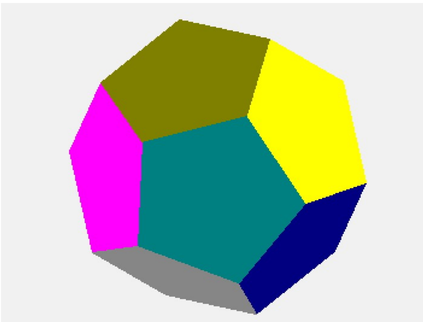
# Solving Partial Differential Equations Using generalized coordinates



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# Contents

## 1. Introduction

After a brief description of some linear partial differential equations and their classification, we shall discuss methods of obtaining solutions which satisfy given boundary and initial conditions. The elementary method of separation of variables and its application to classical boundary value problems is described in section 2. The closely related topics of eigenvalue problems and Greens functions is treated in the article http://olewitthansen.dk/Mathematics/Vector_analysis.pdf

The Examples that will be treated below are

**1. Equation of the vibrating string, or the one dimensional wave equation.**

$$\frac{\partial^2\psi}{\partial x^2}-\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2}=0$$

$c$ is the speed of the wave. For a flexible string $c^2 = F_s/\rho$ where $F_s$ is the tension, and $\rho$ is the density per unit length.

**2. Laplace's equation:**

$$\nabla^2\psi=\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)=0$$

**3. The three dimensional wave equation**

$$\nabla^2\psi-\frac{1}{c^2}\frac{\partial^2\psi}{dt^2}$$

**4. The diffusion equation**

$$\nabla^2\psi-\frac{1}{\kappa}\frac{\partial\psi}{\partial t}=0$$

Here $\psi$ is the temperature, and $\kappa=\frac{K}{C\rho}=\frac{thermal\ conductivity}{(specific\ heat)x(density)}$

**5. The Schrödinger equation**

$$-\frac{\hbar^2}{2m}\nabla^2\psi+V(\vec{r})\psi=i\hbar\frac{\partial\psi}{dt}$$

These are the equations, of which we will mostly occupy ourselves. Note that they are all linear second order differential equations.
The equations above are all homogenous, which means that if $\psi$ is a solution so is any multiple of $\psi$. Many problems involve an inhomogenous equation containing a term corresponding to

"applied" forces or sources. For example, if a force *f*(*x,t*) is applied to a vibrating string the equation is an inhomogenous one.

$$\frac{\partial^2\psi}{\partial x^2}-\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2}=-\frac{1}{F_s}f(x,t)$$

A problem may be inhomogenous because of the boundary conditions as well as because of the equation itself. The criterion for a homogenous boundary value problem, is the one stated above, that is, if $\psi$ is the solution of the equation and the boundary conditions then is also a multiple of $\psi$.

An example of an inhomogenous boundary condition is the vibrating string for which the end is prescribed to move in a definite way. $\psi(0,t)=f(t)$. The general solution to an inhomogenous equation is composed of a particular solution plus the complete solution to the homogenous equation

## 2. General discussion. (May be bypassed. Not relevant for the examples)

Before proceeding to concrete methods for solving equations like those just given, we shall briefly discuss the general linear second order partial differential equation. We shall make one restriction, however, and consider only two independent variables. This is done in order to simplify matters and to draw understandable pictures. Most of the reasoning can be generalized to equations with more independent variables.

We have then a function $\psi(x,y)$ to be evaluated in some region of the (*x,y*) plane. The partial differential equation will certainly need to be supplemented by boundary conditions of some sort. We will suppose these to involve $\psi$ and/or some of its derivatives which encloses the region within which, we are trying to solve the equation.

There are three common types of boundary conditions.

1. Dirichlet conditions: $\psi$ is specified at each point at the boundary.

4. Neumann condition: $(\nabla\psi)_n$ the normal component of the gradient of $\psi$ is specified at each point of the boundary.

3. Cauchy conditions: $\psi$ and $(\nabla\psi)_n$ are specified at each point of the boundary.

By analogy with ordinary second order differential equations, we would expect that Cauchy conditions along a line would be the most natural set of boundary conditions. However things are not so simple.

For an ordinary (that is one dimensional) second order differential equation for $\psi(x)$ the specification of $\psi$ and $\psi'$ at an ordinary point $x_0$ together with higher derivatives at $x_0$. and thus ensure the existence of a solution in the form of a Taylor series near the curve.

We now investigate the corresponding question for second order partial differential equations, namely, whether the specification of $\psi$ and $(\nabla\psi)_n$. Along a boundary curve together with the differential equation itself is sufficient to determine the second and higher derivatives of $\psi$ on the boundary curve, and thus ensure the existence of a solution in the form of a Taylor series near the curve. Let us suppose that our boundary curve is described parametrically by the equations

$x = x(s) \quad y = y(s)$, where $s$ is the arc length along the boundary. Figure (8.1). We shall suppose that we are given $\psi(s)$ and its normal derivative $N(s)$ along the boundary. The components of the unit normal $\vec{n}$ are $-\left(\frac{dy}{ds}\right),\left(\frac{dx}{ds}\right)$ , so that

$$N(s) = -\frac{\partial \psi}{\partial x}\frac{dy}{ds} + \frac{\partial \psi}{\partial y}\frac{dx}{ds}$$

$$\frac{d}{ds}\psi(s) = \frac{\partial \psi}{\partial x}\frac{dx}{ds} + \frac{\partial \psi}{\partial y}\frac{dy}{ds}$$

May be solved for the first partial derivative of $\psi$ :

$$\frac{\partial \psi}{\partial x} = -N(s)\frac{dy}{ds} + \left[\frac{d}{ds}\psi(s)\right]\frac{dx}{ds}$$

$$\frac{\partial \psi}{\partial y} = -N(s)\frac{dx}{ds} + \left[\frac{d}{ds}\psi(s)\right]\frac{dy}{ds}$$

The trouble comes with the second derivatives. There are three:

$$\frac{\partial^2 \psi}{\partial x^2} \qquad \frac{\partial^2 \psi}{\partial x \partial y} \qquad \frac{\partial^2 \psi}{\partial y^2}$$

Two equations for these are found by differentiating the known first derivatives along the boundary.

$$\frac{d}{ds}\frac{\partial \psi}{\partial x} = \frac{\partial^2 \psi}{\partial x^2}\frac{dx}{ds} + \frac{\partial^2 \psi}{\partial y^2}\frac{dy}{ds}$$

$$\frac{d}{ds}\frac{\partial \psi}{\partial y} = \frac{\partial^2 \psi}{\partial x \partial y}\frac{dx}{ds} + \frac{\partial^2 \psi}{\partial y^2}\frac{dy}{ds}$$

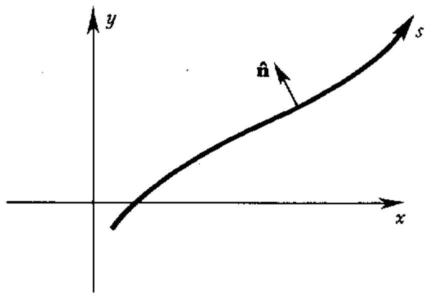



**Figure 8–1 A boundary curve and unit vector n̂ normal to it**

A third equation is provided by the original differential equation, which we shall write in the form

$$A\frac{\partial^2\psi}{\partial x^2}+2B\frac{\partial^2\psi}{\partial x\partial y}+C\frac{\partial^2\psi}{\partial y^2}=f(x,y,\frac{\partial\psi}{\partial x},\frac{\partial\psi}{\partial y})$$

Where $f(x,y,\frac{\partial\psi}{\partial x},\frac{\partial\psi}{\partial y})$ is some function. These three (inhomogenous) equations can be solved for the second partial derivative of $\psi$ unless the determinant of the coefficients vanishes.

$$\begin{vmatrix} \frac{dx}{ds} & \frac{dy}{ds} & 0 \\ 0 & \frac{dx}{ds} & \frac{dy}{ds} \\ A & 2B & C \end{vmatrix}=0 \quad \text{or} \quad A\left(\frac{dy}{ds}\right)^2-2B\frac{dx}{ds}\frac{dy}{ds}+C\left(\frac{ds}{ds}\right)^2=0$$

At each point in the *xy*-plane this equation determines two directions, the so called characteristic direction at that point. Curves in the *xy*-plane whose tangents at each point lie along characteristic directions are called characteristics of the partial differential equation.
Thus the second derivatives are determined except in the case where the boundary curve is tangent to a characteristic somewhere. By further differentiations a similar set of simultaneous equations for the third (and higher) derivatives may be found, and the condition for a solution involves a determinant which is exactly the one above. Thus Cauchy boundary conditions will determine the solution if the boundary curve is nowhere tangent to a characteristic.
Returning to the equation (1.15) for the characteristics, if the characteristics are to be real curves , we clearly must have $B^2 > AC$. Partial differential equations obeying are called hyperbolic equations. If $B^2 = AC$ the equation is said to by parabolic, if $B^2 < AC$ the equation is elliptic. of the examples in the beginning numbers 1 and 3 are hyperbolic, number 2 is elliptic and number 4 and 5 are parabolic. The Schrödinger equation is a little unusual, however, since not all the coefficients are real.
Let us discuss the choice of boundary conditions which is appropriate for each of the three types of equation, beginning with the hyperbolic. We have seen above, generally speaking, Cauchy conditions along a curve, which is not a characteristic is sufficient are sufficient to specify the solution near the curve. A useful picture for visualizing the role of the characteristics and boundary conditions is obtained by thinking of the characteristics as curves along which the partial information about the solution propagates. The meaning of this statement and the way in which it works are most easily understood with the aid of an elementary example.

## Example

Consider the simplest hyperbolic equation, having $A = 1$, $B = 0$ and $C$ = constant = $1/c^2$, that is, the one dimensional wave equation.

$$\frac{\partial^2\psi}{\partial x^2}-\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2}=0$$

For which the equation of characteristic is

$$\left(\frac{\partial t}{\partial s}\right)^2 - \frac{1}{c^2}\left(\frac{\partial x}{\partial s}\right)^2 = 0 \qquad \text{or} \qquad \left(\frac{\partial x}{\partial t}\right)^2 = c^2$$

Thus the characteristics are straight lines. $(x-ct)=\xi$ and $(x+ct)=\eta$.
The families of lines are shown in the figure below.

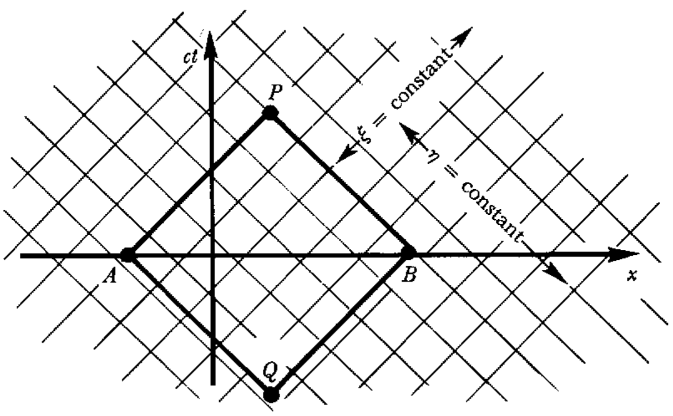



**Figure 8–2 Characteristics for the one-dimensional wave equation**

The characteristics form a natural set of coordinates for a hyperbolic equation. For example if we transform equation to the new coordinates $\xi,\eta$, defined by (1.17), we obtain the equation in so called normal form.

$$\frac{\partial^2\psi}{\partial\xi\partial\eta} = 0$$

The solution is immediate:

$$\psi = f(\varsigma) + g(\eta)$$

where *f* and *g* are arbitrary functions.
Now, if we know $\psi(x)$ and its normal derivative $N(x) = c^{-1}(\partial\psi/\partial t)$ along the line segment *AB* of figure 8-2, we can find the individual functions $f(\varsigma), g(\eta)$ specifically,

$$\psi(x,t=0) = f(x) + g(x)$$

And

$$\frac{1}{c}\frac{\partial\psi}{\partial t}(x,t=0) = -f'(x) + g'(x)$$

From which

$$f(x) = \tfrac{1}{2}\psi(x) - \tfrac{1}{2c}\int\frac{\partial\psi}{\partial t}dx$$

$$g(x) = \tfrac{1}{2}\psi(x) + \tfrac{1}{2c}\int\frac{\partial\psi}{\partial t}dx$$

The arbitrary constant is of no importance since it cancels in the sum $\psi == f + g$ everywhere.

The values of $f(x)$ along the line segment determine $f(\xi)$ along all the characteristics $\xi =$ constant, which intersects *AB*. Similarly the values of $g(x)$ determine $g(\eta)$ along the curves $\eta =$ constant which intersects *AB*.
Both $f(\xi)$ and $g(\eta)$, and thus $\psi(x,t)$ are determined within the common region traversed by both kinds of characteristics, which is the rectangle *AQBP* in figure 8-4.
The results obtained for the simple example above hold generally for hyperbolic equations.
Suppose the net of characteristics as is shown in figure 8 – 3, where *SS'* is a boundary curve.
Cauchy condition along an arc *AB* of the boundary determine the solution within the "triangular" – shaped regions on each side, bounded by characteristics through *A* and *B*.

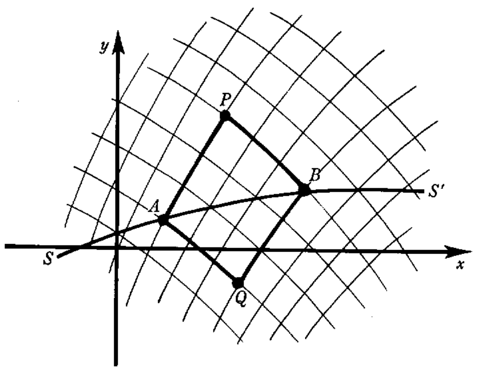
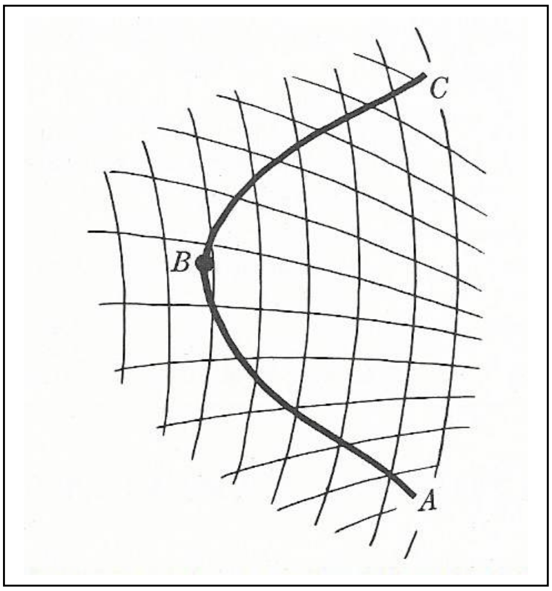



**Figure 8–3** **Characteristics for a hyperbolic equation, and a boundary curve *SS'* not tangent to a characteristic. Cauchy conditions along the arc *AB* of *SS'* fix the solution within the region *AQBP***




The above picture enables us to discuss more complicated situations. For example the boundary of net shown in figure 8 – 4. Cauchy conditions from *A* to *B* determine the behaviour along all the vertical characteristics which intersects the boundary *ABC,* and along the horizontal characteristics which intersect the arc *AB*. All that is left is the specification of the behaviour along the horizontal characteristics, starting between *B* and *C*. Thus Dirichlet or Neumann conditions along *BC* suffice. Cauchy conditions are here too much to over determine the solution.
Rather than elaborating further on the formal theory of partial differential equations, we shall illustrate the ideas, by doing some well known examples.

Reference: Jon Mathews and R.L. Walker: Mathematical methods of physics

## 3.1 Wave in one dimension

The wave equation in one dimension reads

$$\frac{\partial^2\psi}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2\psi}{dt^2} = 0 \qquad (3.1)$$

The general method to solve this kind of equation is separation of variables.

$$\psi(x,t) = X(x)T(t)$$

This leads to

$$T\frac{\partial^2 X}{\partial x^2} = \frac{1}{c^2} X \frac{\partial^2 T}{\partial t^2}$$

And by dividing by $XT$

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = \frac{1}{c^2}\frac{1}{T}\frac{\partial^2 T}{\partial t^2}$$

Since the left side depends only on $x$, and the right side depends only on $t$, then both sides must be equal to the same constant, say $-\omega^2$. A positive constant would lead to exponential increasing or decreasing functions. Although such solutions appear in the physical world, we shall only treat the "wave" solutions.

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = \frac{1}{c^2}\frac{1}{T}\frac{\partial^2 T}{\partial t^2} = -\omega^2 \quad \Rightarrow \quad \frac{1}{X}\frac{\partial^2 X}{\partial x^2} = -\omega^2 \quad \wedge \quad \frac{1}{c^2}\frac{1}{T}\frac{\partial^2 T}{\partial t^2} = -\omega^2$$

(3.2) $$\frac{\partial^2 X}{\partial x^2} = -X\omega^2 \quad \wedge \quad \frac{\partial^2 T}{\partial t^2} = -c^2\omega^2 T$$

The solutions to these equations are the familiar trigonometric functions.

(3.3) $$X = Ae^{i\omega x+\varphi} \quad \text{or} \quad X = A\cos(\omega t+\varphi) \quad \text{and}$$
$$T = Ae^{-ic\omega t+\varphi} \quad \text{or} \quad T = A\cos(c\omega t+\varphi)$$

Giving the solution

$$\psi = XT = Ae^{i\omega(x-ct)+\varphi} \quad \text{or} \quad \psi = A\cos(\omega(x-ct)+\varphi)$$

Which are the equivalent equations for propagation of a wave having the speed c.

The solutions to the equations (X.X) may however be much easier accomplished, using the fundamental characteristics of wave propagation.
A wave is characterized by having a constant "shape", but where the shape of the wave moves with a constant speed $v$.
Let the fluctuations of a wave at position $x$, and time $t$ be denoted

(3.4) $$u = u(x,t).$$

Thus the fluctuation at $x = 0$ becomes $u = u(0,t) = f(t)$, where $f(t)$ may be an (almost) arbitrary function of $t$.

Since the shape of the wave is unchanged, then the fluctuation at $x$ at time $t$, must be the same as the fluctuation at $x$, but at an earlier time, namely the time takes the wave to move from $x = 0$ to $x$, which is $x/v$. Thus:

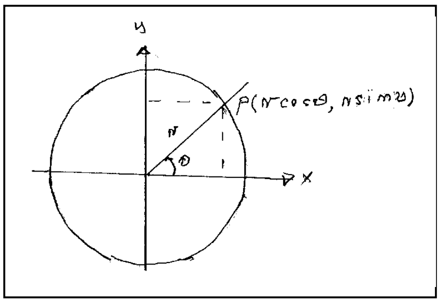
$$u = u(x,t) = u(0, t - \frac{x}{v}) = f(t - \frac{x}{v})$$

It is straightforward to verify, that $f(t - \frac{x}{v})$ is a solution to the wave equation.

$$\frac{\partial^2 \psi}{\partial x^2} - \frac{1}{v^2}\frac{\partial^2 \psi}{dt^2} = 0 \quad \Rightarrow \quad \frac{\partial^2 f}{\partial x^2} - \frac{1}{v^2}\frac{\partial^2 f}{dt^2} = 0 \quad \Leftrightarrow \quad \frac{1}{v^2} f'' - \frac{1}{v^2} f'' = 0$$

If we put $v = \frac{\omega}{k}$ we find the more familiar expression for *f*: $u(x,t) = f(\omega t - kx)$, or if the fluctuations are harmonic. $u(x,t) = A\cos(\omega t - kx + \varphi)$.

## 4. Polar coordinates in the plane and space




The polar coordinates in the plane are usually chosen as $(r, \theta)$ as shown in the figure: We have:

(4.1) $$x = r\cos\theta \quad and \quad y = r\sin\theta$$

The infinitesimal distance vector is seen geometrically to be: $d\vec{s} = (rd\theta, dr)$

Since the direction of $rd\theta$ *and* $dr$ are orthogonal the square of the distance element is.

(4.2) $$ds^2 = r^2 d\theta^2 + dr^2$$

And the area element *dA* is:

(4.3) $$dA = rd\theta dr$$

These results obtained geometrically, may also be formally proven, by making a coordinate transformation.

$$dx = \frac{\partial x}{\partial \theta} d\theta + \frac{\partial x}{\partial r} dr = -r\sin\theta d\theta + \cos\theta dr$$

$$dy = \frac{\partial y}{\partial \theta} d\theta + \frac{\partial y}{\partial r} dr = r\cos\theta d\theta + \sin\theta dr$$

$$ds^2 = dx^2 + dy^2 = (-r\sin\theta d\theta + \cos\theta dr)^2 + (r\cos\theta d\theta + \sin\theta dr)^2 \quad \Rightarrow$$

(4.4) $$ds^2 = r^2 d\theta^2 + dr^2$$

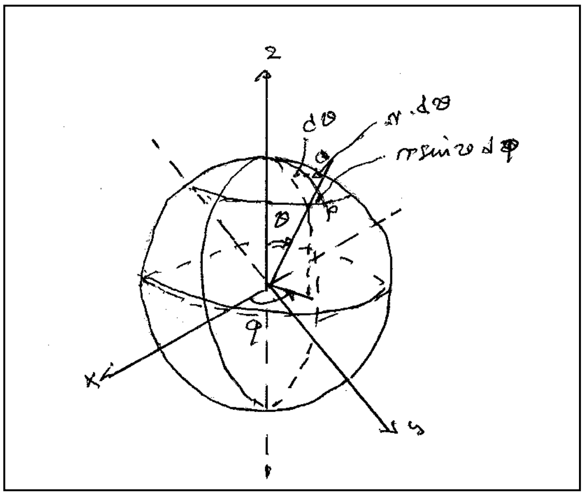
Since we shall consider a rotational symmetric wave, we shall seek the Laplace operator in polar coordinates.

## 5. ***Orthogonal*** curvilinear coordinates

For general *orthogonal* curvilinear coordinates in the plane $(p_1, p_2)$ or in space $(p_1, p_2, p_3)$, the distance element is $d\vec{s} = (g_1 dp_1, g_2 dp_2)$ in the plane, and in space is: $d\vec{s} = (g_1 dp_1, g_2 dp_2, g_3 dp_3)$.
Here the *g's* are generally functions of the coordinates $(p_1, p_2)$ or $(p_1, p_2, p_3)$.
If the curvilinear coordinate displacements are orthogonal we have:

(5.1) $$ds^2 = g_1^{\ 2} dp_1^{\ 2} + g_2^{\ 2} dp_2^{\ 2} \quad \text{and} \quad ds^2 = g_1^{\ 2} dp_1^{\ 2} + g_2^{\ 2} dp_2^{\ 2} + g_3^{\ 2} dp_3^{\ 2}$$

In *space* a point $P(x, y, z)$ has the polar coordinates $(r, \theta, \varphi)$. See the figure below. $\theta$ is the polar angle and $\varphi$ is the azimuth angle.
The coordinates are then, when expressed by the radius and the two angles.



(5.1) $x = r\sin\theta\cos\varphi,\ \ y = r\sin\theta\sin\varphi,\ z = r\cos\theta$

To come from one point $P\ (r,\theta,\varphi)$ to another $Q(r+dr,\ \theta + d\theta,\ \varphi + d\varphi)$, you first go "horizontally" $r\sin\theta\ d\varphi$ then "vertically" the distance $rd\theta$, and finally the radial distance $dr$.
The infinitesimal distance vector therefore becomes

(5.2) $d\vec{s} = (r\sin\theta d\phi,\ rd\theta,\ dr)$

Since the three "steps" are perpendicular to each other, the square of the distance is:

(5.3) $ds^2 = r^2 d\theta^2 + r^2\sin^2\theta d\varphi^2 + dr^2$

Likewise the infinitesimal volume element is the product of the three orthogonal steps.

(5.2) $$dV = r^2\sin\theta d\theta d\varphi dr$$

The gradient of a scalar field in the *plane* is defined as:

(5.3) $$\vec{\nabla} u = \left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right)$$

The significance of the gradient is: $du = \dfrac{\partial u}{\partial x} dx + \dfrac{\partial u}{\partial y} dy = \vec{\nabla} u \cdot (dx, dy)$

That is, the infinitesimal increase in $u$ resulting from the displacement $(dx, dy)$.

The infinitesimal displacement along the curvilinear coordinates is in the plane

$$d\vec{s} = (g_1 dp_1, g_2 dp_2)$$

and in space:

$$d\vec{s} = (g_1 dp_1, g_2 dp_2, g_3 dp_3)$$

Above $dx$ is replaced by $g_1 dp_1$ and so on, and therefore the gradient of a scalar field $U$ in plane curvilinear becomes.

$$\vec{\nabla} U = (\frac{\partial U}{\partial x}, \frac{\partial U}{\partial y}) \qquad \to \qquad \vec{\nabla} U = (\frac{1}{g_1}\frac{\partial U}{\partial p_1}, \frac{1}{g_2}\frac{\partial U}{\partial p_2})$$

And in space:

(5.4) $$\vec{\nabla} U = (\frac{\partial U}{\partial x}, \frac{\partial U}{\partial y}, \frac{\partial U}{\partial z}) \qquad \to \qquad \vec{\nabla} U = (\frac{1}{g_1}\frac{\partial U}{\partial p_1}, \frac{1}{g_2}\frac{\partial U}{\partial p_2}, \frac{1}{g_3}\frac{\partial U}{\partial p_3})$$

Since $d\vec{s} = (rd\theta, dr)$ in polar coordinates in the plane we have:

(5.5) $$\vec{\nabla} U = (\frac{1}{r}\frac{\partial U}{\partial \theta}, \frac{\partial U}{\partial r})$$

And in polar coordinates in space: $d\vec{s} = (r\sin\theta d\varphi, rd\theta, dr)$

(5.6) $$\vec{\nabla} U = (\frac{1}{r\sin\theta}\frac{\partial U}{\partial \varphi}, \frac{1}{r}\frac{\partial U}{\partial d\theta}, \frac{\partial U}{\partial r})$$

Concerning the divergence, things become somewhat more complicated: This comes about because the lines inclosing the "rectangular" square or box in curvilinear coordinates are not straight lines, so the area of the front end and the back end are not necessarily equal.

In space the areas of a box with sides (1-2) (1-3) and (2-3) are

$$\Delta A_{23} = g_2 g_3 \Delta p_2 \Delta p_3 \,, \quad \Delta A_{13} = g_1 g_3 \Delta p_1 \Delta p_3 \,, \quad \Delta A_{12} = g_1 g_2 \Delta p_1 \Delta p_2 \,,$$

So in the calculation of the "change of flux", along one of the coordinates in a Cartesian coordinate system, which is: $\frac{\partial u_x}{\partial x}\Delta x \Delta y \Delta z$ must be replaced by

$\frac{1}{g_1}\frac{\partial}{\partial p_1}(g_2 g_3 u_1) g_1 \Delta p_1 \Delta p_2 \Delta p_3 = \frac{\partial}{\partial p_1}(g_2 g_3 u_1)\Delta p_1 \Delta p_2 \Delta p_3$, because $g_2 g_3$ may depend on $p_1$.

The divergence of a vector field, however, is defined as the flux out of the volume $dV$:

$$\int \vec{\nabla} \cdot \vec{u} dV$$

The flux in curvilinear coordinates calculated in this manner from a "curvelinear" box is, however:

(5.7)
$$\int (\frac{\partial}{\partial p_1}(g_2 g_3 u_1) + \frac{\partial}{\partial p_2}(g_1 g_3 u_2) + \frac{\partial}{\partial p_3}(g_1 g_2 u_3)) dp_1 dp_2 dp_3 =$$
$$\int \frac{1}{g_1 g_2 g_3}(\frac{\partial}{\partial p_1}(g_2 g_3 u_1) + \frac{\partial}{\partial p_2}(g_1 g_3 u_2) + \frac{\partial}{\partial p_3}(g_1 g_2 u_3)) g_1 dp_1 g_2 dp_2 g_3 dp_3$$

Since $dV = g_1 dp_1 g_2 dp_2 g_3 dp_3$ is the correct expression for the volume element, the divergence becomes.

(5.8)
$$\vec{\nabla} \cdot \vec{u} = \frac{1}{g_1 g_2 g_3}\left(\frac{\partial}{\partial p_1}(g_2 g_3 u_1) + \frac{\partial}{\partial p_2}(g_1 g_3 u_2) + \frac{\partial}{\partial p_3}(g_1 g_2 u_3)\right)$$

In the *plane* we get in the same manner:

(5.9)
$$\vec{\nabla} \cdot \vec{u} = \frac{1}{g_1 g_2}\left(\frac{\partial}{\partial p_1}(g_2 u_1) + \frac{\partial}{\partial p_2}(g_1 u_2)\right)$$

Using polar coordinates in the plane we have: $d\vec{s} = (r d\theta, dr)$, so we find:

(5.10)
$$\vec{\nabla} \cdot \vec{u} = \frac{1}{r}\left(\frac{\partial u_1}{\partial \theta} + \frac{\partial}{\partial r}(r u_2)\right) = \frac{1}{r}\frac{\partial u_1}{\partial \theta} + \frac{1}{r}\frac{\partial (r u_2)}{\partial r}$$

And for the Laplace operator in the plane we find:

$$\nabla^2 U = \vec{\nabla} \cdot \vec{\nabla} U = \vec{\nabla} \cdot (\frac{1}{r}\frac{\partial U}{\partial \theta}, \frac{\partial U}{\partial r}) = \frac{1}{r}\frac{\partial}{\partial \theta}(\frac{1}{r}\frac{\partial U}{\partial \theta}) + \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial U}{\partial r})$$

(5.11)
$$\nabla^2 U = \frac{1}{r^2}\frac{\partial^2 U}{\partial \theta^2} + \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial U}{\partial r})$$

## 5.1 The Laplace operator in space

We have already shown using the notation we introduced above:

$d\vec{s} = (g_1 dp_1, g_2 dp_2, g_3 dp_3) = (r \sin\theta d\phi, r d\theta, dr)$ and $ds^2 = r^2 \sin^2\theta d\varphi^2 + r^2 d\theta^2 + dr^2$

So we have: $g_1 = r\sin\theta, g_2 = r, g_3 = 1$

The gradient of a scalar field *U* becomes:

$$\vec{\nabla} U = (\frac{1}{g_1}\frac{\partial U}{\partial p_1}, \frac{1}{g_2}\frac{\partial U}{\partial p_2}, \frac{1}{g_3}\frac{\partial U}{\partial p_3}) \quad = \quad \vec{\nabla} U = (\frac{1}{r\sin\theta}\frac{\partial U}{\partial \varphi}, \frac{1}{r}\frac{\partial U}{\partial \theta}, \frac{\partial U}{\partial r})$$

For the divergence of a vector $\vec{u} = (u_1, u_{2,} u_3)$ we then have

$$\vec{\nabla} \cdot \vec{u} = \frac{1}{g_1 g_2 g_3}\left(\frac{\partial}{\partial p_1}(g_2 g_3 u_1) + \frac{\partial}{\partial p_2}(g_1 g_3 u_2) + \frac{\partial}{\partial p_3}(g_1 g_2 u_3)\right) =$$

$$\vec{\nabla} \cdot \vec{u} = \frac{1}{r^2 \sin\theta}\left(\frac{\partial}{\partial \phi}(r u_1) + \frac{\partial}{\partial \theta}(r \sin\theta\, u_2) + \frac{\partial}{\partial r}(r^2 \sin\theta\, u_3)\right)$$

Then we shall evaluate the Laplace operator by inserting $\vec{\nabla} U$ for $\vec{u}$ in the expression above.

$$\nabla^2 U = \vec{\nabla} \cdot \vec{\nabla} \vec{u} = \vec{\nabla} \cdot \left(\frac{1}{r\sin\theta}\frac{\partial U}{\partial \varphi}, \frac{1}{r}\frac{\partial U}{\partial \theta}, \frac{\partial U}{\partial r}\right) =$$

$$\frac{1}{r^2 \sin\theta}\left(\frac{\partial}{\partial \phi}\left(r \frac{1}{r\sin\theta}\frac{\partial U}{\partial \varphi}\right) + \frac{\partial}{\partial \theta}\left(r\sin\theta \frac{1}{r}\frac{\partial U}{\partial \theta}\right) + \frac{\partial}{\partial r}\left(r^2 \sin\theta \frac{\partial U}{\partial r}\right)\right) =$$

$$\frac{1}{r\sin^2\theta}\frac{\partial^2 U}{\partial \varphi^2} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial U}{\partial \theta}\right) + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial U}{\partial r}\right)$$

$$\frac{1}{r\sin^2\theta}\frac{\partial^2 \psi}{\partial \varphi^2} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial \psi}{\partial \theta}\right) + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \psi}{\partial r}\right)$$

## 6. Solving the wave equation for circular waves in space

(6.1) $$\nabla^2 \psi - \frac{1}{c^2}\frac{\partial^2 \psi}{dt^2} = 0,$$

$$\frac{1}{r\sin^2\theta}\frac{\partial^2 \psi}{\partial \varphi^2} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial \psi}{\partial \theta}\right) + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \psi}{\partial r}\right) - \frac{1}{c^2}\frac{\partial^2 \psi}{dt^2} = 0$$

First we separate the solution in a space part and a time part. $\psi(\vec{r}, t) = \vec{u}(r, \theta, \varphi) w(t)$
Inserted in (c,c) gives:

$$w\nabla^2 u = \frac{u}{c^2}\frac{\partial^2 w}{dt^2} \quad \text{and by division with } uw\text{:} \quad \frac{1}{u}\nabla^2 u = \frac{1}{wc^2}\frac{\partial^2 w}{dt^2}$$

Since the left side depends on $\vec{r} = (x, y, z)$ only, and the right side depends on $t$ only. The two sides of the equation must be equal to the same constant, which we for physical reasons denote $-k^2$.
We then have the two equations:

$$\nabla^2 u = -k^2 u \qquad \text{and} \qquad \frac{\partial^2 w}{dt^2} = -k^2 c^2 w$$

The second equation we put $\omega = kc$ , and it has the well known solution: $w = Ae^{i\omega t}$

In the first expression $\nabla^2 u = -k^2 u$ we insert the Laplace operator in polar coordinates, and separate the coordinates in their dependence on $\theta, \varphi$

(6.2) $$u(r,\theta,\varphi) = R(r)Y(\theta,\varphi)$$

Then we move the factor that does not depend on the other variables outside the differentiation in each term.

(6.3) $$\frac{Y}{r^2}\frac{\partial}{\partial r}r^2\left(\frac{\partial R}{\partial r}\right) + \frac{R}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{R}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2} + k^2 RY = 0$$

Next we multiply the equation by $r^2$ and divide the equation with *YR*, rearranging the terms.

$$\frac{1}{R}\frac{\partial}{\partial r}r^2\left(\frac{\partial R}{\partial r}\right) + \frac{1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{Y\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2} + k^2 = 0$$

We can now see, that the first and the last term do not depend on $(\theta, \varphi)$, whereas the last two middle terms do not depend on *r*. This is only possible if they both are equal to the same constant λ with opposite sign.

(6.4) $$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + k^2 = \lambda \qquad \text{and} \qquad \frac{1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{Y\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2} = -\lambda$$

Multiplying the equations with *R* and *Y* respectively, we have

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + k^2 R - \lambda R = 0 \qquad \text{and} \qquad \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2} + \lambda Y = 0$$

## 6.1 The angular part of the wave equation

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2} + \lambda Y = 0$$

The next step is to separate the dependence on the angle $\theta$ from the angle $\varphi$. Multiplying the second equation by $\sin^2\theta$, and introducing the functions $\Theta(\theta)$ and $\Phi(\varphi)$ by $Y(\theta,\varphi) = \Theta(\theta)\Phi(\varphi)$.

(6.5) $$\Phi\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\Theta\frac{\partial^2\Phi}{\partial\varphi^2}+\lambda\sin^2\theta\Theta\Phi=0$$

Then by division by $\Theta(\theta)\Phi(\varphi)$, we have:

(6.6) $$\frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\lambda\sin^2\theta+\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\varphi^2}=0$$

Since the first two terms depend only on θ and the last term only on φ they must be equal to the same constant κ with opposite sign. We then have the two equations:

$$\frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\lambda\sin^2\theta=-\kappa \qquad \text{and} \qquad \frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\varphi^2}=\kappa$$

$$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\Theta\lambda\sin^2\theta+\kappa\Theta=0 \qquad \text{and} \qquad \frac{\partial^2\Phi}{\partial\varphi^2}-\kappa\Phi=0$$

The differential equation

$$\frac{\partial^2\Phi}{\partial\varphi^2}-\kappa\Phi=0$$

has the solution:

$$\Phi=c_1e^{im\varphi}+c_2e^{-im\varphi}$$

where $m^2=-\kappa$.

Since φ is the azimuth angle we may choose its zero as we wish, and we therefore put $c_2 = 0$ .
So the solution becomes:

(6.7) $$\Phi=c_1e^{im\varphi}$$

The other equation is a bit harder:

(6.8) $$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\Theta\lambda\sin^2\theta-m^2\Theta=0$$

We divide this equation by $\sin^2\theta$ to get:

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\left(\lambda+\frac{\kappa}{\sin^2\theta}\right)\Theta=0$$

We make the substitutions: $x=\cos(\theta)$ *and* $K(x)=\Theta(\theta)$ and carry out the differentiations, since

$$\frac{\partial\Theta}{\partial\theta}=\frac{\partial\Theta}{\partial x}\frac{\partial x}{\partial\theta}=-\sin(\theta)\frac{\partial\Theta}{\partial x}$$

we get:

$$-\frac{\partial}{\partial x}\left(\sin\theta(-\sin x)\frac{\partial\Theta}{\partial x}\right)+\left(\lambda-\frac{m^2}{\sin^2\theta}\right)\Theta=0 \quad \Leftrightarrow$$

$$\frac{\partial}{\partial x}\left(\sin\theta\sin\theta\frac{\partial\Theta}{\partial x}\right)+\left(\lambda-\frac{m^2}{\sin^2\theta}\right)\Theta=0 \quad \Leftrightarrow$$

$$\frac{\partial}{\partial x}\left((1-\cos^2\theta)\frac{\partial\Theta}{\partial x}\right)+\left(\lambda-\frac{m^2}{1-\cos^2\theta}\right)\Theta=0 \quad \Leftrightarrow$$

$$\frac{d}{dx}\left((1-x^2)\frac{\partial P}{dx}\right)+\left(\lambda-\frac{m^2}{1-x^2}\right)P=0 \quad \Leftrightarrow$$

$$(1-x^2)\frac{d^2P}{dx^2}-2x\frac{dP}{dx}+\left(\lambda-\frac{m^2}{1-x^2}\right)P=0$$

To comply with the standard way of writing, we put $\lambda = l(l+1)$

(6.9) $$(1-x^2)\frac{d^2P}{dx^2}-2x\frac{dP}{dx}+\left(l(l+1)-\frac{m^2}{1-x^2}\right)P=0$$

This equation is, however, just the so called associated Legendre equation, which has the solution $P_l^m(x)$.
The Legendre polynomials belong to a rather complex part of university mathematics, and we restricts ourselves to the results that can be found in any textbook on the subject or in the article on my homepage www.olewitthansen.dk**/Mathematics/Legendre_and_associated_Polynomials.pdf**

The Legendre differential equation, which appears in several connections in physics, is:

(6.10) $$(1-x^2)\frac{d^2y}{dx^2}-2x\frac{dy}{dx}+n(n+1)y=0$$

The solution may be given in several different ways but most compactly by Rodrigues formula:

$$P_n(x)=\frac{1}{2^n n!}\left(\frac{d}{dx}\right)^n(x^2-1)^n$$

The first three Legendre polynomials are.

$$P_0(x) = 1,$$
$$P_1(x) = \frac{1}{2}\frac{d}{dx}(x^2 - 1) = x$$
$$P_2(x) = \frac{1}{2^2 2!}\frac{d^2}{dx^2}(x^2 - 1)^2 = \tfrac{1}{2}x^3 - x$$

$P_0(x)$ is trivially a solution, since it gives: $0 - 2x + 2x = 0$

$P_1(x)$ is a solution, since: $0 - 2x + 1(1+1)x = 0$

Then we show that $P_2$ is a solution to: $(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + n(n+1)y = 0$

$$(1-x^2)\frac{1}{2}\frac{d^2}{dx^2}(3x^2-1) - x\frac{d}{dx}(3x^2-1) + 3(3x^2-1) =$$
$$3(1-x^2) - 6x^2 + 9x^2 - 3 = 0$$

To show that the general Legendre polynomial is a solution is more tiresome, however.

We shall now return to the equation for the polar dependence, where $x = \cos(\theta)$, which has the associated Legendre polynomials $P_l^m(x)$ as their solution.

(6.11) $$(1-x^2)\frac{d^2P}{dx^2} - 2x\frac{dP}{dx} + \left(l(l+1) - \frac{m^2}{1-x^2}\right)P = 0$$

The analytic formula for the *associated* Legendre polynomials is:

(6.12) $$P_l^m(x) = (1-x^2)^{\frac{m}{2}}\left(\frac{d}{dx}\right)^m P_l(x)$$

Where $P_l(x)$ is the Legendre polynomial of degree $l$. The *associated* Legendre polynomials have the following series expansion:

(6.12) $$P_l^m(x) = (1-x^2)^{\frac{m}{2}}\left(a_0\sum_{n=0}^{\infty}\frac{a_{2n}}{a_0}x^{2n} + a_1\sum_{n=1}^{\infty}\frac{a_{2n+1}}{a_1}x^{2n+1}\right)$$

By some rather cumbersome calculations leads to the recursion relation.

(6.13) $$a_{n+2} = \frac{(n+m)(m+n+1) - l(l+1)}{(n+1)(n+2)}a_n$$

It is important to notice that when $l = n + m$, then $a_{n+2} = 0$, insuring that $a_{n+4}$, $a_{n+6}$,… are all zero. In any case for integer $l$, $P_l^m(x)$ is a polynomial of degree $l$.

The combination of the solutions to the azimuth and the polar equation $\Theta(\theta)\Phi(\varphi)$ are called spherical harmonics. They are denoted:

(6.14) $$Y_{lm}(\theta,\varphi) = P_l^m(\theta)e^{im\varphi} \qquad l = 0,1,...\ and - l \le m \le l$$

The first few spherical harmonics are:

$$Y_{00} = \sqrt{\frac{1}{4\pi}} \qquad Y_{11} = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\varphi} \qquad Y_{10} = -\sqrt{\frac{3}{4\pi}}\cos\theta \qquad Y_{1,-1} = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\varphi}$$

## 6.2 The radial part of the wave equation

The radial equation is, where we have put: $\lambda = l(l+1)$.

(6.15) $$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + k^2 - l(l+1) = 0$$

And after multiplying with $R$:

(6.15) $$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + k^2r^2R - l(l+1)R = 0$$

It appears that we can come closer to a solution, if we change the dependent variable to $R = \frac{u}{\sqrt{r}}$.

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + k^2r\sqrt{r}u - l(l+1)\frac{u}{\sqrt{r}} = 0$$

We do the differentiation in steps:

$$\frac{dR}{dr} = \frac{d}{dr}\frac{u}{\sqrt{r}} = -\tfrac{1}{2}\frac{1}{r\sqrt{r}}u + \frac{1}{\sqrt{r}}\frac{du}{dr} \qquad \Rightarrow$$

$$r^2\frac{dR}{dr} = -\tfrac{1}{2}\sqrt{r}u + r\sqrt{r}\frac{du}{dr}$$

So

$$\frac{d}{dr}(r^2\frac{dR}{dr}) = \frac{d}{dr}(-\tfrac{1}{2}\sqrt{r}u + r\sqrt{r}\frac{du}{dr}) = -\tfrac{1}{4}\frac{1}{\sqrt{r}}u - \tfrac{1}{2}\sqrt{r}\frac{du}{dr} + \tfrac{3}{2}\sqrt{r}\frac{du}{dr} + r\sqrt{r}\frac{d^2u}{dr^2}$$

The equation then becomes

$$-\tfrac{1}{4}\frac{1}{\sqrt{r}}u-\tfrac{1}{2}\sqrt{r}\frac{du}{dr}+\tfrac{3}{2}\sqrt{r}\frac{du}{dr}+r\sqrt{r}\frac{d^2u}{dr^2}+k^2r\sqrt{r}u-l(l+1)\frac{u}{\sqrt{r}}=0$$

We shall then divide the equation by $r\sqrt{r}$ .

$$-\tfrac{1}{4}\frac{1}{r^2}u-\tfrac{1}{2}\frac{1}{r}\frac{du}{dr}+\tfrac{3}{2}\frac{1}{r}\frac{du}{dr}+\frac{d^2u}{dr^2}+k^2u-l(l+1)\frac{u}{r^2}=0$$

Rearranging the terms

$$\frac{d^2u}{dr^2}+\frac{1}{r}\frac{du}{dr}+k^2u-\frac{\tfrac{1}{4}+l^2+l}{r^2}u=0$$

$$\frac{d^2u}{dr^2}+\frac{1}{r}\frac{du}{dr}+(k^2-\frac{(l+\tfrac{1}{2})^2}{r^2})u=0$$

The Bessel function of order *n* is the solution to the equation:

(6.16) $$\frac{\partial^2u_n}{\partial x^2}+\frac{1}{x}\frac{\partial u_n}{\partial x}+(1-\frac{n^2}{x^2})u_n=0$$

Let $J_n(x)$ be the solution of this differential equation. $J_n(x)$ it is then denoted the Bessel function of order *n*. Or when setting $x = kr$ :

$$\frac{\partial^2u_n}{k^2\partial x^2}+\frac{1}{kr}\frac{\partial u_n}{k\partial r}+(1-\frac{n^2}{k^2r^2})u_n=0$$ And multiplying by $k^2$

$$\frac{\partial^2u_n}{\partial x^2}+\frac{1}{r}\frac{\partial u_n}{\partial r}+(k^2-\frac{n^2}{r^2})u_n=0$$ Which we compare to (6.16)

$$\frac{d^2u}{dr^2}+\frac{1}{r}\frac{du}{dr}+(k^2-\frac{(l+\tfrac{1}{2})^2}{r^2})u=0$$

We recognize that the solution to the radial equation is a Bessel function with $x = kr$, and $n^2 = (l+\tfrac{1}{2})^2$.

(6.17) $$R=\frac{J_{1+\frac{1}{2}}(kr)}{\sqrt{r}}$$

Below is shown the first three Bessel functions

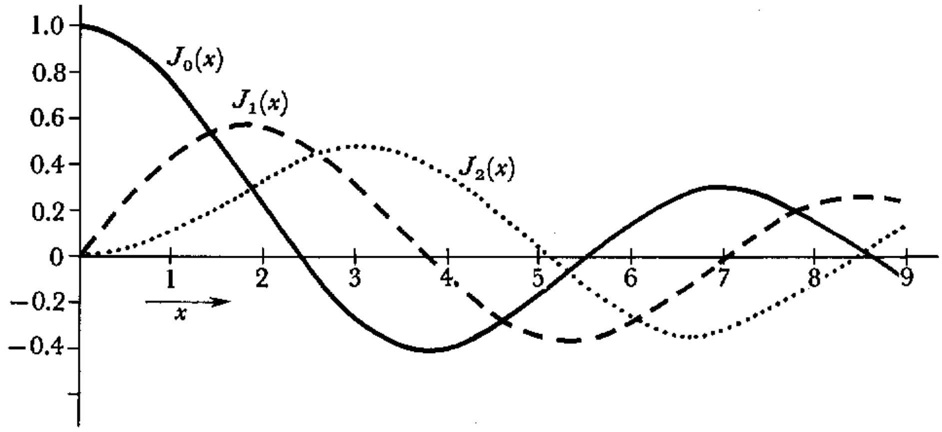



**Figure 7–1 The Bessel functions $J_0(x)$, $J_1(x)$, and $J_2(x)$**

## 7. Solving the wave equation for plane circular waves

The wave equation in the plane $(r,\theta)$ is: $\nabla^2 U = \frac{1}{v^2}\frac{\partial^2 U}{dt^2}$, where $v$ is the speed of propagation is in polar coordinates:

(7.1) $$\frac{1}{r^2}\frac{\partial^2 U}{\partial\theta^2} + \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial U}{\partial r}) = \frac{1}{v^2}\frac{\partial^2 U}{dt^2}$$

Assuming that the time dependence is independent of *r* and θ, we write: $U(r,\theta,t) = u(r,\theta)\psi(t)$. Inserting in (7.1) and subsequently dividing by $u\psi$, we have:

(7.2) $$\psi\frac{1}{r^2}\frac{\partial^2 u}{\partial\theta^2} + \psi\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial u}{\partial r}) = u\frac{1}{v^2}\frac{\partial^2\psi}{dt^2} \quad \Leftrightarrow$$
$$\frac{1}{u}(\frac{1}{r^2}\frac{\partial^2 u}{\partial\theta^2} + \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial u}{\partial r})) = \frac{1}{v^2}\frac{1}{\psi}\frac{\partial^2\psi}{dt^2}$$

In this equation the left side depends only on *r* and θ, whereas the right side depends only on *t*. But that means that they are both equal to the same constant, which we for physical reasons put to $-k^2$, where *k* is the wave number: $k = \frac{\omega}{v}$. So we have the two equations:

(7.3) $$\frac{1}{v^2}\frac{1}{\psi}\frac{\partial^2\psi}{dt^2} = -k^2 \quad \Leftrightarrow \quad \frac{\partial^2\psi}{dt^2} = -k^2v^2\psi \quad \Leftrightarrow$$
$$\psi = Ae^{ikvt} \quad \Leftrightarrow \quad \psi = Ae^{i\omega t}$$

So we are left with

(7.4) $$\frac{1}{r^2}\frac{\partial^2 u}{\partial\theta^2}+\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial u}{\partial r})=-k^2u \quad\Leftrightarrow\quad \frac{1}{r^2}\frac{\partial^2 u}{\partial\theta^2}+\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial u}{\partial r})+k^2u=0$$

If we further assume that $u = u(r, \theta)$ does not depend explicitly on θ, such that: $\frac{\partial u}{\partial\theta}=0$. We have thus the equation:

(7.5) $$\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial u}{\partial r})+k^2u=0 \quad\Leftrightarrow\quad \frac{\partial^2 u}{\partial r^2}+\frac{1}{r}\frac{\partial u}{\partial r}+k^2u=0$$

If we put $\rho = kr$, we may eliminate the constant *k*.

(7.6) $$k^2\frac{\partial^2 u}{\partial\rho^2}+k^2\frac{1}{r}\frac{\partial u}{\partial\rho}+k^2u=0 \quad\Leftrightarrow$$
$$\frac{\partial^2 u}{\partial\rho^2}+\frac{1}{r}\frac{\partial u}{\partial\rho}+u=0$$

The solution to this differential equation cannot be expressed with already known standard functions, but the solution is called the Bessel function of zero order and is denoted $J_0(\rho)$ or as it usually written $J_0(x)$.
For details see: **http://olewitthansen.dk/Physics/Circular_waves_and_the_bessel_function.pdf**

## 8. The diffusion equation

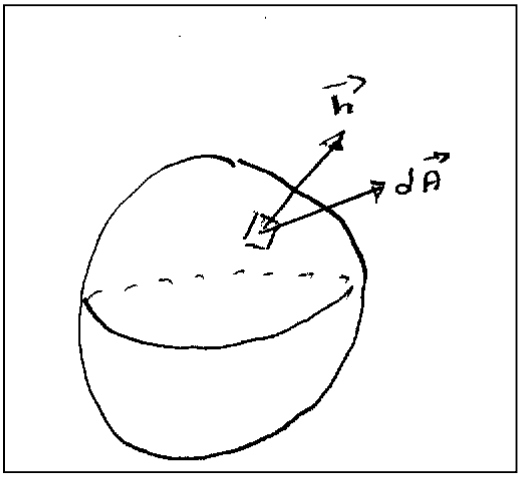
In a heat conducting material, the temperature ψ obeys the diffusion equation:

(8.1) $$\vec{\nabla}^2\psi-\frac{1}{\kappa}\frac{\partial\psi}{\partial t}=0$$

$\vec{\nabla}^2=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$ is the Laplace operator, and $\kappa=\frac{k}{c\rho}$, where *k* is the heat conductivity, *c* is the specific heat and ρ is the density of the material. The connection between the heat conducting vector $\vec{h}$ and the temperature gradient is:

(8.2) $$\vec{h}=-k\vec{\nabla}T$$

## 8.1 Derivation of the diffusion equation




In the figure is shown a mathematical surface in a heat conducting body. The flow of heat per second through the surface is equal to the rate of change of heat in the volume enclosed by the surface. *T* is the temperature.

(1.3) $$\int_{surface}\vec{h}\cdot d\vec{A}=-\frac{\partial}{\partial t}\int_{volume}\rho cTdV$$

If we use Stokes law on the first integral, and then use $\vec{h}=-k\vec{\nabla}T$, we have:

(8.4) $$\int_{surface} \vec{h}\cdot d\vec{A} = \int_{volume} \vec{\nabla}\cdot\vec{h}dV = -k\int_{volume} \vec{\nabla}^2 TdV$$

We then have the equation:

$$-k\int_{volume} \vec{\nabla}^2 TdV = -\frac{\partial}{\partial t}\int_{volume} \rho cTdV$$

Since this equation must hold for all volumes, it must also hold for the infinitesimal volume *dV*, therefore:

(8.5) $$k\vec{\nabla}^2 T = \rho c\frac{\partial T}{\partial t} \quad \text{or} \quad \vec{\nabla}^2 T = \frac{\rho c}{k}\frac{\partial T}{\partial t} \quad \Leftrightarrow \quad \vec{\nabla}^2 T = \frac{1}{\kappa}\frac{\partial T}{\partial t}$$

Our aim is then to solve this equation in some special cases, with radial symmetry.

## 8.2 Solution of the spherical diffusion equation

The spherical coordinates are $(r,\theta,\varphi)$, and when there are no dependence on $\theta,\varphi$, the Laplace operator reduces to:

(8.6) $$\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial U}{\partial r})$$

If we replace the temperature *T* with $\psi$, we then have the equation:

(8.7) $$\vec{\nabla}^2\psi = \frac{1}{\kappa}\frac{\partial\psi}{\partial t} \quad \Leftrightarrow \quad \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial\psi}{\partial r}) = \frac{1}{\kappa}\frac{\partial\psi}{\partial t}$$

Where $\psi = \psi(r,t)$, and where the dependence on *r* and *t* cannot be factorized. We want to eliminate the constant κ, so we make the substitution: $r = \sqrt{\kappa}\rho$ , and then the equation becomes:

(8.8) $$\frac{1}{\kappa\rho^2}\frac{\partial}{\sqrt{k}\partial\rho}(\kappa\rho^2\frac{\partial\psi}{\sqrt{\kappa}\partial\rho}) = \frac{1}{\kappa}\frac{\partial\psi}{\partial t} \quad \Leftrightarrow \quad \frac{1}{\rho^2}\frac{\partial}{\partial\rho}(\rho^2\frac{\partial\psi}{\partial\rho}) = \frac{\partial\psi}{\partial t}$$

There is (as far as I know) no general methods to solve this partial differential equation but 35 years ago, when I first was occupied with this equation, analyzing geothermal heating pipes. I made my way by an educated guess to find the solution:

(8.8) $$\psi(\rho,t) = \frac{\psi_0}{(4\pi t)^{\frac{3}{2}}}e^{-\frac{\rho^2}{4t}}$$

We shall now demonstrate that this is indeed a solution:

$$\frac{1}{\rho^2}\frac{\partial}{\partial\rho}(\rho^2\frac{\partial\psi}{\partial\rho}) = \frac{1}{\rho^2}\frac{\partial}{\partial\rho}(-\frac{\rho^3}{2t}\psi) = -\frac{1}{\rho^2}\frac{1}{2t}(3\rho^2\psi - \frac{\rho^4}{2t}\psi)$$

So we have:

$$\frac{1}{\rho^2}\frac{\partial}{\partial \rho}(\rho^2 \frac{\partial \psi}{\partial \rho}) = (\frac{\rho^2}{4t^2} - \frac{3}{2t})\psi$$

And:

$$\frac{\partial \psi}{\partial t} = -\tfrac{3}{2}\frac{\psi_0}{(4\pi t)^{\frac{3}{2}}}\frac{1}{t}e^{\frac{-\rho^2}{4t}} + \frac{\psi_0}{(4\pi t)^{\frac{3}{2}}}e^{\frac{-\rho^2}{4t}}(\frac{\rho^2}{4t^2}) = (\frac{\rho^2}{4t^2} - \frac{3}{2t})\psi$$

The solution to (8.7) is then, apart from a constant, obtained by substituting $\rho = \frac{r}{\sqrt{k}}$ in (8.8).

And since $\int_0^\infty e^{-\frac{r^2}{4\kappa t}}dr = \sqrt{4\pi\kappa t}$ , we prefer to write the solution in the following form, still making room for a constant, to comply with the boundary conditions.

(8.9)
$$\psi(\frac{r}{\sqrt{\kappa}}, t) = \frac{\psi_0 r_0 t_0}{t\sqrt{4\pi\kappa t}} e^{-\frac{r^2}{4\kappa t}}$$

We notice that if $r \neq 0$ *then* $\psi(\frac{r}{\sqrt{\kappa}}, t) \to 0$ *for* $t \to 0$. This is what we may expect if a heat is released at $r = 0$ for $t = 0$.

But $\psi(0, t) = \frac{\psi_0 r_0 t_0}{t\sqrt{4\pi\kappa t}}$ has a pole at $t = 0$, so a more correct description is:

$$\psi(\frac{r}{\sqrt{\kappa}}, t) = \frac{\psi_0 r_0 t_0}{t\sqrt{4\pi\kappa t}} e^{-\frac{r^2}{4\kappa t}} \quad for \quad r > 0 \quad and \quad \psi(\frac{r}{\sqrt{\kappa}}, t) = \delta(t) \quad for \quad r = 0$$

Where $\delta(t) = \begin{cases} 0 & for \quad t \neq 0 \\ \infty & for \quad t = 0 \end{cases}$ is the Dirac *delta* function.

## 8.3 Solution of the cylindrical diffusion equation

The cylindrical coordinates are: $(r, \theta, z)$. The infinitesimal displacement vector is $d\vec{s} = (dr, rd\theta, dz)$ and the distance element is $ds^2 = dr^2 + r^2 d\theta^2 + dz^2$, (since the three displacements are orthogonal).
In cylindrical coordinates the gradient of a scalar field ψ therefore becomes:

(8.10)
$$\vec{\nabla}\psi = (\frac{1}{r}\frac{\partial \psi}{\partial \theta}, \frac{\partial \psi}{\partial r}, \frac{\partial \psi}{\partial z})$$

And the Laplace operator can be shown to be. (See e.g. www.olewitthansen.dk vector analysis).

(8.11)
$$\nabla^2\psi = \frac{1}{r^2}\frac{\partial^2 \psi}{\partial \theta^2} + \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial \psi}{\partial r}) + \frac{\partial^2 \psi}{\partial z^2}$$

If the field $\psi = \psi(r,t)$ depends neither on $\theta$ nor on $z$, the Laplacian reduces to:

(8.12) $$\nabla^2\psi = \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial\psi}{\partial r})$$

And the diffusion equation $\nabla^2\psi = \frac{1}{\kappa}\frac{\partial\psi}{\partial t}$ reduces to

(8.13) $$\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial\psi}{\partial r}) = \frac{1}{\kappa}\frac{\partial\psi}{\partial t}$$

As we did in the spherical symmetric case, we eliminate the factor $\kappa$ by the substitution $r = \sqrt{\kappa}\rho$, which results in the equation:

(8.14) $$\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial\psi}{\partial\rho}) = \frac{\partial\psi}{\partial t}$$

Neither this equation can be solved by traditional methods, but an educated guess, suggests:

(8.15) $$\psi(\rho,t) = \frac{1}{t}e^{-\frac{\rho^2}{4t}}$$

Proof:

$$\frac{\partial\psi}{d\rho} = \frac{1}{t}(-\frac{2\rho}{4t})e^{-\frac{\rho^2}{4t}} \quad => \quad \rho\frac{\partial\psi}{d\rho} = \frac{1}{t}(-\frac{2\rho^2}{4t})e^{-\frac{\rho^2}{4t}} = -\frac{\rho^2}{2t^2}e^{-\frac{\rho^2}{4t}}$$

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial\psi}{\partial\rho}) = \frac{1}{\rho}\frac{\partial}{\partial\rho}(-\frac{\rho^2}{2t^2}e^{-\frac{\rho^2}{4t}}) = \frac{1}{\rho}(-\frac{\rho}{t^2}e^{-\frac{\rho^2}{4t}} - \frac{\rho^2}{2t^2}(-\frac{\rho}{2t})e^{-\frac{\rho^2}{4t}} = \frac{1}{t^2}(\frac{\rho^2}{4t}-1)e^{-\frac{\rho^2}{4t}}$$

And

$$\frac{\partial\psi}{\partial t} = \frac{\partial}{\partial t}(\frac{1}{t}e^{-\frac{\rho^2}{4t}}) = -\frac{1}{t^2}e^{-\frac{\rho^2}{4t}} + \frac{1}{t}\frac{\rho^2}{4t^2}e^{-\frac{\rho^2}{4t}} = \frac{1}{t^2}(\frac{\rho^2}{4t}-1)e^{-\frac{\rho^2}{4t}}$$

To obtain the correct dimension of the equation, we add two constants

$$\psi(\rho,t) = \psi_0\frac{\rho_0^{\ 2}}{t}e^{-\frac{\rho^2}{4t}}$$

To obtain the solution to the original diffusion equation we reverse the substitution $r = \sqrt{\kappa}\rho$, and we find, when adding two constants.

(8.16) $$\psi(\frac{r}{\sqrt{\kappa}},t) = \frac{\psi_0 r_0^{\ 2}}{\kappa t}e^{-\frac{r^2}{4\kappa t}}$$

Or written with the temperature $T$ instead of ψ.

(8.17) $$T(\frac{r}{\sqrt{\kappa}},t)=\frac{T_0 r_0^{\;2}}{\kappa t}e^{-\frac{r^2}{4\kappa t}}$$

Since $\int_0^\infty e^{-\frac{r^2}{4\kappa t}}dr=\sqrt{4\pi\kappa t}$ we shall write the equation for normalization purposes as:

(8.18) $$T(\frac{r}{\sqrt{\kappa}},t)=\frac{T_0 r_0^{\;2}}{\sqrt{4\pi\kappa t}}e^{-\frac{r^2}{4\kappa t}}$$

As in the spherical symmetric case, we have for $r\neq 0,\quad T(\frac{r}{\sqrt{\kappa}},t)\to 0\quad for\quad t\to 0$,

But $T(\frac{r}{\sqrt{\kappa}},t)=\frac{T_0 r_0^{\;2}}{\sqrt{4\pi\kappa t}}e^{-\frac{r^2}{4\kappa t}}$ has a pole at $t$ = 0, so the correct description is:

(8.19) $$T(\frac{r}{\sqrt{\kappa}},t)=\frac{T_0 r_0^{\;2}}{\sqrt{4\pi\kappa t}}e^{-\frac{r^2}{4\kappa t}}\quad for\ \ r>0\quad and\quad T(0,t)=\delta(t)$$

Where $\delta(t)=\begin{cases}0 & for\quad t\neq 0\\ \infty & for\quad t=0\end{cases}$ is the Dirac *delta* function.

Even having found the mathematical solutions to the diffusion equation, it is not so easy to apply it to the boundary conditions of concrete physical example.

## 8.5. Heating of a body, the stationary situation.

Let us again consider a body, in which we have a closed mathematical surface, but now having inside a heat source. We assume that long time has passed, so we have a quasi stationary situation, in which the heat leaving the closed surface is equal to the heat produced within the surface. We then repeat the steps from section 1. If the power of the heating source per unit volume is $w$, we must have:

(2.1) $$\int_{surface}\vec{h}\cdot d\vec{A}+\int_{volume}wdV=0$$

If we use Stokes law on the first integral using: $\vec{h}=-k\vec{\nabla}T$, we have:

$$\int_{surface}\vec{h}\cdot d\vec{A}=\int_{volume}\vec{\nabla}\cdot\vec{h}dV=-k\int_{volume}\vec{\nabla}^2TdV$$

We then get the equation:

$$-k\int_{volume}\vec{\nabla}^2 T dV+\int_{volume} w dV=0 \quad\Leftrightarrow\quad \int_{volume}\vec{\nabla}^2 T dV=\frac{1}{k}\int_{volume} w dV$$

or

(2.2) $$\vec{\nabla}^2 T=\frac{w}{k}$$

This is formally the same equation as Gauss' law for the electric field of a charge distribution of charge (Maxwell's 1. equation): $\vec{\nabla}^2 E=\frac{\sigma}{\varepsilon_0}$, and for spherical symmetric heat source $W$, placed in the centre of a sphere, it has the solution.

(2.3) $$T=\frac{W}{4\pi k}\frac{1}{r^2}$$

By the same token, we may find the temperature distribution for a cylindrical symmetric heat source:

(2.4) $$T=\frac{W}{2\pi k}\frac{1}{r}$$

## 8.6. Heating a body

The most common situation is, however, not the diffusion of heat from a body to the surroundings, but rather heating of a body from the surroundings.

(-This means that the heat conducting vector $\vec{h}$, is reversed, and a minus is inserted in the equation: $\int_{surface}\vec{h}\cdot d\vec{A}$ -)

This means, however, that the volume is heated, not cooled, so we have $\int_{surface}\vec{h}\cdot d\vec{A}=\frac{\partial}{\partial t}\int_{volume}\rho c T dV$

which results in the diffusion equation:

$$\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial\psi}{\partial r})=-\frac{1}{\kappa}\frac{\partial\psi}{\partial t},$$

It is rather obvious that this equation must have the solution,

$$T(\frac{r}{\sqrt{\kappa}},t)=T_0\frac{r_0^{\,2}}{\kappa t}e^{\frac{r^2}{4\kappa t}}$$

Since in the original equation, the minus sign in the exponent of the exponential function is squared in the second derivative on the left hand side, but not in the right hand side of the equation.

However this equation does not comply with the boundary conditions, $T = T_0$ for $r = r_0$ at $t = 0$. Not even if he solution is supplied with a constant. Furthermore the temperature will drop to zero, after some time.
However this is not applicable to the situation of heating a body, that is, a potato or a thermal heating pipe, where we have a constant adding of heat on the surface.

## 9. The Schrödinger equation

The Schrödinger equation is treated in detail in:

http://olewitthansen.dk/Physics/The_hydrogen_atom.pdf . This section is reproduced here

The Schrödinger equation was proposed in 1925 by the Austrian physicist Kurt Erwin Schrödinger and it is the foundation of classical quantum physics in the same manner as Newton's laws are the foundation of classical mechanics. (In this context classical means non relativistic).
It does not at every instant describe a physical system by its position and momentum as in Newtonian mechanics, but rather by a (complex) wave function $\psi = \psi(\vec{x})$, were the density $|\psi|^2\, d\vec{x}$ is the probability to find the system in a certain state.
According to the uncertainty principle of Heisenberg, it is not possible to determine the position and momentum simultaneously for a quantum mechanical system. Quantum physics may seem very odd, when you encounter it for the first time – and it certainly is.

The Schrödinger equation describes the dynamical development of a physical system by the wave function.
Compared with Newtonian mechanics the mathematics of the Schrödinger equation is far more complex.
The aim of this section is to solve the Schrödinger equation for what ought to be a simple two body system – the Hydrogen atom. But as you will find it requires rather advanced university mathematics.
The Schrödinger equation in polar coordinates is shown below.

(9.1)
$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}r^2\left(\frac{\partial \psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}\right]-\frac{Ze^2}{4\pi\varepsilon_0 r}\psi = E\psi$$

First we divide this equation by $-\frac{\hbar^2}{2m}$ and collect the terms on the left side.

$$\frac{1}{r^2}\frac{\partial}{\partial r}r^2\left(\frac{\partial \psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}+\frac{2m}{\hbar^2}\left(\frac{Ze^2}{4\pi\varepsilon_0 r}+E\right)\psi = 0$$

The first step in solving the Schrödinger equation is to separate it into three equation corresponding to the three variable $(r, \theta, \varphi)$. This is done in two steps. First we put:

(9.2)
$$\psi(r,\theta,\varphi) = R(r)Y(\theta,\varphi)$$

Then we move the factor that does not depend on the other variables outside the differentiation in each term.

(9.3) $$\frac{Y}{r^2}\frac{\partial}{\partial r}r^2\left(\frac{\partial R}{\partial r}\right)+\frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{R}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}+\frac{2m}{\hbar^2}\left(\frac{Ze^2}{4\pi\varepsilon_0 r}+E\right)YR=0$$

Next we multiply the equation by $r^2$ and divide the equation with $YR$, rearranging the terms.

$$\frac{1}{R}\frac{\partial}{\partial r}r^2\left(\frac{\partial R}{\partial r}\right)+\frac{2mr^2}{\hbar^2}\left(\frac{Ze^2}{4\pi\varepsilon_0 r}+E\right)+\frac{1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{Y\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}=0$$

We can now see, that the first two terms do not depend on $(\theta,\varphi)$, whereas the last two terms do not depend on $r$. This is only possible if they both are equal to the same constant $\lambda$ with opposite sign.

(9.4) $$\frac{1}{R}\frac{\partial}{\partial r}r^2\left(\frac{\partial R}{\partial r}\right)+\frac{2mr^2}{\hbar^2}\left(\frac{Ze^2}{4\pi\varepsilon_0 r}+E\right)=\lambda$$

$$\frac{1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{Y\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}=-\lambda$$

Multiplying the equations with $R$ and $Y$ respectively

$$\frac{\partial}{\partial r}r^2\left(\frac{\partial R}{\partial r}\right)+\frac{2mr^2}{\hbar^2}\left(\frac{Ze^2}{4\pi\varepsilon_0 r}+E\right)R-\lambda R=0$$

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}+\lambda Y=0$$

The next step is to separate the dependence on the angle $\theta$ from the angle $\varphi$. Multiplying the second equation by $\sin^2\theta$, and introducing the functions $\Theta(\theta)$ and $\Phi(\varphi)$ by $Y(\theta,\varphi)=\Theta(\theta)\Phi(\varphi)$.

(9.5) $$\Phi\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\Theta\frac{\partial^2\Phi}{\partial\varphi^2}+\lambda\sin^2\theta\Theta\Phi=0$$

Then by division by $\Theta(\theta)\Phi(\varphi)$, we have:

(9.6) $$\frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\lambda\sin^2\theta+\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\varphi^2}=0$$

Since the first two terms depend only on $\theta$ and the last term only on $\varphi$ they must be equal to the same constant $\kappa$ with opposite sign. We then have the two equations:

$$\frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\lambda\sin^2\theta=-\kappa \qquad \text{and} \qquad \frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\varphi^2}=\kappa$$

$$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\lambda\sin^2\theta+\kappa\Theta=0 \qquad \text{and} \qquad \frac{\partial^2\Phi}{\partial\varphi^2}-\kappa\Phi=0$$

The differential equation

$$\frac{\partial^2\Phi}{\partial\varphi^2}-\kappa\Phi=0$$

has the solution:

$$\Phi=c_1e^{im\varphi}+c_2e^{-im\varphi}$$

where $m^2=-\kappa$.

Since φ is the azimuth angle we may choose its zero as we wish, and we therefore put $c_2 = 0$ .
So the solution becomes:

(9.7) $$\Phi=c_1e^{im\varphi}$$

The other equation is a bit harder:

(9.8) $$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\lambda\sin^2\theta-m^2\Theta=0$$

We divide this equation by $\sin^2\theta$ to get:

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\left(\lambda+\frac{\kappa}{\sin^2\theta}\right)\Theta=0$$

We make the substitutions: $x=\cos(\theta) \quad and \; K(x)=\Theta(\theta)$ and carry out the differentiations, since

$$\frac{\partial\Theta}{\partial\theta}=\frac{\partial\Theta}{\partial x}\frac{\partial x}{\partial\theta}=-\sin(\theta)\frac{\partial\Theta}{\partial x}$$

then we get:

$$-\frac{\partial}{\partial x}\left(\sin\theta(-\sin x)\frac{\partial\Theta}{\partial x}\right)+\left(\lambda-\frac{m^2}{\sin^2\theta}\right)\Theta=0 \quad \Leftrightarrow$$

$$\frac{\partial}{\partial x}\left(\sin\theta\sin\theta\frac{\partial\Theta}{\partial x}\right)+\left(\lambda-\frac{m^2}{\sin^2\theta}\right)\Theta=0 \quad \Leftrightarrow$$

$$\frac{\partial}{\partial x}\left((1-\cos^2\theta)\frac{\partial\Theta}{\partial x}\right)+\left(\lambda-\frac{m^2}{1-\cos^2\theta}\right)\Theta=0 \quad \Leftrightarrow$$

$$\frac{d}{dx}\left((1-x^2)\frac{\partial P}{dx}\right)+\left(\lambda-\frac{m^2}{1-x^2}\right)P=0 \qquad \Leftrightarrow$$

$$(1-x^2)\frac{d^2P}{dx^2}-2x\frac{dP}{dx}+\left(\lambda-\frac{m^2}{1-x^2}\right)P=0$$

To comply with the standard way of writing, we put $\lambda = l(l+1)$

(9.9) $$(1-x^2)\frac{d^2P}{dx^2}-2x\frac{dP}{dx}+\left(l(l+1)-\frac{m^2}{1-x^2}\right)P=0$$

This equation is, however, just the associated Legendre equation, which has the solution $P_l^m(x)$. The Legendre polynomials belong to a rather complex part of university mathematics, and we restricts ourselves to the results that can be found in any textbook on the subject or in the article on my homepage www.olewitthansen.dk/Mathematics/Legendre_and_associated_Polynomials.pdf

The Legendre differential equation which appears in several connections in physics is:

$$(1-x^2)\frac{d^2y}{dx^2}-2x\frac{dy}{dx}+n(n+1)y=0$$

The solution may be given in several different ways but most compactly by Rodrigues formula:

$$P_n(x)=\frac{1}{2^n n!}\left(\frac{d}{dx}\right)^n(x^2-1)^n$$

The first three Legendre polynomials are.

$$P_0(x)=1,$$
$$P_1(x)=\frac{1}{2}\frac{d}{dx}(x^2-1)=x$$
$$P_2(x)=\frac{1}{2^2 2!}\frac{d^2}{dx^2}(x^2-1)^2=\tfrac{1}{2}x^3-x$$

$P_0(x)$ is trivially a solution, since it gives: $0-2x+2x=0$

$P_1(x)$ is a solution, since: $0-2x+1(1+1)x=0$

Then we show that $P_2$ is a solution to: $(1-x^2)\frac{d^2y}{dx^2}-2x\frac{dy}{dx}+n(n+1)y=0$

$$(1-x^2)\frac{1}{2}\frac{d^2}{dx^2}(3x^2-1)-x\frac{d}{dx}(3x^2-1)+3(3x^2-1)=$$
$$3(1-x^2)-6x^2+9x^2-3=0$$

To show that the general Legendre polynomial is a solution is more tiresome, however.

We shall now return to the equation for the polar dependence, where $x = \cos(\theta)$, which has the associated Legendre polynomials $P_l^m(x)$ as their solution.

(9.10) $$(1-x^2)\frac{d^2P}{dx^2} - 2x\frac{dP}{dx} + \left(l(l+1) - \frac{m^2}{1-x^2}\right)P = 0$$

The analytic formula for the *associated* Legendre polynomials is:

(9.11) $$P_l^m(x) = (1-x^2)^{\frac{m}{2}}\left(\frac{d}{dx}\right)^m P_l(x)$$

Where $P_l(x)$ is the Legendre polynomial of degree *l*. The *associated* Legendre polynomials have the following series expansion:

(9.12) $$P_l^m(x) = (1-x^2)^{\frac{m}{2}}\left(a_0\sum_{n=0}^{\infty}\frac{a_{2n}}{a_0}x^{2n} + a_1\sum_{n=1}^{\infty}\frac{a_{2n+1}}{a_1}x^{2n+1}\right)$$

Which, by some rather cumbersome calculations leads to the recursion relation.

(9.12) $$a_{n+2} = \frac{(n+m)(m+n+1) - l(l+1)}{(n+1)(n+2)}a_n$$

It is important to notice that when $l = n+m$ , then $a_{n+2} = 0$, insuring that all $a_{n+4}$, $a_{n+6}$,… are zero. In any case for integer $l$, $P_l^m(x)$ is a polynomial of degree *l*.

## 10. The angular part of the Schrödinger equation

We have seen above that the Schrödinger equation can be separated into an angular part and a radial part. The angular part can furthermore be separated into two differential equations corresponding to the polar and azimuth angles. First the azimuth angle.

The equation $\frac{\partial^2\Phi}{\partial\varphi^2} + \kappa\Phi = 0$ has the solution $\Phi = ce^{im\varphi}$ where $\kappa = -m^2$.

Since the state is supposed to be a stationary we must require:

$$\Phi(\phi + 2\pi) = \Phi(\phi) \Leftrightarrow e^{im(\varphi+2\pi)} = e^{im\varphi} \Leftrightarrow e^{im2\pi} = 1 \Leftrightarrow m \in Z$$ (*m* is an integral number).

The quantum *m* is the first of the three quantum numbers which characterize the hydrogen (or any atom). It is called the *magnetic* quantum number.

The differential equation for the polar angle is:

(8.1) $$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\left(l(l+1)-\frac{m^2}{\sin^2\theta}\right)\Theta=0$$

The polar equation has the associated Legendre polynomials $P_l^m(x)$ as its solutions.
We have seen that the solutions are always finite polynomials if *l* is an integer and: $-l \le m \le l$
The second quantum number for the hydrogen (or any) atom is *l*.
The number *l* it is called the angular momentum quantum number.
The combination of the solutions to the azimuth and the polar equation $\Theta(\theta)\Phi(\varphi)$ are called spherical harmonics. They are denoted:

(10.2) $$Y_{lm}(\theta,\varphi)=P_l^m(\theta)e^{im\varphi} \qquad l=0,1,...\ and -l\le m\le l$$

In the operator formulation of the Schrödinger equation, we have:

(10.3) $$H\psi=i\hbar\frac{\partial\psi}{dt}$$

where *H* is the Hamilton operator (the energy).

(10.4) $$H=-\frac{\hbar^2}{2m}(\nabla^2+V(\vec{x}))$$

The spherical harmonics are simultaneous eigenfunctions to the operators $L^2$ and $L_z$, where $\vec{L}=(L_x,L_y,L_z)$ is the angular momentum.

(10.5) $$L^2=\frac{\hbar}{i}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\left(\frac{1}{\sin^2\theta}\right)\right] \quad \text{and} \quad L_z=\frac{\hbar}{i}\frac{\partial}{\partial\varphi}$$

(10.6) $$L^2Y_{lm}(\theta,\varphi)=l(l+1)\hbar^2Y_{lm}(\theta,\varphi) \quad \text{and} \quad L_zY_{lm}(\theta,\varphi)=m\hbar Y_{lm}(\theta,\varphi)$$

The first few spherical harmonics are:

$$Y_{00}=\sqrt{\frac{1}{4\pi}} \qquad Y_{11}=-\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\varphi} \qquad Y_1=-\sqrt{\frac{3}{8\pi}}\sin\ \theta e^{i\varphi} \qquad Y_{1,-1}=-\sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\varphi}$$

## 10.1 The radial part of the Schrödinger equation

(10.7) $$\frac{\partial}{\partial r}r^2\left(\frac{\partial R}{\partial r}\right)+\frac{2mr^2}{\hbar^2}\left(+\frac{Ze^2}{4\pi\varepsilon_0 r}+E\right)R-\lambda R=0$$

$$\frac{\partial}{\partial r} r^2 \left( \frac{\partial R}{\partial r} \right) + \frac{2mr^2}{\hbar^2} \left( \frac{Ze^2}{4\pi\varepsilon_0 r} + E \right) R - l(l+1)R = 0$$

It seems practical to introduce the substitution: $\chi(r) = rR(r) \quad \Leftrightarrow \quad R(r) = \frac{\chi(r)}{r}$

(10.8)

$$\frac{\partial}{\partial r} r^2 \left( \frac{\partial}{\partial r} \frac{\chi(r)}{r} \right) + \frac{2m^2 r^2}{\hbar^2} \left( \frac{Ze^2}{4\pi\varepsilon_0 r} + E \right) \frac{\chi(r)}{r} - l(l+1) \frac{\chi(r)}{r} = 0 \quad \Leftrightarrow$$

$$\frac{\partial}{\partial r} (\chi'(r)r - \chi(r)) + \frac{2m^2 r^2}{\hbar^2} \left( \frac{Ze^2}{4\pi\varepsilon_0 r} + E \right) \frac{\chi(r)}{r} - l(l+1) \frac{\chi(r)}{r} = 0 \quad \Leftrightarrow$$

$$\chi''(r)r + \chi'(r) - \chi'(r) + \frac{2mr^2}{\hbar^2} \left( \frac{Ze^2}{4\pi\varepsilon_0 r} + E \right) \frac{\chi(r)}{r} - l(l+1) \frac{\chi(r)}{r} = 0 \quad \Leftrightarrow$$

$$\chi''(r) + \frac{2m}{\hbar^2} \left( \frac{Ze^2}{4\pi\varepsilon_0 r} + E \right) \chi(r) - \frac{l(l+1)}{r^2} \chi(r) = 0$$

Even if you find that the solution of the polar equation involve rather complex mathematics then the solution of the radial equation turns out to be rather heavy university mathematics.

## 10.2 The Laguerre polynomials and related Laguerre function

The Laguerre differential equation is:

(10.9)
$$x \frac{d^2 L_n}{dx^2} + (1-x) \frac{dL_n}{dx} + nL_n = 0$$

The first five Laguerre polynomials, which are solutions to Laguerre's equation are listed below

$$L_0(x) = 1 \qquad L_1(x) = 1 - x \qquad L_2(x) = x^2 - 4x + 2$$

$$L_3(x) = -x^3 + 9x^2 - 18x + 6 \qquad L_4(x) = x^4 - 16x^3 + 72x^2 - 96x + 24$$

Laguerre polynomials of any order can be calculated, using the generating function:

(10.10)
$$L_n(x) = e^x \frac{d^n}{dx^n} (e^{-x} x^n)$$

As an example, we shall generate $L_2(x)$:

$$\frac{d^2}{dx^2} e^{-x} x^2 = \frac{d}{dx} (-e^{-x} x^2 + e^{-x} 2x) = e^{-x} x^2 - e^{-x} 2x - e^{-x} 2x + e^{-x} 2$$

$$e^x \frac{d^2}{dx^2} e^{-x} x^2 = x^2 - 4x + 2$$

The Laguerre polynomials do not form an orthogonal set, but the related *Laguerre functions* do,

$$\phi_n(x) = e^{-x/2} L_n(x)$$

since they are orthonormal on the interval $0 \le x \le \infty$. The Laguerre functions are not solutions to the Laguerre equation, but they are solutions to an equation which is related.

As it was the case with the Legendre equation the Laguerre equation has a derived associated equation, which contain a second index *k*. The associated Laguerre equation is, (where $L_n^k$ denotes the solutions).

(10.11) $$x\frac{d^2 L_n^k}{dx^2} + (1 - x + k)\frac{dL_n^k}{dx} + nL_n^k = 0$$

It reduces to the Laguerre equation when *k* =0. The first few *associated Laguerre polynomials* are listed below: In general $L_n^0(x) = L_n(x)$.

$$L_0^1(x) = 1, \qquad L_1^1(x) = -2x + 4, \qquad L_2^1(x) = 3x^2 - 18x + 18$$
$$L_0^2(x) = 2, \qquad L_1^2(x) = -6x + 18, \qquad L_2^2(x) = 12x^2 - 96x + 144$$

Associated Laguerre polynomial are not orthogonal, but associated Laguerre functions of the type:

(10.12) $$\phi_n^k(x) = e^{-x/2} x^{k/2} L_n^k(x)$$

Are orthogonal on the interval $0 \le x < \infty$, so the make an orthogonal set. The functions $\phi_n^k(x)$, are not solutions to the associated Laguerre equation, but they are solutions to a *related* equation.

In dealing with the radial part of the Schrödinger equation, we are interested in a slightly different associated Laguerre function, where the only difference is that *k* is replaced with *k*+1, that is the function:

(10.13) $$y_j^k(x) = e^{-x/2} x^{(k+1)/2} L_j^k(x)$$

These are not only solution to the associated Laguerre equation, but they are also solutions to

(10.14) $$\frac{d^2 y_j^k}{dx^2} + \left(-\frac{1}{4} + \frac{2j + k + 1}{2x} x - \frac{k^2 - 1}{4x^2} k\right) y_j^k = 0$$

The main reason for studying this equation, is that the radial equation may be brought in the form, (10.8), where that the radial function *R*(*r*) that we seek is: $R_n^l(r) = \chi_n^l(x)/r$, apart from a normalization constant.
We are now ready to form the connection between the equation above and the radial equation. For simplicity we put $v = L_j^k(x)$, since the indices do not change in the calculations.
We then show that $y_j^k(x) = y = e^{-x/2} x^{(k+1)/2} v$ satisfy (8,14). We find the first derivative:

$$y' = -\tfrac{1}{2}e^{-x/2}x^{(k+1)/2}v + e^{-x/2}(\tfrac{k+1}{2})x^{(k+1)/2}v + \tfrac{1}{2}e^{-x/2}x^{(k+1)/2}v'$$
$$= \left(-\frac{1}{2}v + (\frac{k+1}{2x})v + v'\right)e^{-x/2}x^{(k+1)/2}$$

$$y'' = -\tfrac{1}{2}e^{-x/2}x^{(k+1)/2}\left(-\frac{1}{2}v + (\frac{k+1}{2x})v + v'\right) + e^{-x/2}(\tfrac{k+1}{2})x^{(k+1)/2}\left(-\frac{1}{2}v + (\frac{k+1}{2x})v + v'\right) +$$
$$e^{-x/2}x^{(k+1)/2}\left(-\frac{1}{2}v' - (\frac{k+1}{2x^2})v + (\frac{k+1}{2x})v' + v'\right)$$
$$y'' = e^{-x/2}x^{(k+1)/2}\left[-\tfrac{1}{2}\left(-\frac{1}{2}v + (\frac{k+1}{2x})v + v'\right) + (\frac{k+1}{2x})\left(-\frac{1}{2}v + (\frac{k+1}{2x})v + v'\right) + \left(-\frac{1}{2}v' - (\frac{k+1}{2x^2})v + (\frac{k+1}{2x})v' + v'\right)\right]$$

Inserting the second derivative and the function $y_j^k(x) = y = e^{-x/2}x^{(k+1)/2}v$ into the equation

$$\frac{d^2y_j^k}{dx^2} + (-\frac{1}{4} + \frac{2j+k+1}{2x}x - \frac{k^2-1}{4x^2}k)y_j^k = 0$$

and reducing with the common factor $e^{-x/2}x^{(k+1)/2}$, it still requires some non trivial algebra to arrive at the (correct) result:

(10.15)
$$v'' - v' + \frac{k+1}{x} + \frac{j}{x}v = 0 \quad \Leftrightarrow$$
$$xv'' + (k+1-x)v' + jv = 0$$

Which is the associated Laguerre equation:

(10.16)
$$\frac{d^2L_j^k}{dx^2} + (1-x+k)\frac{dL_j^k}{dx} + jL_j^k = 0$$

Since $y = e^{-x/2}x^{(k+1)/2}v = e^{-x/2}x^{(k+1)/2}L_j^k$ then $y$ must be a solution to (8.14):

(10.17)
$$\frac{d^2y_j^k}{dx^2} + (-\frac{1}{4} + \frac{2j+k+1}{2x}x - \frac{k^2-1}{4x^2}k)y_j^k = 0$$

## 10.3 Finding the energy levels for the hydrogen atom.

We have reduced the radical equation to:

$$\chi''(r) + \frac{2m}{\hbar^2}\left(\frac{Ze^2}{4\pi\varepsilon_0 r} + E\right)\chi(r) - \frac{l(l+1)}{r^2}\chi(r) = 0 \quad \text{where } R(r) = \chi(r)/r$$

(10.18)
$$\frac{d^2\chi}{dr^2} + \left(\frac{2mZe^2}{4\hbar^2\pi\varepsilon_0 r} + \frac{2m}{\hbar^2}E - \frac{l(l+1)}{r^2}\right)\chi(r) = 0$$

To comply with the associated Laguerre equation, we make the following substitution:

$$(\frac{\beta}{2})^2 = -\frac{2mE}{\hbar^2} \qquad \text{(Since } E \text{ is negative)}$$

The last equation becomes:

(10.18) $$\frac{d^2\chi}{dr^2} + \left( \frac{2mZe^2}{4\hbar^2 \pi \varepsilon_0 r} - \frac{\beta^2}{4} - \frac{l(l+1)}{r^2} \right) \chi(r) = 0$$

Then we make a minor change of variables, since we put $x = r\beta \;\Leftrightarrow\; r = \frac{x}{\beta} \;\Rightarrow\; dr = \frac{dx}{\beta}$

Using this substitution the equation reads:

(10.19)
$$\beta^2 \frac{d^2\chi}{dx^2} + \left( \frac{2mZe^2}{4\hbar^2 \pi \varepsilon_0 x} \beta - \frac{\beta^2}{4} - \frac{l(l+1)}{x^2} \beta^2 \right) \chi(r) = 0 \quad \Rightarrow$$
$$\frac{d^2\chi}{dx^2} + \left( \frac{2mZe^2}{4\hbar^2 \pi \varepsilon_0 x \beta} - \frac{1}{4} - \frac{l(l+1)}{x^2} \right) \chi(r) = 0$$

Then equation (10.19) is equal to (10.17)) if

$$l(l+1) = \frac{k^2 - 1}{4} \qquad \text{and} \qquad \frac{2mZe^2}{4\hbar^2 \pi \varepsilon_0 \beta} = \frac{2j + k + 1}{2}$$

$$l(l+1) = \frac{k^2 - 1}{4} \;\Rightarrow\; 4l^2 + 4l + 1 = k^2 \;\Leftrightarrow\; k^2 = (2l+1)^2 \;\Rightarrow\; k = 2l + 1$$

Equation (8,19) gives us the conditions of quantisation of the energy, but it requires some development.

$$\frac{2j + k + 1}{2} = \frac{2j + 2l + 1 + 1}{2} = j + l + 1$$

From the discussion on the associated Laguerre polynomials the indices $j$ and $l$ are non negative integers. $J + l + 1$ can therefore assume any integer value from 1. This integer is traditionally denoted $n$.

$$n = j + l + 1$$

We return to the equation (10.19)

$$\frac{2mZe^2}{4\hbar^2 \pi \varepsilon_0 \beta} = n \;\Rightarrow\; \left( \frac{2mZe^2}{4\hbar^2 \pi \varepsilon_0 n} \right)^2 = \beta^2$$

Since $(\frac{\beta}{2})^2 = -\frac{2mE}{\hbar^2}$, we find: $\left( \frac{2mZe^2}{4\hbar^2 \pi \varepsilon_0 n} \right)^2 = -\frac{8mE}{\hbar^2} \;\Rightarrow$

(10.20)
$$\frac{4m^2Z^2e^4}{16\hbar^4\pi^2{\varepsilon_0}^2n^2}=-\frac{8mE}{\hbar^2}\quad\Rightarrow$$
$$E=-\frac{mZ^2e^4}{32\hbar^2\pi^2{\varepsilon_0}^2n^2}=-\frac{mZ^2e^4}{2\hbar^2(4\pi\varepsilon_0)^2n^2}=\frac{Z^2me^4}{8h^2{\varepsilon_0}^2}\frac{1}{n^2}$$

And for the hydrogen atom, where $Z = 1$

(10.21)
$$E=-\frac{me^4}{8h^2{\varepsilon_0}^2}\frac{1}{n^2}$$

There is a tradition to express the energy by the Rydberg constant.

(10.22)
$$R_H=\frac{me^4}{8ch^3{\varepsilon_0}^2}$$

Then the energy levels become:

(10.23)
$$E=-\frac{hcR_H}{n^2}$$

The constant $hcR_H$ has the value 13.6 eV, so the energy levels of the Hydrogen atom are given by:

(10.24)
$$E=-\frac{13.6\,eV}{n^2}$$

The quantity $\hbar^2/me^2$ has the dimension of a length. It is called the Bohr radius $a_0$.

(10.24)
$$a_0=\frac{\hbar^2}{me^2}=0.529\cdot10^{-8}m=0.529\mathring{A}$$