# Laplace equation and related equations in spherical coordinates

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The spherical coordinates are $(r, \phi, \theta)$, where

$$r \geq 0, \quad 0 \leq \phi \leq \pi, \quad -\pi < \theta \leq \pi,$$

here $r$ is the distance from the origin, and $(\phi, \theta)$ are coordinates on the sphere: $\phi$ is called co-latitude, (the ordinary geographical latitude is $\pi/2 - \phi$), and $\theta$ is the longitude (same as in geography).

The correspondence between spherical and rectangular coordinates is as follows:

$$x = r \sin \phi \cos \theta, \quad y = r \sin \phi \sin \theta, \quad z = r \cos \phi.$$

Draw a picture to visualize this.

The volume element

$$dx \, dy \, dz = r^2 \sin \phi \, dr \, d\phi \, d\theta,$$

and the area element on the sphere of radius $r$ centered at the origin is

$$r^2 \sin \phi \, d\phi \, d\theta.$$

Laplace operator has this form:

$$\Delta u = u_{rr} + \frac{2}{r} u_r + \frac{1}{r^2 \sin \phi} (u_\phi \sin \phi)_\phi + \frac{1}{r^2 \sin^2 \phi} u_{\theta\theta}.$$

It is convenient to write it as a sum

$$\Delta u = \Delta_r u + \frac{1}{r^2} \Delta_s u,$$

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where $\Delta_r$ is the *radial part* containing derivatives with respect to $r$ only, and $\Delta_s$ is the *spherical part* containing derivatives with respect to the angular coordinates.

For future use, it is convenient to consider a more general equation of the form

$$L_r u + \frac{1}{r^2}\Delta_s u = 0, \tag{1}$$

where $L_r$ is any operator involving only derivatives with respect to $r$.

Our first task is to separate the variables, and deal with the spherical part.

Looking for solutions of (1) of the form

$$u(r, \phi, \theta) = R(r)S(\phi, \theta),$$

we obtain

$$r^2 \frac{L_r R}{R} = -\frac{\Delta_s S}{S}.$$

Since the LHS depends only on $r$ and the RHS only on $\phi, \theta$, their common value must be a constant $\lambda$. Then the radial part becomes

$$r^2 L_r R = \lambda R, \tag{2}$$

and the spherical part becomes

$$\Delta_s S + \lambda S = \frac{1}{\sin\phi}(S_\phi \sin\phi)_\phi + \frac{1}{\sin^2\phi}S_{\theta\theta} + \lambda S = 0. \tag{3}$$

Our first main concern will be the spherical part. Notice that in (3) there are no explicitly stated boundary conditions, since the sphere has no boundary. However the very nature of the spherical coordinates imposes some conditions since we are looking for smooth, continuous functions on the sphere. First of them is that $\theta \mapsto S(\phi, \theta)$ must be *periodic*, with period $2\pi$. And there is one more, related to the North and South poles $\phi \in \{0, \pi\}$ which will be discussed below.

## 1. Spherical part of the Laplace operator.

We perform the second separation of variables by setting $S(\phi, \theta) = \Phi(\phi)\Theta(\theta)$ in (3), multiplying on $\sin^2\phi$ and shifting the $\theta$ part to the RHS: and obtain

$$\frac{\sin\phi\,(\Phi' \sin\phi)'}{\Phi} + \lambda \sin^2\phi = -\frac{\Theta''}{\Theta}.$$

since the LHS depends only on $\phi$ and the RHS depends only on $\theta$, we conclude that they are both equal to the same constant which we denote by $m^2$, so the problem for $\Theta$ is of familiar type:

$$\Theta'' + m^2\Theta = 0,$$

with periodic boundary conditions (recall that $\theta$ is the longitude!). We conclude that $m$ is a *non-negative integer*, and eigenfunctions are

$$\Theta_m(\theta) = a_m \cos(m\theta) + b_m \sin(m\theta), \quad m = 0, 1, 2, \ldots,$$

or in complex form

$$\Theta_m(\theta) = c_m e^{im\theta}, \quad m = 0, \pm1, \pm2, \ldots. \tag{4}$$

Now the $\phi$ part becomes, after division on $\sin^2 \phi$:

$$\frac{(\Phi' \sin \phi)'}{\sin \phi} + \left(\lambda - \frac{m^2}{\sin^2 \phi}\right)\Phi = 0. \tag{5}$$

This can be simplified by the change of the independent variable $x = \cos\phi$. As $\phi$ changes between $0$ and $\pi$, $x$ describes the interval $[-1, 1]$, and this correspondence is one-to-one. Concerning derivatives, we have

$$\frac{d}{d\phi} = \frac{d}{dx}\frac{dx}{d\phi} = -\sin\phi\frac{d}{dx}, \quad \text{or} \quad \frac{1}{\sin\phi}\frac{d}{d\phi} = -\frac{d}{dx},$$

so if we set $S(x) = S(\cos\phi) =: \Phi(\phi)$, and notice that $1 - x^2 = \sin^2 \phi$, we obtain

$$\frac{(\Phi' \sin \phi)'}{\sin \phi} = \frac{d}{dx}\left((1 - x^2)S'\right),$$

and our equation (5) becomes

$$\left((1 - x^2)S'\right)' - \frac{m^2 S}{1 - x^2} + \lambda S = 0, \tag{6}$$

which is the *associated Legendre equation* (see the handout "Orthogonal polynomials").

Let us discuss the boundary conditions for (6).

When $m = 0$, the theta part $\Theta(\theta)$ is constant (see (4), so the requirement for $\Phi$ is that it has finite limits for $\phi \to 0, \pi$, which means that $S$ has finite

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limits as $x = \cos\phi \to \pm 1$. Thus in this case the condition is that $S(x)$ tends to finite limits as $x \to \pm 1$, and under this condition, we obtain eigenvalues

$$\lambda_n = n(n+1), \quad n = 0, 1, 2 \ldots \tag{7}$$

and eigenfunctions are $S_n = P_n$, the Legendre polynomials (see "Orthogonal polynomials").

When $m \geq 1$ we have that $\Theta_m(\theta)$ non-constant, so for existence of the limits of $\Theta(\theta)\Phi(\phi)$ as $\phi \to 0$ or $\phi \to \pi$, it is *necessary* that $\Phi(0) = 0$ and $\Phi(\pi) = 0$. The reason is that $\phi = 0$ and $\phi = \pi$ correspond each to one point on the sphere (North and South pole, respectively). So we obtain the boundary conditions $\Phi(0) = \Phi(\pi) = 0$ which translates to $S(\pm 1) = 0$, exactly as required for the associated Legendre equation to have eigenvalues $n(n+1)$ and associated Legendre functions $P_n^m$ as eigenfunctions!

If we use complex form of $\Theta_m$ as in (4), we allow $m$ to be any integer, positive or negative, but since equation (6) contains only $m^2$ we write its eigenfunctions as $P_n^{|m|}$.

The conclusion is that the $\phi$-part always has eigenvalues $\lambda_n$ as in (7), and eigenfunctions $P_n^{|m|}(\cos\phi)$, where $n \geq m$.

Combining the results for $\theta$ and $\phi$ parts, we make the following fundamental conclusion:

**Theorem.** *Eigenvalues for the spherical part of the Laplace operator (3) are* $\lambda_n = n(n+1)$, $n = 0, 1, 2, \ldots$. *To each eigenvalue* $\lambda_n$ *correspond* $2n+1$ *linearly independent eigenfunctions, namely*

$$P_n^{|m|}(\cos\phi)e^{im\theta}, \quad -n \leq m \leq n, \tag{8}$$

*where* $P_n^{|m|}$ *are associated Legendre functions.*

Another (real) basis of eigenfunctions consists of

$$P_n^m(\cos\phi)\cos(n\theta), \quad 0 \leq m \leq n, \tag{9}$$

and

$$P_n^m(\cos\theta)\sin(n\theta), \quad 1 \leq m \leq n, \tag{10}$$

and of course we again have $2n+1$ of them.

It follows from the results about associated Legendre functions stated in "Orthogonal polynomials" that functions (8) form an complete orthogonal system in $L^2$ on the sphere.

Another basis consisted of real functions is formed by functions (9) and (10).

## 2. Applications.

### 2.1. Dirichlet problem for a three-dimensional ball.

$$\Delta u = 0, \quad u(L, \phi, \theta) = f(\phi, \theta), \tag{11}$$

where $f$ is the boundary condition. We have equation (1) with the radial part $L_r u = \Delta_r u$, so (2) becomes

$$r^2 u_{rr} + 2r u_r - n(n+1)u = 0,$$

where $n(n+1)$ are eigenvalues of the spherical part which we found in the previous section, see (7). This is Euler's equation whose characteristic equation is

$$\rho(\rho - 1) + 2\rho - n(n+1) = 0,$$

whose solutions are $\rho_1 = n$, $\rho_2 = -n - 1$. The second solution is rejected because $r^{-n-1}$ will blow up as $r \to 0$, since $n \geq 0$, so only $r^n$ remains, and we obtain the general solution of (11) in the form

$$\sum_{n=0}^{\infty} \sum_{m=-n}^{n} c_{m,n} e^{im\theta} r^n P_n^{|m|}(\cos \phi).$$

To satisfy the boundary condition, we plug $r = L$ and obtain

$$f(\phi, \theta) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} c_{m,n} e^{im\theta} L^n P_n^{|m|}(\cos \phi), \tag{12}$$

which is a generalized Fourier series. Its coefficients are obtained by Fourier formulas, using the values

$$\|P_n^{|m|}\|^2 = \frac{2}{2n+1} \frac{(n+|m|)!}{(n-|m|)!},$$

computed in "Orthogonal polynomials":

$$c_{m,n} = \frac{(2n+1)(n-|m|)!}{4\pi L^n (n+|m|)!} \int_0^\pi \int_{-\pi}^\pi f(\phi, \theta) e^{-im\theta} P_n^{|m|}(\cos \phi) \sin \phi \, d\phi \, d\theta.$$

**Exercise.** Where did $\sin\phi$ under the integral come from?

Remarks.

1. In general, an eigenvalue problem in $k$ dimensions will have eigenfunctions labeled by $k$ subscripts.

2. One can proceed as we did for the Dirichlet problem for the disk, and derive a Poisson formula, which may be more convenient than a series expansion. (It contains only one integral instead of infinitely many in Fourier formula!) Instead of summing a geometric series, as in the derivation of Poisson's formula in 2 dimensions, one would use the *generating function* for Legendre polynomials. The statement is given in Theorem 6.10 in the book.

3. It turns out that each term of the series (12), when expressed in rectangular coordinates, becomes a homogeneous polynomial in $x, y, z$ of degree $n$ and this polynomial satisfies the Laplace equation. These polynomials are called the *spherical harmonics*, and the explicit expression is

$$r^n Y_n^m(\phi, \theta) := r^n P_n^{|m|}(\cos\phi)e^{im\theta}.$$

## 2.2. Eigenvalue problem for Laplace operator in a ball.

It arises when separating the time variable from the space variables in the heat or wave equation for a ball $\|x\| \leq L$.

The space part is

$$\Delta u + E^2 u = 0, \tag{13}$$

subject to boundary conditions, for example, the *Dirichlet boundary condition*

$$u(L, \phi, \theta) = 0, \tag{14}$$

or the *Neumann boundary condition*

$$u_r(L, \phi, \theta) = 0. \tag{15}$$

I denoted the eigenvalue by $E^2$, since I now it is going to be positive, and used another later, to avoid confusion with $\lambda_n = n(n+1)$ is section 1.

Writing $\Delta = \Delta_r + r^{-2}\Delta_s$ in (13) and separating the variables, we obtain the eigenvalue problem for $\Delta_s$, which we solved in section 1, and the radial part (2)s with

$$L_r = \Delta_r + E^2.$$

So we have to solve the radial part

$$r^2 R_{rr} + 2r R_r + (E^2 r^2 - n(n+1)) R = 0,$$

which is (2) with substituted value $\lambda = n(n+1)$ found in the Theorem in Section 1,

This looks very similar to Bessel equation, and indeed can be transformed to Bessel equation by the change of the variable $R(r) = r^{-1/2} y(Er)$, which gives the Bessel equation

$$r^2 y'' + r y' + (r^2 - (n+1/2)^2) g = 0.$$

Since we need a solution which is finite at 0, the solution is

$$R_n(r) = r^{-1/2} J_{n+1/2}(Er).$$

**Exercise**: what is $R_n(0)$, really?

Now the boundary condition (14) gives $J_{n+1/2}(EL) = 0$, so

$$E_{n,k} = x_{n+1/2,k}/L,$$

where $x_{n+1/2,k}$ is the $k$-th zero of Bessel function $J_{n+1/2}$. It is worth recalling that $J_{n+1/2}$ is in fact elementary, so its zeros can be found explicitly, at least in principle. The eigenfunctions corresponding to these eigenvalues are

$$u_{m,n,k}(r, \phi, \theta) = r^{-1/2} J_{n+1/2}(E_{n,k} r) P_n^{|m|}(\cos \phi) e^{im\theta}.$$

The boundary condition (14) translates into $J_{n+1/2}'(EL) = 0$, so this time

$$E_{n,k} = y_{n+1/2,k}/L, \tag{16}$$

where $y_{n+1/2,k}$ is the $k$-th zero of derivative of the Bessel function $J_{n+1/2}$. The eigenfunctions are of the same form using these new values (16).

These eigenvalues and eigenfunctions allow us to solve heat and wave equations for the ball.

## 2.3. Spectrum of the hydrogen atom and the periodic table

It is the following eigenvalue problem[1] in the whole 3-space:

$$\Delta u + \frac{2}{r} u + 2E u = 0,$$

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[1] For simplicity of formulas, we use the units where Planck's constant, mass and charge of the electron are all equal to 1.

where $E < 0$ is the eigenvalue[2], and the boundary condition is that $u \in L^2(\mathbf{R}^3)$ which essentially means that $u(x) \to 0$ when $|x| \to \infty$. And of course $u$ is assumed to be finite everywhere. The problem is to find eigenvalues. Eigenvalues correspond to possible energies of an electron in an atom.

Applying the same approach as in the beginning of this text, we split $\Delta$ into spherical and radial parts (1), and use our solution of the spherical problem is section 2. Eigenvalues of the spherical part are $n(n+1)$ (Theorem in Section 1), so the radial part (2) becomes

$$r^2 R'' + 2r R' + \left(2E r^2 + 2r - n(n+1)\right) R = 0.$$

We are looking for *negative* numbers $E$ for which this equation has a non-trivial solution which is finite at 0 and tends to 0 at $+\infty$. It turns out that the differential equation can be transformed to the Laguerre equation by the following changes of the variables.

First we set

$$\nu = (-2E)^{-1/2}, \quad x = 2r/\nu, \quad S(x) = S(2r/\nu) = R(r).$$

which gives

$$x^2 S'' + 2x S' + \left(\nu x - x^2/4 - n(n+1)\right) S = 0,$$

and then we put $S(x) = x^n e^{-x/2} y(x)$, and obtain

$$x y'' + (2n + 2 - x) y' + (\nu - n - 1) y = 0,$$

which is the Laguerre equation with $\alpha = 2n + 1$ and $n$ replaced by $\nu - n - 1$.

**Exercise.** Verify these changes of the variables.

The boundary conditions imply that the solutions must be the Laguerre polynomials, of degree $n - \nu - 1$, so we conclude that
$\nu \geq n + 1$ is an integer, and thus the eigenvalue $E$ is

$$E_\nu = -\frac{1}{2\nu^2}, \quad \nu = n + 1, n + 2, \dots. \tag{17}$$

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[2]One can show that all eigenvalues are negative, though the set of eigenfunctions is not complete. Eigenvalues correspond to the stationary states of the hydrogen atom.

So
$$R_{n,\nu}(r) = (2r/\nu)^n e^{-r/\nu} L^{2n+1}_{\nu-n-1}(2r/\nu).$$

and the eigenfunctions of the original problem are
$$u_{m,n,\nu}(r,\phi,\theta) = R_{n,\nu}(r) e^{im\theta} P^{|m|}_n(cos\phi).$$

They are indexed by three integers $(m,n,\nu)$ which satisfy
$$0 \le |m| \le n < \nu,$$

and correspond to eigenvalues (17).

To a fixed eigenvalue corresponds fixed $\nu \ge 1$ to this $\nu$ correspond $\nu$ values of $n$, namely $(0, 1, 2, \ldots, \nu-1)$ and to each $n$ correspond $2n+1$ values of $m$, namely $-n, -n+1, \ldots, n-1, n$. Thus the total dimension of the eigenspace corresponding to an eigenvalue $E_\nu = -1/(2\nu^2)$ is

$$\sum_{n=0}^{\nu-1}(2n+1) = \nu^2.$$

This has the following interpretation. To each eigenfunction corresponds a *state* of an electron in an atom, and the eigenvalue $E$ is its energy. Pauli Principle says that there can be at most two electrons in any given state (besides the three integers $(m,n,\nu)$ an electron also characterized by the *spin* which can take only two values $\pm 1/2$. And all electrons in an atom must have distinct triples $(m,n,\nu)$ or different spins.

So the energy level $\nu = 1$ can have at most 2 electrons, $\nu = 2$ at most 8, $\nu = 3$ at most 18. We recognize these numbers $2, 8, 18, \ldots$ as the row lengths of the Periodic Table.

Returning to the hydrogen atom, the energy levels $-1/(2\nu^2)$ has the following meaning. Normally the single electron will occupy the lowest level $\nu = 1$. When the hydrogen atom absorbs light the electron is "excited", that it jumps to some other level $\nu = k$. The absorbed energy is the difference. In general, when an electron jumps from level $n$ to level $k$, the energy difference will be

$$R\left(\frac{1}{n^2} - \frac{1}{k^2}\right),$$

where $R$ is the *Rydberg constant* which depends on the units (in our units it is $1/2$). Since the energy of light quantum is proportional to its frequency, this explains the frequencies of the *Balmer series* in the spectrum of hydrogen.

The computation in this section was made for the first time by the famous mathematician Hermann Weyl, shortly after the discovery of the modern form of quantum mechanics in the work of Heisenberg, Born, Jordan, Schrödinger and Dirac.