QUANTUM MECHANICS

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Classical Mechanics

The Newton's and Eulero-Lagrange's Equations

To simplify the discussion we restrict our considerations to a one dimensional motion of a single material point under a conservative field. If the point has mass m the Newton's equation is given by:

$$F(x) = m\,\ddot{x}$$

where F is the force applied to the point depending on the position x of the point itself and not depending on the time (conservative system). Since the field is conservative it is possible define a potential energy function as:

$$F(x) = -\frac{\partial V(x)}{\partial x} = -V'(x)$$

Furthermore the kinetic energy as known is defined as:

$$T(\dot{x}) = \frac{1}{2} m\,\dot{x}^2 \quad \rightarrow \quad \frac{\partial T(\dot{x})}{\partial \dot{x}} = m\,\dot{x}$$

This allows us to rewrite the Newton's equation as:

$$-\frac{\partial V(x)}{\partial x} = \frac{d}{dt}\frac{\partial T(\dot{x})}{\partial \dot{x}}$$

Since V(x) depends only on x and $T(\dot{x})$ depends only on $\dot{x}$, it is possible define the function $L(x, \dot{x}) = T(\dot{x}) - V(x)$ for which the following Eulero-Lagrange equation holds:

$$\frac{d}{dt}\frac{\partial L(x, \dot{x})}{\partial \dot{x}} - \frac{\partial L(x,\dot{x})}{\partial x} = 0$$

Energy Integral

We have:

$$\frac{d L(x, \dot{x})}{dt} = \frac{\partial L(x,\dot{x})}{\partial x}\dot{x} + \frac{\partial L(x, \dot{x})}{\partial \dot{x}}\ddot{x} + \frac{\partial L(x,\dot{x})}{\partial t} = \left(\begin{array}{c} L \text{ doesn't} \\ \text{depend in} \\ \text{explicit} \\ \text{way by t}\end{array}\right) = \frac{\partial L(x,\dot{x})}{\partial x}\dot{x} + \frac{\partial L(x, \dot{x})}{\partial \dot{x}}\ddot{x} =$$

$$= \left(\begin{array}{c} \text{using} \\ \text{Eulero-} \\ \text{Lagrange's} \\ \text{equation}\end{array}\right) = \frac{d}{dt}\left(\frac{\partial L(x,\dot{x})}{\partial \dot{x}}\right)\dot{x} + \frac{\partial L(x, \dot{x})}{\partial \dot{x}}\ddot{x} = \frac{d}{dt}\left(\frac{\partial L(x,\dot{x})}{\partial \dot{x}}\dot{x}\right) \rightarrow$$

$$\frac{d}{dt}\left(\frac{\partial L(x,\dot{x})}{\partial \dot{x}}\dot{x} - L(x,\dot{x})\right) = 0 \quad \rightarrow \quad \frac{\partial L(x,\dot{x})}{\partial \dot{x}}\dot{x} - L(x,\dot{x}) = \text{cost} = E$$

With $L(x, \dot{x}) = T(\dot{x}) - V(x) = m\dot{x}^2/2 - V(x)$ we obtain the energy conservation principle:

$$m\dot{x}\,\dot{x} - m\dot{x}^2/2 + V(x) = E \quad \rightarrow \quad m\dot{x}^2/2 + V(x) = E \quad \rightarrow \quad T(\dot{x}) + V(x) = E$$

The Hamilton's Equations

Defining $p = \dfrac{\partial L(x, \dot{x})}{\partial \dot{x}}$ the Eulero-Lagrange's equation becomes $\dot{p} = \dfrac{\partial L(x, \dot{x})}{\partial x}$

So we have obtained a pair of asymmetrical equations which can be simplified introducing a new function defined by:

$$H(x, p) = p\,\dot{x} - L(x, \dot{x})$$

For this function we have the following pair of equations (Hamilton's equations):

(I) $$\frac{\partial H(x,p)}{\partial x} = \frac{\partial (p\,\dot{x})}{\partial x} - \frac{\partial L(x, \dot{x})}{\partial x} = \left(\begin{matrix}p\dot{x}\text{ doesn't}\\ \text{depend in}\\ \text{explicit}\\ \text{way by x}\end{matrix}\right) = -\dot{p}$$

(II) $$\frac{\partial H(x,p)}{\partial p} = \frac{\partial (p\,\dot{x})}{\partial p} - \frac{\partial L(x, \dot{x})}{\partial p} = \left(\begin{matrix}L\text{ doesn't}\\ \text{depend in}\\ \text{explicit}\\ \text{way by p}\end{matrix}\right) = \dot{x}$$

Since $L(x, \dot{x}) = T(\dot{x}) - V(x) = m\dot{x}^2/2 - V(x)$ and $p = \partial L(x, \dot{x})/\partial \dot{x} = m\,\dot{x}$, the physical meaning of $H(x, p)$ is the total energy of the system:

$$H(x, p) = p\,\dot{x} - L(x, \dot{x}) = m\,\dot{x}\,\dot{x} - (m\dot{x}^2/2 - V(x)) = m\dot{x}^2/2 + V(x) = T(\dot{x}) + V(x) = E$$

The Classical Harmonic Oscillator

The force, the potential energy and the Lagrange's function of a mass m bound by a spring with characteristic constant k, are given by:

$$F = -k\,x \quad\rightarrow\quad V(x) = \frac{k\,x^2}{2} \quad\rightarrow\quad L(x, \dot{x}) = \frac{1}{2}m\,\dot{x}^2 - \frac{k\,x^2}{2} \quad\rightarrow\quad \text{the energy integral is:}$$

$$\frac{\partial L(x,\dot{x})}{\partial \dot{x}}\dot{x} - L(x,\dot{x}) = E \quad\rightarrow\quad \dot{x}\,m\,\dot{x} - \frac{1}{2}m\,\dot{x}^2 + \frac{k\,x^2}{2} = E \quad\rightarrow\quad \frac{1}{2}m\,\dot{x}^2 + \frac{k\,x^2}{2} = E$$

$$\dot{x} = \pm\sqrt{\frac{2E - kx^2}{m}} \quad\rightarrow\quad \frac{dx}{\pm\sqrt{\dfrac{2E - kx^2}{m}}} = dt \quad\rightarrow\quad \pm\int_0^x \sqrt{\frac{m}{2E - k\xi^2}}\,d\xi = \int_0^t d\tau$$

putting: $\xi = \sqrt{\dfrac{2E}{k}}\cos\theta \quad\rightarrow\quad d\xi = -\sqrt{\dfrac{2E}{k}}\sin\theta\,d\theta$ we obtain:

$$\int\sqrt{\frac{m}{2E - k\xi^2}}\,d\xi = -\int\sqrt{\frac{m}{2E(1 - \cos^2\theta)}}\sqrt{\frac{2E}{k}}\sin\theta\,d\theta = -\sqrt{\frac{m}{k}}\,\theta = -\sqrt{\frac{m}{k}}\,\text{acos}\left(\xi\sqrt{\frac{k}{2E}}\right)$$

$$\pm\int_0^x \sqrt{\frac{m}{2E - k\xi^2}}\, d\xi = \pm\sqrt{\frac{m}{k}}\left(-\frac{\pi}{2} + \mathrm{acos}\left(x\sqrt{\frac{k}{2E}}\right)\right) = t \qquad \text{so finally:}$$

$$x = \sqrt{\frac{2E}{k}}\cos\left(\frac{\pi}{2} \pm \sqrt{\frac{k}{m}}\,t\right) = -\pm\sqrt{\frac{2E}{k}}\sin\left(\sqrt{\frac{k}{m}}\,t\right) = -\pm x_0 \sin(\Omega\, t)$$

where: $\Omega = \frac{2\pi}{T} = \sqrt{\frac{k}{m}}$ is the frequency of the oscillations (T is their period)

$x_0 = \sqrt{\frac{2E}{k}}$ is the maximum value that x can reach

Let face now the problem to find the probability that the mass m is in a given point x at the time t. Since the ball spans the interval $(-x_0,x_0)$ in T/2 time, the probability that it is in the interval (x(t),x(t+dt)) is given by:

$$dP(x(t),x(t+dt)) = \frac{dt}{T/2} \qquad \text{with} \qquad dP(x(t),x(t+dt)) = f(x)\, dx$$

where f(x) is the probability density function. The sign of x can be neglected so we can write:

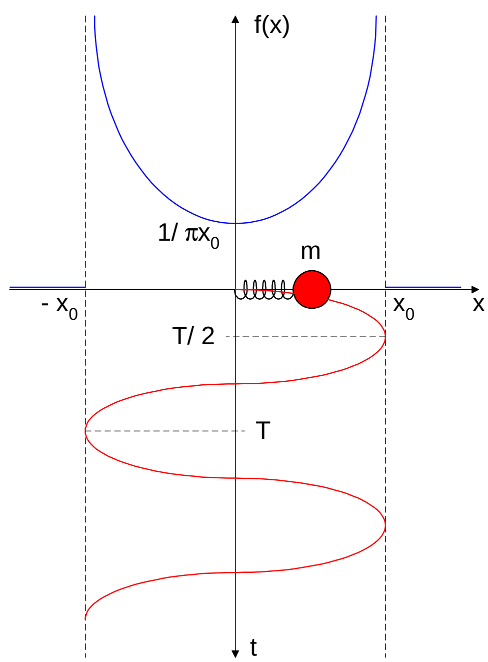
$$x = x_0 \sin\left(\frac{2\pi}{T}t\right) \;\rightarrow\; t = \frac{T}{2\pi}\,\mathrm{asin}\left(\frac{x}{x_0}\right) \;\rightarrow\; dt = \frac{T}{2\pi\, x_0}\frac{1}{\sqrt{1-\frac{x^2}{x_0^2}}}\,dx$$

$$dP = f(x)\,dx = \frac{dt}{T/2} = \frac{1}{\pi\, x_0}\frac{1}{\sqrt{1-\frac{x^2}{x_0^2}}}\,dx \;\rightarrow\; f(x) = \begin{cases} \frac{1}{\pi}\frac{1}{\sqrt{x_0^2 - x^2}} & x < x_0 \\ 0 & x \geq x_0 \end{cases}$$

The probability satisfies obviously the following condition:

$$\int_{-\infty}^{\infty}\frac{dx}{\pi\sqrt{x_0^2 - x^2}} = \int_{-x_0}^{x}\frac{dx}{\pi\sqrt{x_0^2 - x^2}} = 1$$

The following picture shows the parameters and the functions obtained above.



Quantum Mechanics

The De Broglie's Hypothesis

Using the two relativistic formulas:

$$E = m_r c^2 \qquad p = \frac{m v}{\sqrt{1 - \frac{v^2}{c^2}}} \qquad m_r = \frac{m}{\sqrt{1 - \frac{v^2}{c^2}}}$$

we can obtain an expression binding the energy and the momentum of a particle which is true for all relativistic particles including the photons. Here m is the mass at rest of the particle having velocity v and relativistic mass m_r. In fact we can write:

$$p^2c^2 = \frac{m^2 v^2 c^2}{1 - \frac{v^2}{c^2}} = \frac{m^2 \frac{v^2}{c^2} c^4}{1 - \frac{v^2}{c^2}} = \frac{m^2 c^4 \left(\frac{v^2}{c^2} - 1\right)}{1 - \frac{v^2}{c^2}} + \frac{m^2 c^4}{1 - \frac{v^2}{c^2}} = - m^2 c^4 + (m_r c^2)^2 = E^2 - (m c^2)^2$$

so:

$$E = \sqrt{(pc)^2 + (mc^2)^2}$$

in particular for a photon, whose mass at rest is null, we have:

$$E = p c$$

Comparing this relationship with the Plank's formula:

$$E = h \nu$$

where ν is the frequency of the wave associated to the photon, we have the following expression for the momentum of a photon:

$$p = \frac{h \nu}{c} = \frac{h}{\lambda}$$

where λ is the wavelength of the photon.
Basing on the fact that many experiments (e.g. electrons diffraction) show particles with a wave like behaviour, De Broglie formulated the hypothesis that any particle has its own wavelength and that this wavelength and its energy are those just obtained for the photons.

The Schrodinger's Equation

If we consider a monochromatic wave in one dimension with wavelength λ, period T and velocity $v = \lambda/T$:

$$\Psi(x,t) = \sin(k x - \omega t) \qquad \text{where:} \qquad \omega = \frac{2\pi}{T} = 2\pi\nu \qquad k = \frac{2\pi}{\lambda} \qquad v = \frac{\lambda}{T} = \frac{\omega}{k}$$

We have:

$$\frac{\partial \Psi(x,t)}{\partial x} = k \cos(k x - \omega t) \quad \rightarrow \quad \frac{\partial^2 \Psi(x,t)}{\partial x^2} = - k^2 \sin(k x - \omega t) = - k^2 \Psi(x,t)$$

$$\frac{\partial \Psi(x,t)}{\partial t} = - \omega \cos(k x - \omega t) \quad \rightarrow \quad \frac{\partial^2 \Psi(x,t)}{\partial t^2} = - \omega^2 \sin(k x - \omega t) = - \omega^2 \Psi(x,t)$$

so we can argue that Ψ(x,t) satisfies the following differential equation:

$$\omega^2 \frac{\partial^2 \Psi(x,t)}{\partial x^2} = k^2 \frac{\partial^2 \Psi(x,t)}{\partial t^2} \quad \rightarrow \quad \frac{\partial^2 \Psi(x,t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \Psi(x,t)}{\partial t^2}$$

i.e. the wave equation. What we have done is

1) found a wave function Ψ (function able to propagate itself);
2) found an order of the pure temporal derivative proportional to Ψ (in this case the order found is 2);
3) found an order of the pure spatial derivative proportional to Ψ (in this case the order found is 2);
4) satisfied the equation 1=1 or Ψ= Ψ in terms of temporal and spatial derivatives;

A similar approach can be used to obtain the Schrodinger's wave equation for a particle: we have to find a wave equation Ψ whose pure temporal and spatial derivatives can be combined in order to satisfied the equation E=T+V. First of all let try to obtain a more explicit form for the equation E=T+V.

$$E = T + V \quad \rightarrow \quad h\nu = \frac{p^2}{2m} + V = \frac{h^2}{2m\lambda^2} + V \quad \rightarrow \quad \hbar\omega = \frac{\hbar^2 k^2}{2m} + V \quad \rightarrow \quad \hbar\omega\Psi = \frac{\hbar^2 k^2}{2m}\Psi + V\Psi$$

we have only ω (not ω^2 as in the previous canonical wave equation) in the left member of the equation and k^2 in the right member. This means that we cannot use the function Ψ(x,t)=sin(kx−ωt) and its second partial derivatives as in the previous case to satisfies the equation. The presence of ω (instead of ω^2) suggests us to involve only the first temporal derivative at the left member. Furthermore, in order to achieve the more general particular solution, we can try to use the complex wave function Ψ(x,t)=exp[i(kx−ωt)] which has all orders of its derivatives proportional to itself!

$$\frac{\partial \Psi(x,t)}{\partial t} = -i\omega \exp[i(kx - \omega t)] = -i\omega \Psi(x,t)$$

$$\frac{\partial \Psi(x,t)}{\partial x} = ik \exp[i(kx - \omega t)] \quad \rightarrow \quad \frac{\partial^2 \Psi(x,t)}{\partial x^2} = -k^2 \exp[i(kx - \omega t)] = -k^2 \Psi(x,t)$$

substituting:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V\Psi(x,t)$$ (Time-Dependent Schrodinger Equation – TDSE)

When E is constant (the only case we consider) we can avoid to substitute it in the equation E=T+V achieving the equation:

$$E\Psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V\Psi(x,t)$$ (Time-Independent Schrodinger Equation – TISE)

The Born's Interpretation Of The Wave Function

The Born's interpretation of the wave function Ψ is the basic postulate of the quantum mechanics. It states:

$|\Psi(x,t)|^2 dx$ is the probability to find the particle in the segment [x,x+dx] at time t

The quantity $|\Psi(x,t)|^2$ is a probability density and the wave function Ψ(x,t) is called "probability amplitude". This postulate implies that:

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 \, dx = 1$$

being the above integral the probability to find the particle everywhere. This equation is called normalisation condition.

The Born's interpretation of the wave function Ψ leads to a definition of both expected value <x> and variance Δx of the particle position x:

$$\langle x \rangle = \int_{-\infty}^{+\infty} x \, |\Psi(x,t)|^2 \, dx$$

$$(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle = \int_{-\infty}^{+\infty} (x - \langle x \rangle)^2 \, |\Psi(x,t)|^2 \, dx = \langle x^2 \rangle - 2 \langle x \rangle \langle x \rangle + \langle x \rangle^2 = \langle x^2 \rangle - \langle x \rangle^2$$

The Quantum Harmonic Oscillator

Since $V(x)=kx^2/2$, the Schrodinger's equation becomes (here k is the spring constant):

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + \left(\frac{k x^2}{2} - E\right)\Psi(x,t) = 0$$

The presence of x^2 suggests us:

1) the solution can be put in the form A $\exp(-(x/a)^2)$ because its second derivative create a term in x^2 that can be related with the existing term $kx^2/2$ coming from the potential energy;
2) since the potential energy is symmetric for x, after flattening due to $\exp(-(x/a)^2)$ one can consider any symmetric function containing terms like $(x/a)^n$ to be related with the existing term in x^2, i.e. symmetrical polynomials: n^{th}-order polynomials $H_n(x/a)$ containing only even or only odd powers of x/a;

The above considerations enable us to take into account solutions in the form (stationary in time):

$$\Psi(x,t) = A_n H_n\left(\frac{x}{a}\right) \exp\left(-\left(\frac{x}{a}\right)^2\right)$$

where "a" is a constant to be determined just inserting the solution into the equation, whereas A_n can be obtained forcing the solution to respect the normalisation condition. We have:

$$\Psi_x(x,t) = A_n H_n'\left(\frac{x}{a}\right)\frac{1}{a}\exp\left(-\left(\frac{x}{a}\right)^2\right) - A_n H_n\left(\frac{x}{a}\right)\frac{2x}{a^2}\exp\left(-\left(\frac{x}{a}\right)^2\right)$$

$$\Psi_{xx}(x,t) = A_n H_n''\left(\frac{x}{a}\right)\frac{1}{a^2}\exp\left(-\left(\frac{x}{a}\right)^2\right) - A_n H_n'\left(\frac{x}{a}\right)\frac{2x}{a^3}\exp\left(-\left(\frac{x}{a}\right)^2\right) -$$

$$- A_n\left(H_n'\left(\frac{x}{a}\right)\frac{2x}{a^3} + H_n\left(\frac{x}{a}\right)\frac{2}{a^2}\right)\exp\left(-\left(\frac{x}{a}\right)^2\right) + A_n H_n\left(\frac{x}{a}\right)\frac{4x^2}{a^4}\exp\left(-\left(\frac{x}{a}\right)^2\right) =$$

$$= A_n\left(H_n''\left(\frac{x}{a}\right)\frac{1}{a^2} - H_n'\left(\frac{x}{a}\right)\frac{4x}{a^3} - H_n\left(\frac{x}{a}\right)\frac{2}{a^2} + H_n\left(\frac{x}{a}\right)\frac{4x^2}{a^4}\right)\exp\left(-\left(\frac{x}{a}\right)^2\right)$$

substituting into the Schrodinger's equation:

$$-\frac{\hbar^2}{2m}\left(H_n''\left(\frac{x}{a}\right)\frac{1}{a^2} - H_n'\left(\frac{x}{a}\right)\frac{4x}{a^3} - H_n\left(\frac{x}{a}\right)\frac{2}{a^2} + H_n\left(\frac{x}{a}\right)\frac{4x^2}{a^4}\right) + \left(\frac{k x^2}{2} - E\right)H_n\left(\frac{x}{a}\right) = 0$$

that is:

$$-\frac{\hbar^2}{2m}H_n''\left(\frac{x}{a}\right)\frac{1}{a^2} + \left(\frac{\hbar^2}{2m}\frac{4x}{a^3}H_n'\left(\frac{x}{a}\right) + \frac{\hbar^2}{2m}\frac{2}{a^2}H_n\left(\frac{x}{a}\right) - E\,H_n\left(\frac{x}{a}\right)\right) + \left(-\frac{\hbar^2}{2m}\frac{4x^2}{a^4} + \frac{k x^2}{2}\right)H_n\left(\frac{x}{a}\right) = 0$$

the first term has degree n-2, the second term has degree n and the last term has degree n+2. Since:

$$H_n\left(\frac{x}{a}\right) = a_n \left(\frac{x}{a}\right)^n + a_{n-2}\left(\frac{x}{a}\right)^{n-2} + a_{n-4}\left(\frac{x}{a}\right)^{n-4} + \ldots$$

$$H_n'\left(\frac{x}{a}\right) = n\, a_n \left(\frac{x}{a}\right)^{n-1} + (n-2)\, a_{n-2}\left(\frac{x}{a}\right)^{n-3} + (n-4)\, a_{n-4}\left(\frac{x}{a}\right)^{n-5} + \ldots$$

$$H_n''\left(\frac{x}{a}\right) = n\,(n-1)\, a_n \left(\frac{x}{a}\right)^{n-2} + (n-2)\,(n-3)\, a_{n-2}\left(\frac{x}{a}\right)^{n-4} + (n-4)\,(n-5)\, a_{n-4}\left(\frac{x}{a}\right)^{n-6} + \ldots$$

Taking into account that:

$$\frac{x}{a} H_n'\left(\frac{x}{a}\right) = n\, a_n \left(\frac{x}{a}\right)^n + (n-2)\, a_{n-2}\left(\frac{x}{a}\right)^{n-2} + (n-4)\, a_{n-4}\left(\frac{x}{a}\right)^{n-4} + \ldots$$

We obtain:

COEFF of x^{n+2}: $\left(-\frac{\hbar^2}{2m}\frac{4}{a^4} + \frac{k}{2}\right) a_n = 0$

COEFF of x^n: $\left(\frac{\hbar^2}{2m}\frac{4}{a^2}\, n + \frac{\hbar^2}{2m}\frac{2}{a^2} - E\right) a_n + \left(-\frac{\hbar^2}{2m}\frac{4}{a^4} + \frac{k}{2}\right) a_{n-2} = 0$

COEFF of x^{n-2}: $-\frac{\hbar^2}{2m}\frac{1}{a^2}\, n\,(n-1)\, a_n + \left(\frac{\hbar^2}{2m}\frac{4}{a^2}(n-2) + \frac{\hbar^2}{2m}\frac{2}{a^2} - E\right) a_{n-2} + \left(-\frac{\hbar^2}{2m}\frac{4}{a^4} + \frac{k}{2}\right) a_{n-4} = 0$

COEFF of x^{n-4}: $-\frac{\hbar^2}{2m}\frac{1}{a^2}(n-2)\,(n-3)\, a_{n-2} + \left(\frac{\hbar^2}{2m}\frac{4}{a^2}(n-4) + \frac{\hbar^2}{2m}\frac{2}{a^2} - E\right) a_{n-4} + \left(-\frac{\hbar^2}{2m}\frac{4}{a^4} + \frac{k}{2}\right) a_{n-6} = 0$

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Simplifying:

COEFF of x^{n+2}: $-\frac{\hbar^2}{2m}\frac{4}{a^4} + \frac{k}{2} = 0 \quad \rightarrow \quad a^2 = \frac{2\hbar}{\sqrt{m k}}$

COEFF of x^n: $\frac{\hbar^2}{2m}\frac{4}{a^2}\, n + \frac{\hbar^2}{2m}\frac{2}{a^2} - E = 0 \quad \rightarrow \quad E = \frac{\hbar^2}{m}\frac{\sqrt{m k}}{2\hbar}(2n+1) = \hbar\sqrt{\frac{k}{m}}\left(n + \frac{1}{2}\right)$

COEFF of x^{n-2}: $-\frac{\hbar^2}{2m}\frac{1}{a^2}\, n\,(n-1)\, a_n - \frac{\hbar^2}{2m}\frac{4\cdot 2}{a^2}\, a_{n-2} = 0 \quad \rightarrow \quad n\,(n-1)\, a_n + 4\cdot 2\, a_{n-2} = 0$

COEFF of x^{n-4}: $-\frac{\hbar^2}{2m}\frac{1}{a^2}(n-2)\,(n-3)\, a_{n-2} - \frac{\hbar^2}{2m}\frac{4\cdot 4}{a^2}\, a_{n-4} = 0 \quad \rightarrow \quad (n-2)\,(n-3)\, a_{n-2} + 4\cdot 4\, a_{n-4} = 0$

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From the expression for x^n, we can state that only a finite number of energy levels are admitted:

$$E = \hbar\sqrt{\frac{k}{m}}\left(n + \frac{1}{2}\right) = \frac{1}{2}\hbar\sqrt{\frac{k}{m}}\,(2n+1) = E_0\,(2n+1)$$

giving as much as solutions. Where E_0 is the energy level corresponding to the level n=0. Using the value of E_0, from the expression for x^{n+2} we can also write:

$$a^2 = \frac{2\hbar}{\sqrt{m\,k}} = \frac{4\,E_0}{k}$$

From the last two expressions (x^{n-2} and x^{n-4}) we can also argue that:

$$(n-r)\,(n-(r+1))\,a_{n-r} = -4(r+2)\,a_{n-(r+2)} \qquad \rightarrow \qquad \text{putting: } n-r = s+2 \quad \text{we have:}$$

$$(s+2)\,(s+1)\,a_{s+2} = -4(n-s)\,a_s \quad \rightarrow \quad a_{s+2} = \frac{2(s-n)}{(s+2)\,(s+1)}\,a_s$$

This is the recursive definition of the Lagrange polynomials when forcing the coefficient of x^n to be 2^n and compute the others ones, in descending order:

```
n:= …:                                # polynomial order
c:= 2^n:                              # coeff of x^n
p:= c*(x/abs(a))^n:                   # polynomial
for s from n-2 by -2 to 0 do
      c:= c*((s+2)*(s+1))/(2*(s-n)):
      p:= p+c*(x/abs(a))^s:
end do:
```

Some solution (n=0,1,2,3) of the Schrodinger's harmonic oscillator equation are then:

Polynomial degree n	Energy	COEFF a_5	COEFF a_4	COEFF a_3	COEFF a_2	COEFF a_1	COEFF a_0	Coefficient A_n
0	E_0	-	-	-	-	-	1	$\sqrt{\frac{1}{a}\sqrt{\frac{2}{\pi}}}$
1	$3E_0$	-	-	-	-	2	0	$\sqrt{\frac{1}{a}\sqrt{\frac{2}{\pi}}}$
2	$5E_0$	-	-	-	4	0	-2	$\sqrt{\frac{1}{3a}\sqrt{\frac{2}{\pi}}}$
3	$7E_0$	-	-	8	0	-12	0	$\sqrt{\frac{1}{15a}\sqrt{\frac{2}{\pi}}}$
4	$9E_0$	-	16	0	-48	0	12	$\sqrt{\frac{1}{105a}\sqrt{\frac{2}{\pi}}}$
5	$11E_0$	32	0	-160	0	120	0	$\sqrt{\frac{1}{945a}\sqrt{\frac{2}{\pi}}}$

Where the values for A_n have been obtained using the normalisation condition:

$$\int_{-\infty}^{+\infty} \left| A_n\, H_n\left(\frac{x}{a}\right) \exp\left(-\left(\frac{x}{a}\right)^2\right)\right|^2 dx = 1 \quad \rightarrow \quad A_n = \sqrt{\frac{1}{\int_{-\infty}^{+\infty} \left| H_n\left(\frac{x}{a}\right) \exp\left(-\left(\frac{x}{a}\right)^2\right)\right|^2 dx}}$$

Classical and Quantum Harmonic Oscillator: Explicit Solutions

The probability density function can be then expressed as:

$$|\Psi(x,t)|_n^2 = b_n \left(\frac{1}{a}\sqrt{\frac{2}{\pi}}\right) H_n^2\left(\frac{x}{a}\right) \exp\left(-2\left(\frac{x}{a}\right)^2\right) = b_n \sqrt{\frac{k}{2\,E_0\,\pi}}\, H_n^2\left(\frac{x}{2}\sqrt{\frac{k}{E_0}}\right) \exp\left(-\frac{k}{2\,E_0}x^2\right)$$

where b_n is a constant only depending on n (not on a) (b_0=1, b_1=1, b_2=1/3, b_3=1/15, b_4=1/105).
Considering now as examples the cases n=1 ($E=E_0$), n=3 ($E=7E_0$) and n=5 ($E=11E_0$), we obtain the following expressions for the probability density function:

$$f_0(x) := |\Psi(x,t)|_0^2 = \sqrt{\frac{k}{2\,E\,\pi}} \exp\left(-\frac{k}{2\,E}x^2\right)$$

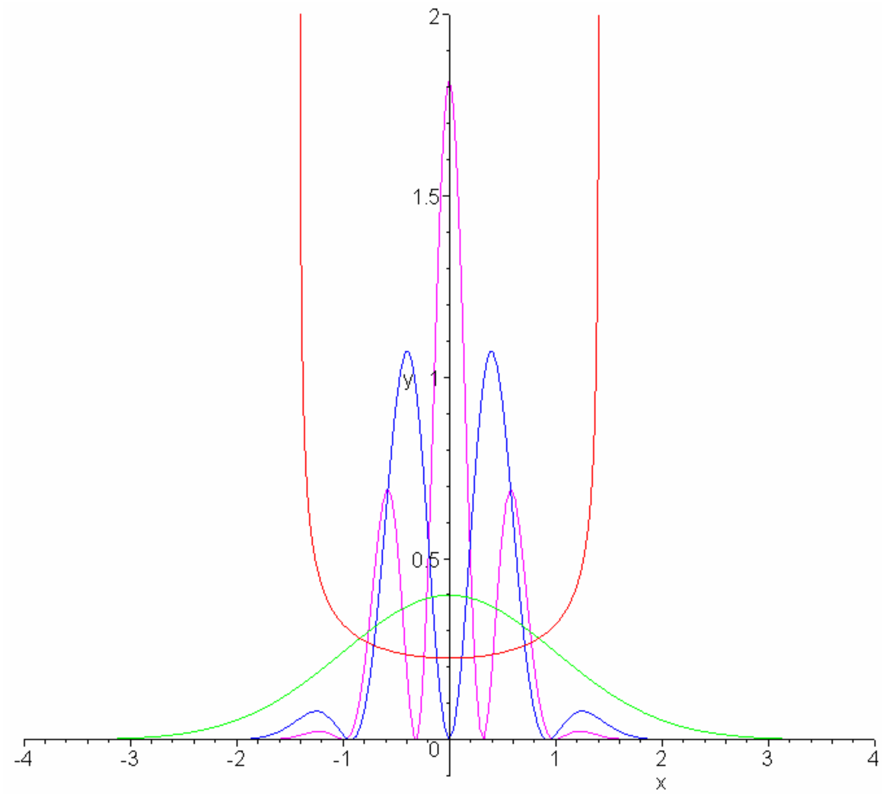
$$f_3(x) := |\Psi(x,t)|_3^2 = \frac{1}{15}\sqrt{\frac{7\,k}{2\,E\,\pi}} \left[8\left(\frac{x}{2}\sqrt{\frac{7\,k}{E}}\right)^3 - 12\left(\frac{x}{2}\sqrt{\frac{7\,k}{E}}\right)\right]^2 \exp\left(-\frac{7\,k}{2\,E}x^2\right)$$

$$f_4(x) := |\Psi(x,t)|_4^2 = \frac{1}{105}\sqrt{\frac{11k}{2\,E\,\pi}} \left[16\left(\frac{x}{2}\sqrt{\frac{11k}{E}}\right)^4 - 48\left(\frac{x}{2}\sqrt{\frac{11k}{E}}\right)^2 + 12\right]^2 \exp\left(-\frac{11k}{2\,E}x^2\right)$$

Recalling that for the classical harmonic oscillator we had:

$$f(x) = \frac{1}{\pi}\frac{1}{\sqrt{\frac{2\,E}{k} - x^2}}$$

setting E/k=1, the graphs of the previous functions are those reported in the next figure (f=red, f_0=green, f_3=blue, f_4=magenta):



The Heisenberg's Uncertainty Principle

The Heisenberg's uncertainty principle can be written as:

$$\Delta x \, \Delta p \geq \frac{\hbar}{2}$$

and its physical meaning is that it is not possible to determine the position x and the momentum p of a particle with an error less than that indicated in the previous formula. The quantities Δx and Δp are defined statistically by the Born's interpretation of the wave function. The mathematical proof of this principle is based on the special relationship existing between the wave function $\Psi(x,t)$ and its Fourier's transform.

It is known that the Fourier's transform of a function f(t) defined in the time domain gives a function $F(\omega)$ in the temporal frequency domain $\omega=2\pi/T$ being T the period of a generic component of f(t). Analogously the Fourier's transform of a function g(x) defined in a spatial domain provides a function G(k) in the spatial frequency domain $k=2\pi/\lambda$ where λ is the spatial period (wavelength) of a generic component of g(x). When the Fourier's transform is applied to a quantum wave function $\Psi(x,t)$ a modified normalisation factor ($1/\sqrt{2\pi\hbar}$ instead of $1/\sqrt{2\pi}$) is normally used:

$$\underline{\Psi}(k,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x,t) \exp(-i\,k\,x)\, dx$$

Since $p=h/\lambda$ we can express k as $k=2\pi/\lambda=2\pi p/h=p/\hbar$ so putting $\Gamma(p,t)=\underline{\Psi}(p/\hbar,t)$ the transformation pair becomes:

$\Gamma(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x,t) \exp(-i\,p\,x/\hbar)\, dx$	$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Gamma(p,t) \exp(i\,p\,x/\hbar)\, dp$

Before give a proof of the uncertainty principle, it is necessary review some properties of the Fourier's transform:

Parseval-Plancherel Theorem (PPT): for any Fourier transform pairs f(x), F(p), g(x), G(p):

$$\int_{-\infty}^{\infty} f(x)\, g^*(x)\, dx = \int_{-\infty}^{\infty} F(p)\, G^*(p)\, dp \qquad \text{in fact:}$$

$$\int_{-\infty}^{\infty} f(x)\, g^*(x)\, dx = \int_{-\infty}^{\infty} f(x) \left(\frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} G^*(p) \exp(-i\,p\,x/\hbar)\, dp \right) dx =$$

$$= \int_{-\infty}^{\infty} G^*(p) \left(\frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} f(x) \exp(-i\,p\,x/\hbar)\, dx \right) dp = \int_{-\infty}^{\infty} G^*(p)\, F(p)\, dp$$

From PPT we also have:

$$1 = \int_{-\infty}^{\infty} |\Psi|^2\, dx = \int_{-\infty}^{\infty} \Psi\, \Psi^*\, dx = \int_{-\infty}^{\infty} \Gamma\, \Gamma^*\, dp = \int_{-\infty}^{\infty} |\Gamma|^2\, dp$$

Complex Inequality (CI): for any two complex numbers z, w:

$$|z\,w| \ge \frac{1}{2}(z\,w^* + z^*\,w)$$

because putting $z = Z\,e^{i\alpha}$ and $w = W\,e^{i\beta}$ it is easy obtain:

$$\frac{1}{2}(z\,w^* + z^*\,w) = \frac{1}{2}\left[ZW\,(e^{i(\alpha-\beta)} + e^{-i(\alpha-\beta)}\right] = ZW\cos(\alpha-\beta) \le ZW = |z\,w|$$

Fourier's Transforms of Differentiated Functions (FTD): for any Fourier transform pair f, F it is easily achieve:

$$FT\{f'(x)\} = \frac{i}{\hbar}\,p\,F(p) \qquad \text{in fact:}$$

$$f'(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} F(p)\,\frac{\partial}{\partial x}\exp(\,i\,p\,x/\hbar\,)\,dp = \frac{i}{\hbar}\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} p\,F(p)\exp(\,i\,p\,x/\hbar\,)\,dp = \frac{i}{\hbar}\,IFT\{p\,F(p)\}$$

Uncertainty Principle Proof: Putting:

$$(\Delta x)^2 = \langle (x - \langle x\rangle)^2\rangle := \langle a^2\rangle \qquad (\Delta p)^2 = \langle (p - \langle p\rangle)^2\rangle := \langle b^2\rangle$$

we can write:

$$(\Delta x)^2(\Delta p)^2 = \langle a^2\rangle\langle b^2\rangle = \int_{-\infty}^{+\infty} a^2\,|\Psi(x,t)|^2\,dx\int_{-\infty}^{+\infty} b^2\,|\Gamma(p,t)|^2\,dp =$$

$$= \int_{-\infty}^{+\infty} a^2\,|\Psi(a-\langle x\rangle,t)|^2\,da\int_{-\infty}^{+\infty} b^2\,|\Gamma(b-\langle p\rangle,t)|^2\,db = \int_{-\infty}^{+\infty}|\,a\,\Psi(a-\langle x\rangle,t)\,|^2\,da\int_{-\infty}^{+\infty}|\,b\,\Gamma(b-\langle p\rangle,t)\,|^2\,db =$$

using FTD on the last integral:

$$= \int_{-\infty}^{+\infty}|\,a\,\Psi(a-\langle x\rangle,t)\,|^2\,da\int_{-\infty}^{+\infty}\left|\,\frac{\hbar}{i}\,FT\{\Psi'(a-\langle x\rangle,t)\}\,\right|^2\,db =$$

using now PPT on the second integral and then the Schwartz inequality:

$$= \hbar^2\int_{-\infty}^{+\infty}|\,a\,\Psi(a-\langle x\rangle,t)\,|^2\,da\int_{-\infty}^{+\infty}|\,\Psi'(a-\langle x\rangle,t)\,|^2\,da \ge \hbar^2\left(\int_{-\infty}^{+\infty}|\,a\,\Psi(a-\langle x\rangle,t)\,\Psi'(a-\langle x\rangle,t)\,|\,da\right)^2 \ge$$

and finally using CI:

$$\ge \hbar^2\left(\int_{-\infty}^{+\infty}\frac{a}{2}\left(\,\Psi^*(a-\langle x\rangle,t)\,\Psi'(a-\langle x\rangle,t) + \Psi(a-\langle x\rangle,t)\,(\Psi')^*(a-\langle x\rangle,t)\,\right)da\right)^2 =$$

$$= \frac{\hbar^2}{4}\left(\int_{-\infty}^{+\infty} a \frac{\partial}{\partial a} \left(\Psi^*(a - \langle x\rangle,t)\, \Psi(a - \langle x\rangle,t) \right) da \right)^2 = \frac{\hbar^2}{4}\left(\int_{-\infty}^{+\infty} a \frac{\partial}{\partial a} |\, \Psi(a - \langle x\rangle,t)\, |^2 \, da \right)^2 =$$

$$= \frac{\hbar^2}{4}\left(\int_{-\infty}^{+\infty} a \, d\, |\, \Psi(a - \langle x\rangle,t)\, |^2 \right)^2 = \frac{\hbar^2}{4}\left(\left[a \,|\, \Psi(a - \langle x\rangle,t)\, |^2 \right]_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} |\, \Psi(a - \langle x\rangle,t)\, |^2 \; da \right)^2 = \frac{\hbar^2}{4}$$

being $\Psi(\pm\infty) = 0$ (wave packets) and the last integral equal to 1.

Time-Energy Uncertainty: If v is the velocity of the particle, since:

$$\Delta x \sim v\, \Delta t \qquad \text{and} \qquad \Delta E \sim \frac{\partial E}{\partial p} \Delta p \sim v\, \Delta p \qquad \rightarrow \qquad \Delta t\, \Delta E \sim \Delta x\, \Delta p = \frac{\hbar}{2}$$

so we find that the uncertainty principle works for the pair time-energy as well as the pair space-momentum.

The Klein-Gordon's Equation

In deriving the Schrodinger's equation we used the classical expression for the total energy E=T+V. When we consider particles with relativistic velocity we have to use the relativistic expression of the energy:

$$E = \sqrt{(pc)^2 + (mc^2)^2} + V$$

We obtain:

$$(E - V)^2 = (pc)^2 + (mc^2)^2 \qquad \rightarrow \qquad (h\nu)^2 - 2\, h\nu \; V + V^2 = (pc)^2 + (mc^2)^2 \qquad \rightarrow$$

$$(\hbar\omega)^2 - 2\, \hbar\omega \; V + V^2 = \frac{h^2\, c^2}{\lambda^2} + (mc^2)^2 = \hbar^2\, c^2\, k^2 + (mc^2)^2 \qquad \rightarrow$$

$$\hbar^2\omega^2\, \Psi - 2\, \hbar\omega\, V\, \Psi + V^2\, \Psi = \hbar^2\, c^2\, k^2\, \Psi + (mc^2)^2\, \Psi$$

Taking into account the complex wave function $\Psi(x,t)=\exp[i(kx-\omega t)]$ whose derivatives have already been obtained:

$$\frac{\partial\, \Psi(x,t)}{\partial\, t} = - i\omega\, \Psi(x,t) \qquad \frac{\partial^2\, \Psi(x,t)}{\partial\, t^2} = - \omega^2\, \Psi(x,t) \qquad \frac{\partial\, \Psi(x,t)}{\partial\, x} = i\, k\, \Psi(x,t) \qquad \frac{\partial^2\, \Psi(x,t)}{\partial\, x^2} = - k^2\, \Psi(x,t)$$

and substituting we obtain the Klein-Gordon equation (KGE):

$$- \hbar^2 \frac{\partial^2\, \Psi(x,t)}{\partial\, t^2} - 2\, i\, \hbar\, V \frac{\partial\, \Psi(x,t)}{\partial\, t} + V^2\, \Psi(x,t) = - \hbar^2\, c^2 \frac{\partial^2\, \Psi(x,t)}{\partial\, x^2} + (mc^2)^2\, \Psi(x,t)$$

In particular for a free photon (V=m=0) it becomes the classical wave equation with propagation velocity equal to c. When E is constant we can avoid substituting it in the previous computation achieving the equation:

$$(E - V)^2\, \Psi(x,t) = - \hbar^2\, c^2 \frac{\partial^2\, \Psi(x,t)}{\partial\, x^2} + (mc^2)^2\, \Psi(x,t)$$

The Klein-Gordon equation allows negative energies as solution explained as energy due to the presence of antimatter. The positron was discovered after the Klein proposed his equation. Furthermore Ψ don't allow for statistical interpretation of $|\Psi|^2$ as being probability density because its integral would not remain constant. This is not really a problem since relativistic quantum mechanical equation has to allow for creation and annihilation of particles so the integral probability doesn't have to stay necessarily constant. The Klein-Gordon equation describes the behaviour of the bosons.

The Dirac's Equation

Dirac's intuition is in trying to achieve a wave-like equation only involving the first order time derivative. In order to preserve the Lorentz's invariance, then also the space derivative must be of the first order.
In both the Schrodinger and Klein-Gordon equations the total energy is a function of the momentum p and of the mass m. In general Dirac tried to find two coefficients α and β such that E was linear in p and m and satisfied the relativistic expression for the energy.

$$E = \alpha\, p + \beta\, m + V \quad \rightarrow \quad (E - V)^2 = (\alpha\, p + \beta\, m)^2 = \alpha^2\, p^2 + \beta^2\, m^2 + (\alpha\beta + \beta\alpha)\, p\, m$$

To be compliant with the relativistic energy equation:

$$(E - V)^2 = (pc)^2 + (mc^2)^2 \qquad \alpha \text{ and } \beta \text{ must satisfy the system: } \begin{cases} \alpha^2 = c^2 \\ \beta^2 = c^4 \\ \alpha\beta + \beta\alpha = 0 \end{cases}$$

This system has no solutions in the field of the complex numbers but it has solution if we consider the coefficients α and β as matrices. In this case, called I the unitary matrix, we want satisfy the system:

$$\begin{cases} \alpha^2 = c^2\, I \\ \beta^2 = c^4\, I \\ \alpha\beta + \beta\alpha = 0\, I \end{cases} \qquad \text{In fact, defining:} \qquad \alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} \xi & 0 \\ 0 & -\xi \end{pmatrix}$$

We have:

$$\alpha^2 = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}\begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} = \begin{pmatrix} \sigma^2 & 0 \\ 0 & \sigma^2 \end{pmatrix} = \sigma^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \sigma^2\, I$$

$$\beta^2 = \begin{pmatrix} \xi & 0 \\ 0 & -\xi \end{pmatrix}\begin{pmatrix} \xi & 0 \\ 0 & -\xi \end{pmatrix} = \begin{pmatrix} \xi^2 & 0 \\ 0 & \xi^2 \end{pmatrix} = \xi^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \xi^2\, I$$

$$\alpha\,\beta + \beta\,\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}\begin{pmatrix} \xi & 0 \\ 0 & -\xi \end{pmatrix} + \begin{pmatrix} \xi & 0 \\ 0 & -\xi \end{pmatrix}\begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} = \begin{pmatrix} 0 & -\sigma\xi \\ \sigma\xi & 0 \end{pmatrix} + \begin{pmatrix} 0 & \sigma\xi \\ -\sigma\xi & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = 0\, I$$

so it is enough put σ=c and $\xi=c^2$:

$$\alpha = \begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix} = c \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = c\, I \qquad \beta = \begin{pmatrix} \xi & 0 \\ 0 & -\xi \end{pmatrix} = c^2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = c^2\, L$$

Then we have:

$$\begin{aligned} & E\,\Psi\, I = \alpha\, p\, \Psi + \beta\, m\, \Psi + V\, I = (pc)\,\Psi\, I + (mc^2)\,\Psi\, L + V\, I \\ \rightarrow\quad & h\nu\,\Psi\, I = (hc/\lambda)\,\Psi\, I + (mc^2)\,\Psi\, L + V\, I \\ \rightarrow\quad & \hbar\omega\,\Psi\, I = c\hbar k\,\Psi\, I + (mc^2)\,\Psi\, L + V\, I \end{aligned}$$

so substituting as usual the quantities ωΨ and kΨ we obtain the Dirac's equations (DE):

$$i\,\hbar \frac{\partial\, \Psi(x,t)}{\partial\, t}\, I = -\, i\, c\, \hbar \frac{\partial\, \Psi(x,t)}{\partial\, x}\, I + mc^2\, \Psi(x,t)\, L + V\, \Psi(x,t)\, I$$

The Dirac's equation for mass-less particles (m=0) is called Weyl's equation. Dirac and Weyl equations are used to describe the behaviour of the fermions (leptons and quarks) which often can be considered mass-less.

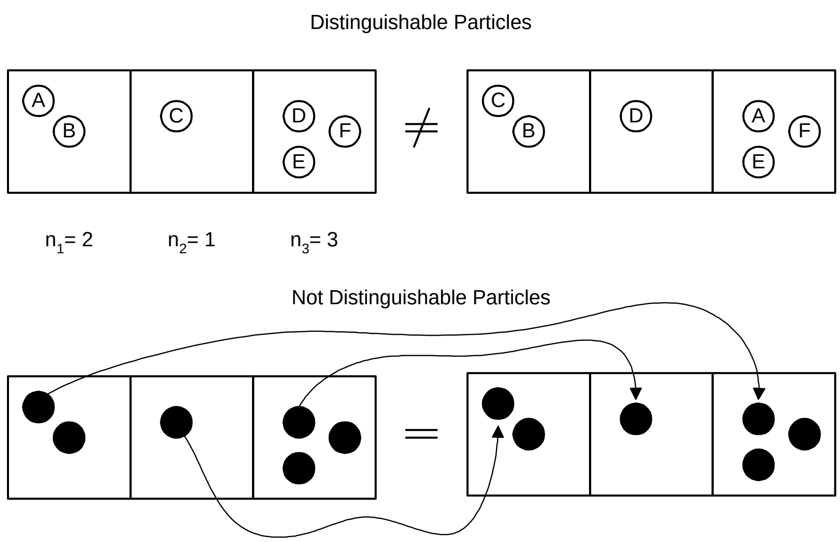
Statistic Mechanics

Introduction

The energy E of a system constituted by a finite number “n” of particles can be divided up in a finite number N of energy levels E_i in order to have n_i particles belonging to each of these levels. The following relationships hold:

$$n = \sum_{i=1}^{N} n_i \qquad E = \sum_{i=1}^{N} n_i E_i$$

A MACROSTATE is a sequence $(n_1, n_2, \ldots, n_N)$ representing the number of particles assigned to the N energy levels $(E_1, E_2, \ldots, E_N)$.
A MICROSTATE, contributing to a given MACROSTATE, is one of possible distributions of the particles realising the sequence $(n_1, n_2, \ldots, n_N)$ of that MACROSTATE. The number of MICROSTATES contributing to the same MACROSTATE $(n_1, n_2, \ldots, n_N)$ is indicated by the function of several variables $\Omega(n_1,n_2,..,n_N)$.
If the particles are not distinguishable we cannot enumerate the MICROSTATES and $\Omega=1$ as shown by the following example:



In case of distinguishable particles we can obtain the same MACROSTATE (2,1,3) with many distributions of the particles (the picture shows at least two of these distributions). Conversely, in case of not distinguishable particles, an exchange between particles cannot be recognised if it leaves unchanged the number of particles in the various energy levels (bottom side of the picture) and only one distribution is highlighted leading to $\Omega=1$.
We can now calculate the number of MICROSTATES $\Omega(n_1,n_2,..,n_N)$ realising a given MACROSTATE $(n_1,n_2,..,n_N)$ in case of distinguishable particles.

$$\Omega(n_1,n_2,..,n_N) = \binom{n}{n_1}\binom{n-n_1}{n_2}\binom{n-n_1-n_2}{n_3}\cdots\binom{n_N+n_{N-1}}{n_{N-1}}\binom{n_N}{n_N} =$$

$$= \frac{n!}{n_1!\,(n-n_1)!}\,\frac{(n-n_1)!}{n_2!\,(n-n_1-n_2)!}\,\frac{(n-n_1-n_2)!}{n_3!\,(n-n_1-n_2-n_3)!}\cdots\frac{(n_N+n_{N-1})!}{n_{N-1}!\,n_N!}\,\frac{n_N!}{n_N!\,0!} = \frac{n!}{\prod_{k=1}^{N} n_k!}$$

To obtain a formula compliant with both the previous situations (distinguishable and not distinguishable particles where $\Omega(n_1,n_2,..,n_N)=1$) we can write the previous relationship as:

$$\Omega(n_1,n_2,..,n_N) = \prod_{k=1}^{N} \frac{\sqrt[N]{n!}}{n_k!} = \prod_{k=1}^{N} f_k(n_1,n_2,..,n_N)$$

where $f_k(n_1,n_2,..,n_N) = 1$ for each k when the particles are not distinguishable.
A further aspect to take into account is that inside each energy level more than one status is admissible and so also the possible distributions of the particles inside each energy level must be computed in determining the number of MICROSTATES that lead to the same MACROSTATE. This computing depends on the model we assume to describe these sublevels. Three models have been proposed which are coherent with the experimental facts in different situations.

- **Maxwell-Boltzmann (MB) statistic:** valid for describing the behaviour of the classical ideal gases and solids;
- **Bose-Einstein (BE) statistics:** valid to describe the behaviour of the bosons in quantum mechanics (particles that can stay in any number in a given quantum state like photons and integer-spin particles);
- **Fermi-Dirac (FD) statistic**: valid to describe the behaviour of the fermions in quantum mechanics (particles that can stay at most one per quantum state like electrons, positrons, quarks and other half-integer-spin particles);

For each statistic model we assume that inside the energy level E_i, a certain number of sub-levels g_i are possible. These sub-levels are necessary to distinguish particles that have the same energy but different states like for example different position in a solid (where the classical MB statistics can be applied) or different spin in an atom (where BE or FD statistics are applied). If $\Theta(g_k,n_k)$ is the function describing the number of MICROSTATES generated scrambling the n_k particles belonging to the energy level E_k over the g_k possible sublevels, then the total number of MICROSTATES contributing to the same MACROSTATE $(n_1,n_2,..,n_N)$ is given by:

$$\Phi(n_1,n_2,..,n_N,g_1,g_2,..,g_N) = \prod_{k=1}^{N} f_k(n_1,n_2,..,n_N)\,\Theta(g_k,n_k)$$

The most probable MACROSTATE is the MACROSTATE realised by the maximum number of MICROSTATES so it is possible determine it maximising the function Φ in the N variables $(n_1,n_2,..,n_N)$ considering the quantities $(g_1,g_2,..,g_N)$ as constants.

Maxwell-Boltzmann's Statistic

Each particle can belong or not to a given state inside the energy level E_k so that, being the particles distinguishable, at each of them can be associated any number included in $1..g_k$. Following these approach, n_k particles provide g_k^{nk} configurations. Next table gives an example for $n_k=2$ (particle A, B) and $g_k=3$ (states 1,2,3), in this case $3^2=9$ configurations are generated.

A	B
1	1
1	2
1	3
2	1
2	2
2	3
3	1
3	2
3	3

$\rightarrow$ $\Theta_{MB}(g_k,n_k) = g_k^{n_k}$

Furthermore, being in this case:

$$f_k(n_1,n_2,..,n_N) = \frac{\sqrt[N]{n!}}{n_k!}$$

for each k, we obtain for Φ_{MB} (Maxwell-Boltzmann Φ):

$$\Phi_{MB}(n_1,n_2,..,n_N,g_1,g_2,..,g_N) = n! \prod_{k=1}^{N} \frac{g_k^{n_k}}{n_k!}$$

Applying the Stirling formula $n! \approx n \log n - n$, and taking into account that $n=\sum n_k$, $\log(\Phi_{MB})$ can be written as:

$$\log\left(\Phi_{MB}(n_1,n_2,..,n_N,g_1,g_2,..,g_N) \right) = n \log(n) - n + \sum_{k=1}^{N} \left(n_k \log(g_k) - n_k \log(n_k) + n_k\right) =$$

$$= \log(n) \sum_{k=1}^{N} n_k + \sum_{k=1}^{N} \left(n_k \log(g_k) - n_k \log(n_k)\right) = \sum_{k=1}^{N} n_k \log \frac{n}{n_k} + \sum_{k=1}^{N} n_k \log(g_k) = \sum_{k=1}^{N} n_k \log \frac{n\, g_k}{n_k}$$

In particular for $g_k=1$ for each k we obtain the so called Boltzmann statistic (no sub-states are foreseen).

$\log\left(\Phi_{MB}(n_1,n_2,..,n_N,g_1,g_2,..,g_N) \right) = \sum_{k=1}^{N} n_k \log \frac{n\, g_k}{n_k}$	$\log\left(\Phi_{B}(n_1,n_2,..,n_N,g_1,g_2,..,g_N) \right) = \sum_{k=1}^{N} n_k \log \frac{n}{n_k}$

Bose-Einstein's Statistic

Being the particles not distinguishable, putting for example $n_k=2$ (particle A, B) and $g_k=3$ (states 1,2,3), the two following configurations must considered only once:

A	-	B

B	-	A

Strictly speaking we couldn't label the particles. Here the labels are used to describe the counting process.
To consider only once the above configurations we can proceed as follows:

1. Fix the order of the particles not admitting the possibility to change their position; for example in case of 6 particles:

A	B	C	D	E	F

2. Insert between the particles g_k-1 barriers in order to create g_k states; for example in case of 6 particles and 3 barriers:

A ▌	B	C ▌	D ▌	E	F

3. Count in how many ways we can insert the g_k-1 identical barriers between (n_k+g_k-1) objects (particles and barriers). Since the barriers are identical, this can be done in a number of ways given by:

$$\Theta_{BE}(g_k,n_k) = \binom{n_k+g_k-1}{g_k-1}$$

Since in Bose-Einstein the particles are not distinguishable we have $f_k(n_1,n_2,..,n_N) = 1$ for each k so:

$$\Phi_{BE}(n_1,n_2,..,n_N,g_1,g_2,..,g_N) = \prod_{k=1}^{N} \binom{n_k+g_k-1}{g_k-1} \approx \prod_{k=1}^{N} \binom{n_k+g_k}{g_k}$$

Applying the Stirling formula $n! \approx n \log n - n$, $\log(\Phi_{BE})$ can be written as:

$$\log\left(\Phi_{BE}(n_1,n_2,..,n_N,g_1,g_2,..,g_N)\right) = \sum_{k=1}^{N} \left((n_k + g_k) \log(n_k + g_k) - (n_k + g_k) - n_k \log(n_k) + n_k - g_k \log(g_k) + g_k \right) =$$

$$= \sum_{k=1}^{N} \left((n_k + g_k) \log(n_k + g_k) - n_k \log(n_k) - g_k \log(g_k) \right) = \sum_{k=1}^{N} n_k \log \frac{n_k + g_k}{n_k} + \sum_{k=1}^{N} g_k \log \frac{n_k + g_k}{g_k}$$

Fermi-Dirac's Statistic

This statistic is based on the same hypotheses of the Bose-Einstein statistic plus the validity of the Pauli exclusion principle: in a given status, belonging to the generic energy level E_k, at most one particle can be present (the hypothesis $n_k<g_k$ is adopted). Considering the example of 4 particles distributed among 6 status:

	•	•		•	

It is easy to deduce that:

$$\Theta_{FD}(g_k,n_k) = \binom{g_k}{n_k} \quad \rightarrow \quad \Phi_{FD}(n_1,n_2,..,n_N,g_1,g_2,..,g_N) = \prod_{k=1}^{N} \binom{g_k}{n_k}$$

Applying the Stirling formula $n! \approx n \log n - n$, $\log(\Phi_{FD})$ can be written as:

$$\log\left(\Phi_{FD}(n_1,n_2,..,n_N,g_1,g_2,..,g_N)\right) = \sum_{k=1}^{N} \left(g_k \log(g_k) - g_k - (g_k - n_k) \log(g_k - n_k) + (g_k - n_k) - n_k \log(n_k) + n_k \right) =$$

$$= \sum_{k=1}^{N} \left(g_k \log(g_k) - (g_k - n_k) \log(g_k - n_k) - n_k \log(n_k) \right) = \sum_{k=1}^{N} n_k \log \frac{g_k - n_k}{n_k} - \sum_{k=1}^{N} g_k \log \frac{g_k - n_k}{g_k}$$

The most probable macrostate

In order to proceed with a common approach for all the statistics defined above, we can define the function:

$$\log\left(\Phi(n_1,n_2,..,n_N)\right) = \sum_{k=1}^{N} n_k \log \frac{\lambda\, g_k + \mu\, n_k}{n_k} - \mu \sum_{k=1}^{N} g_k \log \frac{\lambda\, g_k + \mu\, n_k}{g_k}$$

from which the three different statistics can be obtained assigning to λ and μ the following values:

λ	μ	Φ
n	0	Φ_{MB}
1	1	Φ_{BE}
1	-1	Φ_{FD}

The most probable MACROSTATE can be then obtained maximising the quantity $\log(\Phi(n_1,n_2,..,n_N))$, as function of the variables $(n_1,n_2,..,n_N)$, with the constraints:

$$n = \sum_{i=1}^{N} n_i \qquad\qquad E = \sum_{i=1}^{N} n_i E_i$$

Such a problem can be solved using the Lagrange's multipliers method which suggests us to maximise the following unconstrained function of N+2 variables:

$$\Gamma(n_1,n_2,..,n_N,\alpha,\beta) = \log(\Phi(n_1,n_2,..,n_N)) + \alpha\left(n - \sum_{i=1}^{N} n_i \right) + \beta\left(E - \sum_{i=1}^{N} n_i E_i \right)$$

Following this approach, first of all we have to compute:

$$\frac{\partial\,\Gamma(n_1,n_2,..,n_N,\alpha,\beta)}{\partial\, n_k} = \log\frac{\lambda\, g_k + \mu\, n_k}{n_k} + n_k \frac{n_k}{\lambda\, g_k + \mu\, n_k}\frac{\mu\, n_k - (\lambda\, g_k + \mu\, n_k)}{n_k^2} + \mu\, g_k \frac{g_k}{\lambda\, g_k + \mu\, n_k}\frac{\mu}{g_k} - \alpha - \beta\, E_k =$$

$$= \log\frac{\lambda\, g_k + \mu\, n_k}{n_k} + \frac{-\lambda\, g_k}{\lambda\, g_k + \mu\, n_k} + \mu^2\frac{g_k}{\lambda\, g_k + \mu\, n_k} - \alpha - \beta\, E_k = \log\frac{\lambda\, g_k + \mu\, n_k}{n_k} + \frac{(\mu^2 - \lambda)\, g_k}{\lambda\, g_k + \mu\, n_k} - \alpha - \beta\, E_k =$$

$$= \log\frac{\lambda\, g_k + \mu\, n_k}{n_k} + (\mu^2 - 1) - \alpha - \beta\, E_k$$

where we have used the previous table to simplify the last term. The maximum of the function is obtained making equal to zero this derivative:

$$n_k = \frac{\lambda\, g_k}{e^{\alpha + \beta E_k - (\mu^2 - 1)} - \mu}$$

These are the distributions (for all the statistics varying the parameters λ and μ) of the n particles that realise the most probable MACROSTATE.
Making equal to zero the remaining derivatives $\partial\Gamma/\partial\alpha$ and $\partial\Gamma/\partial\beta$ we obtain back the constraint equations so, substituting the values n_k as expressed by the distribution above, we have a system of transcendental equations like:

$$n = \sum_{i=1}^{N} n_i(\alpha,\beta) \qquad\qquad E = \sum_{i=1}^{N} n_i(\alpha,\beta)\, E_i$$

which has no explicit solution for α and β. These quantities will be determined using arguments from thermodynamic. Nevertheless it is obvious that these solutions are of the type:

$$\alpha = G_\alpha(n,E,N) \qquad\qquad \beta = G_\beta(n,E,N)$$

that is both α and β depend on the values n (total number of particles), E (total energy of the system) and N (number of available volume cells). If we then insert the quantities n_k into the function $\Phi(n_1,n_2,..,n_N)$ we achieve an expression of Φ as function of parameters n, E and N:

$$\Phi = G(n,E,N)$$

Since in thermodynamic the volume is indicated with V, it is convenient change N with V:

$$\Phi = G(n,E,V)$$

Entropy

In thermodynamic the entropy S is defined through the first and second principle as follow:

$$1°)\quad đQ = dE + đL \qquad 2°)\quad đQ = T\,dS \qquad \rightarrow \qquad T\,dS = dE + đL$$

being the system under consideration characterised by a quantity of heat Q at temperature T, an total energy E and a work L carried out when it moves from a state to another.
Since we also have:

$$đL = PdV - \eta dn$$

being P and V the pressure and volume of the system and ηdn the work associated to variation of the total particles number. The expression T dS = dE + đL can be then written as:

$$T\,dS = dE + PdV - \eta dn \qquad \rightarrow \qquad S = F(n,E,V)$$

The analogy between this relation and the expression obtained for $\Phi = G(n,E,V)$ suggests that there exist a function f such that:

$$S = f(\Phi)$$

This function lead to the Boltzmann's relation between entropy and disorder and can be determined as follow.

Let us consider two systems with entropy S_1 and S_2 and disorder Φ_1 and Φ_2. As we know the total disorder of the system (system 1 plus system 2) can be obtained counting the total amount of the possible states that is:

$$\Phi = \Phi_1\,\Phi_2$$

Whereas the total entropy of the system is just (S is defined adding additive quantities E, V, n so it is an additive quantity):

$$S = S_1 + S_2$$

Furthermore the following equation holds:

$$f(\Phi_1\,\Phi_2) = f(\Phi) = S = S_1 + S_2 = f(\Phi_1) + f(\Phi_2)$$

then:

$$\frac{\partial f(\Phi_1)}{\partial \Phi_1} = \frac{\partial f(\Phi_1\Phi_2)}{\partial \Phi_1} - \frac{\partial f(\Phi_2)}{\partial \Phi_1} = \frac{\partial f(\Phi_1\Phi_2)}{\partial (\Phi_1\Phi_2)}\,\Phi_2$$

and:

$$\frac{\partial f(\Phi_2)}{\partial \Phi_2} = \frac{\partial f(\Phi_1\Phi_2)}{\partial \Phi_2} - \frac{\partial f(\Phi_1)}{\partial \Phi_2} = \frac{\partial f(\Phi_1\Phi_2)}{\partial (\Phi_1\Phi_2)}\,\Phi_1$$

so:

$$\Phi_1 \frac{\partial f(\Phi_1)}{\partial \Phi_1} = \Phi_2 \frac{\partial f(\Phi_2)}{\partial \Phi_2} = k \qquad \rightarrow \qquad f(\Phi_1) = k \log \Phi_1 \quad \text{and} \quad f(\Phi_2) = k \log \Phi_2$$

where k is a constant by separation of variables. From these we have the Boltzmann's relation:

$$S = S_1 + S_2 = f(\Phi_1) + f(\Phi_2) = k \log (\Phi_1\Phi_2) = k \log (\Phi)$$

The constant k is the Boltzmann's constant.

The Lagrange's Multipliers

Recalling that for the most probable MACROSTATE we have:

$$\log \frac{\lambda\, g_k + \mu\, n_k}{n_k} + (\mu^2 - 1) - \alpha - \beta\, E_k = 0 \qquad \rightarrow \qquad \log \frac{\lambda\, g_k + \mu\, n_k}{n_k} + (\mu^2 - 1) = \alpha + \beta\, E_k$$

and:

$$\frac{\partial \log \Phi(n_1,n_2,..,n_N)}{\partial\, n_k} = \log \frac{\lambda\, g_k + \mu\, n_k}{n_k} + (\mu^2 - 1) \qquad \rightarrow \qquad \frac{\partial \log \Phi(n_1,n_2,..,n_N)}{\partial\, n_k} = \alpha + \beta\, E_k$$

Using the Boltzmann's formula $S = k \log(\Phi)$, we can write:

$$\frac{\partial\, S}{\partial\, n_k} = k\,(\,\alpha + \beta\, E_k\,)$$

so:

$$dS = \sum_{h=1}^{N} \frac{\partial\, S}{\partial\, n_h} dn_h = k \sum_{h=1}^{N} (\,\alpha + \beta\, E_h\,)\, dn_h = k\,\alpha \sum_{h=1}^{N} dn_h + k\,\beta \sum_{h=1}^{N} E_h\, dn_h =$$

$$= k\,\alpha \sum_{h=1}^{N} dn_h + k\,\beta \sum_{h=1}^{N} d(E_h\, n_h) - k\,\beta \sum_{h=1}^{N} n_h\, dE_h$$

recalling that:

$$n = \sum_{i=1}^{N} n_i \qquad\qquad E = \sum_{i=1}^{N} n_i\, E_i$$

we obtain:

$$T\, dS = T\, k\, \alpha\, dn + T\, k\, \beta\, dE + T\, k\, \beta\, dW$$

Where W is a suitable function. If we consider now the expression previously obtained by the first and second principle of the thermodynamic:

$$T\, dS = dE + PdV - \eta dn$$

We can argue that:

$$T\, k\, \alpha = -\eta; \qquad T\, k\, \beta = 1; \qquad dW = PdV \qquad \rightarrow \qquad \alpha = -\frac{\eta}{k\, T}; \qquad \beta = \frac{1}{k\, T}$$

so finally the distributions can be explicitly written as:

$$n_k = \frac{\lambda\, g_k}{e^{\frac{E_k - \eta}{k\, T} - (\mu^2 - 1)} - \mu}$$

Appendix I: Atomic Physic

Elementary Particles

All the elementary particles can be subdivided into two classes: Fermions and Bosons.

- **Fermions**: any particle that obeys Fermi-Dirac statistics and is subject to the Pauli's exclusion principle. All the particles constituting the nuclear and atomic structure are fermions (including electrons, protons and neutrons). All fermions have half integer spin.
- **Bosons**: any particle that obeys Bose-Einstein statistics but not the Pauli's exclusion principle. All nuclei with an even mass number are bosons. Bosons act to transmit forces between fermions. The photon, gluon, and the *W* and *Z* particles are bosons. All bosons have integer spin.

All the particles that interact strongly with other particles are called **Hadrons** and can be subdivided into two categories:

- **Baryons**: any of the elementary particles having a mass equal to or greater than that of a proton (+1 baryon number). Each baryon is a fermion. Protons and neutrons are baryons. Baryons are constituted by 3 quarks with half-integral spin. Baryons can be stable or unstable.
- **Mesons**: an elementary particle responsible for the forces in the atomic nucleus (0 baryon number). Each meson is a boson. Mesons are constituted by quark-antiquark pairs with integral spin. No meson is stable.

Fermions are the fundamental matter of the universe and can be divided into:

- **Leptons**: an elementary particle that participates in weak interactions (0 baryon number).
- **Quarks**: fundamental particle in mesons and baryons.

FERMIONS matter constituents spin = 1/2, 3/2, 5/2, ...

Leptons spin = 1/2			Quarks spin = 1/2		
Flavor	Mass GeV/c^2	Electric charge	Flavor	Approx. Mass GeV/c^2	Electric charge
ν_e electron neutrino	$<1\times10^{-8}$	0	u up	0.003	2/3
e electron	0.000511	–1	d down	0.006	–1/3
ν_μ muon neutrino	<0.0002	0	c charm	1.3	2/3
μ muon	0.106	–1	s strange	0.1	–1/3
ν_τ tau neutrino	<0.02	0	t top	175	2/3
τ tau	1.7771	–1	b bottom	4.3	–1/3

Baryons qqq and Antibaryons $\bar{q}\bar{q}\bar{q}$

Baryons are fermionic hadrons. There are about 120 types of baryons.

Symbol	Name	Quark content	Electric charge	Mass GeV/c^2	Spin
p	proton	uud	1	0.938	1/2
$\bar{p}$	anti-proton	$\bar{u}\bar{u}\bar{d}$	–1	0.938	1/2
n	neutron	udd	0	0.940	1/2
Λ	lambda	uds	0	1.116	1/2
Ω^-	omega	sss	–1	1.672	3/2

Mesons $q\bar{q}$

Mesons are bosonic hadrons. There are about 140 types of mesons.

Symbol	Name	Quark content	Electric charge	Mass GeV/c^2	Spin
π^+	pion	$u\bar{d}$	+1	0.140	0
K^-	kaon	$s\bar{u}$	–1	0.494	0
ρ^+	rho	$u\bar{d}$	+1	0.770	1
B^0	B-zero	$d\bar{b}$	0	5.279	0
η_c	eta-c	$c\bar{c}$	0	2 .980	0

Fundamental Forces

The fundamental forces can be classified according to the next table:

Force	Description
Gravity	Attractive – acts on all particles
Electromagnetic	Attracts or repels electric charges: bends charges in magnetic fields
Weak	Responsible for transmuting particles: Up→←Down, Electron/Muon→←Neutrino
Strong	Holds hadrons together by gluing quarks: exchanges information between hadrons, e.g. to hold nuclei together

More details are given in the table below:

PROPERTIES OF THE INTERACTIONS

Property \ Interaction	Gravitational	Weak (Electroweak)	Electromagnetic (Electroweak)	Strong: Fundamental	Strong: Residual
Acts on:	Mass – Energy	Flavor	Electric Charge	Color Charge	See Residual Strong Interaction Note
Particles experiencing:	All	Quarks, Leptons	Electrically charged	Quarks, Gluons	Hadrons
Particles mediating:	Graviton (not yet observed)	W^+ W^- Z^0	γ	Gluons	Mesons
Strength relative to electromag for two u quarks at: 10^{-18} m	10^{-41}	0.8	1	25	Not applicable to quarks
Strength relative to electromag for two u quarks at: 3×10^{-17} m	10^{-41}	10^{-4}	1	60	
for two protons in nucleus	10^{-36}	10^{-7}	1	Not applicable to hadrons	20

Whilst classically fields are defined throughout space and act on particles, quantum mechanically, fields are force particles exchanged between matter particles.

In principle, weak force is just another force, however, the major victory of theoretical physics was finding a structure which could include electromagnetism and weak forces in a single set of fields.

The W & Z bosons were discovered in 1981, exactly where they were predicted to be!