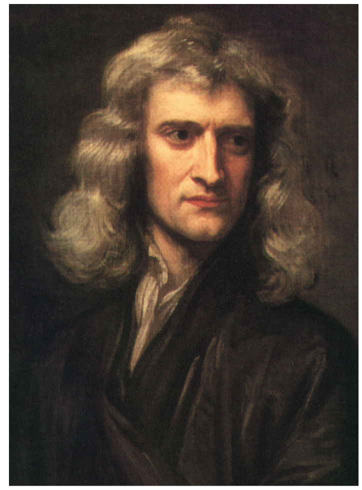
Johannes Kepler (1571–1630)
Founder of celestial mechanics



Sir Isaac Newton (1642–1727)
Founder of modern mechanics

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Classical mechanics and the advent of quantum mechanics

1.1 Newtonian mechanics

The principles of classical mechanics do not provide the correct description of physical processes if very small length or energy scales are involved. ***Classical*** or ***newtonian*** mechanics allows a *continuous* spectrum of energies and allows *continuous* spatial distribution of matter. For example, coffee is distributed homogeneously within a cup. In contrast, quantum mechanical distributions are not continuous but *discrete* with respect to energy, angular momentum, and position. For example, the bound electrons of an atom have discrete energies and the spatial distribution of the electrons has distinct maxima and minima, that is, they are not homogeneously distributed.

Quantum-mechanics does not contradict newtonian mechanics. As will be seen, quantum-mechanics merges with classical mechanics as the energies involved in a physical process increase. In the classical limit, the results obtained with quantum mechanics are identical to the results obtained with classical mechanics. This fact is known as the ***correspondence principle***.

In classical or newtonian mechanics the instantaneous state of a particle with mass m is fully described by the particle's position $[x(t), y(t), z(t)]$ and its *momentum* $[p_x(t), p_y(t), p_z(t)]$. For the sake of simplicity, we consider a particle whose motion is restricted to the x-axis of a cartesian coordinate system. The position and momentum of the particle are then described by $x(t)$ and $p(t) = p_x(t)$. The momentum $p(t)$ is related to the particle's velocity $v(t)$ by $p(t) = m\, v(t) = m\, [\mathrm{d}x(t) / \mathrm{d}t]$. It is desirable to know not only the instantaneous state-variables $x(t)$ and $p(t)$, but also their functional evolution with time. Newton's first and second law enable us to determine this functional dependence. ***Newton's first law*** states that the momentum is a constant, if there are *no forces* acting on the particle, *i. e.*

$$p(t) = m\,v(t) = m\frac{\mathrm{d}x(t)}{\mathrm{d}t} = \text{const.} \tag{1.1}$$

Newton's second law relates an external force, F, to the second derivative of the position $x(t)$ with respect to t,

$$F = m\frac{\mathrm{d}^2 x(t)}{\mathrm{d}t^2} = m\,a \tag{1.2}$$

where a is the acceleration of the particle. Newton's first and second law provide the state variables $x(t)$ and $p(t)$ in the presence of an external force.

For consideration: ***Resistance to Newton's and Kepler's laws***. Newton's laws were greeted with skepticism. Newton postulated that a body continues its uniform motion if there are no forces acting on the body. Opposing contemporaries argued that this would be counter-intuitive and in utter conflict with daily experience: A carriage must be *constantly pulled* by horses for the carriage to move at a *constant velocity* (see ***Fig***. 1.1). They further argued that as soon as the horses would stop pulling the carriage, it would rest!

Fig. 1.1. Did Newton's first law, which postulates that a body maintains a constant velocity if no forces act on the body, contradict intuition and experience? (after Carriage Association of America, 2004).

Kepler was greeted with skepticism as well. Not understood by the citizens of the village he was born in, they turned against his mother and accused her of being a witch. Despite the threat of torture, she did not admit to being a witch. Kepler's intervention helped to set her free after she was kept in jail for 14 months. She died six months after her release.

1.2 Energy

Newton's second law is the basis for the introduction of work and energy. Work done by moving a particle along the x axis from 0 to x by means of the force $F(x)$ is defined as

$$W(x) = \int_0^x F(x)\,\mathrm{d}x \ . \tag{1.3}$$

The energy of the particle *increases* by the (positive) value of the integral given in Eq. (1.3). The total particle energy, E, can be (*i*) purely potential, (*ii*) purely kinetic, or (*iii*) a sum of potential and kinetic energy. If the total energy of the particle is a purely potential energy, $U(x)$, then $W(x) = -\,U(x)$ and one obtains from Eq. (1.3)

$$F(x) = -\frac{\mathrm{d}}{\mathrm{d}x}U(x) \ . \tag{1.4}$$

If, on the other hand, the total energy is purely kinetic, Eq. (1.2) can be inserted in the energy equation, Eq. (1.3), and one obtains with $(\mathrm{d}^2 / \mathrm{d}t^2)\, x = v(\mathrm{d} / \mathrm{d}x)\, v$

$$E_{\text{kin}} = \frac{1}{2} m v^2 = \frac{p^2}{2m} . \tag{1.5}$$

If no external forces act on the particle, then the total energy of the particle is a constant and is the sum of potential and kinetic energy

$$E_{\text{total}} = E_{\text{kin}} + U(x) = \frac{p^2}{2m} + U(x) . \tag{1.6}$$

An example of a one-dimensional potential function is shown in ***Fig***. 1.2. Consider a classical object, *e. g*. a soccer ball, positioned on one of the two slopes of the potential, as shown in ***Fig***. 1.2. Once the ball is released, it will move downhill with increasing velocity, reach the maximum velocity at the bottom, and move up on the opposite slope until it comes to a momentary complete stop at the ***classical turning point***. At the turning point, the energy of the ball is purely potential. The ball then reverses its direction of motion and will move again downhill. In the absence of friction, the ball will continue forever to oscillate between the two classical turning points. The total energy of the ball, *i. e*. the sum of potential and kinetic energy remains constant during the oscillatory motion as long as no external forces act on the object.

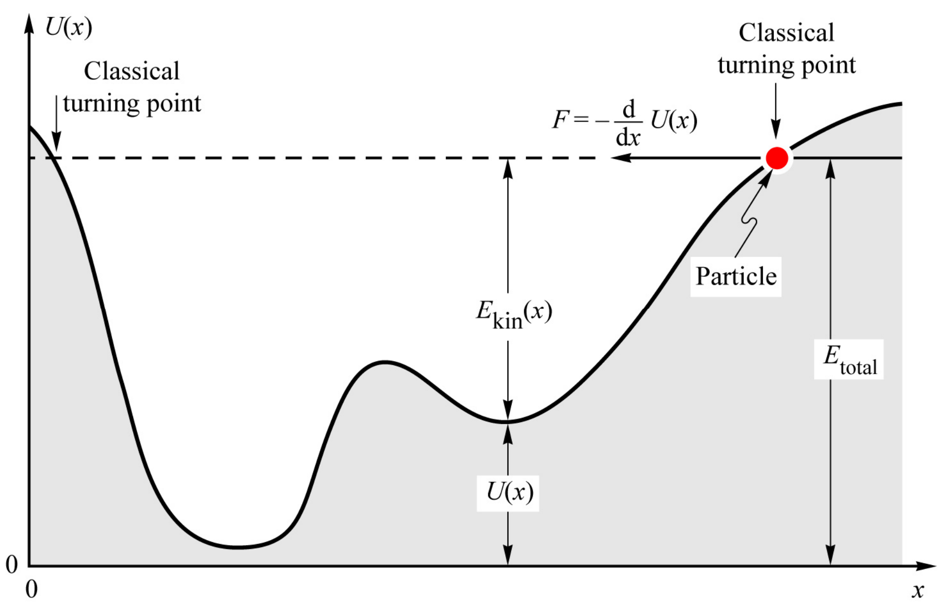

Fig. 1.2. Potential energy as a function of spatial coordinate x. The total energy of the particle shown is the sum of kinetic and potential energies. The force F acting on the particle is the negative derivative of the potential energy with respect to x.

1.3 Hamiltonian formulation of newtonian mechanics

Equations (1.1) and (1.2) are known as the newtonian formulation of classical mechanics. The *hamiltonian formulation* of classical mechanics has the same physical content as the newtonian formulation. However, the hamiltonian formulation focuses on *energy*. The ***hamiltonian function*** $H(x, p)$ is defined as the total energy of a system

$$H(x, p) = \frac{p^2}{2m} + U(x) . \tag{1.7}$$

The partial derivatives of the hamiltonian function with respect to *x* and *p* are given by

$$\frac{\partial}{\partial x} H(x, p) = \frac{\mathrm{d}}{\mathrm{d}x} U(x) \tag{1.8}$$

$$\frac{\partial}{\partial p} H(x, p) = \frac{p}{m} . \tag{1.9}$$

Employing these partial derivatives and Eqs. (1.1) and (1.4), one obtains two equations, which are known as the ***hamiltonian equations of motion***:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\partial}{\partial p} H(x, p) \tag{1.10}$$

$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial}{\partial x} H(x, p) . \tag{1.11}$$

Formally, the linear Eq. (1.1) and the linear, second order differential Eq. (1.2) have been transformed into the *two* linear, first order partial differential Eqs. (1.10) and (1.11). Despite this formal difference, the physical content of the newtonian and the hamiltonian formulation is identical.

1.4 Breakdown of classical mechanics

One of the characteristics of classical mechanics is the continuous, non-discrete nature of its variables position, $x(t)$, and momentum, $p(t)$. That is, a particle can have any (non-relativistic) momentum with no restrictions imposed by the axioms of classical mechanics. A second characteristic of classical mechanics is the deterministic nature of time dependent processes. Once initial conditions of a mechanical problem are known (that is the position and momentum of all particles of the system), the subsequent evolution of particle motion can be *predetermined* according to the hamiltonian or newtonian equations of motion. In its final consequence, determinism would predetermine the entire universe from its birth to its death. However, quantum-mechanics shows, that physical processes are not predetermined in a mathematically exact sense. As will be seen later, the determinism inherent to newtonian mechanics is in conflict with with quantum mechanics.

Quantum mechanical principles were first postulated by Planck to explain the black-body radiation. At the end of the 19th century, scientists tried to explain the emission intensity spectrum of a *black body* with temperature *T*. A black body is defined as a perfectly absorbing, non-reflecting body. The intensity spectrum $I(\lambda)$ (in Watts per unit area and per unit wavelength) was experimentally found to be the same for all black bodies at the same temperature, as predicted by arguments based on thermodynamics. The spectral intensity of black-body radiation as a function of wavelength is shown in ***Fig***. 1.3 for different temperatures.

Rayleigh and Jeans predicted a law based on laws of mechanics, electromagnetic theory and statistical thermodynamics. The Rayleigh-Jeans formula is given by

$$I(\lambda) = \frac{2\pi k T}{\lambda^2} \qquad (1.12)$$

where k is Boltzmann's constant. However, this formula yielded agreement with experiments only for long wavelengths. For short wavelengths, namely in the ultraviolet region, the formula has a singularity, *i. e.* $I(\lambda \to 0) \to \infty$. Thus, the formula cannot be physical meaningful.

Planck (1900) postulated that the oscillating atoms of a black body radiate energy only in the discrete, *i. e.* quantized amounts

$$E = \hbar\,\omega,\ 2\,\hbar\,\omega,\ 3\,\hbar\,\omega,\ \cdots = \hbar\, c\,\frac{2\pi}{\lambda},\ 2\,\hbar\, c\,\frac{2\pi}{\lambda},\ 3\,\hbar\, c\,\frac{2\pi}{\lambda},\ \cdots \qquad (1.13)$$

where $\hbar = h/(2\pi)$ is *Planck's constant* divided by 2π, c is the velocity of light, and $\omega = 2\pi f$ is the intrinsic angular frequency of the radiating oscillators. The quantum constant or Planck's constant has a value of

$$\hbar = h/(2\pi) = 1.05 \times 10^{-34}\,\mathrm{Js}\,. \qquad (1.12)$$

Employing this postulate in the black-body radiation problem, Planck obtained the following formula for the spectral intensity distribution of a black body at temperature T

$$\boxed{I(\lambda) = \frac{4\pi\hbar c^2}{\lambda^5\left(\exp\left(\dfrac{2\pi\hbar c}{\lambda k T}\right) - 1\right)}} \qquad (1.15)$$

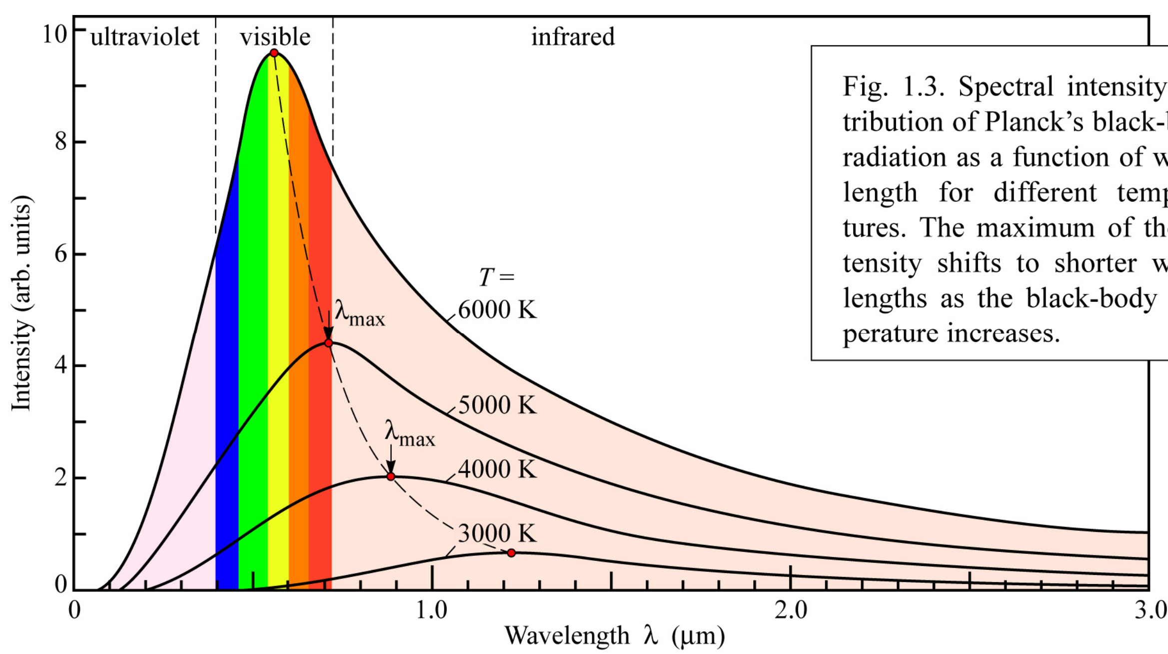

Fig. 1.3. Spectral intensity distribution of Planck's black-body radiation as a function of wavelength for different temperatures. The maximum of the intensity shifts to shorter wavelengths as the black-body temperature increases.

Planck's law of black body radiation was in agreement with experimental observations. The maximum intensity of radiation can be easily deduced from Eq. (1.15) and it occurs at the wavelengths given by ***Wien's law***

$$\lambda_{max}\, T \quad = \quad \text{const.} \quad = \quad 2880\, \mu\text{m K}\,. \tag{1.16}$$

This law predicts that the maximum intensity shifts to the blue spectral region as the temperature of the black body is increased. The energy of the black body radiation at the intensity maximum is given by $E_{max} = h\,c\,/\,\lambda_{max}$ and E_{max} equals about five times the thermal energy, that is $E_{max} = 4.98\; kT$. Several black body radiation spectra are shown in ***Fig***. 1.3.

Planck's postulate of discrete, *allowed* energies of atomic oscillators as well as of *forbidden*, or *disallowed* energies marks the historical origin of quantum mechanics. It took scientists several decades to come to a complete understanding of quantum mechanics. In the following, the basic postulates of quantum mechanics will be summarized and their implications will be discussed.

Exercise: ***The color of hot objects***. If an object gets sufficiently hot, it appears to the human eye, to glow in the red region of the visible spectrum. Assume that the emission spectrum of the hot object peaks at a wavelength of 650 nm. Calculate the temperature of the object.

Solution: The temperature of the hot object is 4431 K.

As the temperature of the object is increased further, the glow changes from the reddish to a yellowish color. At even higher temperatures, the light emitted by the object changes to a white glow. Explain these experimental observations based on the black body radiation.

Solution: As the temperature of the black body increases, the peak wavelength shifts from the infrared into the visible and ultimately into the ultraviolet. At low temperatures, only the short-wavelength tail of the radiation reaches into the visible spectrum and the body therefore appears as red. When the black body is at sufficiently high temperatures, the emission spectrum covers the entire visible spectrum and the body appears as white.

Thermal and night-vision imaging systems can detect the thermal radiation emitted by hot electronic components or by humans, as shown in ***Fig***. 1.4. What is the peak wavelength of planckian emission of a hot electronic component of 100 °C and a human body at 37 °C?

Solution: The peak emission wavelength of the electronic component and human body is 7.7 μm and 9.3 μm, respectively.

Why is a planckian radiator assumed to be perfectly black?

Solution: This assumption is made to ensure that the body does not reflect light. If the body were not perfectly black, it would reflect light thereby appearing in a certain color even if it were at 0 K.

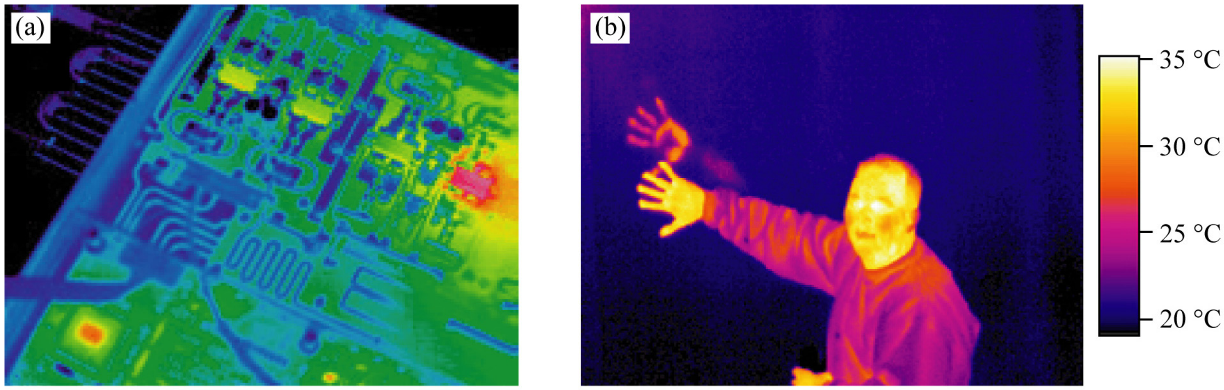

Fig. 1.4. Thermal infrared image obtained in the 3 − 6 μm wavelength range of (a) an electronic circuit and (b) a person having touched a cold wall and leaving a "thermal imprint" (after Sierra Pacific Corp., 2004; Mikron Corp., 2004).