

PHYSICAL SYSTEMS AND LAWS

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Summary

Physical laws in classical physics have a deterministic nature which implies that any isolated system such as the universe as a whole evolves in a deterministic way so that once we know the state of a system at a time states of the system in future will be uniquely predicted. This turns out to be violated by the uncertainty principle of quantum mechanics on the one hand and the presence of chaotic motion even in classical physics on the other.

The energy conservation law and the law of increase of entropy are discussed in an elementary way. They are valid for any isolated system without exceptions, showing the universality and great power of laws of physics. Symmetry principle is an indispensable ingredient in modern physics. Symmetries such as the symmetry under translations in space or time are well shared by the fundamental laws of physics, which lead to the law of energy conservation or momentum conservation. Also the charge conservation law is related to the gauge symmetry of electromagnetic interaction.

The special and general relativities by Einstein based upon the geometrical symmetry principle revealed the space-time structure of the physical world with remarkable outcomes. For example, space and time are interrelated, mass is a kind of energy, and gravity is related to the curvature of the space-time structure of our physical world.

Ordinary matter consists of a huge number of atoms or molecules and there exist quite many microscopic states indistinguishable from each other. Thus, we need a statistical approach to find useful information about ordinary matter. Statistical thermodynamics is such a theory to connect the microscopic and macroscopic worlds. The basic postulate is that every microstate is realized with equal probability for an isolated system. This postulate together with the first and second laws of thermodynamics makes it possible to predict properties of any thermodynamical quantity not only for isolated systems but also for other systems interacting with their surroundings.

Study of complex systems with non-linear interactions among their constituents is a relatively new field out of which some interesting features of the complex systems emerge. For example, even a system with a few degrees of freedom of motion can exhibit chaotic behavior under appropriate conditions. Important concepts in complex phenomena such as attractors, bifurcations, entrainments, fractals, and chaos are described.

Introduction

Any physical system is described by an appropriate set of dynamical variables. A single pointlike particle is described by its position and momentum, and a system consisting of many particles is described by the positions and momenta of all the particles in the system. Any thermodynamical system in equilibrium can be described by an appropriate set of thermodynamical variables such as temperature and pressure. A physical law is a relation among dynamical variables or an equation of motion to determine the time

evolution of dynamical variables through interactions among them.

When something unexpected happens, we feel that there must be some reason for it and try hard to find its cause. When we know something happened, we might speculate on what will occur next. These thoughts are based on a view that past, present, and future are interrelated with each other through causal strings connecting them. If the causal relations were so tight that past determines present and present determines future, we are living in a deterministic physical world.

One of the most prominent features of a physical system is its deterministic nature. When we throw a ball, we know through our experiences that the motion of the ball is uniquely determined by the initial position and velocity of the ball. If we use a technique such as throwing a ball to rotate about its own axis, the ball will take a different path depending on how it was rotated. Even in this case, the motion of the ball is uniquely determined by the position, velocity and rotational motion of the ball at the initial time.

We can choose the initial position and velocity of a body as we like. However, the acceleration of a body is determined by forces such as the gravitational force acting on the body. Then, by solving Newton's equation of motion under the given forces, states of the body afterwards will be uniquely determined. In general, the state of an object or a system in the past uniquely determines the states of present and of future through causal strings connecting them.

In natural as well as social phenomena the time evolution of a system is determined not only by the internal dynamics of the system but also by external circumstances affecting the system. In physics, forces acting on an object are due to the presence of other objects. In the case of the gravitational force, the force depends on the position of the object relative to the others. In case of the frictional force due to air, the force depends on the velocity of the object relative to air. Only when the positions and velocities of all the external objects are precisely known as functions of time, motion of the object can be uniquely determined by solving the equation of motion for the object.

In order to avoid any effect of the outside environment on a system, we may consider an isolated system on which no external body is exerting a force. Such an isolated system must be chosen large enough to accommodate all of mutually interacting bodies in it. Then, the time evolution of the isolated system would be entirely governed by its internal dynamics and is uniquely determined by the initial positions and velocities of all the bodies in the system.

We might ask whether there exists such an isolated system in nature. The whole universe is apparently an isolated system, because we cannot think of any outside world of it. Can we think of any other isolated system besides the whole universe? All of the known forces such as gravitational and electrostatic forces decrease rapidly in strengths with increasing distances between interacting bodies. Therefore, any system which is well separated from others by large distances might be regarded approximately as an isolated system. Even if the system is still acted by weak forces from outside, motion of bodies in the system might be approximately determined by the internal dynamics of the

system. In this respect, there exist quite many isolated systems in nature.

The position and momentum (or velocity) are dynamical variables to describe motion of bodies. Their values can be arbitrarily chosen at an initial time, but their courses in time afterwards are uniquely determined by the equations of motion once the initial conditions are given. Both the position and momentum of a body are a three dimensional vector in space. Therefore, the initial conditions of motion of a body are specified by fixing the values of the three components of the position and momentum at an initial time. We call that the degree of freedom of motion is three for a single object moving in three dimensional space. For a system consisting of N particles, the degree of freedom of motion is $3N$ and the number of dynamical variables is $6N$.

The deterministic nature inherent in Newton's equation of motion was advocated fiercely by his earnest successor Laplace (1749-1827). Laplace expressed a view that the future of our universe as well as the fates of individuals are determined by the initial conditions given at the beginning of the history of our universe, thus either the universe or individuals cannot escape from the fates specified by the initial conditions. He once stated that "*If we can know positions and velocities of all the atoms in our universe at an instant of time, we can predict through analytical methods how the universe has evolved up to now and how it would develop in future*".

There exist a huge number of atoms or elementary particles in our universe. According to our present knowledge, the number of atoms in the whole universe is estimated to be of the order of 10^{78} . Even if we take a small object such as a grain of wheat, the number of atoms in the grain is quite large and almost infinite. This means that the degree of freedom of motion or the number of dynamical variables is extremely large and almost infinite. Therefore, it is practically impossible to know positions and velocities of all the atoms in any macroscopic system. Thus, the deterministic nature of Newton's equation of motion is masked by uncertainties due to our ignorance about initial conditions of a system.

However, conceptually we cannot get rid of a logical assertion that the fate of the universe as well as the fate of our individual life is basically fixed by how our universe started. This is similar to the situation that we are free in our way of living when we are ignorant about social customs and circumstances and that we become less free when we get more knowledge on them. If one's fate is really predetermined through the causal strings coming out from the initial state of the universe, many of us might feel our life dull.

Fortunately, the deterministic nature inherent in the Newtonian physics has become questionable through progress in physics. One of the breakthroughs is the discovery of possible violation of the deterministic nature even within the framework of the Newtonian mechanics and the other is the birth of quantum mechanics in which the uncertainty principle of Heisenberg plays dominant role. Since we shall describe quantum mechanics in a later chapter (see *Quantum Systems*), here we will be only concerned with possible violation of the deterministic nature in classical mechanics.

In the birth of Newtonian mechanics, very ordered motion of the planets in our solar

system had played important roles. Each of the planets circles along its elliptic orbit about the sun with a definite period and its motion is quite stable and likely to last forever. The motion of the planets was fully understood in terms of Newton's laws of motion and gravity, showing us great power of the natural laws governing motion of bodies.

Newton's laws of motion and the resultant ordered motion of the planets in the solar system were quoted as a prototype of the constitutional laws and political order resulting from interplay of the laws and people in England. For example, in 1728 Desagurie wrote a poem to praise the constitutional monarchy of England, in which he quoted the ordered motion of planets about the sun as a prototype of the constitutional political system of England. He compared the sun to the King, the planets to Ministers of the Cabinet, and the laws of motion and gravity to the constitutional laws of England.

The King rules Ministers through his power just like the sun rules motion of the planets through its gravity. In turn, the King is subjected to the acts of Ministers through the constitutional laws just like the sun gets reactions from the planets through their gravities. Planets in the solar system circle about the sun steadily and their ordered motions are likely to continue for ever. Likewise, the political system in England based on the constitutional laws is stable and well ordered, thus likely to last forever.

At the end of the 19th century, Poincare first questioned about stability of the solar system and showed that the system could become unstable even within the framework of the Newtonian mechanics. This is not to say that the sun finally will come to death because of consumption of its fuel (hydrogen nuclei) or that the solar system will become unstable due to strong disturbances by some external bodies. Instead, he discussed instability due to gravitational forces among stars within the solar system. When we consider motion of a system consisting of three bodies such as the sun, the earth and the moon, we cannot solve rigorously Newton's equations of motion for the three bodies interacting with each other through gravity. Therefore, it is difficult for us to predict the long term behavior of the motion of the three bodies and some unexpected instability of the motion may arise.

For two- body problems such as motion of the earth relative to the sun, we can solve exactly the equation of motion. The result is an ordered periodic motion and the earth moves along its elliptic orbit about the sun steadily forever. In the case of three-body or more than three-body problems, even able mathematicians cannot solve rigorously the equations of motion for them. One has to start from an approximate solution and then improve it step by step in order to get better solutions.

As an example, let us consider a three-body system consisting of the sun and two planets. Each of the planets moves along its elliptic orbit about the sun due to the gravity of the sun. When we neglect the relatively weak gravity between the two planets, the above elliptic orbits are stable and the planets will continue moving along their orbits forever.

Next, we take into account the gravity between the two planets as a small perturbation to the motion of the planets. Suppose, for simplicity, one of the planets moves about the

sun with a period of 2 years and the other planet moves with a period of 3 years. Then after every 6 years the relative position of the two planets becomes the same and the gravitational forces between the two are the same in its magnitude and direction. Therefore, small perturbations due to the gravity between the two planets would accumulate additively once for every six years and the perturbations might grow, eventually leading to a large disturbance on the motion of the planets.

In general, when two periodic motions of different bodies coexist in a system with the ratio of the periods equal to a ratio of simple integers, the periodic motions could be sufficiently disturbed in a long run by a weak force between the bodies and the ordered periodic motions might be sufficiently disturbed to change into irregular ones. In particular, when one of the planets in the above three body system is very light, it was shown that the lighter planet will be eventually knocked out and will move away from the system. On the contrary, when the ratio of the periods is an irrational number (a number which cannot be expressed as a ratio of two integers), we do not expect additive accumulation of small perturbations due to the weak gravity between the planets, and the three-body system is likely to maintain the ordered stable motion forever.

There exist quite many small planets called asteroids moving about the sun along orbits located between the orbits of Mars and Jupiter. Jupiter is the most massive planet in the solar system, and asteroids are acted by the gravity of the Jupiter as the largest perturbation to their orbits. In Fig. 2.1 we show the number of observed asteroids as a function of the ratio of the period of the elliptic motion of the Jupiter ($T_J \sim 11.86$ years) to the period T of motion of an asteroid. The figure shows clearly that asteroids with the ratio of simple integers such as 2, 3 and 4 are very scarce.

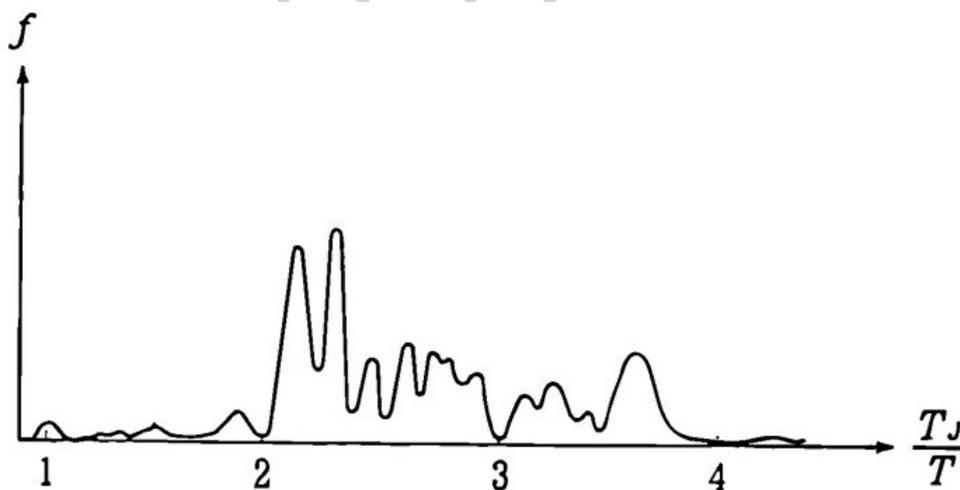


Figure 1. The relative number f of observed asteroids as a function of the ratio of the period of Jupiter to that of an asteroid.

In general, asteroids with the ratio of simple rational numbers seem to be scarce according to the observation of asteroids. This is an indirect evidence for the instability of motion of some of asteroids. There the gravity of the Jupiter acts on asteroids and disturbs their motion, the small disturbances on some of the asteroids accumulate

additively, and finally their orbits are much distorted so that the asteroids get away from their ordered elliptic orbits. Some of meteorites coming to the earth are regarded as those asteroids knocked out from their stable orbits.

As we have shown in the above example, there exists a system where the equation of motion of the system is deterministic, but its asymptotic behaviour is very irregular and hard to predict. This kind of motion is called chaotic motion. Since the 1960s chaotic motion of a system has been studied extensively and various types of chaotic motion have been found in a wide range of systems and phenomena. This was partly because large and fast electronic computers became available to us and the results of numerical calculations using them disclosed the existence of chaotic solutions in many dynamical systems.

Now, we have to ask what chaotic motions really mean. In general, a dynamical system is described by an appropriate set of dynamical variables, which we denote by X_i ($i = 1, 2, \dots, N$). Here, N is the number of the dynamical variables of the system. The general form of a set of equations to determine time evolution of the system is

$$dX_i/dt = F_i(X_1, X_2, \dots, X_N) \quad (i = 1, 2, \dots, N) \quad (1)$$

Here dX_i/dt is the rate of change of X_i in time, i.e. the time derivative of X_i and F_i is a function of all X_i 's. The set of the functions F_i uniquely specifies the system. Since the values of X_i at an instant of time determine the subsequent change of X_i in time, the system described by Eq.(1) is fully deterministic in nature.

For a given set of initial values of X_i , X_{i0} , at an initial time t_0 , we can solve Eq.(1) and obtain X_i as a function of time; $X_i(t)$. In most cases, if we change the initial values X_{i0} by small amounts ΔX_{i0} , $X_i(t)$ also changes by a small amount $\Delta X_i(t)$. Therefore, we expect $\Delta X_i(t) \rightarrow 0$ for $\Delta X_{i0} \rightarrow 0$ at any t . If this is the case, we can allow small errors in the initial values of X_i without spoiling the deterministic nature of the system.

However, it has become known that there exist dynamical systems in which small changes of the initial values ΔX_{i0} lead to large deviations of the dynamical variables, $\Delta X_i(t)$, after long enough time passed. Furthermore, the large deviations $\Delta X_i(t)$ could depend upon ΔX_{i0} in a very sensitive manner. Since we cannot know the initial values ΔX_{i0} with an infinite accuracy in practice, this means that we cannot predict the long-term behavior of the system. Thus the presence of uncontrollable small errors in determination of the initial conditions of the system can lead to violation of the deterministic nature of the system. Such behavior of a system is called the deterministic chaos, because equations of motion are deterministic but long-term behavior of the system is unpredictable and chaotic.

A simple system described by either one or two dynamical variables which change continuously in time does not show any chaotic behavior. In Fig.2b and 2c we show typical trajectories of motion of a system described by only two dynamical variables X_1 and X_2 . Fig.2a shows a trajectory which has a self-crossing point P . This means that the system can change from the same point P into two different directions, which is against

the deterministic nature of the system. Thus a trajectory with self-crossing points such as one in Fig.2a is not allowed for any deterministic system.

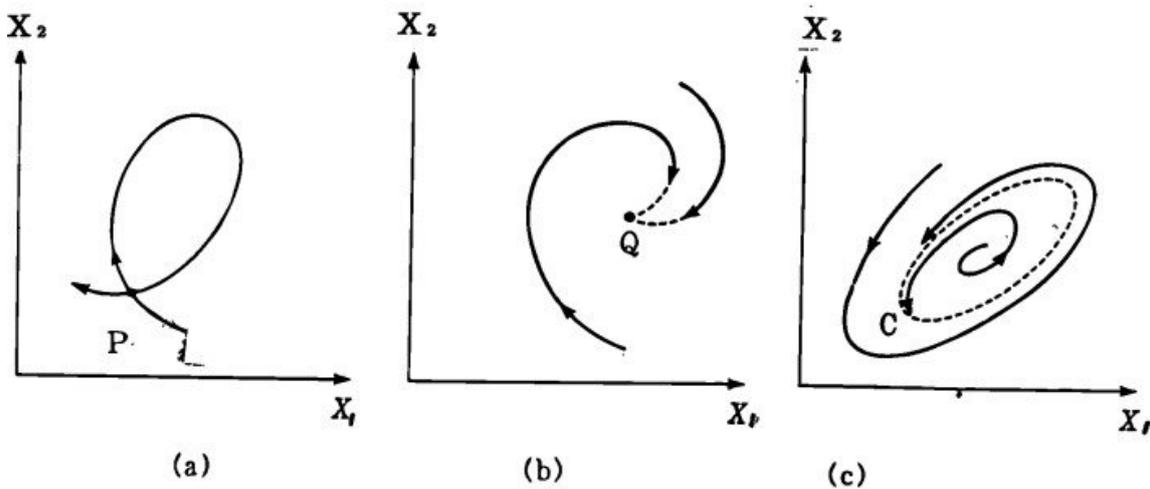


Figure 2. Asymptotic behavior of a system described by two dynamical variables (a) a forbidden trajectory, (b) a fixed point, and (d) a limit cycle

If we draw any continuous trajectory with no self-crossing in a finite region of the two dimensional phase-space (X_1X_2 -space), we can easily convince ourselves that the trajectory asymptotically approaches either a fixed point or a closed curve in the phase-space. In the former case the system approaches the fixed state denoted by the fixed point Q and in the latter case the motion of the system approaches a periodic motion moving repeatedly along the closed curve C with a fixed period. Thus the long-term behavior of the system is predicted as either the fixed state denoted by Q or the periodic motion denoted by C .

When the number of dynamical variables is more than two, chaotic motion becomes possible even in a deterministic system described by a set of equations of the form of Eqs.(1) provided that the equations of motion are nonlinear. This does not mean that motion becomes always chaotic for a system with $N \geq 3$, but means that depending upon the form of F_i s and values of parameters appearing in F_i s motion can become chaotic. We will describe in detail possible chaotic behavior of nonlinear systems in a later chapter (see *Quantum Systems*).

The basic feature of chaotic motion is its extreme sensitivity to the initial conditions of motion. Even if the initial conditions change only a little, the resulting motion afterwards depends very sensitively on the small change of the initial conditions. This is illustrated in Fig.3, in which three trajectories originating from nearby points in the phase-space become far separated from each other after enough time passed even if they are confined in a finite region of the phase space. This can happen even if the separations of the nearby points are infinitesimally small, provided we compare the three trajectories after a sufficiently long time.

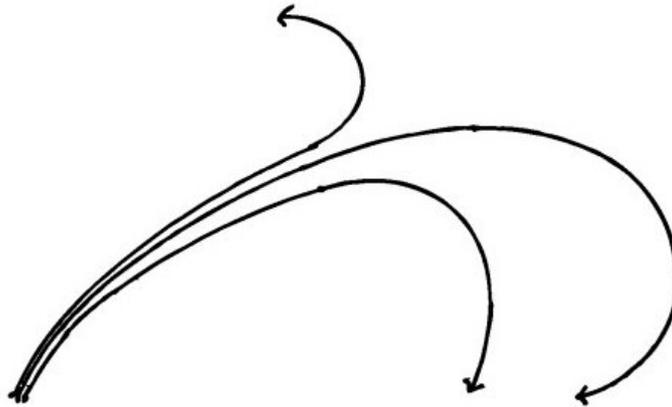


Figure 3. Chaotic motion which is extremely sensitive to the initial conditions of motion

Since we know initial conditions of motion only with a limited accuracy, we cannot predict the long-term behavior of the motion of the system. We should emphasize that there is no logical inconsistency between the presence of chaotic motions and the deterministic nature of the equations of motion.

The word 'chaos' is frequently used in our daily conversation too. There chaos simply means a phenomenon which is so complex that we cannot find any regularity in it or that we cannot think of any explanation for it. The phenomenon just looks like one produced by accidental occurrence of many unknown external disturbances acting upon the system.

When the number of dynamical variables of a system is large, in practice we have to choose a set of small number of appropriate variables to approximately describe behavior of the system, thereby neglecting the others. If that is the case, effects of the neglected dynamical variables might grow up in a long run and modify drastically long-term behavior of the system in an unexpected manner.

The deterministic chaos might look somewhat similar in its appearance to the chaotic behavior of a system due to the omission of a large number of dynamical variables in describing the system. However, the deterministic chaos is fundamentally different from the latter and it occurs for a system where exact equations of motion for all the dynamical variables are given. It can occur even for a system with a low degree of freedom of motion such as $N = 3$. Thus, the presence of chaotic motion in a deterministic system makes us free from the conceptual problem that everything including fates of people are predetermined by how our universe started.

So far we have discussed the deterministic nature of physical processes and its possible violations. Next we shall consider physical laws, in particular, the law of energy conservation and the law of entropy increase which are the most basic laws in physics as well as in natural science in general. Here we will be mainly concerned with what the laws mean to physical phenomena.

Nature changes constantly. Many people tried to find the underlying laws which govern all kinds of complex processes occurring in nature. We know now that the total energy of any isolated system is strictly conserved and that the entropy of any isolated system always increases irrespective of what happens in the system. The law of energy conservation is a law to recognize the presence of a certain physical quantity which is kept constant in any process occurring and the law of entropy increase is a law to give the direction of change of a system when physical processes are occurring in the system.

These laws are called the first and second thermodynamical laws respectively (see *Thermodynamics and Heat Transfer in Development of Fundamentals in Physics*). Not only physical processes but also biological phenomena cannot escape from the restrictions due to these laws. Although the laws alone do not uniquely determine change of states of a system, the laws are valid even when the system is so complex that we do not know equations of motion or initial conditions for the system.

The word 'energy' is used not only in diverse fields of natural science but also in our daily conversations. Energy means, loosely speaking, ability to do work. Without energy one cannot do any work, and we spend a certain amount of energy when we do work. When work is done on a body or a system, it will gain an amount of energy equivalent to the work done on it.

The energy conservation law was formulated by Meyer, Helmholtz, Joule and others and has been shown to be exactly valid without exceptions until today. A moving body has kinetic energy K associated with its motion. In the Newtonian mechanics K is given by $mv^2/2$, where m and v are the mass and velocity of the body respectively. When a body is acted upon by a force, the body has a potential energy V associated with the force. This energy is equivalent to the amount of work done on the body by the force, when we bring the body from a reference position to the present position through the field of the force. When several forces act on a body, the potential energy V is the sum of the potential energies due to each of the forces.

Both the kinetic and potential energies are forms of mechanical energy. The total mechanical energy of an isolated system is conserved in any physical process where neither heat nor radiation energy is involved. There are other kinds of energy besides the mechanical energy, such as thermal energy (heat) or energy of radiation (light). Even the mass of a body at rest has an energy given by $E = mc^2$ according to Einstein's theory of special relativity. Different kinds of energy are convertible to one another in general, yet the total energy of an isolated system is strictly conserved in any process occurring in the system.

The existence of different kinds of energy is analogous to the presence of different currencies in economics. American dollars, Euro dollars, Japanese Yens, and other currencies are convertible to one another. When we exchange one currency with another, the total value of the currencies in hand will not be effected. This is analogous to the energy conservation law in physics. The exchange rate of one currency to another is fixed, just like 1 calorie of heat energy is equal to 4.184 joule of mechanical energy. Of course, the analogy is not complete. In economics the exchange rates of currencies would vary in time and there are some service charges in exchange, while in physics the

mechanical equivalent of heat is fixed forever and no energy is lost in exchange unlike the loss of money in hand due to service charges in money exchange.

Dyson, an eminent theoretical physicist, once quoted the following lines of a poem, "The Marriage of Heaven and Hell" by William Blake's (1789), as the best description of what energy is:

"Man has no Body distinct from his Soul; for that call'd Body is a portion of Soul discern'd by the five Senses, the chief inlets of Soul in this age. Energy is the only life and is from the Body and Reason is the bound or outward circumference of Energy. Energy is Eternal Delight".

From Newton's equations of motion one can derive the conservation of the total mechanical energy of an isolated system, and one can assign a fixed value of energy to each isolated system. Conversely we can derive the equations of motion from the energy of the system. For example, in the Hamilton formalism of classical mechanics, the Hamiltonian of the system is the total mechanical energy expressed in terms of the momenta and positions of particles constituting the system. If we know the Hamiltonian as a function of the momenta and positions, we can derive Hamilton's equations of motion which are fully equivalent with Newton's equations of motion (see *Newtonian Mechanics* in *Development of Fundamentals in Physics*). In this sense, energy is the quantity to determine time evolution of a system and is the only cause for physical phenomena occurring in the system.

Different kinds of energy can be regarded as the different aspects of energy carried by microscopic constituents of matter and radiation. According to the kinetic theory of gases, the temperature of a gas is related to the random motion of a large number of molecules in the gas and the thermal energy (heat) of the gas is the sum of kinetic energies of the molecules in random motion. Thus, the thermal energy can be regarded as a kind of mechanical energy in the microscopic point of view. If each molecule in a gas changes its state according to Newton's equations of motion, the sum of the mechanical and thermal energies must be conserved, because they are all mechanical in nature.

Quantum physics has brought about some basic changes in our concept of energy. Although we will discuss quantum physics in a later Chapter (see *Quantum systems*), we will briefly outline the basic changes brought by quantum physics. First, energy is related to time translation of the system. The translation in time is defined as the displacement of the origin of time coordinate; $t \Rightarrow t - \tau$, where τ is a constant. Since forces acting upon bodies do not explicitly depend on time and accelerations of the bodies do not change by the time translation, Newton's equations of motion remain the same after the time translation. If the equations of motion or dynamical laws for a system are invariant under the time translation, the energy conservation law follows (see the section on *Symmetry Principles* in this chapter). This is true in classical as well as quantum mechanics, but in quantum mechanics energy has an additional meaning of being an operation on a system to translate it in temporal direction. This point will be discussed in a later chapter (see *Quantum Mechanical Laws* in *Quantum Systems*).

Second, there exist uncertainties as to values of energy of a system because of Heisenberg's uncertainty principle, which is a fundamental principle of quantum physics. According to the principle, the position and momentum of a particle cannot take definite values at the same instant of time. They are subject to certain uncertainties and their values are only given by some probability distributions specified by the state of the particle.

In particular, whatever the state is, the uncertainties of position and momentum at an instant of time, $\Delta \mathbf{r}$ and $\Delta \mathbf{p}$, must satisfy the following uncertainty relations:

$$\Delta x \Delta p_x \sim h, \quad \Delta y \Delta p_y \sim h, \quad \Delta z \Delta p_z \sim h \quad (2)$$

where h is the Planck constant. Therefore, we cannot have $\Delta x = 0$ or $\Delta p_x = 0$ at an instant of time unless $\Delta p_x = \infty$ or $\Delta x = \infty$. (More rigorous uncertainty relations than Eqs.(2) will be described in a later chapter (see *Quantum Systems*).

When we measure the energy of a system, we cannot measure the energy E instantaneously but spend a certain length of time Δt for measuring it. The value of energy obtained has an uncertainty ΔE , which is related to Δt through the uncertainty relation:

$$\Delta E \Delta t \sim h \quad (3)$$

The value of the Planck constant h is very small in the ordinary scales of energy and time, which is given by $h = 6.62 \times 10^{-34}$ joule-sec. Therefore, the uncertainties can be safely neglected for macroscopic systems, but they become important for microscopic ones such as atoms and elementary particles. When we measure any physical quantity, there always exist experimental errors due to measuring devices or method employed. Furthermore, even if we repeat measurements under the same conditions, there exist statistical fluctuations in the measured values and we do not obtain the same value for the quantity to be measured. In classical physics we can improve measuring devices and methods to reduce experimental errors, and we can repeat measurements many times to reduce statistical errors. Thus, at least in principle, ΔE can be made arbitrarily small in classical physics.

We should stress that the uncertainties in quantum systems expressed by Eqs. (2) and (3) are not the ones which we can reduce through further improvement of experimental devices or methods, or through averaging over many repeated measurements. Instead, they are the uncertainties which originated from the fundamental principle of quantum physics and they are valid irrespective of how we measure the physical quantities.

We shall draw the following analogy to understand what the uncertainty relation between energy and time means. Suppose one borrows money from a friend. When the sum of money is 1,000\$, he can borrow it only for one day. If the sum is 100\$, he might be able to borrow it longer, e.g. 10 days. If there is no guarantee or interest, one can borrow larger sum of money for shorter length of time in general. In the above example, the amount of debt is inversely proportional to the length of time one can borrow money.

In order to buy something or even to do some work, we usually need money. If money in hand is not enough, we have to borrow money from someone or a bank. If we compare the sum of money in hand to the energy E , the sum of debt (or loan) to the energy uncertainty ΔE , and the length of time in debt to Δt , the uncertainty relation between ΔE and Δt is quite analogous to the relation between the amount of debt and the length of time in debt.

Of course, there exists some difference between the two cases. When one borrows money, one needs someone to lend him money. In quantum physics, a body does not need any other object to transfer energy to the body. The energy of the body itself is uncertain in principle by an amount ΔE specified by the uncertainty principle. Therefore, it looks like as if the body can borrow energy from vacuum.

Now we shall ask what implication the uncertainty in energy has on physical processes. Suppose a body is at rest at the bottom A of a valley shown in Fig.4. In classical physics the body has to stay there forever. If the body can borrow enough amount of energy, it can climb to the top B of the hill and then move down to the bottom C of the next valley. The minimum energy required for the body to go over the hill is equal to the difference between the potential energies at the points A and B . In quantum physics, if the energy uncertainty ΔE of the body is larger than the minimum energy for a period of time Δt long enough for the body to climb up the hill, the body can move from A to C .

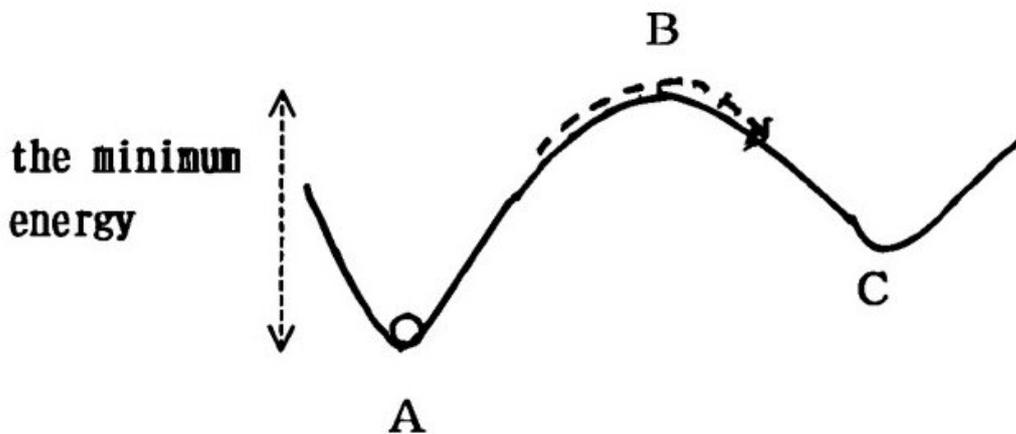


Figure 4. Can the body go over the hill of potential energy?

Since the Planck constant h is very small, the product of the debt in energy and the length of time in the debt is too small for any macroscopic body to climb up any hill of a macroscopic scale. The situation would be totally different when we consider a microscopic object such as an electron. Suppose an electron moves in an electrostatic potential due to the positively charged nuclei of two neighbouring atoms as shown in Fig.5. The potential has two valleys corresponding to states in which the electron is trapped in either one of the two atoms. The height of the peak of the potential between the two valleys is of the order of one electron volt ($1\text{eV} = 1.60 \times 10^{-19}$ joule), which is the energy scale characterizing microscopic systems. The distance R between the two atoms

is of the order of 10^{-10} m.

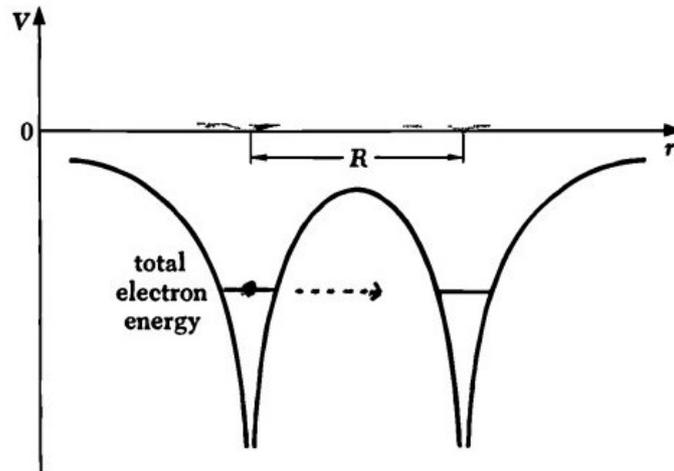


Figure 5. An electron can move from one valley to another due to the uncertainty principle

To move from one valley to the other, the electron has to climb up the hill between the valleys and must have an energy uncertainty of the order of $\Delta E \sim 1\text{eV} \sim 1.6 \times 10^{-19}$ joule. From the uncertainty relation (3), the time required for the electron to climb up the hill is of the order of $\Delta t \sim h/\Delta E \sim 4 \times 10^{-15}$ s or less. The velocity of the electron with kinetic energy of $\Delta E \sim 1\text{eV}$ is of the order of one thousandth of the light velocity c , and then the time needed for the electron to climb up the hill is about $a/(c/1000) \sim 3 \times 10^{-16}$ s, which is a little shorter than Δt . Thus, the electron can move from one valley to the next one due to the energy uncertainty in quantum physics. In classical physics the electron cannot climb up the hill, because its kinetic energy is less than the energy difference between the peak and the valley of the potential.

Thus, electrons in matter can move from the site of one atom to neighbouring sites of other atoms due to the energy uncertainty in quantum systems. It is known that electric currents in metals are carried by electrons, which can more or less freely move in the metal because of the effect of the uncertainty principle described above.

Now, we shall ask how we understand the law of energy conservation under the circumstance of having the uncertainty relations. If we measure the energy of a system by spending an infinite time, then there is no energy uncertainty and the energy conservation law is not affected at all. Even if the measuring time is of the order of 1 second, the expected energy uncertainty is $\Delta E \sim h/\Delta t \sim 4 \times 10^{-15}$ eV, which is extremely small even in the microscopic energy scale. Thus, in macroscopic physics we can safely assume that the energy conservation law is strictly valid for any physical process occurring in nature.

In modern physics any force is known to be mediated by some appropriate particles exchanged between the interacting particles (see *Types of Interactions in Particles and Fields*). The electromagnetic force is mediated by exchange of massless photons. The nuclear force between protons and neutrons is mediated by exchange of massive

particles such as pions and the weak force is mediated by exchange of very massive particles called weak bosons.

The energy mc^2 associated with the mass m of a massive particle is large, and these massive particles exchanged between interacting particles can exist only when the energy uncertainty ΔE of the system is greater than mc^2 . Therefore, the massive particle mediating force can exist for only a short time period given by $\Delta t \sim h/\Delta E \sim h/mc^2$. These particles are called virtual particles because they exist only for a short time allowed by virtue of the uncertainty in energy. Even if a virtual particle moves with the speed of light, it can move at most a distance of the order of h/mc . Therefore, the force mediated by exchange of a massive particle with mass m is action at a short distance and can act only between particles which are apart less than the distance h/mc from each other.

The Law of Entropy Increase

As was mentioned before, existence of different kinds of energy is analogous to existence of different currencies such as American dollars, Euros or Japanese Yens. Different kinds of energy are convertible to one another just like different currencies are interchangeable with one another. If there is no service charge for exchange, the sum of values of the holding currencies is unaffected by the exchange, which might correspond to the energy conservation law in physics.

We know that there exist differences in qualities of currencies which depend upon economical circumstances at the time. Some currencies are good ones, because one can change these currencies to others at any time, anywhere and by any amount without any trouble. Some currencies are bad ones, because they are not easily changeable to good currencies at the normal exchange rates, except at a higher exchange rate in black markets thereby losing some of the values of currencies in hands.

Similarly, there exist differences in qualities of energies. Energy of good quality can be easily converted into energy of bad quality by any amount without any restriction. On the contrary, energy of bad quality is not easily convertible into energy of good quality, and, when it is converted, only a limited fraction of the energy can be converted. For example, the mechanical energy and the electromagnetic energy are of good quality and the thermal energy is of bad quality. As we learned in *Thermodynamics and Heat Transfer* in *Development of Fundamentals in Physics*, any heat engine which works between two heat reservoirs at temperatures T_1 and T_2 ($T_2 < T_1$) can convert heat energy into mechanical energy with an efficiency less than $(T_1 - T_2)/T_1 (< 1)$, meaning that we cannot convert heat into mechanical energy without disposing of some fraction of heat to the lower temperature heat reservoir.

The existence of quality in energy is related to the existence of the preferred direction in which physical processes occur or to the law of increase of entropy which tells us the direction of change of physical systems. Most of physical processes occurring in nature are irreversible except possibly simple idealized motion such as oscillation of a pendulum with no frictional force acting upon it or quasistatic processes occurring at infinitely slow speed. Therefore, in general, there exists a preferred direction in change of states of a physical system.

When we have two bodies at different temperatures in close contact with each other, heat is always transferred from the hotter body to the colder one and finally they become equal in temperature. It never occurs that two bodies with the same temperature spontaneously become different in temperature. Thus, the heat conduction is an irreversible process in which heat flows from hotter bodies to colder ones and not vice versa.

As another example, consider an actual oscillatory motion of a pendulum in a box as shown in Fig.6. We know that the amplitude of oscillation gradually decreases and the pendulum will finally stop due to frictional force between the pendulum and air surrounding it. The mechanical energy of motion of the pendulum was transferred to the heat energy of the air and we can find out a little increase of temperature of air if we measure its temperature.

This simple phenomenon can be regarded as a process in which the energy carried by the pendulum is transferred to the kinetic energy of random motion of molecules in the air. The degree of freedom of motion is one for the pendulum and $3N$ for the molecules in the air, where N is the total number of molecules in the air. Thus, the process means that the energy concentrated in one degree of freedom is dispersed and redistributed over the $3N$ degrees of freedom of motion. In general, a state of a system in which the energy is concentrated in a small degree of freedom of motion would likely to change into states where the energy is distributed over many degrees of freedom.

In 1865, Clausius introduced a quantity called entropy. The change of entropy S of a body at temperature T was defined as $\Delta S = \Delta Q/T$, when the body gets an amount of heat ΔQ from its surroundings. As we described in *Thermodynamics and Heat Transfer in Development of Fundamentals in Physics*, the second thermodynamical law tells us that the entropy of any isolated system should increase in any process occurring in the system.

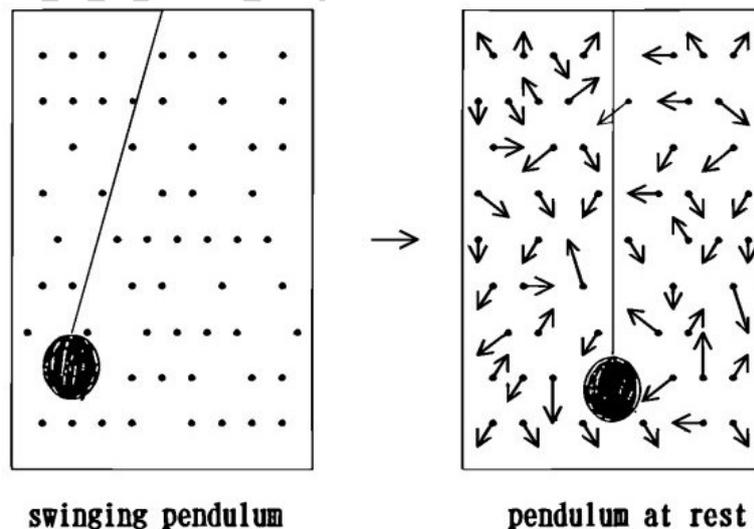


Figure 6. The irreversible motion of a pendulum (dots denote the calm air molecules and the arrows signify their state of agitation)

In thermodynamics, the state of a macroscopic system (macrostate) in thermal equilibrium is described by a set of small number of macroscopic thermodynamical variables such as temperature, pressure, volume, internal energy and entropy. These variables are related to one another through the equation of state and only two of them are independent variables in most cases.

However, any macroscopic system consists of a huge number of atoms and molecules, and the degree of freedom of motion is extremely large and almost infinite. Therefore, there are quite many microscopic states (microstates) which cannot be differentiated from each other by the small set of the macroscopic dynamical variables. This means that there exist a large number of different microstates which belong to a single macrostate specified by a set of values of the thermodynamical variables. Let us denote the number of different microstates for a given macrostate by Ω , and define the entropy S of that macrostate by

$$S = k \ln \Omega \quad (4)$$

Here, k is the Boltzmann constant and $\ln \Omega$ is the natural logarithm of Ω . The entropy introduced above turns out to be identical with the entropy introduced by Clausius as we shall see later. Thus, the formula $S = k \ln \Omega$ gives the meaning of entropy based on the microscopic point of view.

Suppose that in thermal equilibrium every microstate is realized with an equal probability as far as the state is compatible with the energy conservation law or any other constraints imposed on the system. Then, each macrostate will be realized with a probability proportional to its Ω . If Ω for a certain macrostate is overwhelmingly large compared with Ω of other macrostates, we can safely assume that the particular macrostate is realized in thermal equilibrium, thereby neglecting presence of other macrostates which occur with exceedingly small probabilities. If the system starts from a macrostate with a small value of Ω , it will change into states with larger values of Ω and finally settle in the macrostate with the maximum value of Ω . Thus, the direction of change of states of the system should be in the direction of increasing Ω , i.e., increasing entropy of the system.

As an example, let us consider a gas contained in a box. The number of molecules in the gas is N , which is much larger than 1. For example, if the volume of the gas is 22.4 liters, N is equal to the Avogadro number 6×10^{23} for the gas at the normal pressure and temperature (1atm and 0°C). We imagine that the box is divided into two compartments of equal volume as shown in Fig.7. Each molecule in the gas is moving fast and changes its position from one compartment to the other very rapidly. Thus, each molecule is equally likely to be in the right or left compartment.

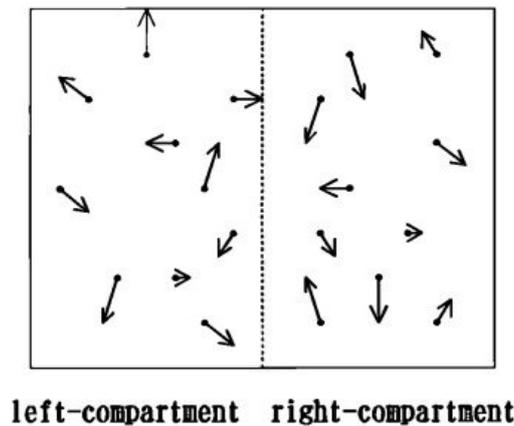


Figure 7. Motion of molecules in a gas (the dots denotes molecules while the arrow indicates the direction of motion of the molecule)

At an instant of time, we may find $N/2 + m$ molecules in the right-compartment and $N/2 - m$ molecules in the left-one. The number of different ways to choose $N/2 + m$ molecules out of the N molecules is

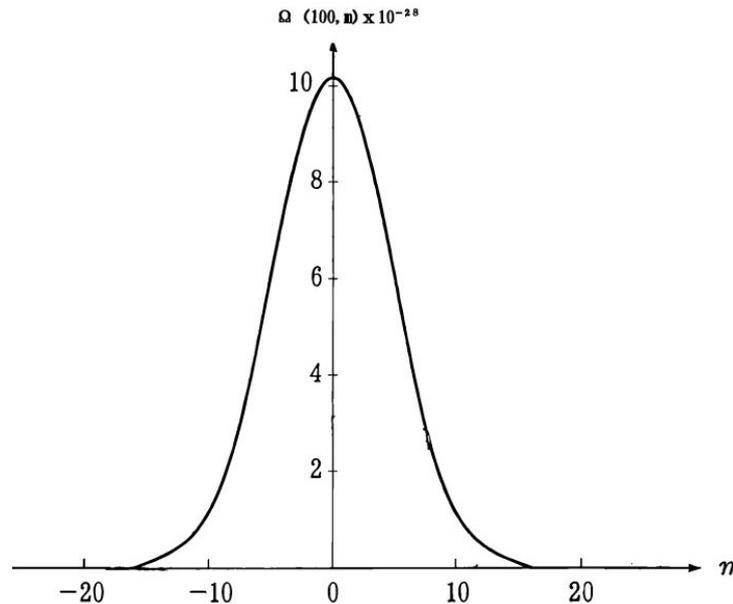
$$\Omega(N, m) = {}_N C_{N/2+m} = N!/((N/2) + m)!(N/2 - m)!$$

The number $2m$ represents the unbalance in number of molecules between the right and left compartments. The deviation $\delta\rho$ of density of the gas in each compartment from the average density ρ is given by $\delta\rho/\rho = \pm 2m/N$.

For small values of N , one can easily calculate $\Omega(N, m)$. For large values of N , we can use the mathematical formula called Sterling's formula to obtain an approximately correct value of Ω . The formula is

$$\Omega(N, m) \sim 2^N (2/N)^{1/2} \exp(-2m^2/N) \quad (5)$$

which is well valid for $N \gg m$ and $m \gg 1$. The calculated result for $N = 100$ is shown in Fig.8. We can see from the figure that the values of $\Omega(N, m)$ are quite large for small values of $|m|$ and that Ω decreases rapidly when $|m|$ increases beyond $N^{1/2}$ ($= 10$).

Figure 8. $\Omega(100, m) 10^{-24}$

We define a microstate by specifying the position of each of molecules to be either in the right- or left-compartment. Since every molecule is equally likely to be in either one of the compartments, it is expected that each microstate thus defined is realized with an equal probability. A macrostate can be defined by the value of the density unbalance $\delta\rho/\rho$ between the two compartments. Since we cannot measure positions of individual molecules, we can only find $\delta\rho/\rho$ as the macroscopic variable to describe the state of gas in the box.

For a given macrostate specified by $\delta\rho/\rho (= 2m/N)$, the number of corresponding microstates is given by $\Omega(N, m)$. Since N is large and of the order of the Avogadro number N_A , only those macrostates with $|m|$ less than $N^{1/2}$ have large enough Ω to be realized with an appreciable probability. Thus, the density variation between the two compartment, $\delta\rho/\rho$, is of the order of $N^{-1/2}$ or less and for $N = N_A$ it is about 10^{-12} or less. This means that the density of the gas in thermal equilibrium is homogeneous.

In Fig.9a we show two macrostates in which all molecules exist exclusively in either one of the right or left compartments ($\delta\rho/\rho = \pm 1$). After enough time passed, both the states would change into the same state of uniform density as shown in the figure. Instead of dividing the box into two compartments, we can imagine to divide the box into many small compartments of equal volume as shown in Fig.9b. In this case too, we can find that states of the gas change into a thermal equilibrium state with its density being homogeneous throughout the whole compartments, if the size of the small compartment is large enough to contain a large number of molecules much larger than 1.

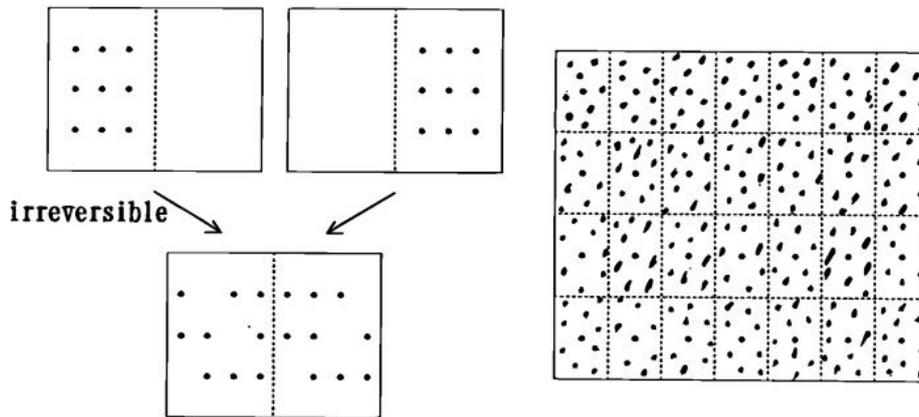


Figure 9. The state of a gas in thermal equilibrium is uniformity in density

When a box is filled with a gas, the gas will diffuse from high-density regions to lower density regions in the box and the state of the gas changes into a state of uniform density everywhere in the box. Likewise, if we make a hole on the wall of the box, the gas will spread out to open space through the hole. No reversed processes take place. All these phenomena are diffusion processes in which a gas moves from higher density regions to lower ones accompanied with increase in the entropy of the system.

One of the characteristic features associated with irreversible processes is the loss of memory of the history. Since a large number of different macrostates lead to the same equilibrium state with maximum entropy, we cannot tell from which state the system has evolved into the present macrostate in thermal equilibrium.

We can measure macroscopic properties of a system such as pressure, temperature and matter density, through which we know the macroscopic state of the system. However, we do not know which one of the possible microstates is actually realized at a time. In general, the microstate of a system changes very rapidly from one to another with time. We can observe only those macroscopic quantities which do not depend on a microstate but depend on time-averaged properties over many microstates.

If Ω or the entropy of a macrostate is large, the system takes within a short time interval a large number of microstates which we cannot differentiate from each other. Thus, a macrostate with a large value of entropy is really a quite complex system, more complex for larger values of entropy. On the contrary, a macrostate with a small value of entropy is an ordered state which is a mixture of a small number of microstates. If $S = 0$ and $\Omega = 1$, one can tell what the microstate is for the given macrostate. Thus, the concept of entropy is related to the concept of degree of order in the structure of matter through the microscopic interpretation of entropy ($S = k \ln \Omega$).

In order to evaluate entropy, we have to know what microstates are and how we calculate the number of microstates compatible with a given macrostate. For a classical system it is sufficient to know at a time t the positions and momenta of all the constituent particles of the system to uniquely specify the state of motion of the system.

Then, a microstate of a system composed of N particles can be represented by a set of values (q_i, p_i) ($i = 1, 2, \dots, 3N$), where q_i and p_i denote each component of the position and momentum vectors of the N particles. The set (q_i, p_i) can be understood as a point in the $6N$ -dimensional phase space.

We can subdivide the entire phase space into small volume elements $d^{3N}q d^{3N}p$. For a 2-dimensional phase space (one coordinate and one momentum) this is illustrated in Fig.10. The phase space element $d^{3N}q d^{3N}p$, which can be of finite size, is called a phase space cell.

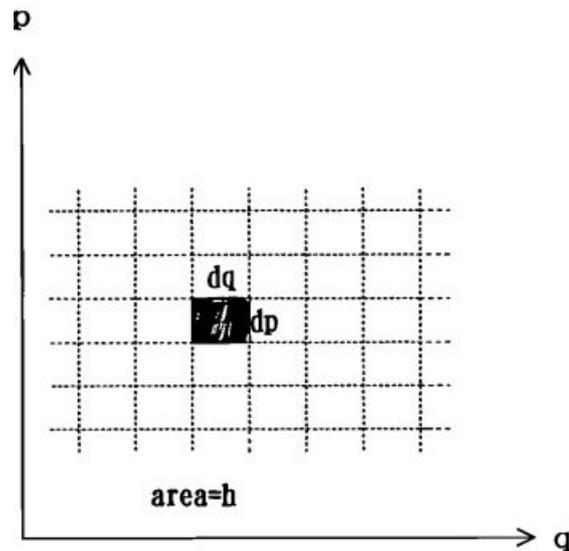


Figure 10. Phase space cells

In the course of time, a system started from a point in the phase space will move to different points and draw a continuous trajectory in the phase space. Let us consider a phase space volume element ΔV and assume that each point in the volume is the starting point of a phase space trajectory. Through the bundle of trajectories started from points in the volume ΔV , the volume ΔV at the initial time is mapped onto another volume element $\Delta V(t)$ at a later time t as shown in Fig.11. For any conservative system, it can be shown that the phase space volume does not change with time; $\Delta V(t) = \text{constant}$. This is called the Liouville's theorem.

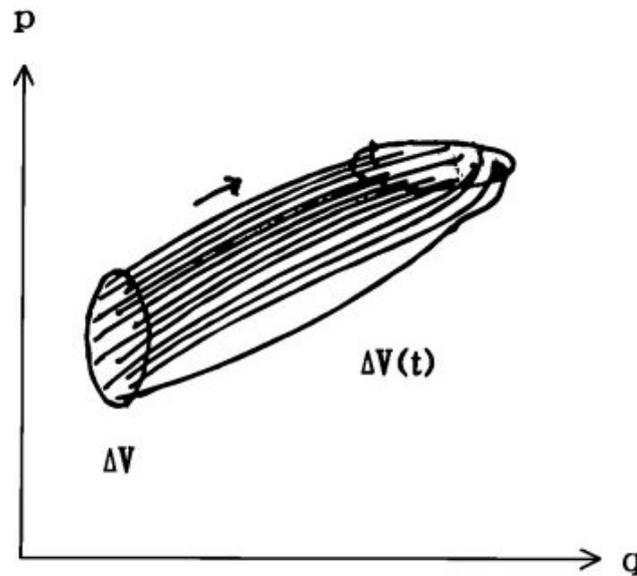


Figure 11. Liouville's theorem

Suppose we divide the entire phase space into small phase space cells of equal volume. Liouville's theorem assures us that this way of division is time-independent. If we take the volume of a cell small enough so that any two points in the cell cannot be differentiated by actual measurements of positions and momenta, we can reasonably specify a microstate by a cell in which the state is. Since in classical physics there is no limitation in accuracies of measurements of these variables in principle, we can even take infinitely small cells to represent microstates.

In quantum physics, there are the uncertainties in values of positions and momenta of particles in principle. The uncertainty relation between the corresponding components of the position and momentum of a particle is $\Delta q \Delta p = h$, where h is the Planck constant. Thus, the natural choice for the volume of the phase space cell is h^{3N} and each cell specifies a quantum microstate of the system (see the topic 4).

Once we specify the microstate by a cell it belongs to, it is straightforward to calculate the number of microstate for a given macrostate. For example, when the energy of a macrostate is between E and $E + \Delta E$, the number of corresponding microstates is given by the ratio of the volume of phase space with energy between E and $E + \Delta E$ and the volume of the unit cell.

Another basic problem related to the concept of entropy is the plausibility of the equal probability of all microstates, which can only be justified by experimental studies of its consequences. In a closed system of finite size, a large number of constituent particles exert forces on one another and constantly change their positions and momenta. Therefore, in thermal equilibrium the system is expected to take any of microstates compatible with the macrostate in the course of time evolution and, if we average over an appropriate time interval, all microstates compatible with the macrostate will be realized with equal probability.

In order to check the equal probability of all microstates, one has to study time evolution of each individual system. In principle, we can follow the change of a microstate if we assume an appropriate internal dynamics of the system. In fact, by use of modern computers we can compute the time evolution of a microstate of a system which consists of not too many constituent particles. In most cases calculated results are affirmative for the equal probability of all microstates.

When the strength of force between the particles is made weaker, it takes longer time for the system to reach thermal equilibrium and realize equal probability of all microstates. The characteristic time for a system to reach a thermal equilibrium is called the relaxation time.

As an important application of the relation $S = k \ln \Omega$, we shall consider the thermal motion of molecules in a gas. As shown in Fig.12, a gas contained in a box is in close contact with a large heat reservoir of temperature T . Heat exchange between the gas and the heat reservoir takes place constantly through the boundary surface between the two. After enough time passed, the temperature of the gas will become equal to T through the heat exchange, and the gas and the heat reservoir are in thermal equilibrium relative to each other.

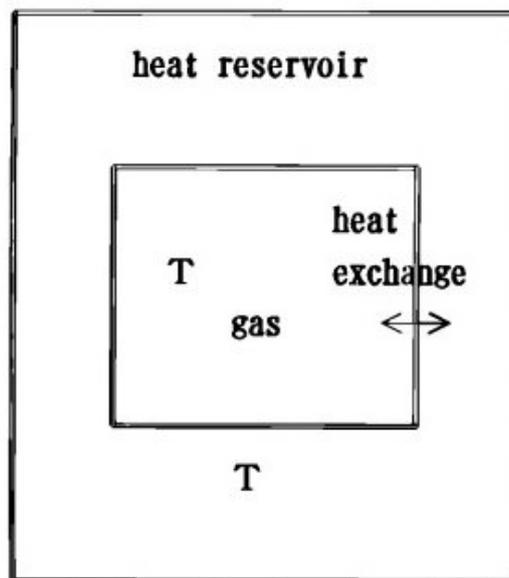


Figure 12. The gas and the heat reservoir in thermal equilibrium

Even in thermal equilibrium, there are heat flows microscopically, but the amount of heat coming into the gas from the reservoir is just cancelled by the heat coming out from the gas into the reservoir in average. The gas in the box is not an isolated system because of heat exchange with the reservoir, but it can be called as a closed system because of no net flow of heat between the gas and the reservoir.

Now, let us consider the energy distribution of molecules in the gas. The heat reservoir is a large system with a large heat capacity so that its temperature T will be kept

constant in spite of heat exchange with the gas. The number of microstates $\Omega(E)$ of the reservoir with energy E is very large and increases with increasing E . Since the large heat reservoir consists of a huge number of particles, there should be many different ways to divide E into energies of the particles in the reservoir and the number of different ways should certainly increase if we add more energy to the reservoir.

Suppose that a molecule in the gas gets energy ε through its heat exchange with the reservoir. Then, the energy of the reservoir becomes $E - \varepsilon$ because of the energy conservation law. The energy ε is of a microscopic magnitude which is very small compared to E . Thus, the entropy of the reservoir of energy $E - \varepsilon$ can be approximated by

$$S(E - \varepsilon) = S(E) - \varepsilon dS(E)/dE \quad (6)$$

In Fig.13 we show the entropy S as a function of E . The derivative dS/dE is given by the inclination of the tangential line of the curve $S(E)$ at the point E .

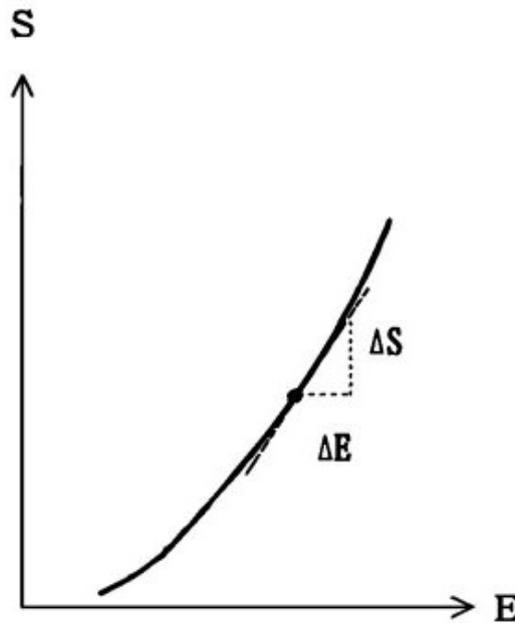


Figure 13. Entropy S as a function of E .

The number of microstates of the whole system composed of the reservoir and the single atom with energy ε is given by the number of microstates $\Omega(E - \varepsilon)$ of the reservoir with energy $E - \varepsilon$: $\Omega(E - \varepsilon) = \exp(S(E - \varepsilon)/k)$ which depends on ε as

$$\Omega(E - \varepsilon) \sim \exp(-(\varepsilon/k) dS(E)/dE)$$

If we define the temperature of the reservoir by

$$dS(E)/dE = 1/T \quad (7)$$

the probability for finding a molecule in a state of energy ε is proportional to the factor $\exp(-\varepsilon/kT)$, which is called the Boltzmann factor:

$$\Omega \sim \exp(-\varepsilon/kT) \quad (8)$$

The relation (7) is equivalent to the relation $\Delta S = \Delta Q/T$ introduced by Clausius, thus showing that the entropy defined by $S = k \ln \Omega$ is equal to the entropy in classical thermodynamics. We have derived the energy distribution of a molecule in the gas through the heat exchange between the heat reservoir and a single molecule in the gas. Since every molecule behaves in the same way, the energy distribution is common to all molecules and it can be taken as the statistical distribution of energy averaged over all molecules in the gas.

Although we derived the distribution function (8) by taking into account heat exchange between a single molecule and the heat reservoir, each molecule exchanges energy not only with the heat reservoir but also with other molecules in the system. If we consider the reservoir plus all other molecules as a heat reservoir, the same distribution function is obtained as the energy distribution of a molecule. Also the same distribution is obtained for a molecule in any system in thermal equilibrium irrespective of whether the system is in a gas, a liquid, or a solid phase.

We have discussed microscopic interpretation of entropy and of the second law of thermodynamics. Even it gives the definition of the absolute temperature T in terms of entropy. Statistical mechanics which we shall describe in a later chapter (see *Statistical Physics* in this chapter) will give us a more comprehensive relation between thermodynamics and microscopic theory of matter.

The law of entropy increase is a basic law in physics which determines the direction of change of physical systems or the direction of flow of time. In Fig.14 we show some typical physical phenomena which increase the entropy of the system. Increasing number of molecules in the system, addition of heat energy, increasing volume of the system, dissociation of molecules into its constituents, deformations of molecules from a simpler form into more complex forms are examples of processes which increase the entropy of the system. Readers will find for themselves that the number of microstates available increases in any of these processes.

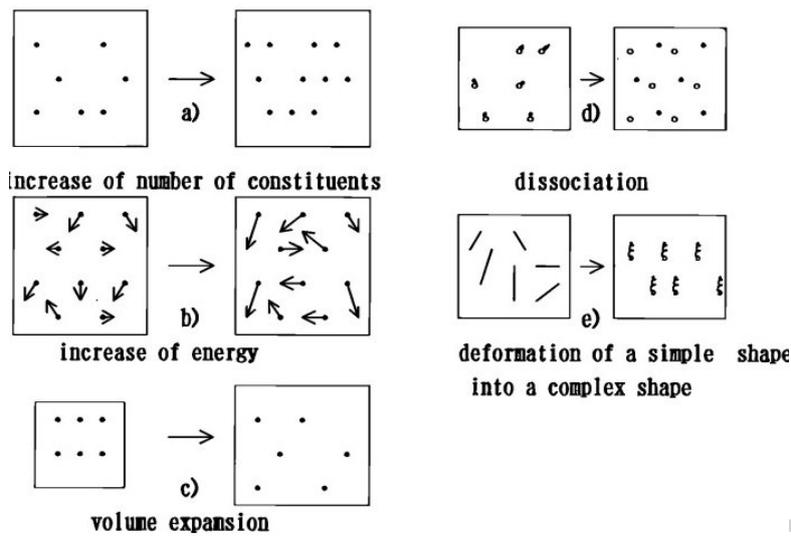


Figure 14. Various processes that increase entropy

Although entropy always increases in any process occurring in an isolated system, it can decrease for an open system, one into which fluxes of energy and matter can come and go, and the state of the open system can change from a less ordered state to a more ordered state. This problem will be discussed in detail in the forthcoming chapter (see *Order and Disorder in Nature*).

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Biographical Sketch

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