: there is the symmetry that acts on the different colors of quarks, and this is an exact gauge symmetry mediated by the gluons, and there is also a flavor symmetry which rotates different flavors of quarks to each other, or *flavor SU(3)*. Flavor SU(3) is an approximate symmetry of the vacuum of QCD, and is not a fundamental symmetry at all. It is an accidental consequence of the small mass of the three lightest quarks.

In the QCD vacuum there are vacuum condensates of all the quarks whose mass is less than the QCD scale. This includes the up and down quarks, and to a lesser extent the strange quark, but not any of the others. The vacuum is symmetric under SU(2) isospin rotations of up and down, and to a lesser extent under rotations of up,down, and strange, or full flavor group SU(3), and the observed particles make isospin and SU(3) multiplets.

The approximate flavor symmetries do have associated gauge bosons, observed particles like the rho and the omega, but these particles are nothing like the gluons and they are not massless. They are emergent gauge bosons in an approximate string description of QCD.

The fields

Quarks are massive spin-1/2 fermions which carry a color charge whose gauging is the content of QCD. Quarks are represented by Dirac fields in the fundamental representation **3** of the gauge group SU(3). They also carry electric charge (either -1/3 or 2/3) and participate in weak interactions as part of weak isospin doublets. They carry global quantum numbers including the baryon number, which is 1/3 for each quark, hypercharge and one of the flavor quantum numbers.

Gluons are spin-1 bosons which also carry color charges, since they lie in the adjoint representation **8** of SU(3). They have no electric charge, do not participate in the weak interactions, and have no flavor. They lie in the singlet representation **1** of all these symmetry groups.

Every quark has its own antiquark. The charge of each antiquark is exactly the opposite of the corresponding quark.

The dynamics

According to the rules of → quantum field theory, and the associated Feynman diagrams, the above theory gives rise to three basic interactions: a quark may emit (or absorb) a gluon, a gluon may emit (or absorb) a gluon, and two gluons may directly interact. This contrasts with QED, in which only the first kind of interaction occurs, since photons have no charge. Diagrams involving Faddeev-Popov ghosts must be considered too.

Methods

Further analysis of the content of the theory is complicated. Various techniques have been developed to work with QCD. Some of them are discussed briefly below.

Perturbative QCD

This approach is based on asymptotic freedom, which allows perturbation theory to be used accurately in experiments performed at very high energies. Although limited in scope, this approach has resulted in the most precise tests of QCD to date.

Lattice QCD

Among non-perturbative approaches to QCD, the most well established one is lattice QCD. This approach uses a discrete set of space-time points (called the lattice) to reduce the analytically intractable path integrals of the continuum theory to a very difficult numerical computation which is then carried out on supercomputers like the QCDOC which was constructed for precisely this purpose. While it is a slow and resource-intensive approach, it has wide applicability, giving insight into parts of the theory inaccessible by other means. Lattice QCD is not, however, useful at high density and low temperature (e.g. nuclear matter or the interior of neutron stars).

1/N expansion

A well-known approximation scheme, the 1/N expansion, starts from the premise that the number of colors is infinite, and makes a series of corrections to account for the fact that it is not. Until now it has been the source of qualitative insight rather than a method for quantitative predictions. Modern variants include the AdS/CFT approach.

Effective theories

For specific problems some theories may be written down which seem to give qualitatively correct results. In the best of cases, these may then be obtained as systematic expansions in some parameter of the QCD Lagrangian. Among the best such effective models one should now count chiral perturbation theory (which expands around light quark masses near zero), heavy quark effective theory (which expands around heavy quark mass near infinity), and soft-collinear effective theory (which expands around large ratios of energy scales). Other less accurate models are the Nambu-Jona-Lasinio model and the chiral model.

Experimental tests

The notion of quark flavours was prompted by the necessity of explaining the properties of hadrons during the development of the quark model. The notion of colour was necessitated by the puzzle of the Δ^{++}. This has been dealt with in the section on the history of QCD.

The first evidence for quarks as real constituent elements of hadrons was obtained in deep inelastic scattering experiments at SLAC. The first evidence for gluons came in three jet events at PETRA.

Good quantitative tests of perturbative QCD are

- the running of the QCD coupling as deduced from many observations
- scaling violation in polarized and unpolarized deep inelastic scattering
- vector boson production at colliders (this includes the Drell-Yan process)
- jet cross sections in colliders
- event shape observables at the LEP
- heavy-quark production in colliders

Quantitative tests of non-perturbative QCD are fewer, because the predictions are harder to make. The best is probably the running of the QCD coupling as probed through lattice computations of heavy-quarkonium spectra. There is a recent claim about the mass of the heavy meson B_c [4]. Other non-perturbative tests are currently at the level of 5% at best. Continuing work on masses and form factors of hadrons and their weak matrix elements are promising candidates for future quantitative tests. The whole subject of quark matter and the quark-gluon plasma is a non-perturbative test bed for QCD which still remains to be properly exploited.

See also

- For overviews, see Standard Model, its field theoretical formulation, strong interactions, quarks and gluons, hadrons, confinement, QCD matter, or quark-gluon plasma.
- For details, see gauge theory, quantization procedure including BRST and Faddeev-Popov ghosts. A more general category is → quantum field theory.
- For techniques, see Lattice QCD, 1/N expansion, perturbative QCD, heavy quark effective theory, chiral models, and the Nambu and Jona-Lasinio model.
- For experiments, see quark search experiments, deep inelastic scattering, jet physics, quark-gluon plasma.

Footnotes

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[2] J. Polchinski, M. Strassler (2002). "Hard Scattering and Gauge/String duality". *Physical Review Letters* **88**: 31601. doi: 10.1103/PhysRevLett.88.031601 (http://dx.doi.org/10.1103/PhysRevLett.88.031601).
[3] Brower, Mathur, Tan, *Glueball Spectrum for QCD from AdS Supergravity duality*, arXiv:hep-th/0003115.
[4] http://www.aip.org/pnu/2005/split/731-1.html

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- Greiner, Walter;Schäfer, Andreas (1994). *Quantum Chromodynamics*. Springer. ISBN 0-387-57103-5.
- Halzen, Francis; Martin, Alan (1984). *Quarks & Leptons: An Introductory Course in Modern Particle Physics*. John Wiley & Sons. ISBN 0-471-88741-2.

- Creutz, Michael (1985). *Quarks, Gluons and Lattices*. Cambridge University Press. ISBN 978-0521315357.

External links

- Particle data group (http://pdg.lbl.gov/)
- The millennium prize (http://www.claymath.org/millennium/) for proving confinement (http://www.claymath.org/millennium/)
- Ab Initio Determination of Light Hadron Masses (http://www.sciencemag.org/cgi/content/abstract/322/5905/1224)
- Andreas S Kronfeld (http://www.sciencemag.org/cgi/content/summary/322/5905/1198) *The Weight of the World Is Quantum Chromodynamics*
- Andreas S Kronfeld (http://www.iop.org/EJ/article/1742-6596/125/1/012067/jpconf8_125_012067.pdf?request-id=f9ccdf0d-ee26-4856-99fb-ce5bfef07c4c) *Quantum chromodynamics with advanced computing*
- Standard model gets right answer (http://www.sciencenews.org/view/generic/id/38788/title/Standard_model_gets_right_answer_for_proton,_neutron_masses)

Quantum field theory

Quantum field theory or **QFT**[1] provides a theoretical framework for constructing → quantum mechanical models of systems classically described by fields or of many-body systems. It is widely used in → particle physics and condensed matter physics. Most theories in modern particle physics, including the Standard Model of elementary particles and their interactions, are formulated as relativistic quantum field theories. In condensed matter physics, quantum field theories are used in many circumstances, especially those where the number of particles is allowed to fluctuate—for example, in the BCS theory of superconductivity.

In quantum field theory (QFT) the forces between particles are mediated by other particles. The electromagnetic force between two electrons is caused by an exchange of photons. Intermediate vector bosons mediate the weak force and → gluons mediate the strong force. There is currently no complete quantum theory of the remaining fundamental force, gravity, but many of the proposed theories postulate the existence of a graviton particle which mediates it. These force-carrying particles are virtual particles and, by definition, cannot be detected while carrying the force, because such detection will imply that the force is not being carried.

In QFT photons are not thought of as 'little billiard balls', they are considered to be field quanta - necessarily chunked ripples in a field that 'look like' particles. Fermions, like the electron, can also be described as ripples in a field, where each kind of fermion has its own field. In summary, the classical visualisation of "everything is particles and fields", in quantum field theory, resolves into "everything is particles", which then resolves into "everything is fields". In the end, particles are regarded as excited states of a field (field quanta).

History

Quantum field theory originated in the 1920s from the problem of creating a → quantum mechanical theory of the electromagnetic field. In 1926, Max Born, Pascual Jordan, and Werner Heisenberg constructed such a theory by expressing the field's internal degrees of freedom as an infinite set of harmonic oscillators and by employing the usual procedure for quantizing those oscillators (canonical quantization). This theory assumed that no electric charges or currents were present and today would be called a free field theory. The first reasonably complete theory of quantum electrodynamics, which included both the electromagnetic field and electrically charged matter (specifically, electrons) as quantum mechanical objects, was created by Paul Dirac in 1927. This quantum field theory could be used to model important processes such as the emission of a photon by an electron dropping into a quantum state of lower energy, a process in which the *number of particles changes* — one atom in the initial state becomes an atom plus a photon in the final state. It is now understood that the ability to describe such processes is one of the most important features of quantum field theory.

It was evident from the beginning that a proper quantum treatment of the electromagnetic field had to somehow incorporate Einstein's relativity theory, which had after all grown out of the study of classical electromagnetism. This need to *put together relativity and quantum mechanics* was the second major motivation in the development of quantum field theory. Pascual Jordan and Wolfgang Pauli showed in 1928 that quantum fields could be made to behave in the way predicted by special relativity during coordinate transformations (specifically, they showed that the field commutators were Lorentz invariant), and in 1933 Niels Bohr and Leon Rosenfeld showed that this result could be interpreted as a limitation on the ability to measure fields at space-like separations, exactly as required by relativity. A further boost for quantum field theory came with the discovery of the Dirac equation, a single-particle equation obeying both relativity and quantum mechanics, when it was shown that several of its undesirable properties (such as negative-energy states) could be eliminated by reformulating the Dirac equation as a quantum field theory. This work was performed by Wendell Furry, Robert Oppenheimer, Vladimir Fock, and others.

The third thread in the development of quantum field theory was the need to *handle the statistics of many-particle systems* consistently and with ease. In 1927, Jordan tried to extend the canonical quantization of fields to the many-body wavefunctions of identical particles, a procedure that is sometimes called second quantization. In 1928, Jordan and Eugene Wigner found that the quantum field describing electrons, or other fermions, had to be expanded using anti-commuting creation and annihilation operators due to the Pauli exclusion principle. This thread of development was incorporated into many-body theory, and strongly influenced condensed matter physics and nuclear physics.

Despite its early successes, quantum field theory was plagued by several serious theoretical difficulties. Many seemingly-innocuous physical quantities, such as the energy shift of electron states due to the presence of the electromagnetic field, gave infinity — a nonsensical result — when computed using quantum field theory. This "divergence problem" was solved during the 1940s by Bethe, Tomonaga, Schwinger, Feynman, and Dyson, through the procedure known as renormalization. This phase of development culminated with the construction of the modern theory of quantum electrodynamics (QED). Beginning in the 1950s with the work of Yang and Mills, QED was generalized to a class of quantum field theories known as gauge theories. The 1960s and 1970s saw the formulation of a gauge theory now known as the Standard Model of → particle physics, which describes all known elementary particles and the interactions between them. The weak interaction part of the standard model was formulated by Sheldon Glashow, with the Higgs mechanism added by Steven Weinberg and Abdus Salam. The theory was shown to be renormalizable and hence consistent by Gerardus 't Hooft and Martinus Veltman.

Also during the 1970s, parallel developments in the study of phase transitions in condensed matter physics led Leo Kadanoff, Michael Fisher and Kenneth Wilson (extending work of Ernst Stueckelberg, Andre Peterman, Murray Gell-Mann and Francis Low) to a set of ideas and methods known as the renormalization group. By providing a better physical understanding of the renormalization procedure invented in the 1940s, the renormalization group sparked what has been called the "grand synthesis" of theoretical physics, uniting the quantum field theoretical techniques used in particle physics and condensed matter physics into a single theoretical framework.

The study of quantum field theory is alive and flourishing, as are applications of this method to many physical problems. It remains one of the most vital areas of theoretical physics today, providing a common language to many branches of → physics.

Principles of quantum field theory

Classical fields and quantum fields

→ Quantum mechanics, in its most general formulation, is a theory of abstract operators (observables) acting on an abstract state space (Hilbert space), where the observables represent physically-observable quantities and the state space represents the possible states of the system under study. Furthermore, each observable corresponds, in a technical sense, to the classical idea of a degree of freedom. For instance, the fundamental observables associated with the motion of a single quantum mechanical particle are the position and momentum operators $\hat{x}$ and $\hat{p}$. Ordinary quantum mechanics deals with systems such as this, which possess a small set of degrees of freedom.

(It is important to note, at this point, that this article does not use the word "particle" in the context of wave–particle duality. In quantum field theory, "particle" is a generic term for any discrete quantum mechanical entity, such as an electron, which can behave like classical particles or classical waves under different experimental conditions.)

A **quantum field** is a quantum mechanical system containing a large, and possibly infinite, number of degrees of freedom. This is not as exotic a situation as one might think. A classical field contains a set of degrees of freedom at each point of space; for instance, the classical electromagnetic field defines two vectors — the electric field and the magnetic field — that can in principle take on distinct values for each position r. When the field *as a whole* is considered as a quantum mechanical system, its observables form an infinite (in fact uncountable) set, because r is continuous.

Furthermore, the degrees of freedom in a quantum field are arranged in "repeated" sets. For example, the degrees of freedom in an electromagnetic field can be grouped according to the position r, with exactly two vectors for each r. Note that r is an ordinary number that "indexes" the observables; it is not to be confused with the position operator $\hat{x}$ encountered in ordinary quantum mechanics, which is an observable. (Thus, ordinary quantum mechanics is sometimes referred to as "zero-dimensional quantum field theory", because it contains only a single set of observables.) It is also important to note that there is nothing special about r because, as it turns out, there is generally more than one way of indexing the degrees of freedom in the field.

In the following sections, we will show how these ideas can be used to construct a quantum mechanical theory with the desired properties. We will begin by discussing single-particle quantum mechanics and the associated theory of many-particle quantum mechanics. Then, by finding a way to index the degrees of freedom in the many-particle problem, we will construct a quantum field and study its implications.

Single-particle and many-particle quantum mechanics

In ordinary quantum mechanics, the time-dependent one-dimensional Schrödinger equation describing the time evolution of the quantum state of a single non-relativistic particle is

$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(\mathbf{x})\right]|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle,$$

where m is the particle's mass, V is the applied potential, and $|\psi\rangle$ denotes the quantum state (we are using bra-ket notation).

We wish to consider how this problem generalizes to N particles. There are two motivations for studying the many-particle problem. The first is a straightforward need in condensed matter physics, where typically the number of particles is on the order of Avogadro's number (6.0221415 x 10^{23}). The second motivation for the many-particle problem arises from → particle physics and the desire to incorporate the effects of special relativity. If one attempts to include the relativistic rest energy into the above equation, the result is either the Klein-Gordon equation or the Dirac equation. However, these equations have many unsatisfactory qualities; for instance, they possess energy eigenvalues which extend to –∞, so that there seems to be no easy definition of a ground state. It turns out that such inconsistencies arise from neglecting the possibility of dynamically creating or destroying particles, which is a crucial aspect of relativity. Einstein's famous mass-energy relation predicts that sufficiently massive particles can decay into several lighter particles, and sufficiently energetic particles can combine to form massive particles. For example, an electron and a positron can annihilate each other to create photons. Thus, a consistent relativistic quantum theory must be formulated as a many-particle theory.

Furthermore, we will assume that the N particles are indistinguishable. As described in the article on identical particles, this implies that the state of the entire system must be either symmetric (bosons) or antisymmetric (fermions) when the coordinates of its constituent particles are exchanged. These multi-particle states are rather complicated to write. For example, the general quantum state of a system of N bosons is written as

$$|\phi_1 \cdots \phi_N\rangle = \sqrt{\frac{\prod_j N_j!}{N!}} \sum_{p\in S_N} |\phi_{p(1)}\rangle \cdots |\phi_{p(N)}\rangle,$$

where $|\phi_i\rangle$ are the single-particle states, N_j is the number of particles occupying state j, and the sum is taken over all possible permutations p acting on N elements. In general, this is a sum of $N!$ (N factorial) distinct terms, which quickly becomes unmanageable as N increases. The way to simplify this problem is to turn it into a quantum field theory.

Second quantization

In this section, we will describe a method for constructing a quantum field theory called **second quantization**. This basically involves choosing a way to index the quantum mechanical degrees of freedom in the space of multiple identical-particle states. It is based on the Hamiltonian formulation of quantum mechanics; several other approaches exist, such as the Feynman path integral[2] , which uses a Lagrangian formulation. For an overview, see the article on quantization.

Second quantization of bosons

For simplicity, we will first discuss second quantization for bosons, which form perfectly symmetric quantum states. Let us denote the mutually orthogonal single-particle states by $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle,$ and so on. For example, the 3-particle state with one particle in state $|\phi_1\rangle$ and two in state $|\phi_2\rangle$ is

$$\frac{1}{\sqrt{3}} \left[|\phi_1\rangle|\phi_2\rangle|\phi_2\rangle + |\phi_2\rangle|\phi_1\rangle|\phi_2\rangle + |\phi_2\rangle|\phi_2\rangle|\phi_1\rangle \right].$$

The first step in second quantization is to express such quantum states in terms of **occupation numbers**, by listing the number of particles occupying each of the single-particle states $|\phi_1\rangle, |\phi_2\rangle,$ etc. This is simply another way of labelling the states. For instance, the above 3-particle state is denoted as

$$|1, 2, 0, 0, 0, \cdots\rangle.$$

The next step is to expand the N-particle state space to include the state spaces for all possible values of N. This extended state space, known as a Fock space, is composed of the state space of a system with no particles (the so-called vacuum state), plus the state space of a 1-particle system, plus the state space of a 2-particle system, and so forth. It is easy to see that there is a one-to-one correspondence between the occupation number representation and valid boson states in the Fock space.

At this point, the quantum mechanical system has become a quantum field in the sense we described above. The field's elementary degrees of freedom are the occupation numbers, and each occupation number is indexed by a number $j \cdots$, indicating which of the single-particle states $|\phi_1\rangle, |\phi_2\rangle, \cdots |\phi_j\rangle \cdots$ it refers to.

The properties of this quantum field can be explored by defining creation and annihilation operators, which add and subtract particles. They are analogous to "ladder operators" in the quantum harmonic oscillator problem, which added and subtracted energy quanta. However, these operators literally create and annihilate particles of a given quantum state. The bosonic annihilation operator a_2 and creation operator $a_2^\dagger$ have the following effects:

$$a_2 |N_1, N_2, N_3, \cdots\rangle = \sqrt{N_2} \mid N_1, (N_2 - 1), N_3, \cdots\rangle,$$
$$a_2^\dagger |N_1, N_2, N_3, \cdots\rangle = \sqrt{N_2 + 1} \mid N_1, (N_2 + 1), N_3, \cdots\rangle.$$

It can be shown that these are operators in the usual quantum mechanical sense, i.e. linear operators acting on the Fock space. Furthermore, they are indeed Hermitian conjugates, which justifies the way we have written them. They can be shown to obey the commutation relation

$$[a_i, a_j] = 0 \quad , \quad \left[a_i^\dagger, a_j^\dagger\right] = 0 \quad , \quad \left[a_i, a_j^\dagger\right] = \delta_{ij},$$

where δ stands for the Kronecker delta. These are precisely the relations obeyed by the ladder operators for an infinite set of independent quantum harmonic oscillators, one for each single-particle state. Adding or removing bosons from each state is therefore analogous to exciting or de-exciting a quantum of energy in a harmonic oscillator.

The Hamiltonian of the quantum field (which, through the Schrödinger equation, determines its dynamics) can be written in terms of creation and annihilation operators. For instance, the Hamiltonian of a field of free (non-interacting) bosons is

$$H = \sum_k E_k \, a_k^\dagger \, a_k,$$

where E_k is the energy of the k -th single-particle energy eigenstate. Note that

$$a_k^\dagger \, a_k | \cdots, N_k, \cdots \rangle = N_k | \cdots, N_k, \cdots \rangle.$$

Second quantization of fermions

It turns out that a different definition of creation and annihilation must be used for describing fermions. According to the Pauli exclusion principle, fermions cannot share quantum states, so their occupation numbers N_i can only take on the value 0 or 1. The fermionic annihilation operators c and creation operators $c^\dagger$ are defined by

$$c_j | N_1, N_2, \cdots, N_j = 0, \cdots \rangle = 0$$
$$c_j | N_1, N_2, \cdots, N_j = 1, \cdots \rangle = (-1)^{(N_1 + \cdots + N_{j-1})} | N_1, N_2, \cdots, N_j = 0, \cdots \rangle$$
$$c_j^\dagger | N_1, N_2, \cdots, N_j = 0, \cdots \rangle = (-1)^{(N_1 + \cdots + N_{j-1})} | N_1, N_2, \cdots, N_j = 1, \cdots \rangle$$
$$c_j^\dagger | N_1, N_2, \cdots, N_j = 1, \cdots \rangle = 0$$

These obey an anticommutation relation:

$$\{c_i, c_j\} = 0 \quad , \quad \left\{c_i^\dagger, c_j^\dagger\right\} = 0 \quad , \quad \left\{c_i, c_j^\dagger\right\} = \delta_{ij}$$

One may notice from this that applying a fermionic creation operator twice gives zero, so it is impossible for the particles to share single-particle states, in accordance with the exclusion principle.

Field operators

We have previously mentioned that there can be more than one way of indexing the degrees of freedom in a quantum field. Second quantization indexes the field by enumerating the single-particle quantum states. However, as we have discussed, it is more natural to think about a "field", such as the electromagnetic field, as a set of degrees of freedom indexed by position.

To this end, we can define *field operators* that create or destroy a particle at a particular point in space. In particle physics, these operators turn out to be more convenient to work with, because they make it easier to formulate theories that satisfy the demands of relativity.

Single-particle states are usually enumerated in terms of their momenta (as in the particle in a box problem.) We can construct field operators by applying the Fourier transform to the creation and annihilation operators for these states. For example, the bosonic field annihilation operator $\phi(\mathbf{r})$ is

$$\phi(\mathbf{r}) \stackrel{\mathrm{def}}{=} \sum_j e^{i\mathbf{k}_j \cdot \mathbf{r}} a_j$$

The bosonic field operators obey the commutation relation

$$[\phi(\mathbf{r}), \phi(\mathbf{r'})] = 0 \quad , \quad \left[\phi^\dagger(\mathbf{r}), \phi^\dagger(\mathbf{r'})\right] = 0 \quad , \quad \left[\phi(\mathbf{r}), \phi^\dagger(\mathbf{r'})\right] = \delta^3(\mathbf{r} - \mathbf{r'})$$

where $\delta(x)$ stands for the Dirac delta function. As before, the fermionic relations are the same, with the commutators replaced by anticommutators.
It should be emphasized that the field operator is *not* the same thing as a single-particle wavefunction. The former is an operator acting on the Fock space, and the latter is just a scalar field. However, they are closely related, and are indeed commonly denoted with the same symbol. If we have a Hamiltonian with a space representation, say

$$H = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{i<j} U(|\mathbf{r}_i - \mathbf{r}_j|)$$

where the indices i and j run over all particles, then the field theory Hamiltonian is

$$H = -\frac{\hbar^2}{2m} \int d^3r \; \phi^\dagger(\mathbf{r}) \nabla^2 \phi(\mathbf{r}) + \int d^3r \int d^3r' \; \phi^\dagger(\mathbf{r}) \phi^\dagger(\mathbf{r}') U(|\mathbf{r} - \mathbf{r}'|) \phi(\mathbf{r}') \phi(\mathbf{r})$$

This looks remarkably like an expression for the expectation value of the energy, with ϕ playing the role of the wavefunction. This relationship between the field operators and wavefunctions makes it very easy to formulate field theories starting from space-projected Hamiltonians.

Implications of quantum field theory

Unification of fields and particles

The "second quantization" procedure that we have outlined in the previous section takes a set of single-particle quantum states as a starting point. Sometimes, it is impossible to define such single-particle states, and one must proceed directly to quantum field theory. For example, a quantum theory of the electromagnetic field *must* be a quantum field theory, because it is impossible (for various reasons) to define a wavefunction for a single photon. In such situations, the quantum field theory can be constructed by examining the mechanical properties of the classical field and guessing the corresponding quantum theory. The quantum field theories obtained in this way have the same properties as those obtained using second quantization, such as well-defined creation and annihilation operators obeying commutation or anticommutation relations.

Quantum field theory thus provides a unified framework for describing "field-like" objects (such as the electromagnetic field, whose excitations are photons) and "particle-like" objects (such as electrons, which are treated as excitations of an underlying electron field).

Physical meaning of particle indistinguishability

The second quantization procedure relies crucially on the particles being identical. We would not have been able to construct a quantum field theory from a distinguishable many-particle system, because there would have been no way of separating and indexing the degrees of freedom.

Many physicists prefer to take the converse interpretation, which is that *quantum field theory explains what identical particles are*. In ordinary quantum mechanics, there is not much theoretical motivation for using symmetric (bosonic) or antisymmetric (fermionic) states, and the need for such states is simply regarded as an empirical fact. From the point of view of quantum field theory, particles are identical if and only if they are excitations of the same underlying quantum field. Thus, the question "why are all electrons identical?" arises from mistakenly regarding individual electrons as fundamental objects, when in fact it is only the electron field that is fundamental.

Particle conservation and non-conservation

During second quantization, we started with a Hamiltonian and state space describing a fixed number of particles (N), and ended with a Hamiltonian and state space for an arbitrary number of particles. Of course, in many common situations N is an important and perfectly well-defined quantity, e.g. if we are describing a gas of atoms sealed in a box. From the point of view of quantum field theory, such situations are described by quantum states that are eigenstates of the number operator $\hat{N}$, which measures the total number of particles present. As with any quantum mechanical observable, $\hat{N}$ is conserved if it commutes with the Hamiltonian. In that case, the quantum state is trapped in the N -particle subspace of the total Fock space, and the situation could equally well be described by ordinary N-particle quantum mechanics.

For example, we can see that the free-boson Hamiltonian described above conserves particle number. Whenever the Hamiltonian operates on a state, each particle destroyed by an annihilation operator a_k is immediately put back by the creation operator $a_k^\dagger$.

On the other hand, it is possible, and indeed common, to encounter quantum states that are *not* eigenstates of $\hat{N}$, which do not have well-defined particle numbers. Such states are difficult or impossible to handle using ordinary quantum mechanics, but they can be easily described in quantum field theory as quantum superpositions of states having different values of N. For example, suppose we have a bosonic field whose particles can be created or destroyed by interactions with a fermionic field. The Hamiltonian of the combined system would be given by the Hamiltonians of the free boson and free fermion fields, plus a "potential energy" term such as

$$H_I = \sum_{k,q} V_q (a_q + a_{-q}^\dagger) c_{k+q}^\dagger c_k,$$

where $a_k^\dagger$ and a_k denotes the bosonic creation and annihilation operators, $c_k^\dagger$ and c_k denotes the fermionic creation and annihilation operators, and V_q is a parameter that describes the strength of the interaction. This "interaction term" describes processes in which a fermion in state k either absorbs or emits a boson, thereby being kicked into a different eigenstate $k+q$. (In fact, this type of Hamiltonian is used to describe interaction between conduction electrons and phonons in metals. The interaction between electrons and photons is treated in a similar way, but is a little more complicated because the role of spin must be taken into account.) One thing to notice here is that even if we start out with a fixed number of bosons, we will typically end up with a superposition of states with different numbers of bosons at later times. The number of fermions, however, is conserved in this case.

In condensed matter physics, states with ill-defined particle numbers are particularly important for describing the various superfluids. Many of the defining characteristics of a superfluid arise from the notion that its quantum state is a superposition of states with different particle numbers.

Axiomatic approaches

The preceding description of quantum field theory follows the spirit in which most physicists approach the subject. However, it is not mathematically rigorous. Over the past several decades, there have been many attempts to put quantum field theory on a firm mathematical footing by formulating a set of axioms for it. These attempts fall into two broad classes.

The first class of axioms, first proposed during the 1950s, include the Wightman, Osterwalder-Schrader, and Haag-Kastler systems. They attempted to formalize the physicists' notion of an "operator-valued field" within the context of functional analysis, and enjoyed limited success. It was possible to prove that any quantum field theory satisfying these axioms satisfied certain general theorems, such as the spin-statistics theorem and the CPT theorem. Unfortunately, it proved extraordinarily difficult to show that any realistic field theory, including the Standard Model, satisfied these axioms. Most of the theories that could be treated with these analytic axioms were physically trivial, being restricted to low-dimensions and lacking interesting dynamics. The construction of theories satisfying one of these sets of axioms falls in the field of constructive quantum field theory. Important work was done in this area in the 1970s by Segal, Glimm, Jaffe and others.

During the 1980s, a second set of axioms based on geometric ideas was proposed. This line of investigation, which restricts its attention to a particular class of quantum field theories known as topological quantum field theories, is associated most closely with Michael Atiyah and Graeme Segal, and was notably expanded upon by Edward Witten, Richard Borcherds, and Maxim Kontsevich. However, most physically-relevant quantum field theories, such as the Standard Model, are not topological quantum field theories; the quantum field theory of the fractional quantum Hall effect is a notable exception. The main impact of axiomatic topological quantum field theory has been on mathematics, with important applications in representation theory, algebraic topology, and differential geometry.

Finding the proper axioms for quantum field theory is still an open and difficult problem in mathematics. One of the Millennium Prize Problems—proving the existence of a mass gap in Yang-Mills theory—is linked to this issue.

Phenomena associated with quantum field theory

In the previous part of the article, we described the most general properties of quantum field theories. Some of the quantum field theories studied in various fields of theoretical physics possess additional special properties, such as renormalizability, gauge symmetry, and supersymmetry. These are described in the following sections.

Renormalization

Early in the history of quantum field theory, it was found that many seemingly innocuous calculations, such as the perturbative shift in the energy of an electron due to the presence of the electromagnetic field, give infinite results. The reason is that the perturbation theory for the shift in an energy involves a sum over all other energy levels, and there are infinitely many levels at short distances which each give a finite contribution.

Many of these problems are related to failures in classical electrodynamics that were identified but unsolved in the 19th century, and they basically stem from the fact that many of the supposedly "intrinsic" properties of an electron are tied to the electromagnetic field which it carries around with it. The energy carried by a single electron—its self energy—is not simply the bare value, but also includes the energy contained in its electromagnetic field, its attendant cloud of photons. The energy in a field of a spherical source diverges in both classical and quantum mechanics, but as discovered by Weisskopf, in quantum mechanics the divergence is much milder, going only as the logarithm of the radius of the sphere.

The solution to the problem, presciently suggested by Stueckelberg, independently by Bethe after the crucial experiment by Lamb, implemented at one loop by Schwinger, and systematically extended to all loops by Feynman and Dyson, with converging work by Tomonaga in isolated postwar Japan, is called renormalization. The technique of renormalization recognizes that the problem is essentially purely mathematical, that extremely short distances are at fault. In order to define a theory on a continuum, first place a cutoff on the fields, by postulating that quanta cannot have energies above some extremely high value. This has the effect of replacing continuous space by a structure where very short wavelengths do not exist, as on a lattice. Lattices break rotational symmetry, and one of the crucial contributions made by Feynman, Pauli and Villars, and modernized by 't Hooft and Veltman, is a symmetry preserving cutoff for perturbation theory. There is no known symmetrical cutoff outside of perturbation theory, so for rigorous or numerical work people often use an actual lattice.

The rule is that one computes physical quantities in terms of the observable parameters such as the physical mass, not the bare parameters such as the bare mass. The main point is not that of getting finite quantities (any regularization procedure does that), but to eliminate the regularization parameters by a suitable addition of counterterms to the original Lagrangian. The main requirements on the counterterms are a) Locality (polynomials in the fields and their derivatives) and b) Finiteness (number of monomials in the Lagrangian that remain finite after the introduction of all the necessary counterterms). The reason for (b) is that each new counterterm leaves behind a free parameter of the theory (like physical mass). There is no way such a parameter can be fixed other than by its experimental value, so one gets not a single theory but a family of theories parameterized by as many free parameters as the counterterms added to the Lagrangian. Since a theory with an infinite number of free parameters has virtually no predictive power the finiteness of the number of counterterms is required.

On a lattice, every quantity is finite but depends on the spacing. When taking the limit of zero spacing, we make sure that the physically-observable quantities like the observed electron mass stay fixed, which means that the constants in the Lagrangian defining the theory depend on the spacing. Hopefully, by allowing the constants to vary with the lattice spacing, all the results at long distances become insensitive to the lattice, defining a continuum limit.

The renormalization procedure only works for a certain class of quantum field theories, called **renormalizable quantum field theories**. A theory is **perturbatively renormalizable** when the constants in the Lagrangian only diverge at worst as logarithms of the lattice spacing for very short spacings. The continuum limit is then well defined in perturbation theory, and even if it is not fully well defined non-perturbatively, the problems only show up at distance scales which are exponentially small in the inverse coupling for weak couplings. The Standard Model of → particle physics is perturbatively renormalizable, and so are its component theories (quantum electrodynamics/electroweak theory and →

quantum chromodynamics). Of the three components, quantum electrodynamics is believed to not have a continuum limit, while the asymptotically free SU(2) and SU(3) weak hypercharge and strong color interactions are nonperturbatively well defined.

The renormalization group describes how renormalizable theories emerge as the long distance low-energy effective field theory for any given high-energy theory. Because of this, renormalizable theories are insensitive to the precise nature of the underlying high-energy short-distance phenomena. This is a blessing because it allows physicists to formulate low energy theories without knowing the details of high energy phenomenon. It is also a curse, because once a renormalizable theory like the standard model is found to work, it gives very few clues to higher energy processes. The only way high energy processes can be seen in the standard model is when they allow otherwise forbidden events, or if they predict quantitative relations between the coupling constants.

Gauge freedom

A gauge theory is a theory that admits a symmetry with a local parameter. For example, in every → quantum theory the global phase of the wave function is arbitrary and does not represent something physical. Consequently, the theory is invariant under a global change of phases (adding a constant to the phase of all wave functions, everywhere); this is a global symmetry. In quantum electrodynamics, the theory is also invariant under a *local* change of phase, that is - one may shift the phase of all wave functions so that the shift may be different at every point in space-time. This is a *local* symmetry. However, in order for a well-defined derivative operator to exist, one must introduce a new field, the gauge field, which also transforms in order for the local change of variables (the phase in our example) not to affect the derivative. In quantum electrodynamics this gauge field is the electromagnetic field. The change of local gauge of variables is termed gauge transformation.

In quantum field theory the excitations of fields represent particles. The particle associated with excitations of the gauge field is the gauge boson, which is the photon in the case of quantum electrodynamics.

The degrees of freedom in quantum field theory are local fluctuations of the fields. The existence of a gauge symmetry reduces the number of degrees of freedom, simply because some fluctuations of the fields can be transformed to zero by gauge transformations, so they are equivalent to having no fluctuations at all, and they therefore have no physical meaning. Such fluctuations are usually called "non-physical degrees of freedom" or *gauge artifacts*; usually some of them have a negative norm, making them inadequate for a consistent theory. Therefore, if a classical field theory has a gauge symmetry, then its quantized version (i.e. the corresponding quantum field theory) will have this symmetry as well. In other words, a gauge symmetry cannot have a quantum anomaly. If a gauge symmetry is anomalous (i.e. not kept in the quantum theory) then the theory is non-consistent: for example, in quantum electrodynamics, had there been a gauge anomaly, this would require the appearance of photons with longitudinal polarization and polarization in the time direction, the latter having a negative norm, rendering the theory inconsistent; another possibility would be for these photons to appear only in intermediate processes but not in the final products of any interaction, making the theory non unitary and again inconsistent (see optical theorem).

In general, the gauge transformations of a theory consist several different transformations, which may not be commutative. These transformations are together described by a mathematical object known as a gauge group. Infinitesimal gauge transformations are the gauge group generators. Therefore the number of gauge bosons is the group dimension (i.e. number of generators forming a basis).

All the fundamental interactions in nature are described by gauge theories. These are:

- Quantum electrodynamics, whose gauge transformation is a local change of phase, so that the gauge group is U(1). The gauge boson is the photon.
- → Quantum chromodynamics, whose gauge group is SU(3). The gauge bosons are eight gluons.
- The electroweak Theory, whose gauge group is $U(1) \times SU(2)$ (a direct product of U(1) and SU(2)).
- Gravity, whose classical theory is general relativity, admits the equivalence principle which is a form of gauge symmetry.

Supersymmetry

Supersymmetry assumes that every fundamental fermion has a superpartner that is a boson and vice versa. It was introduced in order to solve the so-called Hierarchy Problem, that is, to explain why particles not protected by any symmetry (like the Higgs boson) do not receive radiative corrections to its mass driving it to the larger scales (GUT, Planck...). It was soon realized that supersymmetry has other interesting properties: its gauged version is an extension of general relativity (Supergravity), and it is a key ingredient for the consistency of string theory.

The way supersymmetry protects the hierarchies is the following: since for every particle there is a superpartner with the same mass, any loop in a radiative correction is cancelled by the loop corresponding to its superpartner, rendering the theory UV finite.

Since no superpartners have yet been observed, if supersymmetry exists it must be broken (through a so-called soft term, which breaks supersymmetry without ruining its helpful features). The simplest models of this breaking require that the energy of the superpartners not be too high; in these cases, supersymmetry is expected to be observed by experiments at the Large Hadron Collider.

See also

- List of quantum field theories
- Feynman path integral
- Quantum chromodynamics
- Quantum electrodynamics
- Quantum flavordynamics
- Quantum geometrodynamics
- Quantum hydrodynamics
- Quantum magnetodynamics
- Quantum triviality
- Relationship between string theory and quantum field theory
- Abraham-Lorentz force
- Photon polarization
- Theoretical and experimental justification for the Schrödinger equation
- Invariance mechanics
- Green–Kubo relations
- Green's function (many-body theory)
- Common integrals in quantum field theory

- Schwinger-Dyson equation
- Relation between Schrödinger's equation and the path integral formulation of quantum mechanics

Notes

[1] Weinberg, S. Quantum Field Theory, Vols. I to III, 2000, Cambridge University Press: Cambridge, UK.
[2] Abraham Pais, *Inward Bound: Of Matter and Forces in the Physical World* ISBN 0198519974. Pais recounts how his astonishment at the rapidity with which Feynman could calculate using his method. Feynman's method is now part of the standard methods for physicists.

Suggested reading for the layman

- Gribbin, John ; *Q is for Quantum: Particle Physics from A to Z*, Weidenfeld & Nicolson (1998) [ISBN 0297817523] (http://www.amazon.com/Q-QUANTUM-Encyclopedia-Particle-Physics/dp/0684863154/)
- Feynman, Richard ; The Character of Physical Law (http://www.amazon.com/Character-Physical-Messenger-Lectures-1964/dp/0262560038/)
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Suggested reading

- Wilczek, Frank ; *Quantum Field Theory*, Review of Modern Physics 71 (1999) S85-S95. Review article written by a master of Q.C.D., *Nobel laureate 2003* (http://nobelprize.org/physics/laureates/2004/wilczek-autobio.html). Full text available at : *hep-th/9803075* (http://fr.arxiv.org/abs/hep-th/9803075)
- Ryder, Lewis H. ; *Quantum Field Theory* (Cambridge University Press, 1985), ISBN 0-521-33859-X. Introduction to relativistic Q.F.T. for particle physics.
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- Gordon L. Kane (1987). *Modern Elementary Particle Physics*. Perseus Books. ISBN 0-201-11749-5.
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- Kleinert, Hagen and Verena Schulte-Frohlinde, *Critical Properties of φ^4-Theories*, World Scientific (Singapur, 2001) (http://www.worldscibooks.com/physics/4733.html); Paperback ISBN 981-02-4658-7 *(also available online (http://www.physik.fu-berlin.de/~kleinert/re.html#B6))*
- Kleinert, Hagen, *Multivalued Fields in in Condensed Matter, Electrodynamics, and Gravitation*, World Scientific (Singapore, 2008) (http://www.worldscibooks.com/physics/6742.html) (also available online (http://www.physik.fu-berlin.de/~kleinert/re.html#B9))
- Itzykson, Claude and Zuber, Jean Bernard (1980). *Quantum Field Theory*. McGraw-Hill International Book Co.,. ISBN 0-07-032071-3.
- Bogoliubov, Nikolay, Shirkov, Dmitry (1982). *Quantum Fields*. Benjamin-Cummings Pub. Co. ISBN 0805309837.

Advanced reading

- N. N. Bogoliubov, A. A. Logunov, A. I. Oksak, I. T. Todorov (1990): *General Principles of Quantum Field Theory*. Dordrecht; Boston, Kluwer Academic Publishers. ISBN 079230540X. ISBN 978-0792305408.

External links

- Siegel, Warren ; *Fields* (http://insti.physics.sunysb.edu/~siegel/errata.html) (also available from arXiv:hep-th/9912205)
- 't Hooft, Gerard ; *The Conceptual Basis of Quantum Field Theory*, Handbook of the Philosophy of Science, Elsevier (to be published). Review article written by a master of gauge theories, laureate 1999 (http://nobelprize.org/physics/laureates/1999/thooft-autobio.html''Nobel). Full text available in (http://www.phys.uu.nl/~thooft/lectures/basisqft.pdf''here'').
- Srednicki, Mark ; *Quantum Field Theory* (http://gabriel.physics.ucsb.edu/~mark/qft.html)
- Kuhlmann, Meinard ; *Quantum Field Theory* (http://plato.stanford.edu/entries/quantum-field-theory/), Stanford Encyclopedia of Philosophy
- Quantum field theory textbooks: a list with links to amazon.com (http://motls.blogspot.com/2006/01/qft-didactics.html)
- Pedagogic Aids to Quantum Field Theory (http://quantumfieldtheory.info). Click on the link "Introduction" for a simplified introduction to QFT suitable for someone familiar with quantum mechanics.

Introduction

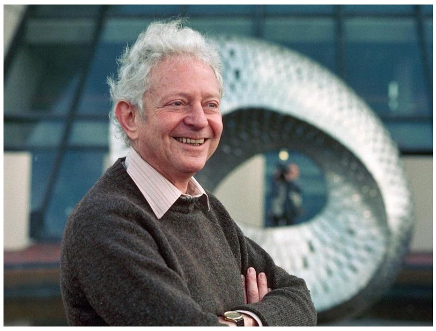
Outline of physics

This **outline of physics** covers much of → physics, the science concerned with the discovery and understanding of the fundamental laws which govern matter, energy, space, and time. Physics deals with the elementary constituents of the Universe and their interactions, as well as the analysis of systems best understood in terms of these fundamental principles. Because physics treats the core workings of the universe, including the → quantum mechanical details which underpin all atomic interactions, it can be thought of as the foundational science, upon which stands "the central science" of chemistry, the earth sciences, biological sciences, and social sciences. Discoveries in basic physics have important ramifications for all of science.

The following outline is provided as an overview of and topical guide to physics:

Where to start

> *See: Portal:Physics*.
>
> *For those seeking an overview of the fundamental categories of physics, see the subcategories of Category:Fundamental physics concepts.*



Leon M. Lederman

For students, there is a school course which starts with Physics First. In the words of Nobel laureate Leon Lederman, students can then "see that we live in an orderly and rational universe";[1] Lederman is one of the physicists behind Physics First. The Physical Science Study Committee (1956) committed to production of the textbook PSSC *Physics* (1960)[2] [3] [4] [5] [6] [7] . Other efforts include the Berkeley Physics Course and the *Feynman Lectures on Physics*.

In addition, it is helpful to prepare for the act of study. See Study skills in the category:Learning methods.

Essence of physics

Main article: → Physics

Physics started with a philosophical commitment to simplicity. It should not be considered a difficult subject (although it is deep); one can learn classical physics on a playground, which describes the motion of balls, swings, slides and merry-go-rounds.

Theory	Major subtopics	Concepts
Classical mechanics	Newton's laws of motion, Lagrangian mechanics, Hamiltonian mechanics, Kinematics, Statics, Dynamics, Chaos theory, Acoustics, Fluid dynamics, Continuum mechanics	Density, Dimension, Gravity, Space, Time, Motion, Length, Position, Velocity, Acceleration, Mass, Momentum, Force, Energy, Angular momentum, Torque, Conservation law, Harmonic oscillator, Wave, Work, Power
Electromagnetism	Electrostatics, Electrodynamics, Electricity, Magnetism, Maxwell's equations, Optics	Capacitance, Electric charge, Electric current, Electrical conductivity, Electric field, Electric permittivity, Electrical resistance, Electromagnetic field, Electromagnetic induction, Electromagnetic radiation, Gaussian surface, Magnetic field, Magnetic flux, Magnetic monopole, Magnetic permeability
Theory of relativity	Special relativity, General relativity, Einstein field equations	Covariance, Einstein manifold, Equivalence principle, Four-momentum, Four-vector, General principle of relativity, Geodesic motion, Gravity, Gravitoelectromagnetism, Inertial frame of reference, Invariance, Length contraction, Lorentzian manifold, Lorentz transformation, Metric, Minkowski diagram, Minkowski space, Principle of Relativity, Proper length, Proper time, Reference frame, Rest energy, Rest mass, Relativity of simultaneity, Spacetime, Special principle of relativity, Speed of light, Stress-energy tensor, Time dilation, Twin paradox, World line
→ Thermodynamics and → Statistical mechanics	Heat engine, Kinetic theory	Boltzmann's constant, Conjugate variables, Enthalpy, Entropy, Equation of state, Equipartition theorem, First Law of Thermodynamics, Free energy, Heat, Ideal gas law, Internal energy, Irreversible process, Partition function, Pressure, Reversible process, Second Law of Thermodynamics, Spontaneous process, State function, Statistical ensemble, Temperature, Thermodynamic equilibrium, Thermodynamic potential, Thermodynamic processes, Thermodynamic state, Thermodynamic system, Third Law of Thermodynamics, Viscosity, Zeroth Law of Thermodynamics

→ Quantum mechanics	Path integral formulation, Scattering theory, Schrödinger equation, → Quantum field theory, Quantum statistical mechanics	Adiabatic approximation, Correspondence principle, Free particle, Hamiltonian, Hilbert space, Identical particles, Matrix Mechanics, Planck's constant, Operators, Quanta, Quantization, Quantum entanglement, Quantum harmonic oscillator, Quantum number, Quantum tunneling, Schrödinger's cat, Dirac equation, Spin, Wavefunction, Wave mechanics, Wave-particle duality, Zero-point energy, Pauli Exclusion Principle, Heisenberg Uncertainty Principle

Branches of physics

- Astrophysics
- Atomic physics
- Biophysics
- Chemical Physics
- Optical physics
- Particle Physics
- Quantum Physics
- Thermodynamics
- Classical physics
- Condensed matter physics
- Molecular physics
- Nuclear Physics

Field	Subfields	Major theories	Concepts
Astrophysics	Cosmology, Gravitation physics, High-energy astrophysics, Planetary astrophysics, Plasma physics, Space physics, Stellar astrophysics	Big Bang, Lambda-CDM model, Cosmic inflation, General relativity, Law of universal gravitation	Black hole, Cosmic background radiation, Cosmic string, Cosmos, Dark energy, Dark matter, Galaxy, Gravity, Gravitational radiation, Gravitational singularity, Planet, Solar system, Star, Supernova, Universe
→ Atomic, molecular, and optical physics	Atomic physics, Molecular physics, Atomic and Molecular astrophysics, Chemical physics, Optics, Photonics	Quantum optics, Quantum chemistry, Quantum information science	Atom, Molecule, Diffraction, Electromagnetic radiation, Laser, Polarization, Spectral line, Casimir effect
→ Particle physics	Accelerator physics, Nuclear physics, Nuclear astrophysics, Particle astrophysics, Particle physics phenomenology	Standard Model, → Quantum field theory, → Quantum chromodynamics, Electroweak theory, Effective field theory, Lattice field theory, Lattice gauge theory, Gauge theory, Supersymmetry, Grand unification theory, Superstring theory, M-theory	Fundamental force (gravitational, electromagnetic, weak, strong), Elementary particle, Spin, Antimatter, Spontaneous symmetry breaking, Brane, String, Quantum gravity, Theory of everything, Vacuum energy

Condensed matter physics	Solid state physics, High pressure physics, Low-temperature physics, Nanoscale and mesoscopic physics, Polymer physics	BCS theory, Bloch wave, Fermi gas, Fermi liquid, Many-body theory	Phases (gas, liquid, solid, Bose-Einstein condensate, superconductor, superfluid), Electrical conduction, Magnetism, Self-organization, Spin, Spontaneous symmetry breaking

History of physics

Main article: History of physics

General physics concepts

- General concepts

  Gravity - Light - Physical system - Physical observation - Physical quantity - Physical state - Physical unit - Physical theory - Physical experiment -

- Theoretical concepts

  Mass-energy equivalence - Particle - Physical field - Physical interaction - Physical law - Fundamental force - Physical constant - Wave

- Basic quantities

  Space - Length - Time - Mass - Electric charge - Energy - Matter - Potential - Force - Momentum - Velocity - Acceleration - Entropy - Temperature

- Subfields

  Acoustics - Aerodynamics - Classical mechanics - Condensed matter physics - Cosmology - Dynamics - Electromagnetism - Hydrodynamics - Kinematics - Mathematical physics - Mechanics - Optics - plasma physics - → Quantum mechanics - Relativity - Statics - → Thermodynamics

Famous physicists

Main list: List of physicists

- Ibn al-Haytham - Father of optics and discovered reflection and refraction.
- Archimedes - Laid down the laws of flotation and developed Archimedes' principle.[8]
- Niels Bohr - made fundamental contributions to understanding atomic structure and → quantum mechanics. Widely considered one of the greatest physicists of the twentieth century.
- Albert Einstein - Greatest scientist of the 20th century, and possibly of all time. Developed both the Special and General Theories of Relativity.
- Richard Feynman - Expanded the theory of quantum electrodynamics, and developed the tool known as Feynman diagrams.
- Isaac Newton - Laid the groundwork for classical mechanics.
- Robert Oppenheimer - "Father of the atomic bomb."

Physics lists

Main article: List of physics topics

- List of Common Physics Abbreviations
- List of games using physics engines
- List of important publications in physics
- List of noise topics
- List of optical topics
- List of physicists
- List of physics-based computer and video games
- List of scientific journals in physics

See also

- Category:Fundamental physics concepts
- Category:Physics lists
- Glossary of classical physics

Notes

[1] Leon Lederman, Address to the 2008 Sigma Pi Sigma Quadrennial Congress, November 8, 2008, Fermilab, Illinois
[2] PSSC *Physics* 2nd ed., 1965
[3] PSSC *Physics* 3rd ed., ISBN 070151552X
[4] PSSC *Physics* 5th ed., 1981, ISBN 0-669-03113-5
[5] PSSC *Physics* 6th ed., 1986
[6] PSSC *Physics* Lab Guide, 7th ed., 1997 , ISBN 0840360266
[7] PSSC *Physics* 7th ed., 1997, ISBN 0669069108
[8] Eminent scientists, Published by scholastic India pvt. Ltd.

External links

- AIP.org (http://www.aip.org/index.html) is the website of the American Institute of Physics
- IOP.org (http://www.iop.org) is the website of the Institute of Physics
- APS.org (http://www.aps.org) is the website of the American Physical Society
- SPS National (http://www.spsnational.org) is the website of the American Society of Physics Students
- CAP.ca (http://www.cap.ca/) is the website of the Canadian Association of Physicists
- EPS.org (http://www.eps.org/) is the website of the European Physical Society

Quantum mechanics

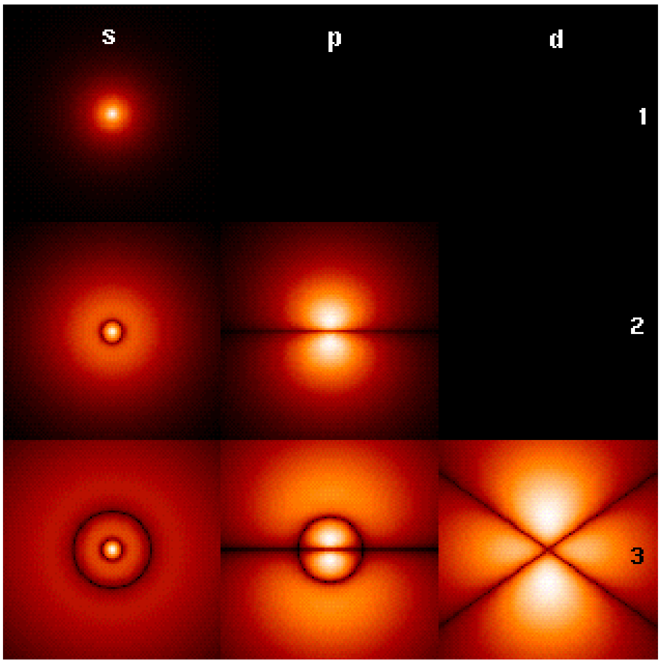


Fig. 1: Probability densities corresponding to the wavefunctions of an electron in a hydrogen atom possessing definite energy (increasing downward: n = 1, 2, 3, ...) and angular momentum (increasing across: s, p, d,...). Brighter areas correspond to higher probability density in a position measurement. Wavefunctions like these are directly comparable to Chladni's figures of acoustic modes of vibration in classical physics and are indeed modes of oscillation as well: they possess a sharp energy and thus a keen frequency. The angular momentum and energy are quantized, and only take on discrete values like those shown (as is the case for resonant frequencies in acoustics).

Quantum mechanics is a set of principles underlying the most fundamental known description of all physical systems at the submicroscopic scale (at the atomic level). Notable among these principles are both a dual wave-like and particle-like behavior of matter and radiation, and prediction of probabilities in situations where classical physics predicts certainties. Classical physics can be derived as a good *approximation* to quantum physics, typically in circumstances with large numbers of particles. Thus quantum phenomena are particularly relevant in systems whose dimensions are close to the atomic scale, such as molecules, atoms, electrons, protons and other subatomic particles. Exceptions exist for certain systems which exhibit quantum mechanical effects on macroscopic scale; superfluidity is one well-known example. Quantum theory provides accurate descriptions for many previously unexplained phenomena such as black body radiation and stable electron orbits. It has also given insight into the workings of many different biological systems, including smell receptors and protein structures.[1]

Overview

The word *quantum* is Latin for "how great" or "how much."[2] In quantum mechanics, it refers to a discrete unit that quantum theory assigns to certain physical quantities, such as the energy of an atom at rest (see Figure 1, at right). The discovery that waves have discrete energy packets (called quanta) that behave in a manner similar to particles led to the branch of physics that deals with atomic and subatomic systems which we today call quantum mechanics. It is the underlying mathematical framework of many fields of → physics and chemistry, including condensed matter physics, solid-state physics, atomic physics, molecular physics, computational chemistry, quantum chemistry, → particle physics, and nuclear physics. The foundations of quantum mechanics were established during the first half of the twentieth century by Werner Heisenberg, Max Planck, Louis de Broglie, Albert Einstein, Niels Bohr, Erwin Schrödinger, Max Born, John von Neumann, Paul Dirac, Wolfgang Pauli, William Hamilton, David Hilbert, and others.[3] Some fundamental aspects of the theory are still actively studied[4] .

Quantum mechanics is essential to understand the behavior of systems at atomic length scales and smaller. For example, if classical mechanics governed the workings of an atom, electrons would rapidly travel towards and collide with the nucleus, making stable atoms impossible. However, in the natural world the electrons normally remain in an unknown orbital path around the nucleus, defying classical electromagnetism.

Quantum mechanics was initially developed to provide a better explanation of the atom, especially the spectra of light emitted by different atomic species. The quantum theory of the atom was developed as an explanation for the electron's staying in its orbital, which could not be explained by Newton's laws of motion and by Maxwell's laws of classical electromagnetism.

In the formalism of quantum mechanics, the state of a system at a given time is described by a complex wave function (sometimes referred to as orbitals in the case of atomic electrons), and more generally, elements of a complex vector space. This abstract mathematical object allows for the calculation of probabilities of outcomes of concrete experiments. For example, it allows one to compute the probability of finding an electron in a particular region around the nucleus at a particular time. Contrary to classical mechanics, one can never make simultaneous predictions of conjugate variables, such as position and momentum, with arbitrary accuracy. For instance, electrons may be considered to be located somewhere within a region of space, but with their exact positions being unknown. Contours of constant probability, often referred to as “clouds” may be drawn around the nucleus of an atom to conceptualize where the electron might be located with the most probability. Heisenberg's uncertainty principle quantifies the inability to precisely locate the particle.

The other exemplar that led to quantum mechanics was the study of electromagnetic waves such as light. When it was found in 1900 by Max Planck that the energy of waves could be described as consisting of small packets or quanta, Albert Einstein exploited this idea to show that an electromagnetic wave such as light could be described by a particle called the photon with a discrete energy dependent on its frequency. This led to a theory of unity between subatomic particles and electromagnetic waves called wave–particle duality in which particles and waves were neither one nor the other, but had certain properties of both. While quantum mechanics describes the world of the very small, it also is needed to explain certain “macroscopic quantum systems” such as superconductors and superfluids.

Broadly speaking, quantum mechanics incorporates four classes of phenomena that classical physics cannot account for: (I) the quantization (discretization) of certain physical quantities, (II) wave-particle duality, (III) the uncertainty principle, and (IV) quantum entanglement. Each of these phenomena is described in detail in subsequent sections.

History

The **history of quantum mechanics**[5] began essentially with the 1838 discovery of cathode rays by Michael Faraday, the 1859 statement of the black body radiation problem by Gustav Kirchhoff, the 1877 suggestion by Ludwig Boltzmann that the energy states of a physical system could be discrete, and the 1900 quantum hypothesis by Max Planck that any energy is radiated and absorbed in quantities divisible by discrete ‘energy elements’, E, such that each of these energy elements is proportional to the frequency ν with which they each individually radiate energy, as defined by the following formula:

$$E = h\nu = \hbar\omega$$

where *h* is Planck's Action Constant. Planck insisted[6] that this was simply an aspect of the processes of absorption and emission of radiation and had nothing to do with the physical reality of the radiation itself. However, this did not explain the photoelectric effect (1839), i.e. that shining light on certain materials can function to eject electrons from the material. In 1905, basing his work on Planck’s quantum hypothesis, Albert Einstein[7] postulated that light itself consists of individual quanta. These later came to be called photons (1926). From Einstein's simple postulation was born a flurry of debating, theorizing and testing, and thus, the entire field of quantum physics...

Relativity and quantum mechanics

The modern world of physics is founded on the two tested and demonstrably sound theories of general relativity and quantum mechanics —theories which appear to contradict one another. The defining postulates of both Einstein's theory of relativity and quantum theory are indisputably supported by rigorous and repeated empirical evidence. However, while they do not directly contradict each other theoretically (at least with regard to primary claims), they are resistant to being incorporated within one cohesive model.

Einstein himself is well known for rejecting some of the claims of quantum mechanics. While clearly inventive in this field, he did not accept the more philosophical consequences and interpretations of quantum mechanics, such as the lack of deterministic causality and the assertion that a single subatomic particle can occupy numerous areas of space at one time. He also was the first to notice some of the apparently exotic consequences of entanglement and used them to formulate the Einstein-Podolsky-Rosen paradox, in the hope of showing that quantum mechanics had unacceptable implications. This was 1935, but in 1964 it was shown by John Bell (see Bell inequality) that Einstein's assumption was correct, but had to be completed by *hidden variables* and thus based on wrong philosophical assumptions. According to the paper of J. Bell and the Copenhagen interpretation (the common interpretation of quantum mechanics by physicists for decades), and contrary to Einstein's ideas, quantum mechanics was

- neither a "realistic" theory (since quantum measurements do not *state* pre-existing properties, but rather they *prepare* properties)
- nor a *local* theory (essentially not, because the state vector $|\psi\rangle$ determines simultaneously the probability amplitudes at all sites, $|\psi\rangle \rightarrow \psi(\mathbf{r}), \forall \mathbf{r}$).

The Einstein-Podolsky-Rosen paradox shows in any case that there exist experiments by which one can measure the state of one particle and instantaneously change the state of its entangled partner, although the two particles can be an arbitrary distance apart; however, this effect does not violate causality, since no transfer of information happens. These experiments are the basis of some of the most topical applications of the theory, quantum cryptography, which works well, although at small distances of typically $\leq$ 1000 km, being on the market since 2004.

There do exist quantum theories which incorporate *special* relativity—for example, quantum electrodynamics (QED), which is currently the most accurately tested physical theory [8] —and these lie at the very heart of modern → particle physics. Gravity is negligible in many areas of particle physics, so that unification between general relativity and quantum mechanics is not an urgent issue in those applications. However, the lack of a correct theory of quantum gravity is an important issue in cosmology.

Attempts at a unified theory

Inconsistencies arise when one tries to join the quantum laws with general relativity, a more elaborate description of spacetime which incorporates gravitation. Resolving these inconsistencies has been a major goal of twentieth- and twenty-first-century physics. Many prominent physicists, including Stephen Hawking, have labored in the attempt to discover a "Grand Unification Theory" that combines not only different models of subatomic physics, but also derives the universe's four forces—the strong force, electromagnetism, weak force, and gravity— from a single force or phenomenon. Leading the charge in this field is Edward Witten, a physicist that formulated the groundbreaking M-theory which is an attempt at describing the supersymmetrical based string theory.

Quantum mechanics and classical physics

Predictions of quantum mechanics have been verified experimentally to a very high degree of accuracy. Thus, the current logic of correspondence principle between classical and quantum mechanics is that all objects obey laws of quantum mechanics, and classical mechanics is just a quantum mechanics of large systems (or a statistical quantum mechanics of a large collection of particles). Laws of classical mechanics thus follow from laws of quantum mechanics at the limit of large systems or large quantum numbers.

The main differences between classical and quantum theories have already been mentioned above in the remarks on the Einstein-Podolsky-Rosen paradox. Essentially the difference boils down to the statement that quantum mechanics is coherent (addition of *amplitudes*), whereas classical theories are incoherent (addition of *intensities*). Thus, such quantities as *coherence lengths* and *coherence times* come into play. For microscopic bodies the extension of the system is certainly much smaller than the coherence length; for macroscopic bodies one expects that it should be the other way round.

This is in accordance with the following observations:

Many “macroscopic” properties of “classic” systems are direct consequences of quantum behavior of its parts. For example, stability of bulk matter (which consists of atoms and molecules which would quickly collapse under electric forces alone), rigidity of this matter, mechanical, thermal, chemical, optical and magnetic properties of this matter—they are all results of interaction of electric charges under the rules of quantum mechanics.

While the seemingly exotic behavior of matter posited by quantum mechanics and relativity theory become more apparent when dealing with extremely fast-moving or extremely tiny particles, the laws of classical “Newtonian” physics still remain accurate in predicting the behavior of surrounding (“large”) objects—of the order of the size of large molecules and bigger—at velocities much smaller than the velocity of light.

Theory

There are numerous mathematically equivalent formulations of quantum mechanics. One of the oldest and most commonly used formulations is the transformation theory proposed by Cambridge theoretical physicist Paul Dirac, which unifies and generalizes the two earliest formulations of quantum mechanics, matrix mechanics (invented by Werner Heisenberg)[9] and wave mechanics (invented by Erwin Schrödinger).

In this formulation, the instantaneous state of a quantum system encodes the probabilities of its measurable properties, or "observables". Examples of observables include energy, position, momentum, and angular momentum. Observables can be either continuous (e.g., the position of a particle) or discrete (e.g., the energy of an electron bound to a hydrogen atom).

Generally, quantum mechanics does not assign definite values to observables. Instead, it makes predictions about probability distributions; that is, the probability of obtaining each of the possible outcomes from measuring an observable. Oftentimes these results are skewed by many causes, such as dense probability clouds or quantum state nuclear attraction. Much of the time, these small anomalies are attributed to different causes such as quantum dislocation. Naturally, these probabilities will depend on the quantum state at the instant of the measurement. When the probability amplitudes of four or more quantum nodes are similar, it is called a quantum parallelism. There are, however, certain states that are associated with a definite value of a particular observable. These are known as "eigenstates" of the observable ("eigen" can be roughly translated from German as inherent or as a characteristic). In the everyday world, it is natural and intuitive to think of everything being in an eigenstate of every observable. Everything appears to have a definite position, a definite momentum, and a definite time of occurrence. However, quantum mechanics does not pinpoint the exact values for the position or momentum of a certain particle in a given space in a finite time; rather, it only provides a range of probabilities of where that particle might be. Therefore, it became necessary to use different words for (a) the state of something having an *uncertainty relation* and (b) a state that has a *definite* value. The latter is called the "eigenstate" of the property being measured.

For example, consider a free particle. In quantum mechanics, there is wave-particle duality so the properties of the particle can be described as a wave. Therefore, its quantum state can be represented as a wave, of arbitrary shape and extending over all of space, called a wave function. The position and momentum of the particle are observables. The Uncertainty Principle of quantum mechanics states that both the position and the momentum cannot simultaneously be known with infinite precision at the same time. However, one can measure just the position alone of a moving free particle creating an eigenstate of position with a wavefunction that is very large at a particular position x, and almost zero everywhere else. If one performs a position measurement on such a wavefunction, the result x will be obtained with almost 100% probability. In other words, the position of the free particle will almost be known. This is called an eigenstate of position (mathematically more precise: a *generalized eigenstate (eigendistribution)*). If the particle is in an eigenstate of position then its momentum is completely unknown. An eigenstate of momentum, on the other hand, has the form of a plane wave. It can be shown that the wavelength is equal to h/p, where h is Planck's constant and p is the momentum of the eigenstate. If the particle is in an eigenstate of momentum then its position is completely blurred out.

Usually, a system will not be in an eigenstate of whatever observable we are interested in. However, if one measures the observable, the wavefunction will instantaneously be an eigenstate (or generalized eigenstate) of that observable. This process is known as wavefunction collapse. It involves expanding the system under study to include the measurement device, so that a detailed quantum calculation would no longer be feasible and a classical description must be used. If one knows the corresponding wave function at the instant before the measurement, one will be able to compute the probability of collapsing into each of the possible eigenstates. For example, the free particle in the previous example will usually have a wavefunction that is a wave packet centered around some mean position x_0, neither an eigenstate of position nor of momentum. When one measures the position of the particle, it is impossible to predict with certainty the result that we will obtain. It is probable, but not certain, that it will be near x_0, where the amplitude of the wave function is large. After the measurement is performed, having obtained some result x, the wave function collapses into a position eigenstate centered at x.

Wave functions can change as time progresses. An equation known as the Schrödinger equation describes how wave functions change in time, a role similar to Newton's second law in classical mechanics. The Schrödinger equation, applied to the aforementioned example of the free particle, predicts that the center of a wave packet will move through space at a constant velocity, like a classical particle with no forces acting on it. However, the wave packet will also spread out as time progresses, which means that the position becomes more uncertain. This also has the effect of turning position eigenstates (which can be thought of as infinitely sharp wave packets) into broadened wave packets that are no longer position eigenstates.

Some wave functions produce probability distributions that are constant in time. Many systems that are treated dynamically in classical mechanics are described by such "static" wave functions. For example, a single electron in an unexcited atom is pictured classically as a particle moving in a circular trajectory around the atomic nucleus, whereas in quantum mechanics it is described by a static, spherically symmetric wavefunction surrounding the nucleus (Fig. 1). (Note that only the lowest angular momentum states, labeled *s*, are spherically symmetric).

The time evolution of wave functions is deterministic in the sense that, given a wavefunction at an initial time, it makes a definite prediction of what the wavefunction will be at any later time. During a measurement, the change of the wavefunction into another one is not deterministic, but rather unpredictable, i.e., random.

The probabilistic nature of quantum mechanics thus stems from the act of measurement. This is one of the most difficult aspects of quantum systems to understand. It was the central topic in the famous Bohr-Einstein debates, in which the two scientists attempted to clarify these fundamental principles by way of thought experiments. In the decades after the formulation of quantum mechanics, the question of what constitutes a "measurement" has been extensively studied. Interpretations of quantum mechanics have been formulated to do away with the concept of "wavefunction collapse"; see, for example, the relative state interpretation. The basic idea is that when a quantum system interacts with a measuring apparatus, their respective wavefunctions become entangled, so that the original quantum system ceases to exist as an independent entity. For details, see the article on measurement in quantum mechanics.

Mathematical formulation

In the mathematically rigorous formulation of quantum mechanics, developed by Paul Dirac[10] and John von Neumann[11] , the possible states of a quantum mechanical system are represented by unit vectors (called "state vectors") residing in a complex separable Hilbert space (variously called the "state space" or the "associated Hilbert space" of the system) well defined up to a complex number of norm 1 (the phase factor). In other words, the possible states are points in the projectivization of a Hilbert space, usually called the complex projective space. The exact nature of this Hilbert space is dependent on the system; for example, the state space for position and momentum states is the space of square-integrable functions, while the state space for the spin of a single proton is just the product of two complex planes. Each observable is represented by a maximally-Hermitian (precisely: by a self-adjoint) linear operator acting on the state space. Each eigenstate of an observable corresponds to an eigenvector of the operator, and the associated eigenvalue corresponds to the value of the observable in that eigenstate. If the operator's spectrum is discrete, the observable can only attain those discrete eigenvalues.

The time evolution of a quantum state is described by the Schrödinger equation, in which the Hamiltonian, the operator corresponding to the total energy of the system, generates time evolution.

The inner product between two state vectors is a complex number known as a probability amplitude. During a measurement, the probability that a system collapses from a given initial state to a particular eigenstate is given by the square of the absolute value of the probability amplitudes between the initial and final states. The possible results of a measurement are the eigenvalues of the operator - which explains the choice of *Hermitian* operators, for which all the eigenvalues are real. We can find the probability distribution of an observable in a given state by computing the spectral decomposition of the corresponding operator. Heisenberg's uncertainty principle is represented by the statement that the operators corresponding to certain observables do not commute.

The Schrödinger equation acts on the entire probability amplitude, not merely its absolute value. Whereas the absolute value of the probability amplitude encodes information about probabilities, its phase encodes information about the interference between quantum states. This gives rise to the wave-like behavior of quantum states.

It turns out that analytic solutions of Schrödinger's equation are only available for a small number of model Hamiltonians, of which the quantum harmonic oscillator, the particle in a box, the hydrogen molecular ion and the hydrogen atom are the most important representatives. Even the helium atom, which contains just one more electron than hydrogen, defies all attempts at a fully analytic treatment. There exist several techniques for generating approximate solutions. For instance, in the method known as perturbation theory one uses the analytic results for a simple quantum mechanical model to generate results for a more complicated model related to the simple model by, for example, the addition of a weak potential energy. Another method is the "semi-classical equation of motion" approach, which applies to systems for which quantum mechanics produces weak deviations from classical behavior. The deviations can be calculated based on the classical motion. This approach is important for the field of quantum chaos.

An alternative formulation of quantum mechanics is Feynman's path integral formulation, in which a quantum-mechanical amplitude is considered as a sum over histories between initial and final states; this is the quantum-mechanical counterpart of action principles in classical mechanics.

Interactions with other scientific theories

The fundamental rules of quantum mechanics are very deep. They assert that the state space of a system is a Hilbert space and the observables are Hermitian operators acting on that space, but do not tell us which Hilbert space or which operators, or if it even exists. These must be chosen appropriately in order to obtain a quantitative description of a quantum system. An important guide for making these choices is the correspondence principle, which states that the predictions of quantum mechanics reduce to those of classical physics when a system moves to higher energies or equivalently, larger quantum numbers. In other words, classic mechanics is simply a quantum mechanics of large systems. This "high energy" limit is known as the *classical* or *correspondence limit*. One can therefore start from an established classical model of a particular system, and attempt to guess the underlying quantum model that gives rise to the classical model in the correspondence limit.

→ Unsolved problems in physics: *In the correspondence limit of **quantum mechanics**: Is there a preferred interpretation of quantum mechanics? How does the quantum description of reality, which includes elements such as the "superposition of states" and "wavefunction collapse", give rise to the reality we perceive?*

When quantum mechanics was originally formulated, it was applied to models whose correspondence limit was non-relativistic classical mechanics. For instance, the well-known model of the quantum harmonic oscillator uses an explicitly non-relativistic expression for the kinetic energy of the oscillator, and is thus a quantum version of the classical harmonic oscillator.

Early attempts to merge quantum mechanics with special relativity involved the replacement of the Schrödinger equation with a covariant equation such as the Klein-Gordon equation or the Dirac equation. While these theories were successful in explaining many experimental results, they had certain unsatisfactory qualities stemming from their neglect of the relativistic creation and annihilation of particles. A fully relativistic quantum theory required the development of → quantum field theory, which applies quantization to a field rather than a fixed set of particles. The first complete quantum field theory, quantum electrodynamics, provides a fully quantum description of the electromagnetic interaction.

The full apparatus of quantum field theory is often unnecessary for describing electrodynamic systems. A simpler approach, one employed since the inception of quantum mechanics, is to treat charged particles as quantum mechanical objects being acted on by a classical electromagnetic field. For example, the elementary quantum model of the hydrogen atom describes the electric field of the hydrogen atom using a classical $-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$ Coulomb potential. This "semi-classical" approach fails if quantum fluctuations in the electromagnetic field play an important role, such as in the emission of photons by charged particles.

Quantum field theories for the strong nuclear force and the weak nuclear force have been developed. The quantum field theory of the strong nuclear force is called → quantum chromodynamics, and describes the interactions of the subnuclear particles: quarks and gluons. The weak nuclear force and the electromagnetic force were unified, in their quantized forms, into a single quantum field theory known as electroweak theory, by the physicists Abdus Salam, Sheldon Glashow and Steven Weinberg.

It has proven difficult to construct quantum models of gravity, the remaining fundamental force. Semi-classical approximations are workable, and have led to predictions such as Hawking radiation. However, the formulation of a complete theory of quantum gravity is hindered by apparent incompatibilities between general relativity, the most accurate theory of gravity currently known, and some of the fundamental assumptions of quantum theory. The resolution of these incompatibilities is an area of active research, and theories such as string theory are among the possible candidates for a future theory of quantum gravity.

Example

The particle in a 1-dimensional potential energy box is the most simple example where restraints lead to the quantization of energy levels. The box is defined as zero potential energy inside a certain interval and infinite everywhere outside that interval. For the 1-dimensional case in the x direction, the time-independent Schrödinger equation can be written as:[12]

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi.$$

The general solutions are:

$$\psi = Ae^{ikx} + Be^{-ikx} \qquad E = \frac{\hbar^2 k^2}{2m}$$

or

$$\psi = C\sin kx + D\cos kx$$ (by Euler's formula).

The presence of the walls of the box restricts the acceptable solutions of the wavefunction. At each wall:

$$\psi = 0 \text{ at } \ x = 0,\ x = L.$$

Consider $x = 0$

- sin 0 = 0, cos 0 = 1. To satisfy $\psi=0$ the cos term has to be removed. Hence $D = 0$.

Now consider: $\psi=C\sin kx$

- at $x = L$, $\psi=C\sin kL=0$
- If $C = 0$ then $\psi=0$ for all x. This would conflict with the Born interpretation
- therefore sin $kL = 0$ must be satisfied, yielding the condition.

$$kL = n\pi \quad n = 1, 2, 3, 4, 5, ...$$

In this situation, n must be an integer showing the quantization of the energy levels.

Applications

Quantum mechanics has had enormous success in explaining many of the features of our world. The individual behaviour of the subatomic particles that make up all forms of matter—electrons, protons, neutrons, photons and others—can often only be satisfactorily described using quantum mechanics. Quantum mechanics has strongly influenced string theory, a candidate for a theory of everything (see reductionism) and the multiverse hypothesis. It is also related to → statistical mechanics.

Quantum mechanics is important for understanding how individual atoms combine covalently to form chemicals or molecules. The application of quantum mechanics to chemistry is known as quantum chemistry. (Relativistic) quantum mechanics can in principle mathematically describe most of chemistry. Quantum mechanics can provide quantitative insight into ionic and covalent bonding processes by explicitly showing which molecules are energetically favorable to which others, and by approximately how much. Most of the calculations performed in computational chemistry rely on quantum mechanics.

Much of modern technology operates at a scale where quantum effects are significant. Examples include the laser, the transistor, the electron microscope, and magnetic resonance imaging. The study of semiconductors led to the invention of the diode and the transistor, which are indispensable for modern electronics.

Researchers are currently seeking robust methods of directly manipulating quantum states. Efforts are being made to develop quantum cryptography, which will allow guaranteed secure transmission of information. A more distant goal is the development of quantum computers, which are expected to perform certain computational tasks exponentially faster than classical computers. Another active research topic is quantum teleportation, which deals with techniques to transmit quantum states over arbitrary distances.

In many devices, even the simple light switch, quantum tunneling is vital, as otherwise the electrons in the electric current could not penetrate the potential barrier made up, in the case of the light switch, of a layer of oxide. Flash memory chips found in USB drives also use quantum tunneling to erase their memory cells.

Philosophical consequences

Since its inception, the many counter-intuitive results of quantum mechanics have provoked strong philosophical debate and many interpretations. Even fundamental issues such as Max Born's basic rules concerning probability amplitudes and probability distributions took decades to be appreciated.

The Copenhagen interpretation, due largely to the Danish theoretical physicist Niels Bohr, is the interpretation of quantum mechanics most widely accepted amongst physicists. According to it, the probabilistic nature of quantum mechanics predictions cannot be explained in terms of some other deterministic theory, and does not simply reflect our limited knowledge. Quantum mechanics provides probabilistic results because the physical universe is itself probabilistic rather than deterministic.

Albert Einstein, himself one of the founders of quantum theory, disliked this loss of determinism in measurement (this dislike is the source of his famous quote, "God does not play dice with the universe."). Einstein held that there should be a local hidden variable theory underlying quantum mechanics and that, consequently, the present theory was incomplete. He produced a series of objections to the theory, the most famous of which has become known as the EPR paradox. John Bell showed that the EPR paradox led to experimentally testable differences between quantum mechanics and local realistic theories. Experiments have been performed confirming the accuracy of quantum mechanics, thus demonstrating that the physical world cannot be described by local realistic theories.

The *Bohr-Einstein debates* provide a vibrant critique of
the Copenhagen Interpretation from an epistemological point of view.

The Everett many-worlds interpretation, formulated in 1956, holds that all the possibilities described by quantum theory simultaneously occur in a "multiverse" composed of mostly independent parallel universes. This is not accomplished by introducing some new axiom to quantum mechanics, but on the contrary by *removing* the axiom of the collapse of the wave packet: All the possible consistent states of the measured system and the measuring apparatus (including the observer) are present in a *real* physical (not just formally mathematical, as in other interpretations) quantum superposition. (Such a superposition of consistent state combinations of different systems is called an entangled state.) While the multiverse is deterministic, we perceive non-deterministic behavior governed by probabilities, because we can observe only the universe, i.e. the consistent state contribution to the mentioned superposition, we inhabit. Everett's interpretation is perfectly consistent with John Bell's experiments and makes them intuitively understandable. However, according to the theory of quantum decoherence, the parallel universes will never be accessible to us. This inaccessibility can be understood as follows: once a measurement is done, the measured system becomes entangled with both the physicist who measured it and a huge number of other particles, some of which are photons flying away towards the other end of the universe; in order to prove that the wave function did not collapse one would have to bring all these particles back and measure them again, together with the system that was measured originally. This is completely impractical, but even if one could theoretically do this, it would destroy any evidence that the original measurement took place (including the physicist's memory).

See also

- Combinatorics and physics
- Copenhagen interpretation
- Correspondence rules
- Fine-structure constant
- Interpretation of quantum mechanics
- Introduction to quantum mechanics
- Many-worlds interpretation
- Measurement in quantum mechanics
- Measurement problem
- Photon dynamics in the double-slit experiment
- Photon polarization
- Quantum chemistry
- → Quantum chromodynamics
- Quantum computers
- Quantum decoherence
- Quantum electrochemistry
- Quantum electronics
- → Quantum field theory
- Quantum information
- Quantum mind
- Quantum optics
- Quantum pseudo-telepathy
- Quantum thermodynamics
- Quantum triviality

- Quantum Zeno effect
- Quasi-set theory
- Relation between Schrödinger's equation and the path integral formulation of quantum mechanics
- Schrödinger's cat
- Theoretical and experimental justification for the Schrödinger equation
- Theoretical chemistry

Notes

[1] http://discovermagazine.com/2009/feb/13-is-quantum-mechanics-controlling-your-thoughts/article_view?b_start:int=1&-C
[2] http://www.merriam-webster.com/dictionary/quantum
[3] http://mooni.fccj.org/~ethall/quantum/quant.htm
[4] Compare the list of conferences presented here http://ysfine.com.
[5] J. Mehra and H. Rechenberg, *The historical development of quantum theory*, Springer-Verlag, 1982.
[6] e.g. T.S. Kuhn, *Black-body theory and the quantum discontinuity 1894-1912*, Clarendon Press, Oxford, 1978.
[7] A. Einstein, *Über einen die Erzeugung und Verwandlung des Lichtes betreffenden heuristischen Gesichtspunkt (On a heuristic point of view concerning the production and transformation of light)*, Annalen der Physik **17** (1905) 132-148 (reprinted in *The collected papers of Albert Einstein,* John Stachel, editor, Princeton University Press, 1989, Vol. 2, pp. 149-166, in German; see also *Einstein's early work on the quantum hypothesis,* ibid. pp. 134-148).
[8] Life on the lattice: The most accurate theory we have (http://latticeqcd.blogspot.com/2005/06/most-accurate-theory-we-have.html)
[9] Especially since Werner Heisenberg was awarded the Nobel Prize in Physics in 1932 for the creation of quantum mechanics, the role of Max Born has been obfuscated. A 2005 biography of Born details his role as the creator of the matrix formulation of quantum mechanics. This was recognized in a paper by Heisenberg, in 1940, honoring Max Planck. See: Nancy Thorndike Greenspan, "The End of the Certain World: The Life and Science of Max Born" (Basic Books, 2005), pp. 124 - 128, and 285 - 286.
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External links

General

- The Modern Revolution in Physics (http://www.lightandmatter.com/html_books/6mr/ch01/ch01.html) - an online textbook
- J. O'Connor and E. F. Robertson: A history of quantum mechanics (http://www-history.mcs.st-andrews.ac.uk/history/HistTopics/The_Quantum_age_begins.html)
- Introduction to Quantum Theory at Quantiki (http://www.quantiki.org/wiki/index.php/Introduction_to_Quantum_Theory)
- Quantum Physics Made Relatively Simple (http://bethe.cornell.edu/): three video lectures by Hans Bethe
- H is for h-bar (http://www.nonlocal.com/hbar/)

Course material

- MIT OpenCourseWare: Chemistry (http://ocw.mit.edu/OcwWeb/Chemistry/index.htm). See 5.61 (http://ocw.mit.edu/OcwWeb/Chemistry/5-61Fall-2004/CourseHome/index.htm), 5.73 (http://ocw.mit.edu/OcwWeb/Chemistry/5-73Fall-2005/CourseHome/index.htm), and 5.74 (http://ocw.mit.edu/OcwWeb/Chemistry/5-74Spring-2005/CourseHome/index.htm)
- MIT OpenCourseWare: Physics (http://ocw.mit.edu/OcwWeb/Physics/index.htm). See 8.04 (http://ocw.mit.edu/OcwWeb/Physics/8-04Spring-2006/CourseHome/index.htm),

8.05 (http://ocw.mit.edu/OcwWeb/Physics/8-05Fall-2004/CourseHome/index.htm), and 8.06 (http://ocw.mit.edu/OcwWeb/Physics/8-06Spring-2005/CourseHome/index.htm)
- 5½ Examples in Quantum Mechanics (http://www.physics.csbsju.edu/QM/)
- Imperial College Quantum Mechanics Course to Download (http://www.imperial.ac.uk/quantuminformation/qi/tutorials)
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- Doron Cohen: Lecture notes in Quantum Mechanics (comprehensive, with advanced topics) (http://arxiv.org/abs/quant-ph/0605180)
- Quantum Physics Online : interactive introduction to quantum mechanics (RS applets) (http://www.quantum-physics.polytechnique.fr)
- Experiments to the foundations of quantum physics with single photons (http://www.quantumlab.de)

FAQs

- Many-worlds or relative-state interpretation (http://www.hedweb.com/manworld.htm)
- Measurement in Quantum mechanics (http://www.mtnmath.com/faq/meas-qm.html)

Media

- Everything you wanted to know about the quantum world (http://www.newscientist.com/channel/fundamentals/quantum-world) — archive of articles from *New Scientist* magazine.
- Quantum Physics Research (http://www.sciencedaily.com/news/matter_energy/quantum_physics/) from Science Daily
- "Quantum Trickery: Testing Einstein's Strangest Theory" (http://www.nytimes.com/2005/12/27/science/27eins.html?ex=1293339600&en=caf5d835203c3500&ei=5090). The New York Times. December 27, 2005. http://www.nytimes.com/2005/12/27/science/27eins.html?ex=1293339600&en=caf5d835203c3500&ei=5090.

Philosophy

- Quantum Mechanics (http://plato.stanford.edu/entries/qm) entry in the *Stanford Encyclopedia of Philosophy* by Jenann Ismael
- David Mermin on the future directions of physics (http://www.physicstoday.org/pt/vol-54/iss-2/p11.html)

Statistical mechanics

Statistical mechanics (or **statistical thermodynamics**[1]) is the application of probability theory, which includes mathematical tools for dealing with large populations, to the field of mechanics, which is concerned with the motion of particles or objects when subjected to a force. It provides a framework for relating the microscopic properties of individual atoms and molecules to the macroscopic or bulk properties of materials that can be observed in everyday life, therefore explaining → thermodynamics as a natural result of statistics and mechanics (classical and quantum) at the microscopic level.

It provides a molecular-level interpretation of thermodynamic quantities such as work, heat, free energy, and entropy, allowing the thermodynamic properties of bulk materials to be related to the spectroscopic data of individual molecules. This ability to make macroscopic predictions based on microscopic properties is the main advantage of statistical mechanics over classical thermodynamics. Both theories are governed by the second law of thermodynamics through the medium of entropy. However, entropy in → thermodynamics can only be known empirically, whereas in statistical mechanics, it is a function of the distribution of the system on its micro-states.

Statistical thermodynamics was born in 1870 with the work of Austrian physicist Ludwig Boltzmann, much of which was collectively published in Boltzmann's 1896 *Lectures on Gas Theory*.[2] Boltzmann's original papers on the statistical interpretation of thermodynamics, the H-theorem, transport theory, thermal equilibrium, the equation of state of gases, and similar subjects, occupy about 2,000 pages in the proceedings of the Vienna Academy and other societies. The term "statistical thermodynamics" was proposed for use by the American thermodynamicist and physical chemist J. Willard Gibbs in 1902. According to Gibbs, the term "statistical", in the context of mechanics, i.e. statistical mechanics, was first used by the Scottish physicist James Clerk Maxwell in 1871.

Overview

The essential problem in statistical thermodynamics is to determine the distribution of a given amount of energy E over N identical systems.[3] The goal of statistical thermodynamics is to understand and to interpret the measurable macroscopic properties of materials in terms of the properties of their constituent particles and the interactions between them. This is done by connecting thermodynamic functions to quantum-mechanic equations. Two central quantities in statistical thermodynamics are the Boltzmann factor and the partition function.

Fundamentals

Central topics covered in statistical thermodynamics include:

- Microstates and configurations
- Boltzmann distribution law
- Partition function, Configuration integral or configurational partition function
- Thermodynamic equilibrium - thermal, mechanical, and chemical.
- Internal degrees of freedom - rotation, vibration, electronic excitation, etc.
- Heat capacity – Einstein solids, polyatomic gases, etc.
- Nernst heat theorem
- Fluctuations
- Gibbs paradox
- Degeneracy

Lastly, and most importantly, the formal definition of entropy of a thermodynamic system from a statistical perspective is called statistical entropy, and is defined as:

$$S = k_B \ln \Omega$$

where

k_B is Boltzmann's constant 1.38066×10^{-23} J K^{-1} and

Ω is the number of microstates corresponding to the observed thermodynamic macrostate.

A common mistake is taking this formula as a hard general definition of entropy. This equation is valid only if each microstate is equally accessible (each microstate has an equal probability of occurring).

Boltzmann Distribution

If the system is large the Boltzmann distribution could be used (the Boltzmann distribution is an approximate result)

$$n_i \propto e^{-\frac{U_i}{k_B T}}.$$

This can now be used with $\rho_i = \frac{n_i}{N}$:

$$\rho_i = \frac{n_i}{N} = \frac{e^{-\frac{U_i}{k_B T}}}{\sum_{i=1}^{\text{all levels}} e^{-\frac{U_i}{k_B T}}}.$$

History

In 1738, Swiss physicist and mathematician Daniel Bernoulli published *Hydrodynamica* which laid the basis for the kinetic theory of gases. In this work, Bernoulli positioned the argument, still used to this day, that gases consist of great numbers of molecules moving in all directions, that their impact on a surface causes the gas pressure that we feel, and that what we experience as heat is simply the kinetic energy of their motion.

In 1859, after reading a paper on the diffusion of molecules by Rudolf Clausius, Scottish physicist James Clerk Maxwell formulated the Maxwell distribution of molecular velocities, which gave the proportion of molecules having a certain velocity in a specific range. This was the first-ever statistical law in physics.[4] Five years later, in 1864, Ludwig Boltzmann, a young student in Vienna, came across Maxwell’s paper and was so inspired by it that he spent much of his long and distinguished life developing the subject further.

Hence, the foundations of statistical thermodynamics were laid down in the late 1800s by those such as Maxwell, Ludwig Boltzmann, Max Planck, Rudolf Clausius, and Willard Gibbs who began to apply statistical and quantum atomic theory to ideal gas bodies. Predominantly, however, it was Maxwell and Boltzmann, working independently, who reached similar conclusions as to the statistical nature of gaseous bodies. Yet, one must consider Boltzmann to be the "father" of statistical thermodynamics with his 1875 derivation of the relationship between entropy S and multiplicity Ω, the number of microscopic arrangements (microstates) producing the same macroscopic state (macrostate) for a particular system.[5]

Fundamental postulate

The fundamental postulate in statistical mechanics (also known as the *equal a priori probability postulate*) is the following:

> *Given an isolated system in equilibrium, it is found with equal probability in each of its accessible microstates.*

This postulate is a fundamental assumption in statistical mechanics - it states that a system in equilibrium does not have any preference for any of its available microstates. Given Ω microstates at a particular energy, the probability of finding the system in a particular microstate is $p = 1/\Omega$.

This postulate is necessary because it allows one to conclude that for a system at equilibrium, the thermodynamic state (macrostate) which could result from the largest number of microstates is also the most probable macrostate of the system.

The postulate is justified in part, for classical systems, by Liouville's theorem (Hamiltonian), which shows that if the distribution of system points through accessible phase space is uniform at some time, it remains so at later times.

Similar justification for a discrete system is provided by the mechanism of detailed balance.

This allows for the definition of the *information function* (in the context of information theory):

$$I = -\sum_i \rho_i \ln \rho_i = \langle \ln \rho \rangle.$$

When all the probabilities (rhos) are equal, I is maximal, and we have minimal information about the system. When our information is maximal (i.e., one rho is equal to one and the rest to zero, such that we know what state the system is in), the function is minimal.

This "information function" is the same as the **reduced entropic function** in thermodynamics.

Statistical ensembles

Microcanonical ensemble

In microcanonical ensemble N, V and E are fixed. Since the second law of thermodynamics applies to isolated systems, the first case investigated will correspond to this case. The *Microcanonical ensemble* describes an isolated system.

The entropy of such a system can only increase, so that the maximum of its entropy corresponds to an equilibrium state for the system.

Because an isolated system keeps a constant energy, the total energy of the system does not fluctuate. Thus, the system can access only those of its micro-states that correspond to a given value *E* of the energy. The internal energy of the system is then strictly equal to its energy.

Let us call $\Omega(E)$ the number of micro-states corresponding to this value of the system's energy. The macroscopic state of maximal entropy for the system is the one in which all micro-states are equally likely to occur, with probability $1/\Omega(E)$, during the system's fluctuations.

$$S = -k_B \sum_{i=1}^{\Omega(E)} \left\{ \frac{1}{\Omega(E)} \ln \frac{1}{\Omega(E)} \right\} = k_B \ln \left(\Omega(E) \right)$$

where

S is the system entropy, and

k_B is Boltzmann's constant.

Canonical ensemble

In canonical ensemble N, V and T are fixed. Invoking the concept of the canonical ensemble, it is possible to derive the probability P_i that a macroscopic system in thermal equilibrium with its environment, will be in a given microstate with energy E_i according to the Boltzmann distribution:

$$P_i = \frac{e^{-\beta E_i}}{\sum_j^{j_{\max}} e^{-\beta E_j}}$$

where $\beta = \frac{1}{kT}$,

The temperature T arises from the fact that the system is in thermal equilibrium with its environment. The probabilities of the various microstates must add to one, and the normalization factor in the denominator is the canonical partition function:

$$Z = \sum_j^{j_{max}} e^{-\beta E_j}$$

where E_i is the energy of the ith microstate of the system. The partition function is a measure of the number of states accessible to the system at a given temperature. The article canonical ensemble contains a derivation of Boltzmann's factor and the form of the partition function from first principles.

To sum up, the probability of finding a system at temperature T in a particular state with energy E_i is

$$P_i = \frac{e^{-\beta E_i}}{Z}.$$

Thermodynamic Connection

The partition function can be used to find the expected (average) value of any microscopic property of the system, which can then be related to macroscopic variables. For instance, the expected value of the microscopic energy E is *interpreted* as the microscopic definition of the thermodynamic variable internal energy U, and can be obtained by taking the derivative of the partition function with respect to the temperature. Indeed,

$$\langle E\rangle = \frac{\sum_i E_i e^{-\beta E_i}}{Z} = -\frac{1}{Z}\frac{dZ}{d\beta}$$

implies, together with the interpretation of $\langle E\rangle$ as U, the following microscopic definition of internal energy:

$$U := -\frac{d\ln Z}{d\beta}.$$

The entropy can be calculated by (see Shannon entropy)

$$\frac{S}{k} = -\sum_i p_i \ln p_i = \sum_i \frac{e^{-\beta E_i}}{Z}(\beta E_i + \ln Z) = \ln Z + \beta U$$

which implies that

$$-\frac{\ln(Z)}{\beta} = U - TS = F$$

is the free energy of the system or in other words,

$$Z = e^{-\beta F}$$

Having microscopic expressions for the basic thermodynamic potentials U (internal energy), S (entropy) and F (free energy) is sufficient to derive expressions for other thermodynamic quantities. The basic strategy is as follows. There may be an intensive or extensive quantity that enters explicitly in the expression for the microscopic energy E_i, for instance magnetic field (intensive) or volume (extensive). Then, the conjugate thermodynamic variables are derivatives of the internal energy. The macroscopic magnetization (extensive) is the derivative of U with respect to the (intensive) magnetic field, and the pressure (intensive) is the derivative of U with respect to volume (extensive).

The treatment in this section assumes no exchange of matter (i.e. fixed mass and fixed particle numbers). However, the volume of the system is variable which means the density is also variable.

This probability can be used to find the average value, which corresponds to the macroscopic value, of any property, J, that depends on the energetic state of the system by using the formula:

$$\langle J\rangle = \sum_i p_i J_i = \sum_i J_i \frac{e^{-\beta E_i}}{Z}$$

where $\langle J\rangle$ is the average value of property J. This equation can be applied to the internal energy, U:

$$U = \sum_i E_i \frac{e^{-\beta E_i}}{Z}$$

Subsequently, these equations can be combined with known thermodynamic relationships between U and V to arrive at an expression for pressure in terms of only temperature, volume and the partition function. Similar relationships in terms of the partition function can be derived for other thermodynamic properties as shown in the following table; see also the detailed explanation in configuration integral [6].

Helmholtz free energy:	$F = -\frac{\ln Z}{\beta}$
Internal energy:	$U = -\left(\frac{\partial \ln Z}{\partial \beta}\right)_{N,V}$
Pressure:	$P = -\left(\frac{\partial F}{\partial V}\right)_{N,T} = \frac{1}{\beta}\left(\frac{\partial \ln Z}{\partial V}\right)_{N,T}$
Entropy:	$S = k(\ln Z + \beta U)$
Gibbs free energy:	$G = F + PV = -\frac{\ln Z}{\beta} + \frac{V}{\beta}\left(\frac{\partial \ln Z}{\partial V}\right)_{N,T}$
Enthalpy:	$H = U + PV$
Constant volume heat capacity:	$C_V = \left(\frac{\partial U}{\partial T}\right)_{N,V}$
Constant pressure heat capacity:	$C_P = \left(\frac{\partial H}{\partial T}\right)_{N,P}$
Chemical potential:	$\mu_i = -\frac{1}{\beta}\left(\frac{\partial \ln Z}{\partial N_i}\right)_{T,V,N}$

To clarify, this is not a grand canonical ensemble.

It is often useful to consider the energy of a given molecule to be distributed among a number of modes. For example, translational energy refers to that portion of energy associated with the motion of the center of mass of the molecule. Configurational energy refers to that portion of energy associated with the various attractive and repulsive forces between molecules in a system. The other modes are all considered to be internal to each molecule. They include rotational, vibrational, electronic and nuclear modes. If we assume that each mode is independent (a questionable assumption) the total energy can be expressed as the sum of each of the components:

$$E = E_t + E_c + E_n + E_e + E_r + E_v$$

Where the subscripts t, c, n, e, r, and v correspond to translational, configurational, nuclear, electronic, rotational and vibrational modes, respectively. The relationship in this equation can be substituted into the very first equation to give:

$$Z = \sum_i e^{-\beta(E_{ti}+E_{ci}+E_{ni}+E_{ei}+E_{ri}+E_{vi})}$$

$$= \sum_i e^{-\beta E_{ti}} e^{-\beta E_{ci}} e^{-\beta E_{ni}} e^{-\beta E_{ei}} e^{-\beta E_{ri}} e^{-\beta E_{vi}}$$

If we can assume all these modes are completely uncoupled and uncorrelated, so all these factors are in a probability sense completely independent, then

$$Z = Z_t Z_c Z_n Z_e Z_r Z_v$$

Thus a partition function can be defined for each mode. Simple expressions have been derived relating each of the various modes to various measurable molecular properties, such as the characteristic rotational or vibrational frequencies.

Expressions for the various molecular partition functions are shown in the following table.

Nuclear	$Z_n = 1 \qquad (T < 10^8 K)$

Electronic	$Z_e = W_0 e^{kTD_e + W_1 e^{-\theta_{e1}/T} + \cdots}$
Vibrational	$Z_v = \prod_j \frac{e^{-\theta_{vj}/2T}}{1 - e^{-\theta_{vj}/T}}$
Rotational (linear)	$Z_r = \frac{T}{\sigma}\theta_r$
Rotational (non-linear)	$Z_r = \frac{1}{\sigma}\sqrt{\frac{\pi T^3}{\theta_A \theta_B \theta_C}}$
Translational	$Z_t = \frac{(2\pi mkT)^{3/2}}{h^3}$
Configurational (ideal gas)	$Z_c = V$

These equations can be combined with those in the first table to determine the contribution of a particular energy mode to a thermodynamic property. For example the "rotational pressure" could be determined in this manner. The total pressure could be found by summing the pressure contributions from all of the individual modes, ie:

$$P = P_t + P_c + P_n + P_e + P_r + P_v$$

Grand canonical ensemble

In grand canonical ensemble V, T and chemical potential are fixed. If the system under study is an open system, (matter can be exchanged), *but* particle number is not conserved, we would have to introduce chemical potentials, μ_j, j = 1,...,n and replace the canonical partition function with the grand canonical partition function:

$$\Xi(V,T,\mu) = \sum_i \exp\left(\beta\left[\sum_{j=1}^n \mu_j N_{ij} - E_i\right]\right)$$

where N_{ij} is the number of j^{th} species particles in the i^{th} configuration. Sometimes, we also have other variables to add to the partition function, one corresponding to each conserved quantity. Most of them, however, can be safely interpreted as chemical potentials. In most condensed matter systems, things are nonrelativistic and mass is conserved. However, most condensed matter systems of interest also conserve particle number approximately (metastably) and the mass (nonrelativistically) is none other than the sum of the number of each type of particle times its mass. Mass is inversely related to density, which is the conjugate variable to pressure. For the rest of this article, we will ignore this complication and pretend chemical potentials don't matter. See grand canonical ensemble.

Let's rework everything using a grand canonical ensemble this time. The volume is left fixed and does not figure in at all in this treatment. As before, j is the index for those particles of species j and i is the index for microstate i:

$$U = \sum_i E_i \frac{\exp(-\beta(E_i - \sum_j \mu_j N_{ij}))}{\Xi}$$

$$N_j = \sum_i N_{ij} \frac{\exp(-\beta(E_i - \sum_j \mu_j N_{ij}))}{\Xi}$$

Grand potential:	$\Phi_G = -\frac{\ln \Xi}{\beta}$
Internal energy:	$U = -\left(\frac{\partial \ln \Xi}{\partial \beta}\right)_\mu + \sum_i \frac{\mu_i}{\beta}\left(\frac{\partial \ln \Xi}{\partial \mu_i}\right)_\beta$

Particle number:	$N_i = \frac{1}{\beta}\left(\frac{\partial \ln \Xi}{\partial \mu_i}\right)_\beta$
Entropy:	$S = k(\ln \Xi + \beta U - \beta \sum_i \mu_i N_i)$
Helmholtz free energy:	$F = \Phi_G + \sum_i \mu_i N_i = -\frac{\ln \Xi}{\beta} + \sum_i \frac{\mu_i}{\beta}\left(\frac{\partial \ln \Xi}{\partial \mu_i}\right)_\beta$

Equivalence between descriptions at the thermodynamic limit

All of the above descriptions differ in the way they allow the given system to fluctuate between its configurations.

In the micro-canonical ensemble, the system exchanges no energy with the outside world, and is therefore not subject to energy fluctuations; in the canonical ensemble, the system is free to exchange energy with the outside in the form of heat.

In the thermodynamic limit, which is the limit of large systems, fluctuations become negligible, so that all these descriptions converge to the same description. In other words, the macroscopic behavior of a system does not depend on the particular ensemble used for its description.

Given these considerations, the best ensemble to choose for the calculation of the properties of a macroscopic system is that ensemble which allows the result to be derived most easily.

Random walks

The study of long chain polymers has been a source of problems within the realms of statistical mechanics since about the 1950s. One of the reasons however that scientists were interested in their study is that the equations governing the behaviour of a polymer chain were independent of the chain chemistry. What is more, the governing equation turns out to be a random (diffusive) walk in space. Indeed, the Schrödinger equation is itself a diffusion equation in imaginary time, $t' = it$.

Random walks in time

The first example of a random walk is one in space, whereby a particle undergoes a random motion due to external forces in its surrounding medium. A typical example would be a pollen grain in a beaker of water. If one could somehow "dye" the path the pollen grain has taken, the path observed is defined as a random walk.

Consider a toy problem, of a train moving along a 1D track in the x-direction. Suppose that the train moves either a distance of + or - a fixed distance **b**, depending on whether a coin lands heads or tails when flipped. Lets start by considering the statistics of the steps the toy train takes (where S_i is the ith step taken):

$\langle S_i \rangle = 0$; due to *a priori* equal probabilities
$\langle S_i S_j \rangle = b^2 \delta_{ij}$

The second quantity is known as the correlation function. The delta is the kronecker delta which tells us that if the indices *i* and *j* are different, then the result is 0, but if *i* = *j* then the kronecker delta is 1, so the correlation function returns a value of b^2. This makes sense, because if *i* = *j* then we are considering the same step. Rather trivially then it can be shown that the average displacement of the train on the x-axis is 0;

$$x = \sum_{i=1}^{N} S_i$$

$$\langle x \rangle = \langle \sum_{i=1}^{N} S_i \rangle$$

$$\langle x \rangle = \sum_{i=1}^{N} \langle S_i \rangle$$

As stated $\langle S_i \rangle$ is 0, so the sum of 0 is still 0. It can also be shown, using the same method demonstrated above, to calculate the root mean square value of problem. The result of this calculation is given below

$$x_{rms} = \sqrt{\langle x^2 \rangle} = b\sqrt{N}$$

From the diffusion equation it can be shown that the distance a diffusing particle moves in a media is proportional to the root of the time the system has been diffusing for, where the proportionality constant is the root of the diffusion constant. The above relation, although cosmetically different reveals similar physics, where *N* is simply the number of steps moved (is loosely connected with time) and *b* is the characteristic step length. As a consequence we can consider diffusion as a random walk process.

Random walks in space

Random walks in space can be thought of as snapshots of the path taken by a random walker in time. One such example is the spatial configuration of long chain polymers.

There are two types of random walk in space: *self-avoiding random walks*, where the links of the polymer chain interact and do not overlap in space, and *pure random* walks, where the links of the polymer chain are non-interacting and links are free to lie on top of one another. The former type is most applicable to physical systems, but their solutions are harder to get at from first principles.

By considering a freely jointed, non-interacting polymer chain, the end-to-end vector is $\mathbf{R} = \sum_{i=1}^{N} \mathbf{r}_i$ where $\mathbf{r}_i$ is the vector position of the *i*-th link in the chain. As a result of the central limit theorem, if N >> 1 then we expect a Gaussian distribution for the end-to-end vector. We can also make statements of the statistics of the links themselves;

$\langle \mathbf{r}_i \rangle = 0$; by the isotropy of space

$\langle \mathbf{r}_i \cdot \mathbf{r}_j \rangle = 3b^2\delta_{ij}$; all the links in the chain are uncorrelated with one another

Using the statistics of the individual links, it is easily shown that $\langle \mathbf{R} \rangle = 0$ and $\langle \mathbf{R} \cdot \mathbf{R} \rangle = 3Nb^2$. Notice this last result is the same as that found for random walks in time.

Assuming, as stated, that that distribution of end-to-end vectors for a very large number of identical polymer chains is gaussian, the probability distribution has the following form

$$P = \frac{1}{\left(\frac{2\pi Nb^2}{3}\right)^{3/2}} \exp \frac{-3\mathbf{R} \cdot \mathbf{R}}{2Nb^2}$$

What use is this to us? Recall that according to the principle of equally likely *a priori* probabilities, the number of microstates, Ω, at some physical value is directly proportional to the probability distribution at that physical value, *viz*;

$$\Omega\left(\mathbf{R}\right) = cP\left(\mathbf{R}\right)$$

where c is an arbitrary proportionality constant. Given our distribution function, there is a maxima corresponding to $\mathbf{R} = 0$. Physically this amounts to there being more microstates which have an end-to-end vector of 0 than any other microstate. Now by considering

$$S(\mathbf{R}) = k_B \ln \Omega(\mathbf{R})$$
$$\Delta S(\mathbf{R}) = S(\mathbf{R}) - S(0)$$
$$\Delta F = -T \Delta S(\mathbf{R})$$

where F is the Helmholtz free energy it is trivial to show that

$$\Delta F = k_B T \frac{3R^2}{2Nb^2} = \frac{1}{2} K R^2 \quad ; K = \frac{3k_B T}{Nb^2}$$

A Hookian spring!

This result is known as the **Entropic Spring Result** and amounts to saying that upon stretching a polymer chain you are doing work on the system to drag it away from its (preferred) equilibrium state. An example of this is a common elastic band, composed of long chain (rubber) polymers. By stretching the elastic band you are doing work on the system and the band behaves like a conventional spring. What is particularly astonishing about this result however, is that the work done in stretching the polymer chain can be related entirely to the change in entropy of the system as a result of the stretching.

Classical thermodynamics vs.statistical thermodynamics

As an example, from a classical thermodynamics point of view one might ask what is it about a thermodynamic system of gas molecules, such as ammonia NH_3, that determines the free energy characteristic of that compound? Classical thermodynamics does not provide the answer. If, for example, we were given spectroscopic data, of this body of gas molecules, such as bond length, bond angle, bond rotation, and flexibility of the bonds in NH_3 we should see that the free energy could not be other than it is. To prove this true, we need to bridge the gap between the microscopic realm of atoms and molecules and the macroscopic realm of classical thermodynamics. From physics, → statistical mechanics provides such a bridge by teaching us how to conceive of a thermodynamic *system* as an assembly of *units*. More specifically, it demonstrates how the thermodynamic parameters of a system, such as temperature and pressure, are interpretable in terms of the parameters descriptive of such constituent atoms and molecules.[7]

In a bounded system, the crucial characteristic of these microscopic units is that their energies are quantized. That is, where the energies accessible to a macroscopic system form a virtual continuum of possibilities, the energies open to any of its submicroscopic components are limited to a discontinuous set of alternatives associated with integral values of some quantum number.

See also

- Chemical thermodynamics
- Configuration entropy
- Dangerously irrelevant
- Paul Ehrenfest
- Equilibrium thermodynamics
- Fluctuation dissipation theorem
- Important Publications in Statistical Mechanics
- Ising Model
- Mean field theory
- Nanomechanics
- Non-equilibrium thermodynamics
- Quantum thermodynamics
- Statistical physics
- Thermochemistry
- Widom insertion method

A Table of Statistical Mechanics Articles

	Maxwell Boltzmann	**Bose-Einstein**	**Fermi-Dirac**
Particle		Boson	Fermion
Statistics	Partition function Statistical properties Microcanonical ensemble | Canonical ensemble | Grand canonical ensemble		
Statistics	Maxwell-Boltzmann statistics Maxwell-Boltzmann distribution Boltzmann distribution Gibbs paradox	Bose-Einstein statistics	Fermi-Dirac statistics
Thomas-Fermi approximation	gas in a box gas in a harmonic trap		
Gas	Ideal gas	Bose gas Debye model Bose-Einstein condensate Planck's law of black body radiation	Fermi gas Fermion condensate
Chemical Equilibrium	Classical Chemical equilibrium		

Notes

[1] The terms "Statistical mechanics" and "statistical thermodynamics" are used interchangeably. "Statistical physics" is a broader term which includes statistical mechanics, but is sometimes also used as a synonym for statistical mechanics

[2] On history of fundamentals of statistical thermodynamics (http://www.worldscibooks.com/phy_etextbook/2012/2012_chap01.pdf) (section 1.2)

[3] Schrodinger, Erwin (1946). *Statistical Thermodynamics*. Dover Publications, Inc.. ISBN 0-486-66101-6. OCLC 20056858 (http://worldcat.org/oclc/20056858).

[4] Mahon, Basil (2003). *The Man Who Changed Everything – the Life of James Clerk Maxwell*. Hoboken, NJ: Wiley. ISBN 0-470-86171-1. OCLC 52358254 62045217 (http://worldcat.org/oclc/52358254+62045217).

[5] Perrot, Pierre (1998). *A to Z of Thermodynamics*. Oxford University Press. ISBN 0-19-856552-6. OCLC 123283342 38073404 (http://worldcat.org/oclc/123283342+38073404).

[6] http://clesm.mae.ufl.edu/wiki.pub/index.php/Configuration_integral_%28statistical_mechanics%29

[7] Nash, Leonard K. (1974). *Elements of Statistical Thermodynamics, 2nd Ed.*. Dover Publications, Inc.. ISBN 0-486-44978-5. OCLC 61513215 (http://worldcat.org/oclc/61513215).

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- Dill, Ken; Bromberg, Sarina (2003). *Molecular Driving Forces*. Garland Science. ISBN 0-8153-2051-5. OCLC 47915710 (http://worldcat.org/oclc/47915710).
- List of notable textbooks in statistical mechanics

Further reading

- Ben-Naim, Arieh (2007). *Statistical Thermodynamics Based on Information*. ISBN 978-981-270-707-9
- Boltzmann, Ludwig; and Dieter Flamm (2000). *Entropie und Wahrscheinlichkeit*. ISBN 978-3817132867
- Boltzmann, Ludwig (1896, 1898). *[Lectures on gas theory]*. New York: Dover. ISBN 0486684555. OCLC 31434905 (http://worldcat.org/oclc/31434905). translated by Stephen G. Brush (1964) Berkeley: University of California Press; (1995) New York: Dover ISBN 0-486-68455-5
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- Landau, Lev Davidovich; and Lifshitz, Evgeny Mikhailovich (1980) [1976]. *Statistical Physics*. **5** (3 ed.). Oxford: Pergamon Press. ISBN 0-7506-3372-7. Translated by J.B. Sykes and M.J. Kearsley
- Reichl, Linda E (1998) [1980]. *A modern course in statistical physics* (2 ed.). Chichester: Wiley. ISBN 0-471-59520-9.

External links

- Philosophy of Statistical Mechanics (http://plato.stanford.edu/entries/statphys-statmech/) article by Lawrence Sklar for the Stanford Encyclopedia of Philosophy.
- Sklogwiki - Thermodynamics, statistical mechanics, and the computer simulation of materials. (http://www.sklogwiki.org/) SklogWiki is particularly orientated towards liquids and soft condensed matter.
- Statistical Thermodynamics (http://history.hyperjeff.net/statmech.html) - Historical Timeline

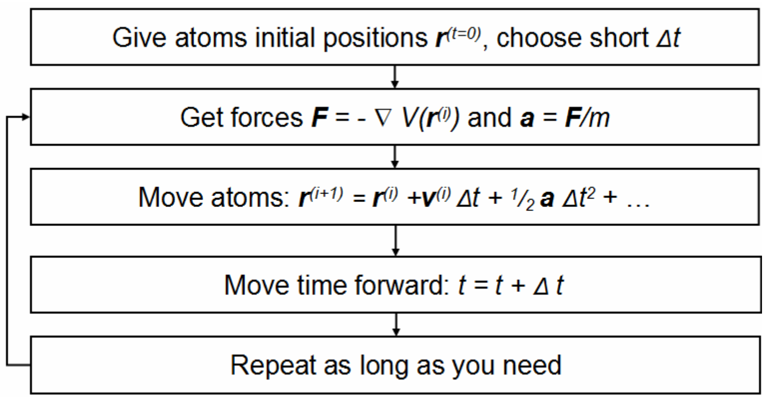
Molecular dynamics

Molecular dynamics (**MD**) is a form of computer simulation in which atoms and molecules are allowed to interact for a period of time by approximations of known physics, giving a view of the motion of the atoms. Because molecular systems generally consist of a vast number of particles, it is impossible to find the properties of such complex systems analytically. When the number of bodies are more than two no analytical solutions can be found and result in chaotic motion (see n-body problem). MD simulation circumvents this problem by using numerical methods. It represents an interface between laboratory experiments and theory, and can be understood as a "virtual experiment". MD probes the relationship between molecular structure, movement and function. Molecular dynamics is a multidisciplinary method. Its laws and theories stem from mathematics, physics, and chemistry, and it employs algorithms from computer science and information theory. It was originally conceived within theoretical physics in the late 1950s[1] and early 1960s [2] , but is applied today mostly in materials science and modeling of biomolecules.

Before it became possible to simulate molecular dynamics with computers, some undertook the hard work of trying it with physical models such as macroscopic spheres. The idea was to arrange them to replicate the properties of a liquid. J.D. Bernal said, in 1962: "... I took a number of rubber balls and stuck them together with rods of a selection of different lengths ranging from 2.75 to 4 inches. I tried to do this in the first place as casually as possible, working in my own office, being interrupted every five minutes or so and not remembering what I had done before the interruption."[3] Fortunately, now computers keep track of bonds during a simulation.

Molecular dynamics is a specialized discipline of molecular modeling and computer simulation based on → statistical mechanics; the main justification of the MD method is that statistical ensemble averages are equal to time averages of the system, known as the ergodic hypothesis. MD has also been termed "statistical mechanics by numbers" and "Laplace's vision of Newtonian mechanics" of predicting the future by animating nature's forces[4] [5] and allowing insight into molecular motion on an atomic scale. However, long MD simulations are mathematically ill-conditioned, generating cumulative errors in numerical integration that can be minimized with proper selection of algorithms and parameters, but not eliminated entirely. Furthermore, current potential functions are, in many cases, not sufficiently accurate to reproduce the dynamics of molecular systems, so the much more computationally demanding Ab Initio Molecular Dynamics method must be used. Nevertheless, molecular dynamics techniques allow detailed time and space resolution into representative behavior in phase space.

Areas of Application



Highly simplified description of the molecular dynamics simulation algorithm. The simulation proceeds iteratively by alternatively calculating forces and solving the equations of motion based on the accelerations obtained from the new forces. In practise, almost all MD codes use much more complicated versions of the algorithm, including two steps (predictor and corrector) in solving the equations of motion and many additional steps for e.g. temperature and pressure control, analysis and output.

There is a significant difference between the focus and methods used by chemists and physicists, and this is reflected in differences in the jargon used by the different fields. In chemistry and biophysics, the interaction between the particles is either described by a "force field" (**classical MD**), a quantum chemical model, or a mix between the two. These terms are not used in physics, where the interactions are usually described by the name of the theory or approximation being used and called the potential energy, or just "potential".

Beginning in theoretical → physics, the method of MD gained popularity in materials science and since the 1970s also in biochemistry and → biophysics. In chemistry, MD serves as an important tool in protein structure determination and refinement using experimental tools such as X-ray crystallography and NMR. It has also been applied with limited success as a method of refining protein structure predictions. In physics, MD is used to examine the dynamics of atomic-level phenomena that cannot be observed directly, such as thin film growth and ion-subplantation. It is also used to examine the physical properties of nanotechnological devices that have not or cannot yet be created.

In applied mathematics and theoretical physics, molecular dynamics is a part of the research realm of dynamical systems, ergodic theory and → statistical mechanics in general. The concepts of energy conservation and molecular entropy come from → thermodynamics. Some techniques to calculate conformational entropy such as principal components analysis come from information theory. Mathematical techniques such as the transfer operator become applicable when MD is seen as a Markov chain. Also, there is a large community of mathematicians working on volume preserving, symplectic integrators for more computationally efficient MD simulations.

MD can also be seen as a special case of the discrete element method (DEM) in which the particles have spherical shape (e.g. with the size of their van der Waals radii.) Some authors in the DEM community employ the term MD rather loosely, even when their simulations do not model actual molecules.

Design Constraints

Design of a molecular dynamics simulation should account for the available computational power. Simulation size (n=number of particles), timestep and total time duration must be selected so that the calculation can finish within a reasonable time period. However, the simulations should be long enough to be relevant to the time scales of the natural processes being studied. To make statistically valid conclusions from the simulations, the time span simulated should match the kinetics of the natural process. Otherwise, it is analogous to making conclusions about how a human walks from less than one footstep. Most scientific publications about the dynamics of proteins and DNA use data from simulations spanning nanoseconds (1E-9 s) to microseconds (1E-6 s). To obtain these simulations, several CPU-days to CPU-years are needed. Parallel algorithms allow the load to be distributed among CPUs; an example is the spatial decomposition in LAMMPS.

During a classical MD simulation, the most CPU intensive task is the evaluation of the potential (force field) as a function of the particles' internal coordinates. Within that energy evaluation, the most expensive one is the non-bonded or non-covalent part. In Big O notation, common molecular dynamics simulations scale by $O(n^2)$ if all pair-wise electrostatic and van der Waals interactions must be accounted for explicitly. This computational cost can be reduced by employing electrostatics methods such as Particle Mesh Ewald ($O(n\log(n))$) or good spherical cutoff techniques ($O(n)$).

Another factor that impacts total CPU time required by a simulation is the size of the integration timestep. This is the time length between evaluations of the potential. The timestep must be chosen small enough to avoid discretization errors (i.e. smaller than the fastest vibrational frequency in the system). Typical timesteps for classical MD are in the order of 1 femtosecond (1E-15 s). This value may be extended by using algorithms such as SHAKE, which fix the vibrations of the fastest atoms (e.g. hydrogens) into place. Multiple time scale methods have also been developed, which allow for extended times between updates of slower long-range forces.[6] [7] [8]

For simulating molecules in a solvent, a choice should be made between explicit solvent and implicit solvent. Explicit solvent particles (such as the TIP3P and SPC/E water models) must be calculated expensively by the force field, while implicit solvents use a mean-field approach. Using an explicit solvent is computationally expensive, requiring inclusion of about ten times more particles in the simulation. But the granularity and viscosity of explicit solvent is essential to reproduce certain properties of the solute molecules. This is especially important to reproduce kinetics.

In all kinds of molecular dynamics simulations, the simulation box size must be large enough to avoid boundary condition artifacts. Boundary conditions are often treated by choosing fixed values at the edges, or by employing periodic boundary conditions in which one side of the simulation loops back to the opposite side, mimicking a bulk phase.

Microcanonical ensemble (NVE)

In the **microcanonical**, or **NVE** ensemble, the system is isolated from changes in moles (N), volume (V) and energy (E). It corresponds to an adiabatic process with no heat exchange. A microcanonical molecular dynamics trajectory may be seen as an exchange of potential and kinetic energy, with total energy being conserved. For a system of N particles with coordinates X and velocities V, the following pair of first order differential equations may be written in Newton's notation as

$$F(X) = -\nabla U(X) = M\dot{V}(t)$$
$$V(t) = \dot{X}(t).$$

The potential energy function $U(X)$ of the system is a function of the particle coordinates X . It is referred to simply as the "potential" in Physics, or the "force field" in Chemistry. The first equation comes from Newton's laws; the force F acting on each particle in the system can be calculated as the negative gradient of $U(X)$.

For every timestep, each particle's position X and velocity V may be integrated with a symplectic method such as Verlet. The time evolution of X and V is called a trajectory. Given the initial positions (e.g. from theoretical knowledge) and velocities (e.g. randomized Gaussian), we can calculate all future (or past) positions and velocities.

One frequent source of confusion is the meaning of temperature in MD. Commonly we have experience with macroscopic temperatures, which involve a huge number of particles. But temperature is a statistical quantity. If there is a large enough number of atoms, statistical temperature can be estimated from the *instantaneous temperature*, which is found by equating the kinetic energy of the system to $nk_BT/2$ where n is the number of degrees of freedom of the system.

A temperature-related phenomenon arises due to the small number of atoms that are used in MD simulations. For example, consider simulating the growth of a copper film starting with a substrate containing 500 atoms and a deposition energy of 100 eV. In the real world, the 100 eV from the deposited atom would rapidly be transported through and shared among a large number of atoms (10^{10} or more) with no big change in temperature. When there are only 500 atoms, however, the substrate is almost immediately vaporized by the deposition. Something similar happens in biophysical simulations. The temperature of the system in NVE is naturally raised when macromolecules such as proteins undergo exothermic conformational changes and binding.

Canonical ensemble (NVT)

In the canonical ensemble, moles (N), volume (V) and temperature (T) are conserved. It is also sometimes called constant temperature molecular dynamics (CTMD). In NVT, the energy of endothermic and exothermic processes is exchanged with a thermostat.

A variety of thermostat methods are available to add and remove energy from the boundaries of an MD system in a realistic way, approximating the canonical ensemble. Popular techniques to control temperature include the Nosé-Hoover thermostat, the Berendsen thermostat, and Langevin dynamics. Note that the Berendsen thermostat might introduce the flying ice cube effect, which leads to unphysical translations and rotations of the simulated system.

Isothermal-Isobaric (NPT) ensemble

In the isothermal-isobaric ensemble, moles (N), pressure (P) and temperature (T) are conserved. In addition to a thermostat, a barostat is needed. It corresponds most closely to laboratory conditions with a flask open to ambient temperature and pressure.

In the simulation of biological membranes, isotropic pressure control is not appropriate. For lipid bilayers, pressure control occurs under constant membrane area (NPAT) or constant surface tension "gamma" (NPγT).

Generalized ensembles

The replica exchange method is a generalized ensemble. It was originally created to deal with the slow dynamics of disordered spin systems. It is also called parallel tempering. The replica exchange MD (REMD) formulation [9] tries to overcome the multiple-minima problem by exchanging the temperature of non-interacting replicas of the system running at several temperatures.

Potentials in MD simulations

A molecular dynamics simulation requires the definition of a potential function, or a description of the terms by which the particles in the simulation will interact. In chemistry and biology this is usually referred to as a force field. Potentials may be defined at many levels of physical accuracy; those most commonly used in chemistry are based on molecular mechanics and embody a classical treatment of particle-particle interactions that can reproduce structural and conformational changes but usually cannot reproduce chemical reactions.

The reduction from a fully quantum description to a classical potential entails two main approximations. The first one is the Born-Oppenheimer approximation, which states that the dynamics of electrons is so fast that they can be considered to react instantaneously to the motion of their nuclei. As a consequence, they may be treated separately. The second one treats the nuclei, which are much heavier than electrons, as point particles that follow classical Newtonian dynamics. In classical molecular dynamics the effect of the electrons is approximated as a single potential energy surface, usually representing the ground state.

When finer levels of detail are required, potentials based on → quantum mechanics are used; some techniques attempt to create hybrid classical/quantum potentials where the bulk of the system is treated classically but a small region is treated as a quantum system, usually undergoing a chemical transformation.

Empirical potentials

Empirical potentials used in chemistry are frequently called force fields, while those used in materials physics are called just empirical or analytical potentials.

Most force fields in chemistry are empirical and consist of a summation of bonded forces associated with chemical bonds, bond angles, and bond dihedrals, and non-bonded forces associated with van der Waals forces and electrostatic charge. Empirical potentials represent quantum-mechanical effects in a limited way through ad-hoc functional approximations. These potentials contain free parameters such as atomic charge, van der Waals parameters reflecting estimates of atomic radius, and equilibrium bond length, angle, and dihedral; these are obtained by fitting against detailed electronic calculations (quantum chemical simulations) or experimental physical properties such as elastic constants, lattice parameters and spectroscopic measurements.

Because of the non-local nature of non-bonded interactions, they involve at least weak interactions between all particles in the system. Its calculation is normally the bottleneck in the speed of MD simulations. To lower the computational cost, force fields employ numerical approximations such as shifted cutoff radii, reaction field algorithms, particle mesh Ewald summation, or the newer Particle-Particle Particle Mesh (P3M).

Chemistry force fields commonly employ preset bonding arrangements (an exception being *ab-initio* dynamics), and thus are unable to model the process of chemical bond breaking and reactions explicitly. On the other hand, many of the potentials used in physics, such as those based on the bond order formalism can describe several different coordinations of a system and bond breaking. Examples of such potentials include the Brenner potential[10] for hydrocarbons and its further developments for the C-Si-H and C-O-H systems. The ReaxFF potential[11] can be considered a fully reactive hybrid between bond order potentials and chemistry force fields.

Pair potentials vs.many-body potentials

The potential functions representing the non-bonded energy are formulated as a sum over interactions between the particles of the system. The simplest choice, employed in many popular force fields, is the "pair potential", in which the total potential energy can be calculated from the sum of energy contributions between pairs of atoms. An example of such a pair potential is the non-bonded Lennard-Jones potential (also known as the 6-12 potential), used for calculating van der Waals forces.

$$U(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

Another example is the Born (ionic) model of the ionic lattice. The first term in the next equation is Coulomb's law for a pair of ions, the second term is the short-range repulsion explained by Pauli's exclusion principle and the final term is the dispersion interaction term. Usually, a simulation only includes the dipolar term, although sometimes the quadrupolar term is included as well.

$$U_{ij}(r_{ij}) = \sum \frac{z_i z_j}{4\pi\epsilon_0}\frac{1}{r_{ij}} + \sum A_l \exp\frac{-r_{ij}}{p_l} + \sum C_l r_{ij}^{-n_j} + \cdots$$

In many-body potentials, the potential energy includes the effects of three or more particles interacting with each other. In simulations with pairwise potentials, global interactions in the system also exist, but they occur only through pairwise terms. In many-body potentials, the potential energy cannot be found by a sum over pairs of atoms, as these interactions are calculated explicitly as a combination of higher-order terms. In the statistical view, the dependency between the variables cannot in general be expressed using only pairwise products of the degrees of freedom. For example, the Tersoff potential[12] , which was originally used to simulate carbon, silicon and germanium and has since been used for a wide range of other materials, involves a sum over groups of three atoms, with the angles between the atoms being an important factor in the potential. Other examples are the embedded-atom method (EAM)[13] and the Tight-Binding Second Moment Approximation (TBSMA) potentials[14] , where the electron density of states in the region of an atom is calculated from a sum of contributions from surrounding atoms, and the potential energy contribution is then a function of this sum.

Semi-empirical potentials

Semi-empirical potentials make use of the matrix representation from quantum mechanics. However, the values of the matrix elements are found through empirical formulae that estimate the degree of overlap of specific atomic orbitals. The matrix is then diagonalized to determine the occupancy of the different atomic orbitals, and empirical formulae are used once again to determine the energy contributions of the orbitals.

There are a wide variety of semi-empirical potentials, known as tight-binding potentials, which vary according to the atoms being modeled.

Polarizable potentials

Most classical force fields implicitly include the effect of polarizability, e.g. by scaling up the partial charges obtained from quantum chemical calculations. These partial charges are stationary with respect to the mass of the atom. But molecular dynamics simulations can explicitly model polarizability with the introduction of induced dipoles through different methods, such as Drude particles or fluctuating charges. This allows for a dynamic redistribution of charge between atoms which responds to the local chemical environment.

For many years, polarizable MD simulations have been touted as the next generation. For homogenous liquids such as water, increased accuracy has been achieved through the inclusion of polarizability.[15] Some promising results have also been achieved for proteins.[16] However, it is still uncertain how to best approximate polarizability in a simulation.

Ab-initio methods

In classical molecular dynamics, a single potential energy surface (usually the ground state) is represented in the force field. This is a consequence of the Born-Oppenheimer approximation. If excited states, chemical reactions or a more accurate representation is needed, electronic behavior can be obtained from first principles by using a quantum mechanical method, such as Density Functional Theory. This is known as Ab Initio Molecular Dynamics (AIMD). Due to the cost of treating the electronic degrees of freedom, the computational cost of this simulations is much higher than classical molecular dynamics. This implies that AIMD is limited to smaller systems and shorter periods of time.

Ab-initio quantum-mechanical methods may be used to calculate the potential energy of a system on the fly, as needed for conformations in a trajectory. This calculation is usually made in the close neighborhood of the reaction coordinate. Although various approximations may be used, these are based on theoretical considerations, not on empirical fitting. *Ab-Initio* calculations produce a vast amount of information that is not available from empirical methods, such as density of electronic states or other electronic properties. A significant advantage of using *ab-initio* methods is the ability to study reactions that involve breaking or formation of covalent bonds, which correspond to multiple electronic states.

A popular software for *ab-initio* molecular dynamics is the Car-Parrinello Molecular Dynamics (CPMD) package based on the density functional theory.

Hybrid QM/MM

QM (quantum-mechanical) methods are very powerful. However, they are computationally expensive, while the MM (classical or molecular mechanics) methods are fast but suffer from several limitations (require extensive parameterization; energy estimates obtained are not very accurate; cannot be used to simulate reactions where covalent bonds are broken/formed; and are limited in their abilities for providing accurate details regarding the chemical environment). A new class of method has emerged that combines the good points of QM (accuracy) and MM (speed) calculations. These methods are known as mixed or hybrid quantum-mechanical and molecular mechanics methods (hybrid QM/MM). The methodology for such techniques was introduced by Warshel and coworkers. In the recent years have been pioneered by several groups including: Arieh Warshel (University of Southern California), Weitao Yang (Duke University), Sharon Hammes-Schiffer (The Pennsylvania State University), Donald Truhlar and Jiali Gao (University of Minnesota) and Kenneth Merz (University of Florida).

The most important advantage of hybrid QM/MM methods is the speed. The cost of doing classical molecular dynamics (MM) in the most straightforward case scales $O(n^2)$, where N is the number of atoms in the system. This is mainly due to electrostatic interactions term (every particle interacts with every other particle). However, use of cutoff radius, periodic pair-list updates and more recently the variations of the particle-mesh Ewald's (PME) method has reduced this between O(N) to $O(n^2)$. In other words, if a system with twice many atoms is simulated then it would take between twice to four times as much computing power. On the other hand the simplest *ab-initio* calculations typically scale $O(n^3)$ or worse (Restricted Hartree-Fock calculations have been suggested to scale $\sim O(n^{2.7})$). To overcome the limitation, a small part of the system is treated quantum-mechanically (typically active-site of an enzyme) and the remaining system is treated classically.

In more sophisticated implementations, QM/MM methods exist to treat both light nuclei susceptible to quantum effects (such as hydrogens) and electronic states. This allows generation of hydrogen wave-functions (similar to electronic wave-functions). This methodology has been useful in investigating phenomenon such as hydrogen tunneling. One example where QM/MM methods have provided new discoveries is the calculation of hydride transfer in the enzyme liver alcohol dehydrogenase. In this case, tunneling is important for the hydrogen, as it determines the reaction rate.[17]

Coarse-graining and reduced representations

At the other end of the detail scale are coarse-grained and lattice models. Instead of explicitly representing every atom of the system, one uses "pseudo-atoms" to represent groups of atoms. MD simulations on very large systems may require such large computer resources that they cannot easily be studied by traditional all-atom methods. Similarly, simulations of processes on long timescales (beyond about 1 microsecond) are prohibitively expensive, because they require so many timesteps. In these cases, one can sometimes tackle the problem by using reduced representations, which are also called coarse-grained models.

Examples for coarse graining (CG) methods are discontinuous molecular dynamics (CG-DMD)[18] [19] and Go-models[20] . Coarse-graining is done sometimes taking larger pseudo-atoms. Such united atom approximations have been used in MD simulations of biological membranes. The aliphatic tails of lipids are represented by a few pseudo-atoms by gathering 2-4 methylene groups into each pseudo-atom.

The parameterization of these very coarse-grained models must be done empirically, by matching the behavior of the model to appropriate experimental data or all-atom simulations. Ideally, these parameters should account for both enthalpic and entropic contributions to free energy in an implicit way. When coarse-graining is done at higher levels, the accuracy of the dynamic description may be less reliable. But very coarse-grained models have been used successfully to examine a wide range of questions in structural biology.

Examples of applications of coarse-graining in biophysics:

- protein folding studies are often carried out using a single (or a few) pseudo-atoms per amino acid;
- DNA supercoiling has been investigated using 1-3 pseudo-atoms per basepair, and at even lower resolution;
- Packaging of double-helical DNA into bacteriophage has been investigated with models where one pseudo-atom represents one turn (about 10 basepairs) of the double helix;
- RNA structure in the ribosome and other large systems has been modeled with one pseudo-atom per nucleotide.

The simplest form of coarse-graining is the "united atom" (sometimes called "extended atom") and was used in most early MD simulations of proteins, lipids and nucleic acids. For example, instead of treating all four atoms of a CH_3 methyl group explicitly (or all three atoms of CH_2 methylene group), one represents the whole group with a single pseudo-atom. This pseudo-atom must, of course, be properly parameterized so that its van der Waals interactions with other groups have the proper distance-dependence. Similar considerations apply to the bonds, angles, and torsions in which the pseudo-atom participates. In this kind of united atom representation, one typically eliminates all explicit hydrogen atoms except those that have the capability to participate in hydrogen bonds ("polar hydrogens"). An example of this is the Charmm 19 force-field.

The polar hydrogens are usually retained in the model, because proper treatment of hydrogen bonds requires a reasonably accurate description of the directionality and the electrostatic interactions between the donor and acceptor groups. A hydroxyl group, for example, can be both a hydrogen bond donor and a hydrogen bond acceptor, and it would be impossible to treat this with a single OH pseudo-atom. Note that about half the atoms in a protein or nucleic acid are nonpolar hydrogens, so the use of united atoms can provide a substantial savings in computer time.

Examples of applications

Molecular dynamics is used in many fields of science.

- First macromolecular MD simulation published (1977, Size: 500 atoms, Simulation Time: 9.2 ps=0.0092 ns, Program: CHARMM precursor) Protein: Bovine Pancreatic Trypsine Inhibitor. This is one of the best studied proteins in terms of folding and kinetics. Its simulation published in Nature magazine paved the way for understanding protein motion as essential in function and not just accessory.[21]
- MD is the standard method to treat collision cascades in the heat spike regime, i.e. the effects that energetic neutron and ion irradiation have on solids an solid surfaces.[22] [23]

The following two biophysical examples are not run-of-the-mill MD simulations. They illustrate almost heroic efforts to produce simulations of a system of very large size (a complete virus) and very long simulation times (500 microseconds):

- MD simulation of the complete satellite tobacco mosaic virus (**STMV**) (2006, Size: 1 million atoms, Simulation time: 50 ns, program: NAMD) This virus is a small, icosahedral plant virus which worsens the symptoms of infection by Tobacco Mosaic Virus (TMV). Molecular dynamics simulations were used to probe the mechanisms of viral assembly. The entire STMV particle consists of 60 identical copies of a single protein that make up the viral capsid (coating), and a 1063 nucleotide single stranded RNA genome. One key finding is that the capsid is very unstable when there is no RNA inside. The simulation would take a single 2006 desktop computer around 35 years to complete. It was thus done in many processors in parallel with continuous communication between them.[24]
- Folding Simulations of the Villin Headpiece in All-Atom Detail (2006, Size: 20,000 atoms; Simulation time: 500 μs = 500,000 ns, Program: folding@home) This simulation was run in 200,000 CPU's of participating personal computers around the world. These computers had the folding@home program installed, a large-scale distributed computing effort coordinated by Vijay Pande at Stanford University. The kinetic properties of the Villin Headpiece protein were probed by using many independent, short trajectories run by CPU's without continuous real-time communication. One technique employed was the Pfold value analysis, which measures the probability of folding before unfolding of a specific starting conformation. Pfold gives information about transition state structures and an ordering of conformations along the folding pathway. Each trajectory in a Pfold calculation can be relatively short, but many independent trajectories are needed.[25]

Molecular dynamics algorithms

Integrators

- Verlet integration
- Beeman's algorithm
- Gear predictor - corrector
- Constraint algorithms (for constrained systems)
- Symplectic integrator

Short-range interaction algorithms

- Cell lists
- Verlet list
- Bonded interactions

Long-range interaction algorithms

- Ewald summation
- Particle Mesh Ewald (PME)
- Particle-Particle Particle Mesh P3M
- Reaction Field Method

Parallelization strategies

- Domain decomposition method (Distribution of system data for parallel computing)
- Molecular Dynamics - Parallel Algorithms [26]

Major software for MD simulations

- Abalone (classical, implicit water)
- ABINIT (DFT)
- ADUN [27] (classical, P2P database for simulations)
- AMBER (classical)
- Ascalaph [28] (classical, GPU accelerated)
- CASTEP (DFT)
- CPMD (DFT)
- CP2K [29] (DFT)
- CHARMM (classical, the pioneer in MD simulation, extensive analysis tools)
- COSMOS [30] (classical and hybrid QM/MM, quantum-mechanical atomic charges with BPT)
- Desmond [31] (classical, parallelization with up to thousands of CPU's)
- DL_POLY [32] (classical)
- ESPResSo (classical, coarse-grained, parallel, extensible)
- Fireball [33] (tight-binding DFT)
- GROMACS (classical)
- GROMOS (classical)
- GULP (classical)
- Hippo [34] (classical)
- LAMMPS (classical, large-scale with spatial-decomposition of simulation domain for parallelism)
- MDynaMix (classical, parallel)
- MOLDY [35] (classical, parallel) latest release [36]
- Materials Studio [37] (Forcite MD using COMPASS, Dreiding, Universal, cvff and pcff forcefields in serial or parallel, QMERA (QM+MD), ONESTEP (DFT), etc.)
- MOSCITO (classical)
- NAMD (classical, parallelization with up to thousands of CPU's)
- NEWTON-X [38] (ab initio, surface-hopping dynamics)
- ProtoMol [39] (classical, extensible, includes multigrid electrostatics)
- PWscf (DFT)
- S/PHI/nX [40] (DFT)
- SIESTA (DFT)
- VASP (DFT)
- TINKER (classical)
- YASARA [41] (classical)
- ORAC [42] (classical)
- XMD (classical)

Related software

- VMD - MD simulation trajectories can be visualized and analyzed.
- PyMol - Molecular Visualization software written in python
- Packmol [43] Package for building starting configurations for MD in an automated fashion
- Sirius - Molecular modeling, analysis and visualization of MD trajectories
- esra [44] - Lightweight molecular modeling and analysis library (Java/Jython/Mathematica).
- Molecular Workbench [45] - Interactive molecular dynamics simulations on your desktop
- BOSS - MC in OPLS

Specialized hardware for MD simulations

- Anton - A specialized, massively parallel supercomputer designed to execute MD simulations.
- MDGRAPE - A special purpose system built for molecular dynamics simulations, especially protein structure prediction.

See also

- Molecular modeling
- Computational chemistry
- Energy drift
- Force field in Chemistry
- Force field implementation
- Monte Carlo method
- Molecular Design software
- Molecular mechanics
- Molecular modeling on GPU
- Protein dynamics
- Implicit solvation
- Car-Parrinello method
- Symplectic numerical integration
- Software for molecular mechanics modeling
- Dynamical systems
- Theoretical chemistry
- → Statistical mechanics
- Quantum chemistry
- Discrete element method
- List of nucleic acid simulation software

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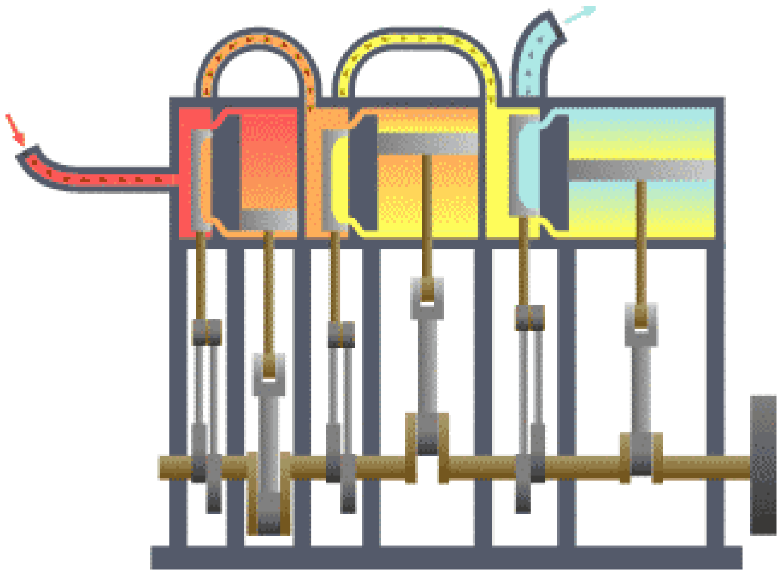
External links

- The Blue Gene Project (http://researchweb.watson.ibm.com/bluegene/) (IBM)
- D. E. Shaw Research (http://deshawresearch.com/) (D. E. Shaw Research)
- Molecular Physics (http://www.tandf.co.uk/journals/titles/00268976.asp)
- Statistical mechanics of Nonequilibrium Liquids (http://www.phys.unsw.edu.au/~gary/book.html) Lecture Notes on non-equilibrium MD
- Introductory Lecture on Classical Molecular Dynamics (http://www.fz-juelich.de/nic-series/volume10/sutmann.pdf) by Dr. Godehard Sutmann, NIC, Forschungszentrum Jülich, Germany
- Introductory Lecture on Ab Initio Molecular Dynamics and Ab Initio Path Integrals (http://www.fz-juelich.de/nic-series/volume10/tuckerman2.pdf) by Mark E. Tuckerman, New York University, USA
- Introductory Lecture on Ab initio molecular dynamics: Theory and Implementation (http://www.fz-juelich.de/nic-series/Volume1/marx.pdf) by Dominik Marx, Ruhr-Universität Bochum and Jürg Hutter, Universität Zürich
- Atomic-scale Friction Research and Education Synergy Hub (AFRESH) (http://nsfafresh.org) an Engineering Virtual Organization for the atomic-scale friction community to share, archive, link, and discuss data, knowledge and tools related to atomic-scale friction.
  - AFRESH (http://nsfafresh.org/wiki/index.php?title=Computational_Tribology) also provides detailed information regarding computational methods such as Molecular Dynamics as it relates to atomic-scale friction research.

Thermodynamics

In → physics, **thermodynamics** (from the Greek *θερμ-<θερμότης*, *therme,* meaning "heat"[1] and δυναμις, *dynamis,* meaning "power") is the study of the conversion of energy into work and heat and its relation to macroscopic variables such as temperature and pressure. Its underpinnings, based upon statistical predictions of the collective motion of particles from their microscopic behavior, is the field of statistical thermodynamics, a branch of → statistical mechanics.[2] [3] [4] . Historically, thermodynamics developed out of need to increase the efficiency of early steam engines.[5]

Starting point and relevance



Typical **thermodynamic system**, showing input from a heat source (boiler) on the left and output to a heat sink (condenser) on the right. Work is extracted, in this case by a series of pistons.

The starting point for most thermodynamic considerations are the laws of thermodynamics, which postulate that energy can be exchanged between physical systems as heat or work.[6] They also postulate the existence of a quantity named entropy, which can be defined for any system.[7] In thermodynamics, interactions between large ensembles of objects are studied and categorized. Central to this are the concepts of *system* and *surroundings*. A system is composed of particles, whose average motions define its properties, which in turn are related to one another through equations of state. Properties can be combined to express internal energy and thermodynamic potentials, which are useful for determining conditions for equilibrium and spontaneous processes.

With these tools, the usage of thermodynamics describes how systems respond to changes in their surroundings. This can be applied to a wide variety of topics in science and engineering, such as engines, phase transitions, chemical reactions, transport phenomena, and even black holes. The results of thermodynamics are essential for other fields of → physics and for chemistry, chemical engineering, aerospace engineering, mechanical engineering, cell biology, biomedical engineering, materials science, and economics to name a few.[8] [9]

History

Sadi Carnot (1796-1832): was the father of thermodynamics

The history of thermodynamics as a scientific discipline generally begins with Otto von Guericke who, in 1650, built and designed the world's first vacuum pump and demonstrated a vacuum using his Magdeburg hemispheres. Guericke was driven to make a vacuum in order to disprove Aristotle's long-held supposition that 'nature abhors a vacuum'. Shortly after Guericke, the Irish physicist and chemist Robert Boyle had learned of Guericke's designs and, in 1656, in coordination with English scientist Robert Hooke, built an air pump.[10] Using this pump, Boyle and Hooke noticed a correlation between pressure, temperature, and volume. In time, Boyle's Law was formulated, which states that pressure and volume are inversely proportional. Then, in 1679, based on these concepts, an associate of Boyle's named Denis Papin built a bone digester, which was a closed vessel with a tightly fitting lid that confined steam until a high pressure was generated.

Later designs implemented a steam release valve that kept the machine from exploding. By watching the valve rhythmically move up and down, Papin conceived of the idea of a piston and a cylinder engine. He did not, however, follow through with his design. Nevertheless, in 1697, based on Papin's designs, engineer Thomas Savery built the first engine. Although these early engines were crude and inefficient, they attracted the attention of the leading scientists of the time.

Their work led 127 years later to Sadi Carnot, the "father of thermodynamics", who, in 1824, published *Reflections on the Motive Power of Fire*, a discourse on heat, power, and engine efficiency. The paper outlined the basic energetic relations between the Carnot engine, the Carnot cycle, and Motive power. This marks the start of thermodynamics as a modern science.[3]

The term *thermodynamics* was coined by James Joule in 1849 to designate the science of relations between heat and power.[3] By 1858, "thermo-dynamics", as a functional term, was used in William Thomson's paper *An Account of Carnot's Theory of the Motive Power of Heat*.[11] The first thermodynamic textbook was written in 1859 by William Rankine, originally trained as a physicist and a civil and mechanical engineering professor at the University of Glasgow.[12]

The laws of thermodynamics

In thermodynamics, there are four laws that do not depend on the details of the systems under study or how they interact. Hence these laws are very generally valid, can be applied to systems about which one knows nothing other than the balance of energy and matter transfer. Examples of such systems include Einstein's prediction, around the turn of the 20th century, of spontaneous emission, and ongoing research into the thermodynamics of black holes.

These four laws are:

- Zeroth law of thermodynamics, about thermal equilibrium:

  > If two thermodynamic systems are separately in thermal equilibrium with a third, they are also in thermal equilibrium with each other.

  If we grant that all systems are (trivially) in thermal equilibrium with themselves, the Zeroth law implies that thermal equilibrium is an equivalence relation on the set of thermodynamic systems. This law is tacitly assumed in every measurement of temperature. Thus, if we want to know if two bodies are at the same temperature, it is not necessary to bring them into contact and to watch whether their observable properties change with time.[13]

- First law of thermodynamics, about the conservation of energy:

  > The change in the internal energy of a closed thermodynamic system is equal to the sum of the amount of heat energy supplied to the system and the work done on the system.

- Second law of thermodynamics, about entropy:

  > The total entropy of any isolated thermodynamic system tends to increase over time, approaching a maximum value.

- Third law of thermodynamics, about the absolute zero of temperature:

  > As a system asymptotically approaches absolute zero of temperature all processes virtually cease and the entropy of the system asymptotically approaches a minimum value; also stated as: "the entropy of all systems and of all states of a system is zero at absolute zero" or equivalently "it is impossible to reach the absolute zero of temperature by any finite number of processes".

The following has sometimes been called the "Fourth Law of Thermodynamics", about the transfer of heat energy between systems.

- Onsager reciprocal relations:

  > In connected thermodynamic systems which are in equilibrium neither for pressure nor temperature, heat flow between is caused by forces proportional with unit of pressure difference, and equal to the proportional density flow caused per unit of temperature difference.
  >
  > *See also:* Bose–Einstein condensate and negative temperature.

Thermodynamic potentials

As can be derived from the energy balance equation (or Burks' equation) on a thermodynamic system there exist energetic quantities called thermodynamic potentials, being the quantitative measure of the stored energy in the system. The five most well known potentials are:

Internal energy	U
Helmholtz free energy	$A = U - TS$
Enthalpy	$H = U + pV$
Gibbs free energy	$G = U + pV - TS$
Grand potential	$\Phi_G = U - TS - \mu N$

Other thermodynamic potentials can be obtained through Legendre transformation. Potentials are used to measure energy changes in systems as they evolve from an initial state to a final state. The potential used depends on the constraints of the system, such as constant temperature or pressure. Internal energy is the internal energy of the system, enthalpy is the internal energy of the system plus the energy related to pressure-volume work, and Helmholtz and Gibbs energy are the energies available in a system to do useful work when the temperature and volume or the pressure and temperature are fixed, respectively.

Classical thermodynamics

Classical thermodynamics is the original early 1800s variation of thermodynamics concerned with thermodynamic states, and properties as energy, work, and heat, and with the laws of thermodynamics, all lacking an atomic interpretation. In precursory form, classical thermodynamics derives from chemist Robert Boyle's 1662 postulate that the pressure P of a given quantity of gas varies inversely as its volume V at constant temperature; i.e. in equation form: $PV = k$, a constant. From here, a semblance of a thermo-science began to develop with the construction of the first successful atmospheric steam engines in England by Thomas Savery in 1697 and Thomas Newcomen in 1712. The first and second laws of thermodynamics emerged simultaneously in the 1850s, primarily out of the works of William Rankine, Rudolf Clausius, and William Thomson (Lord Kelvin).

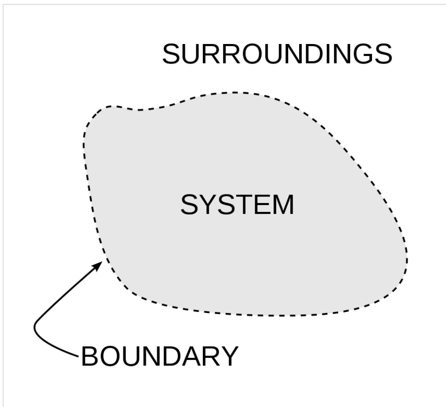
Statistical thermodynamics

With the development of atomic and molecular theories in the late 1800s and early 1900s, thermodynamics was given a molecular interpretation. This field is called **statistical thermodynamics**, which can be thought of as a bridge between macroscopic and microscopic properties of systems. Essentially, statistical thermodynamics is an approach to thermodynamics situated upon → statistical mechanics, which focuses on the derivation of macroscopic results from first principles. It can be opposed to its historical predecessor phenomenological thermodynamics, which gives scientific descriptions of phenomena with avoidance of microscopic details. The statistical approach is to derive all macroscopic properties (temperature, volume, pressure, energy, entropy, etc.) from the properties of moving constituent particles and the interactions between them (including quantum phenomena). It was found to be very successful and thus is commonly used.

Chemical thermodynamics

Chemical thermodynamics is the study of the interrelation of energy with chemical reactions or with a physical change of state within the confines of the laws of thermodynamics. During the years 1873-76 the American mathematical physicist Josiah Willard Gibbs published a series of three papers, the most famous being *On the Equilibrium of Heterogeneous Substances*, in which he showed how thermodynamic processes could be graphically analyzed, by studying the energy, entropy, volume, temperature and pressure of the thermodynamic system, in such a manner to determine if a process would occur spontaneously.[14] During the early 20th century, chemists such as Gilbert N. Lewis, Merle Randall, and E. A. Guggenheim began to apply the mathematical methods of Gibbs to the analysis of chemical processes.[15]

Thermodynamic systems



An important concept in thermodynamics is the "system". Everything in the universe except the system is known as surroundings. A system is the region of the universe under study. A system is separated from the remainder of the universe by a boundary which may be imaginary or not, but which by convention delimits a finite volume. The possible exchanges of work, heat, or matter between the system and the surroundings take place across this boundary. Boundaries are of four types: fixed, moveable, real, and imaginary.

Basically, the "boundary" is simply an imaginary dotted line drawn around a volume of *something* when there is going to be a change in the internal energy of that *something*. Anything that passes across the boundary that effects a change in the internal energy of the *something* needs to be accounted for in the energy balance equation. That *something* can be the volumetric region surrounding a single atom resonating energy, such as Max Planck defined in 1900; it can be a body of steam or air in a steam engine, such as Sadi Carnot defined in 1824; it can be the body of a tropical cyclone, such as Kerry Emanuel theorized in 1986 in the field of atmospheric thermodynamics; it could also be just one nuclide (i.e. a system of quarks) as some are theorizing presently in quantum thermodynamics.

For an engine, a fixed boundary means the piston is locked at its position; as such, a constant volume process occurs. In that same engine, a moveable boundary allows the piston to move in and out. For closed systems, boundaries are real while for open system boundaries are often imaginary. There are five dominant classes of systems:

1. *Isolated Systems* – matter and energy may not cross the boundary
2. *Adiabatic Systems* – heat must not cross the boundary
3. *Diathermic Systems* - heat may cross boundary
4. *Closed Systems* – matter may not cross the boundary
5. *Open Systems* – heat, work, and matter may cross the boundary (often called a control volume in this case)

As time passes in an isolated system, internal differences in the system tend to even out and pressures and temperatures tend to equalize, as do density differences. A system in which all equalizing processes have gone practically to completion, is considered to be in a state of thermodynamic equilibrium.

In thermodynamic equilibrium, a system's properties are, by definition, unchanging in time. Systems in equilibrium are much simpler and easier to understand than systems which are not in equilibrium. Often, when analysing a thermodynamic process, it can be assumed that each intermediate state in the process is at equilibrium. This will also considerably simplify the situation. Thermodynamic processes which develop so slowly as to allow each intermediate step to be an equilibrium state are said to be reversible processes.

Conjugate variables

The central concept of thermodynamics is that of energy, the ability to do work. By the First Law, the total energy of a system and its surroundings is conserved. Energy may be transferred into a system by heating, compression, or addition of matter, and extracted from a system by cooling, expansion, or extraction of matter. In mechanics, for example, energy transfer equals the product of the force applied to a body and the resulting displacement.

Conjugate variables are pairs of thermodynamic concepts, with the first being akin to a "force" applied to some thermodynamic system, the second being akin to the resulting "displacement," and the product of the two equalling the amount of energy transferred. The common conjugate variables are:

- Pressure-volume (the mechanical parameters);
- Temperature-entropy (thermal parameters);
- Chemical potential-particle number (material parameters).

Thermodynamic instruments

There are two types of thermodynamic instruments, the **meter** and the **reservoir**. A thermodynamic meter is any device which measures any parameter of a thermodynamic system. In some cases, the thermodynamic parameter is actually defined in terms of an idealized measuring instrument. For example, the zeroth law states that if two bodies are in thermal equilibrium with a third body, they are also in thermal equilibrium with each other. This principle, as noted by James Maxwell in 1872, asserts that it is possible to measure temperature. An idealized thermometer is a sample of an ideal gas at constant pressure. From the ideal gas law $PV=nRT$, the volume of such a sample can be used as an indicator of temperature; in this manner it defines temperature. Although pressure is defined mechanically, a pressure-measuring device, called a barometer may also be constructed from a sample of an ideal gas held at a constant temperature. A calorimeter is a device which is used to measure and define the internal energy of a system.

A thermodynamic reservoir is a system which is so large that it does not appreciably alter its state parameters when brought into contact with the test system. It is used to impose a particular value of a state parameter upon the system. For example, a pressure reservoir is a system at a particular pressure, which imposes that pressure upon any test system that it is mechanically connected to. The Earth's atmosphere is often used as a pressure reservoir.

It is important that these two types of instruments are distinct. A meter does not perform its task accurately if it behaves like a reservoir of the state variable it is trying to measure. If, for example, a thermometer were to act as a temperature reservoir it would alter the temperature of the system being measured, and the reading would be incorrect. Ideal meters have no effect on the state variables of the system they are measuring.

Thermodynamic states

When a system is at equilibrium under a given set of conditions, it is said to be in a definite *state*. The state of the system can be described by a number of intensive variables and extensive variables. The properties of the system can be described by an equation of state which specifies the relationship between these variables. State may be thought of as the instantaneous quantitative description of a system with a set number of variables held constant.

Thermodynamic processes

A **thermodynamic process** may be defined as the energetic evolution of a thermodynamic system proceeding from an initial state to a final state. Typically, each thermodynamic process is distinguished from other processes, in energetic character, according to what parameters, as temperature, pressure, or volume, etc., are held fixed. Furthermore, it is useful to group these processes into pairs, in which each variable held constant is one member of a conjugate pair. The seven most common thermodynamic processes are shown below:

1. An isobaric process occurs at constant pressure.
2. An isochoric process, or *isometric/isovolumetric process*, occurs at constant volume.
3. An isothermal process occurs at a constant temperature.
4. An adiabatic process occurs without loss or gain of energy by heat.
5. An isentropic process (reversible adiabatic process) occurs at a constant entropy.
6. An isenthalpic process occurs at a constant enthalpy.
7. A steady state process occurs without a change in the internal energy of a system.

See also

Approaches and applied fields

- Atmospheric thermodynamics
- Biological thermodynamics
- Black hole thermodynamics
- Chemical thermodynamics
- Classical thermodynamics
- Psychrometrics
- Quantum thermodynamics
- Statistical thermodynamics
- Thermoeconomics
- Equilibrium thermodynamics
- Maximum entropy thermodynamics
- Non-equilibrium thermodynamics
- Philosophy of thermal and statistical physics

Other

Lists and timelines:

- List of important publications in thermodynamics
- List of textbooks in statistical mechanics
- List of thermal conductivities
- List of thermodynamic properties
- Table of thermodynamic equations
- Timeline of thermodynamics, statistical mechanics, and random processes

Thermodynamic:

- Boundary
- Component
- Conjugate variables
  - Temperature / Entropy
  - Pressure / Volume
  - (Stress / Strain)
  - Chemical potential / Particle number
- Constant:
  - Avogadro's N_A
  - Boltzmann k
  - Ideal gas R
  - Stefan-Boltzmann σ
- Critical line
- Cycle
  - External combustion engine
  - Internal combustion engine
  - Atkinson
  - Bell Coleman
  - Brayton
  - Carnot
  - Combined
  - Diesel
  - Ericsson
  - Hampson-Linde
  - Heat engine
    - Carnot
  - HEHC
  - Hot air engine
  - Heat pump & refrigeration
  - Kalina
  - Kleemenko
  - Lenoir
  - Miller
  - Mixed/Dual
  - Otto
  - Rankine
  - Regenerative
  - Siemens
  - Stirling
  - Stoddard
- Ensemble
  - Canonical
- Equilibrium
  - Chemical
  - Dynamic
  - Local
  - Phase
- History
- Instruments
  - Barometer
  - Calorimeter
  - Dynamometer
  - Thermometer
- Laws:
  - Zeroth
  - First
  - Second
  - Third
  - Charles's
  - Dulong-Petit
  - Fundamental relation
  - Gas laws
    - Ideal gas
  - Joule's
  - Onsager reciprocal relations
  - Stefan-Boltzmann
- Limit
- Material properties
  - Bulk modulus K
  - Compressibility β
  - Specific heat capacity c
  - Thermal expansion α
- Potential
  - Internal energy
  - Entropy
  - Gibbs free energy
  - Grand
  - Helmholtz free energy
- Process
  - Adiabatic
  - Isenthalpic
  - Isentropic
  - Isobaric
  - Isochoric

Variable:

- Chemical potential μ
- Density
- Energy
  - Conservation of
  - Conversion efficiency
  - Electrical
  - Free
  - Gibbs free G
  - Helmholtz free A
  - Internal U
  - Kinetic
  - Potential
  - Specific
- Enthalpy H
- Entropy S
  - & information theory
  - As energy dispersal
  - Introduction to
  - Residual
  - Shannon
  - Statistical
- Exergy
  - Efficiency
- Mass
- Mole (unit)
- Particle number N
- Pressure P
- Temperature T
- Volume V
- Work W
  - Mechanical

- Grand canonical
- Isoenthalpic-isobaric
- Isothermal-isobaric
- Microcanonical
- Equations
  - Boltzmann
  - Bridgman
  - Churchill-Bernstein
  - Clausius-Clapeyron relation
  - Debye-Hückel
  - Equation of state
  - Exact differential
  - Gibbs-Duhem
  - Gibbs-Helmholtz
  - Green-Kubo relations
  - Maxwell relations
  - Onsager reciprocal relations

- Isothermal
- Quasistatic
- Spontaneous
- Steady state
- State
  - Excited
  - Function
  - Ground
  - Standard
  - Stationary
  - Steady
- System
  - Closed
  - Dissipative
  - Isolated
- Temperature
  - Negative
  - Range

Theorem:

- Carnot's
- Clausius
- Equipartition
- Bolzmann's H
- Nernst heat
- Virial

Other Related Topics

Heat:

- Critical heat flux
- Heat of combustion
- Heat transfer
  - Convective
- Latent heat
- Mechanical equivalent
- Theory of heat
- Volumetric heat capacity

Thermal:

- Analysis
- Conductivity
- Contact
- Efficiency

Physical chemistry:

- Autocatalytic reactions and order creation
- Boiling point
- Calorimetry
- Chemical energetics
- Chemical kinetics
- Endergonic reaction
- Endothermic
- Exothermic
- Gibbs phase rule
- Melting point
- Phase diagram
  - Calphad
- Phase transition

Statistical Mechanics:

- Boltzmann distribution
- Boltzmann distribution law
- Boltzmann factor
- Bose-Einstein condensate
- Bose-Einstein statistics
- Brownian motion
- Configuration integral
- Degeneracy
- Degrees of freedom
- Fermi-Dirac statistics
- Fluctuations
- Gibbs paradox
- Ideal gas

Sundry:

- Absolute zero
- Arrow of time
- Black body
- Dissipation
- Ettingshausen effect
- Extensive quantity
- Intensive quantity
- Legendre transformation
- Loschmidt's paradox
- Mass-energy equivalence
- Physical information
- Piezoelectric effect
- Pressure volume diagram

- Energy
- Equilibrium
- Expansion
  - Negative
- Mass
- Motion
- Radiation
- Science
- Thermodynamic databases for pure substances
- Triple point
- Vapor-liquid equilibrium
- Irreversibility
- Kinetic theory
- Macrostate
- Maxwell-Boltzmann statistics
- Microstate
- Molecular chaos
- Partition function
- Pyroelectric effect
- Quality of a fluid
- Refrigeration
  - Gas asbsorption
  - Cycle
  - Thermoelectric cooling
  - Vapor compression
- Standard conditions for temperature and pressure
- T-symmetry
- Two dimensional gas

Thermoelectricity:

- Nernst effect
- Peltier effect
- Seebeck effect
- Thermionic emission
- Thermoelectric effect
- Thermoelectricity
- Thermogenerator
- Thermophotovoltaic
- Thermopower
- Thomson effect

Wikibooks

- Engineering Thermodynamics [16]
- Entropy for Beginners

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Further reading

- Goldstein, Martin, and Inge F. (1993). *The Refrigerator and the Universe*. Harvard University Press. ISBN 0-674-75325-9. OCLC 32826343 (http://worldcat.org/oclc/32826343). A nontechnical introduction, good on historical and interpretive matters.

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External links

- Thermodynamics Data & Property Calculation Websites (http://tigger.uic.edu/~mansoori/Thermodynamic.Data.and.Property_html)
- Thermodynamics Educational Websites (http://tigger.uic.edu/~mansoori/Thermodynamics.Educational.Sites_html)
- Thermodynamics at *ScienceWorld* (http://scienceworld.wolfram.com/physics/topics/Thermodynamics.html)
- History of Thermodynamics (http://thermohistory.org/)
- Shakespeare & Thermodynamics (http://www.shakespeare2ndlaw.com)
- Biochemistry Thermodynamics (http://www.wiley.com/legacy/college/boyer/0470003790/reviews/thermo/thermo_intro.htm)
- Thermodynamics and Statistical Mechanics (http://farside.ph.utexas.edu/teaching/sm1/lectures/lectures.html)
- Free Steam Tables Online (http://www.steamtablesonline.com) calculator based on IAPWS-IF97

Experimental Physics

1. REDIRECT Experimental physics

This is a redirect from a title with another method of capitalisation. It leads to the title in accordance with the Wikipedia naming conventions for capitalisation, and can help writing, searching, and international language issues.

Pages linking to any of these redirects may be updated to link directly to the target page. However, do not replace these redirected links with a piped link unless the page is updated for another reason.

For more information, see Category:Redirects from other capitalisations.

Related Research fields

Atomic, molecular, and optical physics

Atomic, molecular, and optical → physics is the study of matter-matter and light-matter interactions on the scale of single atoms or structures containing a few atoms. The three areas are grouped together because of their interrelationships, the similarity of methods used, and the commonality of the energy scales that are relevant. Physicists sometimes abbreviate the field as *AMO physics*. All three areas include both classical and quantum treatments.

Atomic physics

Atomic physics studies the electron hull of atoms. This branch of → physics is distinct from nuclear physics, despite their association in the public consciousness. Atomic physics is not concerned with the intra-nuclear processes studied in nuclear physics, although properties of the nucleus can be important in atomic physics (e.g., hyperfine structure). Current research focuses on activities in quantum control, cooling and trapping of atoms and ions, low-temperature collision dynamics, the collective behavior of atoms in weakly interacting gases (Bose-Einstein Condensates and dilute Fermi degenerate systems), precision measurements of fundamental constants, and the effects of electron correlation on structure and dynamics.Atomic physics is that branch of physics which deals with the study of atom, particularly extra-nuclear particles like electrons and their behaviour in atom-like interactions with protons, neutrons in the nucleus.

Molecular physics

Molecular physics focuses on multi-atomic structures and their internal and external interactions with matter and light.

Optical physics

Optical physics is distinct from optics in that it tends to focus not on the control of classical light fields by microscopic objects, but on the fundamental properties of optical fields and their interactions with matter in the microscopic realm.

See the Wikipedia page on optical physics.

See also

- subfields: atomic physics, molecular physics, spectroscopy, physical chemistry, classical optics, quantum optics, photonics
- related fields: → quantum mechanics, quantum chemistry, nano sciences, → biophysics
- important publications in atomic, molecular, and optical physics

References

External links

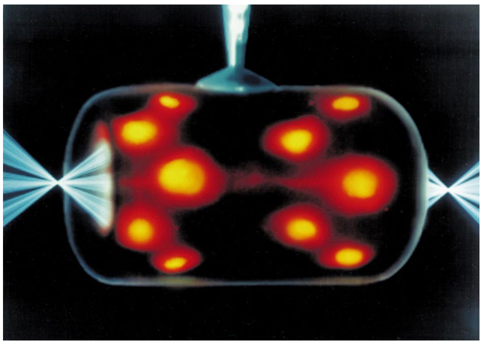
X-ray microscope

An **X-ray microscope** uses electromagnetic radiation in the soft X-ray band to produce images of very small objects.

Unlike visible light, X-rays do not reflect or refract easily, and they are invisible to the human eye. Therefore the basic process of an X-ray microscope is to expose film or use a charge-coupled device (CCD) detector to detect X-rays that pass through the specimen. It is a contrast imaging technology using the difference in absorption of soft x-ray in the water window region (wavelength region: 2.3 - 4.4 nm, photon energy region: 0.28 - 0.53 keV) by the carbon atom (main element composing the living cell) and the oxygen atom (main element for water).

Early X-ray microscopes by Paul Kirkpatrick and Albert Baez used grazing-incidence reflective optics to focus the X-rays, which grazed X-rays off parabolic curved mirrors at a very high angle of incidence. An alternative method of focusing X-rays is to use a tiny fresnel zone plate of concentric gold or nickel rings on a silicon dioxide substrate. Sir Lawrence Bragg produced some of the first usable X-ray images with his apparatus in the late 1940's.

In the 1950's Newberry produced a shadow X-ray microscope which placed the specimen between the source and a target plate, this became the basis for the first commercial X-ray microscopes from the General Electric Company.



Indirect drive laser inertial confinement fusion uses a "hohlraum" which is irradiated with laser beam cones from either side on it its inner surface to bathe a fusion microcapsule inside with smooth high intensity X-rays. The highest energy X-rays which penetrate the hohlraum can be visualized using an X-ray microscope such as here, where X-radiation is represented in orange/red.

The Advanced Light Source (ALS)[1] in Berkeley CA is home to XM-1 (http://www.cxro.lbl.gov/BL612/), a full field soft X-ray microscope operated by the Center for X-ray Optics [2] and dedicated to various applications in modern nanoscience, such as nanomagnetic materials, environmental and materials sciences and biology. XM-1 uses an X-ray lens to focus X-rays on a CCD, in a manner similar to an optical microscope. XM-1 still holds the world record in spatial resolution with Fresnel zone plates down to 15nm and is able to combine high spatial resolution with a sub-100ps time resolution to study e.g. ultrafast spin dynamics.

The ALS is also home to the world's first soft x-ray microscope designed for biological and biomedical research. This new instrument, XM-2 was designed and built by scientists from the National Center for X-ray Tomography (http://ncxt.lbl.gov). XM-2 is capable of producing 3-Dimensional tomograms of cells.

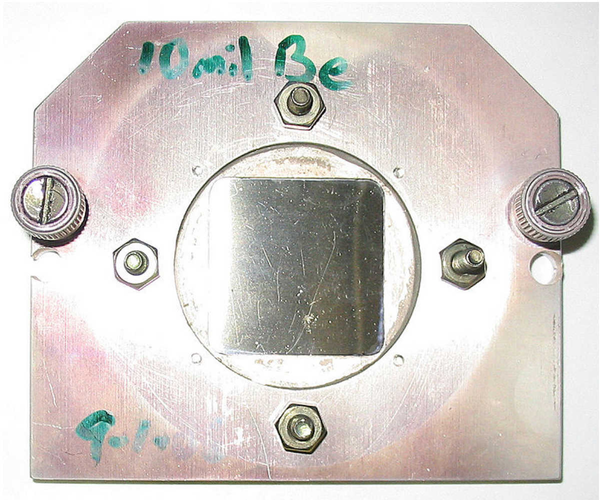
Sources of soft X-rays suitable for microscopy, such as synchrotron radiation sources, have fairly low brightness of the required wavelengths, so an alternative method of image formation is scanning transmission soft X-ray microscopy. Here the X-rays are focused to a point and the sample is mechanically scanned through the produced focal spot. At each point the transmitted X-rays are recorded with a detector such as a proportional counter or an avalanche photodiode. This type of Scanning Transmission X-ray Microscope (STXM) was first developed by researchers at Stony Brook University and was employed at the National Synchrotron Light Source at Brookhaven National Laboratory.

The resolution of X-ray microscopy lies between that of the optical microscope and the electron microscope. It has an advantage over conventional electron microscopy in that it can view biological samples in their natural state. Electron microscopy is widely used to obtain images with nanometer level resolution but the relatively thick living cell cannot be observed as the sample has to be chemically fixed, dehydrated, embedded in resin, then sliced ultra thin. However, it should be mentioned that cryo-electron microscopy allows the observation of biological specimens in their hydrated natural state. Until now, resolutions of 30 nanometer are possible using the Fresnel zone plate lens which forms the image using the soft x-rays emitted from a synchrotron. Recently, more researchers have begun to use the soft x-rays emitted from laser-produced plasma rather than synchrotron radiation.

Additionally, X-rays cause fluorescence in most materials, and these emissions can be analyzed to determine the chemical elements of an imaged object. Another use is to generate diffraction patterns, a process used in X-ray crystallography. By analyzing the internal reflections of a diffraction pattern (usually with a computer program), the three-dimensional structure of a crystal can be determined down to the placement of individual atoms within its molecules. X-ray microscopes are sometimes used for these analyses because the samples are too small to be analyzed in any other way.

See also

- Synchrotron X-ray tomographic microscopy



A square beryllium foil mounted in a steel case to be used as a window between a vacuum chamber and an X-ray microscope. Beryllium, due to its low Z number is highly transparent to X-rays.

External links

- Application of X-ray microscopy in analysis of living hydrated cells [3]
- Hard X-ray microbeam experiments with a sputtered-sliced Fresnel zone plate and its applications [4]
- Scientific applications of soft x-ray microscopy [5]
- Microarrays products [6]

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[3] http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?cmd=Retrieve&db=pubmed&dopt=Abstract&list_uids=12379938
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2D-FT NMRI and Spectroscopy

2D-FT Nuclear magnetic resonance imaging (**2D-FT NMRI**), or **Two-dimensional Fourier transform** nuclear magnetic resonance imaging (**NMRI**), is primarily a non—invasive imaging technique most commonly used in biomedical research and medical radiology/nuclear medicine/MRI to visualize structures and functions of the living systems and single cells. For example it can provides fairly detailed images of a human body in any selected cross-sectional plane, such as longitudinal, transversal, sagital, etc. The basic NMR phenomenon or physical principle[1] is essentially the same in N(MRI), nuclear magnetic resonance/FT (NMR) spectroscopy, topical NMR, or even in Electron Spin Resonance /EPR; however, the details are significantly different at present for EPR, as only in the early days of NMR the static magnetic field was scanned for obtaining spectra, as it is still the case in many EPR or ESR spectrometers. NMRI, on the other hand, often utilizes a linear magnetic field gradient to obtain an image that combines the visualization of molecular structure and dynamics. It is this dynamic aspect of NMRI, as well as its highest sensitivity for the ^{1}H nucleus that distinguishes it very dramatically from X-ray CAT scanning that 'misses' hydrogens because of their very low X-ray scattering factor.

Thus, NMRI provides much greater contrast especially for the different soft tissues of the body than computed tomography (CT) as its most sensitive option observes the nuclear spin distribution and dynamics of highly mobile molecules that contain the naturally abundant, stable hydrogen isotope ^{1}H as in plasma water molecules, blood, disolved metabolites and fats. This approach makes it most useful in cardiovascular, oncological (cancer), neurological (brain), musculoskeletal, and cartilage imaging. Unlike CT, it uses no ionizing radiation, and also unlike nuclear imaging it does not employ any radioactive isotopes. Some of the first MRI images reported were published in 1973[2] and the first study performed on a human took place on July 3, 1977.[3] Earlier papers were also published by Sir Peter Mansfield[4] in UK (Nobel Laureate in 2003), and R. Damadian in the USA[5] , (together with an approved patent for 'fonar', or magnetic imaging). The detailed physical theory of NMRI was published by Peter Mansfield in 1973[6] . Unpublished 'high-resolution' (50 micron resolution) images of other living systems, such as hydrated wheat grains, were also obtained and communicated in UK in 1977-1979, and were subsequently confirmed by articles published in *Nature* by Peter Callaghan.

NMR Principle

Advanced 4.7 T clinical diagnostics and biomedical research NMR Imaging instrument.

Certain nuclei such as ^{1}H nuclei, or `fermions' have spin-1/2, because there are two spin states, referred to as "up" and "down" states. The nuclear magnetic resonance absorption phenomenon occurs when samples containing such nuclear spins are placed in a static magnetic field and a very short radiofrequency pulse is applied with a center, or carrier, frequency matching that of the transition between the up and down states of the spin-1/2 ^{1}H nuclei that were polarized by the static magnetic field. [7] Very low field schemes have also been recently reported.[8]

Chemical Shifts

NMR is a very useful family of techniques for chemical and biochemical research because of the chemical shift; this effect consists in a frequency shift of the nuclear magnetic resonance for specific chemical groups or atoms as a result of the partial shielding of the corresponding nuclei from the applied, static external magnetic field by the electron orbitals (or molecular orbitals) surrounding such nuclei present in the chemical groups. Thus, the higher the electron density surrounding a specific nucleus the larger the chemical shift will be. The resulting magnetic field at the nucleus is thus lower than the applied external magnetic field and the resonance frequencies observed as a result of such shielding are lower than the value that would be observed in the absence of any electronic orbital shielding. Furthermore, in order to obtain a chemical shift value independent of the strength of the applied magnetic field and allow for the direct comparison of spectra obtained at different magnetic field values, the chemical shift is defined by the ratio of the strength of the local magnetic field value at the observed (electron orbital-shielded) nucleus by the external magnetic field strength, $\mathbf{H}_{loc}/ \mathbf{H}_0$. The first NMR observations of the chemical shift, with the correct physical chemistry interpretation, were reported for ^{19}F containing compounds in the early 1950s by Herbert S. Gutowsky and Charles P. Slichter from the University of Illinois at Urbana (USA).

A related effect in metals is called the Knight shift, which is due only to the conduction electrons. Such conduction electrons present in metals induce an "additional" local field at the nuclear site, due to the spin re-orientation of the conduction electrons in the presence of the applied (constant), external magnetic field. This is only broadly `similar' to the chemical shift in either solutions or diamagnetic solids.

NMR Imaging Principles

A number of methods have been devised for combining magnetic field gradients and radiofrequency pulsed excitation to obtain an image. Two major maethods involve either 2D -FT or 3D-FT[9] reconstruction from projections, somewhat similar to Computed Tomography, with the exception of the image interpretation that in the former case must include dynamic and relaxation/contrast enhancement information as well. Other schemes involve building the NMR image either point-by-point or line-by-line. Some schemes use instead gradients in the rf field rather than in the static magnetic field. The majority of NMR images routinely obtained are either by the Two-Dimensional Fourier Transform (2D-FT) technique [10] (with slice selection), or by the Three-Dimensional Fourier Transform (3D—FT) techniques that are however much more time consuming at present. 2D-FT NMRI is sometime called in common parlance a "spin-warp". An NMR image corresponds to a spectrum consisting of a number of `spatial frequencies' at different locations in the sample investigated, or in a patient.[11] A two–dimensional Fourier transformation of such a "real" image may be considered as a representation of such "real waves" by a matrix of spatial frequencies known as the k–space. We shall see next in some mathematical detail how the 2D-FT computation works to obtain 2D-FT NMR images.

Two-dimensional Fourier transform imaging and spectroscopy

A two-dimensional Fourier transform (2D-FT) is computed numerically or carried out in two stages, both involving `standard', one-dimensional Fourier transforms. However, the second stage Fourier transform is not the inverse Fourier transform (which would result in the original function that was transformed at the first stage), but a Fourier transform in a second variable—which is `shifted' in value—relative to that involved in the result of the first Fourier transform. Such 2D-FT analysis is a very powerful method for both NMRI and two-dimensional nuclear magnetic resonance spectroscopy (2D-FT NMRS)[12] that allows the three-dimensional reconstruction of polymer and biopolymer structures at atomic resolution.[13] for molecular weights (Mw) of dissolved biopolymers in aqueous solutions (for example) up to about 50,000 Mw. For larger biopolymers or polymers, more complex methods have been developed to obtain limited structural resolution needed for partial 3D-reconstructions of higher molecular structures, e.g. for up 900,000 Mw or even oriented microcrystals in aqueous suspensions or single crystals; such methods have also been reported for *in vivo* 2D-FT NMR spectroscopic studies of algae, bacteria, yeast and certain mammalian cells, including human ones. The 2D-FT method is also widely utilized in optical spectroscopy, such as *2D-FT NIR hyperspectral imaging* (2D-FT NIR-HS), or in MRI imaging for research and clinical, diagnostic applications in Medicine. In the latter case, 2D-FT NIR-HS has recently allowed the identification of single, malignant cancer cells surrounded by healthy human breast tissue at about 1 micron resolution, well-beyond the resolution obtainable by 2D-FT NMRI for such systems in the limited time available for such diagnostic investigations (and also in magnetic fields up to the FDA approved magnetic field strength $\mathbf{H}_0$ of 4.7 T, as shown in the top image of the state-of-the-art NMRI instrument). A more precise mathematical definition of the `double' (2D) Fourier transform involved in both 2D NMRI and 2D-FT NMRS is specified next, and a precise example follows this generally accepted definition.

2D-FT Definition

A *2D-FT, or two-dimensional Fourier transform*, is a standard Fourier transformation of a function of two variables, **f**(x_1, x_2), carried first in the first variable x_1, followed by the Fourier transform in the second variable x_2 of the resulting function **F**(s_1,x_2). Note that in the case of both 2D-FT NMRI and 2D-FT NMRS the two independent variables in this definition are in the time domain, whereas the results of the two successive Fourier transforms have, of course, frequencies as the independent variable in the NMRS, and ultimately spatial coordinates for both 2D NMRI and 2D-FT NMRS following computer structural recontructions based on special algorithms that are different from FT or 2D-FT. Moreover, such structural algorithms are different for 2D NMRI and 2D-FT NMRS: in the former case they involve macroscopic, or anatomical structure detrmination, whereas in the latter case of 2D-FT NMRS the atomic structure reconstruction algorithms are based on the quantum theory of a microphysical (quantum) process such as nuclear Overhauser enhancement NOE, or specific magnetic dipole-dipole interactions[14] between neighbor nuclei.

Example 1

A 2D Fourier transformation and phase correction is applied to a set of 2D NMR (FID) signals: **s**(t_1,t_2) yielding a real 2D-FT NMR `spectrum' (collection of 1D FT-NMR spectra) represented by a matrix **S** whose elements are

$$\mathbf{S}\ (\nu_1,\nu_2) = \mathbf{Re}\int\int cos(\nu_1 t_1)exp^{(-i\nu_2 t_2)}s(t_1,t_2)dt_1dt_2$$

where : ν_1 and : ν_2 denote the discrete indirect double-quantum and single-quantum(detection) axes, respectively, in the 2D NMR experiments. Next, the *covariance matrix* is calculated in the frequency domain according to the following equation

$$\mathbf{C}\quad (\nu_2',\nu_2) = S^T S = \sum_{\nu^1}[S(\nu_1,\nu_2')S(\nu_1,\nu_2)],$$

with : ν_2, ν_2' taking all possible single-quantum frequency values and with the summation carried out over all discrete, double quantum frequencies : ν_1.

Example 2

Atomic Structure from 2D-FT STEM Images [15] of electron distributions in a high-temperature cuprate superconductor `paracrystal' reveal both the domains (or `location') and the local symmetry of the 'pseudo-gap' in the electron-pair correlation band responsible for the high—temperature superconductivity effect (obtained at Cornell University). So far there have been three Nobel prizes awarded for 2D-FT NMR/MRI during 1992-2003, and an additional, earlier Nobel prize for 2D-FT of X-ray data (`CAT scans'); recently the advanced possibilities of 2D-FT techniques in Chemistry, Physiology and Medicine [16] received very significant recognition.[17]

Brief explanation of NMRI diagnostic uses in Pathology

As an example, a diseased tissue such as a malign tumor, can be detected by 2D-FT NMRI because the hydrogen nuclei of molecules in different tissues return to their equilibrium spin state at different relaxation rates, and also because of the manner in which a malign tumor spreads and grows rapidly along the blood vessels adjacent to the tumor, also inducing further vascularization to occur. By changing the pulse delays in the RF pulse sequence employed, and/or the RF pulse sequence itself, one may obtain a `relaxation—based contrast', or contrast enhancement between different types of body tissue, such as normal vs. diseased tissue cells for example. Excluded from such diagnostic observations by NMRI are all patients with ferromagnetic metal implants, (e.g., cochlear implants), and all cardiac pacemaker patients who cannot undergo any NMRI scan because of the very intense magnetic and RF fields employed in NMRI which would strongly interfere with the correct functioning of such pacemakers. It is, however, conceivable that future developments may also include along with the NMRI diagnostic treatments with special techniques involving applied magnetic fields and very high frequency RF. Already, surgery with special tools is being experimented on in the presence of NMR imaging of subjects.Thus, NMRI is used to image almost every part of the body, and is especially useful for diagnosis in neurological conditions, disorders of the muscles and joints, for evaluating tumors, such as in lung or skin cancers, abnormalities in the heart (especially in children with hereditary disorders), blood vessels, CAD, atherosclerosis and cardiac infarcts [18] (courtesy of Dr. Robert R. Edelman)

See also

- Nuclear magnetic resonance (NMR)
- Edward Mills Purcell
- Felix Bloch
- Medical imaging
- Paul C. Lauterbur
- Magnetic resonance microscopy
- Peter Mansfield
- Computed tomography (CT)
- FT-NIRS (NIR)
- Magnetic resonance elastography
- Solid-state NMR
- Knight shift
- John Hasbrouck Van Vleck
- Chemical shift
- Herbert S. Gutowsky
- John S. Waugh
- Charles Pence Slichter
- Protein nuclear magnetic resonance spectroscopy
- Kurt Wüthrich
- Nuclear Overhauser effect
- Fourier transform spectroscopy(FTS)
- Jean Jeneer
- Richard R. Ernst
- Relaxation
- Earth's field NMR (EFNMR)
- Robinson oscillator

Footnotes

[1] Antoine Abragam. 1968. *Principles of Nuclear Magnetic Resonance.*, 895 pp., Cambridge University Press: Cambridge, UK.

[2] Lauterbur, P.C., Nobel Laureate in 2003 (1973). "Image Formation by Induced Local Interactions: Examples of Employing Nuclear Magnetic Resonance". *Nature* **242**: 190–1. doi: 10.1038/242190a0 (http://dx.doi.org/10.1038/242190a0).

[3] Howstuffworks "How MRI Works" (http://www.howstuffworks.com/mri.htm/printable)

[4] Peter Mansfield. 2003. Nobel Laureate in Physiology and Medicine for (2D and 3D) MRI (http://www.parteqinnovations.com/pdf-doc/fandr-Gaz1006.pdf)

[5] Damadian, R. V. "Tumor Detection by Nuclear Magnetic Resonance," Science, 171 (March 19, 1971): 1151-1153 (http://www.sciencemag.org/cgi/content/abstract/171/3976/1151)

[6] NMR 'diffraction' in solids? P. Mansfield et al. 1973 J. Phys. C: Solid State Phys. 6 L422-L426 doi: 10.1088/0022-3719 (http://www.iop.org/EJ/article/0022-3719/6/22/007/jcv6i22pL422.pdf)

[7] Antoine Abragam. 1968. *Principles of Nuclear Magnetic Resonance.*, 895 pp., Cambridge University Press: Cambridge, UK.

[8] Raftery D (August 2006). " MRI without the magnet (http://www.pubmedcentral.nih.gov/articlerender.fcgi?tool=pmcentrez&artid=1568902)". *Proc Natl Acad Sci USA.* **103** (34): 12657–8. doi: 10.1073/pnas.0605625103 (http://dx.doi.org/10.1073/pnas.0605625103). PMID 16912110.

[9] Wu Y, Chesler DA, Glimcher MJ, *et al.* (February 1999). " Multinuclear solid-state three-dimensional MRI of bone and synthetic calcium phosphates (http://www.pnas.org/cgi/pmidlookup?view=long&pmid=9990066)". *Proc. Natl. Acad. Sci. U.S.A.* **96** (4): 1574–8. doi: 10.1073/pnas.96.4.1574 (http://dx.doi.org/10.1073/pnas.96.4.1574). PMID 9990066. PMC: 15521 (http://www.pubmedcentral.nih.gov/articlerender.fcgi?tool=pmcentrez&artid=15521). .

[10] http://www.math.cuhk.edu.hk/course/mat2071a/lec1_08.ppt

[11] *Haacke, E Mark; Brown, Robert F; Thompson, Michael; Venkatesan, Ramesh (1999). *Magnetic resonance imaging: physical principles and sequence design*. New York: J. Wiley & Sons. ISBN 0-471-35128-8.

[12] Richard R. Ernst. 1992. Nuclear Magnetic Resonance Fourier Transform (2D-FT) Spectroscopy. Nobel Lecture (http://nobelprize.org/nobel_prizes/chemistry/laureates/1991/ernst-lecture.pdf), on December 9, 1992.

[13] http://en.wikipedia.org/wiki/Nuclear_magnetic_resonance#Nuclear_spin_and_magnets Kurt Wüthrich in 1982-1986 : 2D-FT NMR of solutions

[14] Charles P. Slichter.1996. *Principles of Magnetic Resonance.* Springer: Berlin and New York, Third Edition., 651pp. ISBN 0-387-50157-6.

[15] http://www.physorg.com/news129395045.html

[16] http://nobelprize.org/nobel_prizes/chemistry/laureates/1991/ernst-lecture.pdf

[17] Protein structure determination in solution by NMR spectroscopy (http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?cmd=Retrieve&db=pubmed&dopt=Abstract&list_uids=2266107&query_hl=33&itool=pubmed_docsum) Kurt Wüthrich. J Biol Chem. 1990 December 25;265(36):22059-62.

[18] http://www.mr-tip.com/serv1.php?type=img&img=Cardiac%20Infarct%20Short%20Axis%20Cine%204

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- 2D-FT NMRI Instrument image: A JPG color image of a 2D-FT NMRI `monster' Instrument (http://upload.wikimedia.org/wikipedia/en/b/bf/HWB-NMRv900.jpg).
- Richard R. Ernst. 1992. Nuclear Magnetic Resonance Fourier Transform (2D-FT) Spectroscopy. Nobel Lecture (http://nobelprize.org/nobel_prizes/chemistry/laureates/1991/ernst-lecture.pdf), on December 9, 1992.
- Peter Mansfield. 2003. Nobel Laureate in Physiology and Medicine for (2D and 3D) MRI (http://www.parteqinnovations.com/pdf-doc/fandr-Gaz1006.pdf)
- D. Benett. 2007. PhD Thesis. Worcester Polytechnic Institute. PDF of 2D-FT Imaging Applications to NMRI in Medical Research. (http://www.wpi.edu/Pubs/ETD/Available/etd-081707-080430/unrestricted/dbennett.pdf) Worcester Polytechnic Institute. (Includes many 2D-FT NMR images of human brains.)
- Paul Lauterbur. 2003. Nobel Laureate in Physiology and Medicine for (2D and 3D) MRI. (http://nobelprize.org/nobel_prizes/medicine/laureates/2003/)
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pmid=9990066.

External links

- Cardiac Infarct or "heart attack" Imaged in Real Time by 2D-FT NMRI (http://www.mr-tip.com/exam_gifs/cardiac_infarct_short_axis_cine_6.gif)
- Interactive Flash Animation on MRI (http://www.e-mri.org) - *Online Magnetic Resonance Imaging physics and technique course*
- Herbert S. Gutowsky
- Jiri Jonas and Charles P. Slichter: NMR Memoires at NAS about Herbert Sander Gutowsky; NAS = National Academy of Sciences, USA, (http://books.nap.edu/html/biomems/hgutowsky.pdf)
- 3D Animation Movie about MRI Exam (http://www.patiencys.com/MRI/)
- International Society for Magnetic Resonance in Medicine (http://www.ismrm.org)
- Danger of objects flying into the scanner (http://www.simplyphysics.com/flying_objects.html)

Related Wikipedia websites

- Medical imaging
- Computed tomography
- Magnetic resonance microscopy
- Fourier transform spectroscopy
- FT-NIRS
- Magnetic resonance elastography
- Nuclear magnetic resonance (NMR)
- Chemical shift
- Relaxation
- Robinson oscillator
- Earth's field NMR (EFNMR)
- Rabi cycle

Biophysics and Biophysical Chemistry

Biophysics

Biophysics (also **biological physics**) is an interdisciplinary science that employs and develops theories and methods of the physical sciences for the investigation of biological systems. Studies included under the umbrella of biophysics span all levels of biological organization, from the molecular scale to whole organisms and ecosystems. Biophysical research shares significant overlap with biochemistry, nanotechnology, bioengineering, agrophysics and systems biology.

Molecular biophysics typically addresses biological questions that are similar to those in biochemistry and molecular biology, but the questions are approached quantitatively. Scientists in this field conduct research concerned with understanding the interactions between the various systems of a cell, including the interactions between DNA, RNA and protein biosynthesis, as well as how these interactions are regulated. A great variety of techniques are used to answer these questions.

Fluorescent imaging techniques, as well as electron microscopy, x-ray crystallography, NMR spectroscopy and atomic force microscopy (AFM) are often used to visualize structures of biological significance. Direct manipulation of molecules using optical tweezers or AFM can also be used to monitor biological events where forces and distances are at the nanoscale. Molecular biophysicists often consider complex biological events as systems of interacting units which can be understood through → statistical mechanics, → thermodynamics and chemical kinetics. By drawing knowledge and experimental techniques from a wide variety of disciplines, biophysicists are often able to directly observe, model or even manipulate the structures and interactions of individual molecules or complexes of molecules.

In addition to traditional (i.e. molecular and cellular) biophysical topics like structural biology or enzyme kinetics, modern biophysics encompasses an extraordinarily broad range of research. It is becoming increasingly common for biophysicists to apply the models and experimental techniques derived from → physics, as well as mathematics and statistics, to larger systems such as tissues, organs, populations and ecosystems.

Focus as a subfield

Biophysics often does not have university-level departments of its own, but has presence as groups across departments within the fields of molecular biology, biochemistry, chemistry, computer science, mathematics, medicine, pharmacology, physiology, → physics, and neuroscience. What follows is a list of examples of how each department applies its efforts toward the study of biophysics. This list is hardly all inclusive. Nor does each subject of study belong exclusively to any particular department. Each academic institution makes its own rules and there is much overlap between departments.

- Biology and molecular biology - Almost all forms of biophysics efforts are included in some biology department somewhere. To include some: gene regulation, single protein dynamics, bioenergetics, patch clamping, biomechanics.
- Structural biology - Ångstrom-resolution structures of proteins, nucleic acids, lipids, carbohydrates, and complexes thereof.
- Biochemistry and chemistry - biomolecular structure, siRNA, nucleic acid structure, structure-activity relationships.
- Computer science - Neural networks, biomolecular and drug databases.
- Computational chemistry - → molecular dynamics simulation, molecular docking, quantum chemistry
- Bioinformatics - sequence alignment, structural alignment, protein structure prediction
- Mathematics - graph/network theory, population modeling, dynamical systems, phylogenetics.
- Medicine and neuroscience - tackling neural networks experimentally (brain slicing) as well as theoretically (computer models), membrane permitivity, gene therapy, understanding tumors.
- Pharmacology and physiology - channel biology, biomolecular interactions, cellular membranes, polyketides.
- → Physics - biomolecular free energy, stochastic processes, covering dynamics.
- Agronomy Agriculture

Many biophysical techniques are unique to this field. Research efforts in biophysics are often initiated by scientists who were traditional physicists, chemists, and biologists by training.

Topics in biophysics and related fields

- Theoretical biophysics
- Mathematical biophysics
- Systems biology
- Medical biophysics
- Agrophysics
- Origin of Life

Molecular biophysics

- Biological membranes
- Cell membranes
- Bioenergetics
- Channels, receptors and transporters
- Enzyme kinetics
- Molecular motors
- Phospholipids
- Proteins
- Biofilms
- Supramolecular assemblies
- Nucleic acids

Cellular biophysics

- Cell division
- Cell migration

- Cell signalling
- Dynamical systems
- Electrophysiology
- Signaling
- Biochemical systems theory
- Metabolic control analysis

Techniques used in biophysics

- Atomic force microscopy
- Biophotonics
- Biosensor and Bioelectronics
- Calcium imaging
- Calorimetry
- Circular Dichroism
- Cryobiology
- Electrophysiology
- Fluorescence
- Microscopy
- Neuroimaging
- Neutron spin echo spectroscopy
- Patch clamping
- Nuclear Magnetic Resonance Spectroscopy
- Spectroscopy, imaging, etc.
- x-ray crystallography

Other

- Animal locomotion
- Bioacoustics
- Biomechanics
- Biomineralisation
- Bionics
- Evolution
- Evolutionary algorithms
- Evolutionary computing
- Evolutionary theory
- Gravitational biology
- Mathematical biology
- Morphogenesis
- Muscle and contractility
- Negentropy
- Neural encoding
- Radiobiology
- Sensory systems
- Systems neuroscience
- Tensegrity
- Theoretical biology

Famous biophysicists

- Luigi Galvani, discoverer of bioelectricity
- Hermann von Helmholtz, first to measure the velocity of nerve impulses; studied hearing and vision
- Alan Hodgkin & Andrew Huxley, mathematical theory of how ion fluxes produce nerve impulses
- Georg von Békésy, research on the human ear
- Bernard Katz, discovered how synapses work
- Hermann J. Muller, discovered that X-rays cause mutations
- George Palade Nobel Laureate in physiology or medicine for protein secretion and cell ultra-structure from electron microscopy studies
- Linus Pauling & Robert Corey, co-discoverers of the alpha helix and beta sheet structures in proteins
- J. D. Bernal, X-ray crystallography of plant viruses and proteins
- Rosalind Franklin, Maurice Wilkins, James D. Watson and Francis Crick, pioneers of DNA crystallography and co-discoverers of the structure of DNA. Francis Crick later participated in the Crick, Brenner et al. experiment which established the basis for understanding the genetic code
- Max Perutz & John Kendrew, pioneers of protein crystallography
- Sir John Randall, X-ray and neutron diffraction of proteins and DNA
- Ronald Burge, X-ray diffraction of nerve myelin, bacterial cell walls and membranes
- Allan Cormack & Godfrey Hounsfield, development of computer assisted tomography
- Kurt Wüthrich Nobel Laureate in physiology or medicine for 2D-FT NMR of protein structure in solution[1]
- Paul Lauterbur & Peter Mansfield, development of magnetic resonance imaging
- Stephen D. Levene, DNA-protein Interactions, DNA looping, and DNA topology.
- Seiji Ogawa, development of functional magnetic resonance imaging

Other notable biophysicists

- Adolf Eugen Fick, responsible for Fick's law of diffusion and a method to determine cardiac output.
- Howard Berg, characterized properties of bacterial chemotaxis
- Steven Block, observed the motions of enzymes such as kinesin and RNA polymerase with optical tweezers
- Carlos Bustamante, known for single-molecule biophysics of molecular motors and biological polymer physics
- Steven Chu, Nobel laureate who helped develop optical trapping techniques used by many biophysicists
- Christoph Cremer, overcoming the conventional limit of resolution that applies to light based investigations (the Abbe limit) by a range of different methods
- Friedrich Dessauer, research on radiation, especially X-rays
- Julio Fernandez
- Govindjee, professor emeritus at the University of Illinois, research in photosynthesis and photosynthetic mechanisms by fluorescence and NMR methods
- Enrico Gratton research on frequency domain spectroscopy and correlation spectroscopy on biological and biomedical systems

- Stefan Hell, developed the principle of STED microscopy
- Richard Henderson, scientist at the MRC Laboratory of Molecular Biology, developed the use of cryo-EM to study membrane protein structures.
- John J. Hopfield, worked on error correction in transcription and translation (kinetic proof-reading), and associative memory models (Hopfield net)
- Martin Karplus, research on → molecular dynamical simulations of biological macromolecules.
- Franklin Offner, professor emeritus at Northwestern University of professor of biophysics, biomedical engineering and electronics who developed a modern prototype of the electroencephalograph and electrocardiograph called the dynograph.
- Nicolas Rashevsky,[2] , former Editor of the first journal of mathematical and theoretical biophysics entitled " *The Bulletin of Mathematical Biophysics* " (1940--1973) and author of the two-factor model of neuronal excitation, biotopology and organismic set theory.
- Robert Rosen, theoretical biophysicist and mathematical biologist, author of: metabolic-replication systems, categories of metabolic and genetic networks, quantum genetics in terms of von Neumann's approach, non-reductionist complexity theories, dynamical and anticipatory systems in biology.[3]
- Benoit Roux
- Mikhail Volkenshtein, Revaz Dogonadze & Zurab Urushadze, authors of the first → quantum-mechanical model of enzyme catalysis, supported a theory that enzyme catalysis use quantum-mechanical effects such as tunneling.
- John P. Wikswo, research on biomagnetism
- Douglas Warrick, specializing in bird flight (hummingbirds and pigeons)
- Ernest C. Pollard — founder of the Biophysical Society
- Marvin Makinen, pioneer of the structural basis of enzyme action
- Gopalasamudram Narayana Iyer Ramachandran, developer of the Ramachandran plot and pioneer of the collagen triple-helix structure prediction
- Doug Barrick, repeat protein folding
- Naomi Courtemanche, kinetics of leucine rich repeat protein folding
- Ellen Kloss, salt-dependence of leucine rich repeat protein folding
- Bertrand Garcia Moreno E., Dielectric Constant of Globular Protein 'hydrophobic' core
- Ludwig Brand, Time resolved fluorescence anisotropy decay in Biological systems

See also

- Important publications in **bio**physics
- Important publications in bio**physics**

Notes

[1] http://nobelprize.org/nobel_prizes/chemistry/laureates/2002/wuthrich-autobio.html
[2] http://planetmath.org/encyclopedia/NicolasRashevsky.html
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External links

- Biophysical Society (http://www.biophysics.org/)
- Educational Resources from Biophysical Society (http://www.biophysics.org/education/resources.htm|)
- The European Biophysical Societies Association (http://www.ebsa.org/)
- The Wellcome Trust Physiome Project (http://www.physiome.ox.ac.uk/) - Links

Current research

Unsolved problems in physics

This is a list of some of the major **unsolved problems in → physics**. Some of these problems are theoretical, meaning that existing theories seem incapable of explaining a certain observed phenomenon or experimental result. The others are experimental, meaning that there is a difficulty in creating an experiment to test a proposed theory or investigate a phenomenon in greater detail.

Notation

Some problems are not considered significant enough by some physicists. If so, they are marked as follows:

** Problems marked with two stars are considered by a significant number of physicists to be resolved, though there is still significant debate about them.

*** Problems marked with three stars are considered by some physicists to be outside the purview of physics, more properly philosophical in nature.

**** The existence of problems marked with four stars is disputed.

Basic understanding

- What is subatomic particle spin[1] ?

Theoretical problems

The following problems are either fundamental theoretical problems, or theoretical ideas which lack experimental evidence and are in search of one, or both, as most of them are. Some of these problems are strongly interrelated. For example, extra dimensions or supersymmetry may solve the hierarchy problem. It is thought that a full theory of quantum gravity should be capable of answering most of these problems (other than the Island of stability problem).

Quantum gravity, cosmology, and general relativity

Vacuum catastrophe

Why does the predicted mass of the quantum vacuum have little effect on the expansion of the universe?

Quantum gravity

How can → quantum mechanics and general relativity be realized as a fully consistent → quantum field theory? Is string theory (M-theory) the correct approach? [2]

Black holes, black hole information paradox, and black hole radiation

Do black holes produce thermal radiation, as expected on theoretical grounds? Does this radiation contain information about their inner structure, as suggested by Gauge-gravity duality, or not, as implied by Hawking's original calculation? If not, and black holes can evaporate away, what happens to the information stored in them (→ quantum mechanics does not provide for the destruction of information)? Or does the radiation stop at some point leaving black hole remnants? Is there another way to probe their internal structure somehow, if such a structure even exists?

Extra dimensions

Does nature have more than four spacetime dimensions? If so, what is their size? Are dimensions a fundamental property of the universe or an emergent result of other physical laws? Can we experimentally "see" evidence of higher spatial dimensions?

Cosmic inflation

Is the theory of cosmic inflation correct, and if so, what are the details of this epoch? What is the hypothetical inflaton field giving rise to inflation? If inflation happened at one point, is it self-sustaining through inflation of quantum-mechanical fluctuations, and thus ongoing in some impossibly distant place?

Multiple universes

Are there physical reasons to expect other universes that are fundamentally non-observable? For instance: Are there quantum mechanical "alternative histories"? Are there "other" universes with physical laws resulting from alternate ways of breaking the apparent symmetries of physical forces at high energies, possibly incredibly far away due to cosmic inflation? Is the use of the anthropic principle to resolve global cosmological dilemmas justified? ***

The cosmic censorship hypothesis and the chronology protection conjecture

Can singularities not hidden behind an event horizon, known as "naked singularities", arise from realistic initial conditions, or is it possible to prove some version of the "cosmic censorship hypothesis" of Roger Penrose which proposes that this is impossible?[3] Similarly, will the closed timelike curves which arise in some solutions to the equations of general relativity (and which imply the possibility of backwards time travel) be ruled out by a theory of quantum gravity which unites general relativity with → quantum mechanics, as suggested by the "chronology protection conjecture" of Stephen Hawking?

High energy physics

Higgs mechanism

Does the Higgs particle exist? What if it does not?

Hierarchy problem

Why is gravity such a weak force? It becomes strong for particles only at the Planck scale, around 10^{19} GeV, much above the electroweak scale (100 GeV, the energy scale dominating physics at low energies). Why are these scales so different from each other? What prevents quantities at the electroweak scale, such as the Higgs boson mass, from getting quantum corrections of order of the Planck scale? Is the solution supersymmetry, extra dimensions, or just anthropic fine-tuning?

Island of stability

What is the heaviest possible stable or metastable atom?

Magnetic monopoles

Do particles that carry "magnetic charge" exist? The non-existence of magnetic monopoles is the basis of Classical Electrodynamics and modern technology as we know it.

Proton decay and unification

How do we unify the three different → quantum mechanical fundamental interactions of → quantum field theory? As the lightest baryon, are protons absolutely stable? If not, then what is the proton's half-life?

Supersymmetry

Is spacetime supersymmetry realized in nature? If so, what is the mechanism of supersymmetry breaking? Does supersymmetry stabilize the electroweak scale, preventing high quantum corrections? Does the lightest supersymmetric particle comprise dark matter?

Other problems

→ Quantum mechanics in the correspondence limit

Is there a preferred interpretation of quantum mechanics? How does the quantum description of reality, which includes elements such as the superposition of states and wavefunction collapse or quantum decoherence, give rise to the reality we perceive? ***

Physical information

Are there physical phenomena, such as black holes or wave function collapse, which irrevocably destroy information about their prior states? **

Theory of everything

Is there a theory which explains the values of all fundamental physical constants?[4] Do "fundamental physical constants" vary over time? Is there a theory which explains why the gauge groups of the standard model are as they are, why observed space-time has 3 + 1 dimensions, and why all laws of physics are as they are?

Empirical phenomena lacking clear scientific explanation

Cosmology and Astronomy

Accelerating universe and the Cosmological constant

Why doesn't the zero-point energy of the vacuum cause a large cosmological constant? What cancels it out? Is a non-total cancellation of the cosmological constant responsible for the observed accelerated expansion (deSitter phase) of the Universe? If it is, why is the energy density of the cosmological constant of the same magnitude as the density of matter at present when the two evolve quite differently over time; could it be simply that we are observing at exactly the right time? Or is the nature of the dark energy driving this acceleration differently?

Baryon asymmetry

Why is there far more matter than antimatter in the observable universe?

Dark matter

What is dark matter?[5] Is it related to supersymmetry? Do the phenomena attributed to dark matter point not to some form of matter but actually to an extension of gravity?

Electroweak symmetry breaking

What is the mechanism responsible for breaking the electroweak gauge symmetry, giving mass to the W and Z bosons? Is it the simple Higgs mechanism of the Standard Model,[6] or does nature make use of strong dynamics in breaking electroweak symmetry, as proposed by Technicolor?

Entropy (arrow of time)

Why did the universe have such low entropy in the past, resulting in the distinction between past and future and the second law of thermodynamics?[7]

Neutrino mass

What is the mechanism responsible for generating neutrino masses? Is the neutrino its own antiparticle? Or could it be an antiparticle that simply cannot join and annihilate with a normal particle because of its irregular state?

Inertial mass/gravitational mass ratio of elementary particles

According to the equivalence principle of general relativity, the ratio of inertial mass to gravitational mass of all elementary particles is the same. However, there is no experimental confirmation for many particles. In particular, we do not know what the weight of a macroscopic lump of antimatter of known mass would be.

Proton spin crisis

As initially measured by the European Muon Collaboration, the three main ("valence") quarks of the proton account for about 12% of its total spin. Can the gluons that bind the quarks together, as well as the "sea" of quark pairs that are continually being created and annihilating, properly account for the rest of it?**

→ Quantum chromodynamics (QCD) in the non-perturbative regime

The equations of QCD remain unsolved at energy scales relevant for describing atomic nuclei, and only mainly numerical approaches seem to begin to give answers at this limit. How does QCD give rise to the physics of nuclei and nuclear constituents?

Shape of the Universe

What is the 3-manifold of comoving space, i.e. of a comoving spatial section of the Universe, informally called the "shape" of the Universe? Neither the curvature nor the topology is presently known, though the curvature is known to be "close" to zero on observable scales. The cosmic inflation hypothesis suggests that the shape of the Universe may be unmeasurable, but since 2003, Jean-Pierre Luminet et al. and other groups have suggested that the shape of the Universe may be the Poincaré dodecahedral space. Is the shape unmeasurable, the Poincaré space, or another 3-manifold?

Strong CP problem and axions

Why is the strong nuclear interaction invariant to parity and charge conjugation? Is Peccei-Quinn theory the solution to this problem?

Astronomy and Astrophysics

Accretion disc jets

Why do the accretion discs surrounding certain astronomical objects, such as the nuclei of active galaxies, emit relativistic jets along their polar axes? Why are there Quasi-Periodic Oscillations in many accretion discs? Why does the period of these oscillations scale as the inverse of the mass of the central object? Why are there sometimes overtones, and why do these appear at different frequency ratios in different objects?

Corona heating problem

Why is the Sun's Corona (atmosphere layer) so much hotter than the Sun's surface?****

Gamma ray bursts

How do these short-duration high-intensity bursts originate?[8]

Observational anomalies

Hipparcos anomaly: How far away are the Pleiades, exactly?**

Pioneer anomaly[5] : What causes the apparent residual sunward acceleration of the Pioneer spacecraft?[9] [10] ****

Flyby anomaly: Why is the observed energy of satellites flying by earth different by a minute amount from the value predicted by theory?****

Galaxy rotation problem: Is dark matter responsible for differences in observed and theoretical speed of stars revolving around the center of galaxies, or is it something else?

Supernovae: What is the exact mechanism by which an implosion of a dying star becomes an explosion?

Ultra-high-energy cosmic ray[5]

Why is it that some cosmic rays appear to possess energies that are impossibly high (the so called *Oh-My-God particle*), given that there are no sufficiently energetic cosmic ray sources near the Earth? Why is it that (apparently) some cosmic rays emitted by distant sources have energies above the Greisen-Zatsepin-Kuzmin limit?[11] [12]

Condensed matter physics

Amorphous solids

What is the nature of the glass transition between a fluid or regular solid and a glassy phase? What are the physical processes giving rise to the general properties and the physics of glasses?[13] **

High-temperature superconductors

What is the mechanism that causes certain materials to exhibit superconductivity at temperatures much higher than around 50 Kelvin?[14]

Sonoluminescence

What causes the emission of short bursts of light from imploding bubbles in a liquid when excited by sound?

Turbulence

Is it possible to make a theoretical model to describe the statistics of a turbulent flow (in particular, its internal structures)?[15] Also, under what conditions do smooth solutions to the Navier-Stokes equations exist? This is probably the last unsolved problem in Classical or Newtonian Physics .

Biological problems approached with physics

These fields of research normally belong to biology, and traditionally were not included in physics but are included here because increasingly it is physicists who are researching them using methods and tools more popular in physics research than biology.[16] [17]

Synaptic plasticity

It is necessary for computational and physical models of the brain, but what causes it, and what role does it play in higher-order processing outside the hippocampus and visual cortex?

Axon guidance

How do axons branching out from neurons find their targets? This process is crucial to nervous system development, allowing the building up of the brain.

Stochasticity and robustness to noise in gene expression

How do genes govern our body, withstanding different external pressures and internal stochasticity? Certain models exist for genetic processes, but we are far from understanding the whole picture, in particular in development where gene expression must be tightly regulated.

Quantitative study of the immune system

What are the quantitative properties of immune responses? What are the basic building blocks of immune system networks? What roles are played by stochasticity?

Problems recently solved

Long duration gamma ray bursts (2003)

Long-duration bursts are associated with the deaths of massive stars in a specific kind of supernova-like event commonly referred to as a collapsar.

Solar neutrino problem (2002)

Solved by a new understanding of neutrino physics, requiring a modification of the Standard Model of → particle physics — specifically, neutrino oscillation.

Age Crisis (1990s)

The estimated age of the universe was around 3 to 8 billion years younger than estimates of the ages of the oldest stars in our galaxy. Better estimates for the distances to the stars and the addition of dark energy into the cosmological model reconciled the age estimates.

Quasars (1980s)

The nature of quasars was not understood for decades. They are now accepted as a type of active galaxy where the enormous energy output results from matter falling into a massive black hole in the center of the galaxy.

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[5] 13 things that do not make sense (http://www.newscientist.com/article/mg18524911.600-13-things-that-do-not-make-sense.html) newscientistspace, 19 March 2005, Michael Brooks
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[15] Open Questions, Condensed Matter and Nonlinear Dynamics
[16] The Nobel Prizes in Physics 1901-2000 (http://nobelprize.org/nobel_prizes/physics/articles/karlsson/index.html)
[17] The Office of Science - What is Physics? (http://www.sc.doe.gov/Sub/Newsroom/News_Releases/DOE-SC/2005/What_is_Physics.htm)

External links

- What don't we know? (http://www.sciencemag.org/sciext/125th/) Science journal special project for its 125th anniversary: top 25 questions and 100 more.
- Physics News Update (http://www.aip.org/pnu/) A weekly physics news bulletin hosted by the American Institute of Physics.
- Open Questions in Physics (http://math.ucr.edu/home/baez/physics/General/open_questions.html)
- New Scientist: 13 things that do not make sense. (http://www.newscientist.com/article/mg18524911.600-13-things-that-do-not-make-sense.html)
- List of links to unsolved problems in physics, prizes and research. (http://www.geocities.com/ednitou/)
- Ideas Based On What We'd Like To Achieve (http://www.grc.nasa.gov/WWW/PAO/html/warp/ideachev.htm)
- 2004 SLAC Summer Institute: Nature's Greatest Puzzles (http://www-conf.slac.stanford.edu/ssi/2004/Default.htm)
- http://technology.newscientist.com/article/dn14179-glasss-dual-personality-explained-at-last.html

Table of contents

Introduction

Note. This book is based on the Wikipedia article, "Physics." The supporting articles are those referenced as major expansions of selected sections.

Article Sources and Contributors

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Ric, Dandrake, Dane Gustafun, Daniel Mahu, Daniel Quinlan, Dank, Danski14, DarkFalls, DarkRain, Darkspots, Darkwind, Darth Panda, DarthShrine, Dave001001, Dave6, Davewild, David R. Ingham, DavidLevinson, Davidclifford, Db099221, Deglr6328, Dekisugi, Demerzel, Deor, DerHexer, Deryck Chan, Deskana, Dgrant, Dhc529, Diego pmc, Dina, Dipics, Discospinster, Djr32, Dmr2, Doc glasgow, Docu, Donhalcon, Dori, Dougofborg, Doulos Christos, Downw thesickness, DragonflySixtyseven, Drdaco, Drini, Drumsac, Dtgm, Dudesleeper, DumbAndDumber2000, Dumdumdom, Dupz, Dusty669211, Dyknowsore, Dysprosia, EJF, EPM, ERK, Eager McBeaver, Ed g2s, EdBever, Edgar181, Edward Morgan Blake, Edwardo66, Eeekster, Egil, El C, Eleassar, EllenPetersen, Eloquence, Emarti, Emc2, Ems57fcva, EncycloPetey, Enormousdude, Enviroboy, Epbr123, Erebus555, Eric Herboso, Erik9, Esanchez7587, Estarriol, Eu.stefan, EugeneZelenko, Euryalus, Evan Mayer, Evercat, Everyking, Explicit, FeloniousMonk, Fibonacci, Fieari, Fieldday-sunday, Filll, FiniteTree, Fl, Flashgordon12, Flauto Dolce, Flewis, Flyguy649, Fmiddleton, Frankenpuppy, Freakofnurture, Fred Bauder, Fredbauder, Fredrik, FreplySpang, Frito, Funkydunky9, Fuzheado, G. Campbell, G. Moore, Gaara unleashed, Gaara144, Gabbe, Gabi bart, Gabrielleitao, Gahs, Gail, Galaxiaad, Galluer, Galoubet, Gauze123, General Galavan, General Reader, Geobio, Geometry guy, Georgelikesboys, Georgelulu, Ghaly, Ghurtad1, Ghyll, Giftlite, Gilliam, Gina va gina va, Gioto, Gjd001, Glane23, GlasGhost, Gnixon, Go for it!, Golbez, GoldenMeadows, Goldom, Goozle, Graysen98, Greenguy1090, Grubber, Grunty Thraveswain, Gtg204y, Gunslinger of Gilead, Gurch, Gurchzilla, Guérin Nicolas, Gwernol, HKT, Hadal, Haisch, HalfShadow, Haljolad, Harald88, Harryboyles, Haselhurst, Haus, Hdt83, Headbomb, Hellboy2hell, Herakles01, Herbee, Hermione1980, Heron, Hidaspal, Hike395, Holbergj, Hollyellis, Howcheng, Hrishikesh911, Huangdi, Hungrypoo, Husond, Huwwaters, Hydraton31, Hydrogen Iodide, I already forgot, II MusLiM HyBRiD II, IIsL337, IRP, Icairns, Ice Cold Beer, Ilmari Karonen, ImGladMyMomIsDead, Imadeausrname, Immualkurt, ImperfectlyInformed, Imran, Infilms, Insvik, InvertRect, Inyuki, Ipatrol, Iridescent, Ironholds, Isis, Island, Isomorphic, Itub, Ixfd64, J.delanoy, JForget, JFreeman, JHBrewer, JHMM13, JNW, JRGBruno, JYOuyang, JaGa, JabberWok, Jackelfive, Jackol, JackyR, Jade Knight, Jagged 85, Jake Wartenberg, Jamie fearon, Javainone, Jaydawg89, Jbarta, Jbergquist, Jehochman, Jeronimo, JessBr, Jfdwolff, Jim woz ere, Jim62sch, Jimothytrotter, Jitse Niesen, Jjasi, Jklin, Jmabel, Jmundo, Jni, Joanee Woolee, JoanneB, JoeBlogsDord, John254, JohnCD, JohnOwens, Joke137, Jon Awbrey, Jon513, Jonie2102, Jorend, Jose77, Josh the Nerd, Jossi, Joymmart, Jsc83, Julesd, Juliecoolgirl34, Jumping cheese, Jusjih, Just Call Me Einstein, Justinfr, Justup2002, KLHS6, Kaihsu, Karada, Karen Holman, Karlthegreat, Karlwick, Karol Langner, Kasparov, Katalaveno, Katieh5584, Kazvorpal, Kbh3rd, Keegan, Keesiewonder, Keith-07, Kelvin Case, Kenosis, Keo, Kevin Breitenstein, Kevin aylward, Kf4bdy, Kgasso, Kiba, King of Hearts, KingTT, Kmizzledabombdizzle, KnowledgeOfSelf, Knulclunk, Kornfan71, Koyaanis Qatsi, Koyn, KrakatoaKatie, Krea, Kribbeh, Kubigula, Kungfuadam, KurtRaschke, Kuru, Kushal one, Kville105125, Kwekubo, Kwsn, Kyoko, LAX, Lagrangian, Lambertian, Lantonov, Laplace's Demon, LaszloWalrus, Laurascudder, Laverty-j2, Laxragaza, Lcarsdata, Leafyplant, LeaveSleaves, Lee Daniel Crocker, Lenticel, Leobyun, LexCorp, Lexor, Lightmouse, Lights, Lisatwo, Little_guru, Littlealien182, Livilou517, Llull, Logan, Logologist, Lokal Profil, Loodog, Loom91, Looxix, Lseixas, Lumidek, Luna Santin, Lupin, Lupo, Lycurgus, M, M C Y 1008, MASQUERAID, MER-C, MLauba, MONGO, MPerel, Maddemo, Madesfuga, Madman, Maganjeanthrower, Magic5227, Magnus Manske, Makewater, Malafaya, Malhonen, Mannafredo, MarSch, Marijuanaboy, Markan, Markashley1990, Marnanel, Marsrocks09, Martin Hogbin, Masamunecyrus, MassimoAr, Master shepherd, Matthead, Mattmac, Maurice Carbonaro, Maurreen, Mav, MaxSem, Maximus Rex, Maxis ftw, Mayumashu, McSly, McVities, Mdd, MearsMan, Meelar, Melchoir, Men99999, Meno25, MercuryBlue, Mets501, MetsFan76, Mic, Michael C Price, Michael Hardy, Michael K. 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Ingham, David.Mestel, Dawn Bard, Deathcrap, Deglr6328, Delldot, DerHexer, Destroyer 65, Diberri, Discospinster, DocWatson42, Doomcookie222, Doulos Christos, Dr.Science, Drilnoth, Drunkenmonkey, Dsjeisl, Dspradau, Dstrozzi, Dysepsion, EDUCA33E, EJF, Edgar181, Edivorce, Eiland, El C, Elassint, Elenseel, Elfguy, Ellywa, Enormousdude, Enviroboy, Epbr123, Eric-Wester, ErkDemon, Erkcan, EronMain, Euyyn, Everyking, EvocativeIntrigue, Excirial, Faradayplank, Fastfission, Finestblade33, Fingers-of-Pyrex, Finlay McWalter, Firsfron, Fite ez then, FlyingToaster, Foxbull, Frankw101, FreeKresge, Frehley, Fuhghettaboutit, Furrykef, Fusion Power, Gameboy lbl, Gene Nygaard, Gentgeen, Gerweck, Ghewgill, Giacona, Giftlite, Gioto, Glen, Glenn, Gravitan, Grebaldar, GrimFang4, Grunt, Gurch, Gurchzilla, Hadal, Hairy Dude, Headbomb, Heron, Hippojazz, HoudiniMan, Hubert Wan, ILovePlankton, Imaglang, InShaneee, Indon, Infobloat, Inmate20, Inter, Iridescent, Irpen, IstvanWolf, Itinerant1, Itmakesmehappy, Ixfd64, J.delanoy, JFreeman, JLKrause, Jadahl, Jag123, JakeDodd, Jamous77, JedRothwell, Jedidan747, JimVC3, Jklin, Jkominek, Jni, John, JohnAspinall, JohnOwens, Johnb96, Johnfos, Jojhutton, Jordan 1972, Jorfer, JoshuaZ, Jpk, Jpr2x, Jrockley, Juliancolton, Justanyone, JustinFLeighton, Jwilson14, K-UNIT, Kaihsu, Kaiserkarl13, Kaisershatner, Karelj, Karol Langner, Kcordina, Killface55, KingTT, Kirk Grabowski, Kopovoi, Kostisl, Kozuch, KyuuA4, La goutte de pluie, Lahiru k, Larklight, Lcolson, LiamE, Linkman21, Litefantastic, Little Mountain 5, Loboguy, Longhair, Looxix, Loupeter, Lradrama, Luna Santin, Luzu, MBisanz, MGTom, Maddiemoo39, MadmanNova, Magma828, Magnus Manske, Makelifecheap, Makemi, Mani1, MarkGallagher, Markus Poessel, Martinevos, Matt Gies, Matticus78, Maurice Carbonaro, Maury Markowitz, Mav, Maxtitan, MessiahBenDavid, Mg1967cup20011, Mhking, Midgley, Mifter, Mihaip, Mike J., Miquonranger03, Mjj4, Mlouns, Mmxx, Mo0, Moonphase95, Mooquackwooftweetmeow, Moshe Constantine Hassan Al-Silverburg, Mschel, MuhalaC, Mulad, Mundo0987, Murderbydeath222, Nad, Naddy, Nakon, Neil916, Neilc, Nekura, Nemu, Neurolysis, NewEnglandYankee, Nextai13, Nihiltres, Nivix, Nk, Noclevername, Noren, Nottrue, Nsaa, Nuclear fusion man, Nuno Tavares, Objectivist, Oblivious, ObsidianOrder, Obuolys, OldakQuill, OllieFury, Omegatron, Onebravemonkey, Oo64eva, Opelio, Orionus, Ouishoebean, Ozzah, PanagosTheOther, Pandawelch, Panoptical, Panoptik, Pascal.Tesson, Patrick, Pcarbonn, Peterlin, Petri Krohn, PhySusie, Pie Man 360, Pifactorial, Piperh, Pitt, Pizza Puzzle, Pladask, Polio18, Postglock, PranksterTurtle, ProfessorToomin, Pstudier, Puddle, Quinsareth, Qxz, Rachel McPhearson, Ragesoss, RainbowOfLight, Razorflame, Rdsmith4, Rei, Remi0o, Res2216firestar, Rex360, RexNL, Rhinocerous Ranger, Riana, Rich Farmbrough, Riotrocket8676, Rjanson, Rje, Rob.derosa, Roberta F., RockMaster, Rockcutter88, Rod57, RonaldHayden, Rotational, RoyBoy, Rror, Ryryrules100, SMC, SMesser, Sadi Carnot, Sangwine, Saravask, Sbharris, SchfiftyThree, Schumi555, Sdkochman, SeanTater, Searmemcmxciii, Securiger, Serendipodous, Setoor g, Sfacets, Sharkface217, Shawnhath, Sheeson, Sheliak, Shoemaker's Holiday, Sikkema, Sillybilly, Skier Dude, Skinny McGee, SkyLined, Slipstream@npj, Slowking Man, Smithbrenon, SoSaysChappy, Solitude, SpLoT, Special-T, Spitfire, Splash, Splendidtorch, Srikeit, StaanJacobsen, Star controller, Stepan Roucka, StevenBKrivit, Stevertigo, Stickboy42, SunDragon34, Susan118, Sverdrup, Syndicate, T.C.Thornberry, TOO9, Tanaats, Taqi Haider, Taw, Ted Longstaffe, Tellyaddict, That Guy, From That Show!, The Anome, The Original Wildbear, Thechangster, Theron110, Thingg, Think outside the box, Thisnamestaken, Tim Starling, TimTim, Tobin Richard, Tos, Tr-the-maniac, Travelbird, Trelvis, Tsemii, Tylerdfreeze11, Ufundo, Ulric1313, Ultramarine, Uncle Dick, UncleDouggie, Until It Sleeps, Urhixidur, Uruk2008, Useight, Utcursch, Valermos, Vary, Venny85, Verloren, Vianello, Viewgray3, Vorn, Vsmith, Wdfarmer, Wdyoung, Wesino, WhaleyTim, Whitepaw, Why My Fleece?, Wiki alf, Wikibob, Wikidsoup, Wikipedia brown, William M. 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