3.3. Laplace's equation

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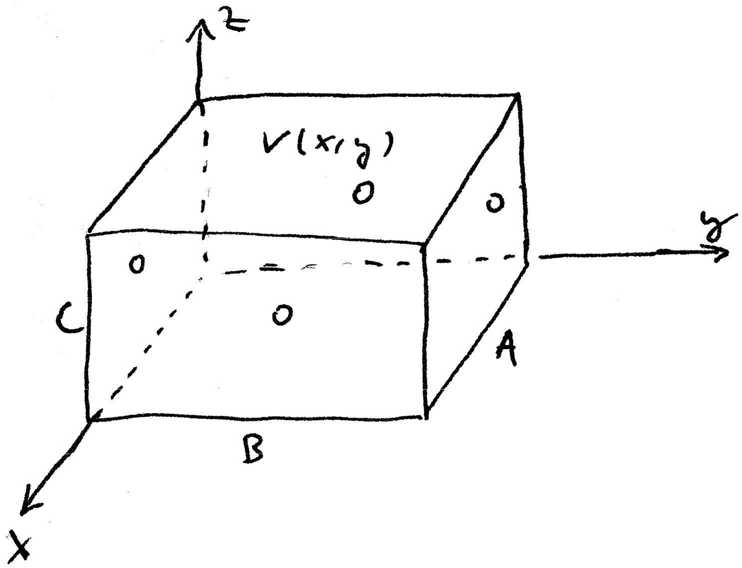
3.3.1 Example : Cartesian coordinates

Calculate potential inside a hollow box with the prescribed boundary conditions:



Ansatz: Separation of variables : $\phi = X(x)\,Y(y)\,Z(z)$

leads to

$$\vec{\nabla}^2 \phi = 0 \implies \frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z} = 0 .$$

Solve $\quad \frac{X''}{X} = \lambda_x = \text{const}.$

two linearly independent solutions:

$X = e^{ikx}$, with $k^2 = -\lambda_x$.

k can be purely real or purely imaginary.

Because of the boundary conditions,

$\phi(x=0) = \phi(x=A) \stackrel{!}{=} 0$, the appropriate

linear combination is

$X = \sin kx = \sin(\sqrt{-\lambda_x}\, x)$, with

$\sqrt{-\lambda_x}\, A = m\pi, \quad m = 1, 2, \ldots$

it follows that the solutions that

satisfy the bc are

$X_m = X_0^{(m)} \sin(\sqrt{-\lambda_x^{(m)}}\, x)$ with $\lambda_x^{(m)} = -\frac{m^2 \pi^2}{A^2}$.

For Y we get analogous solutions:

$Y_n = Y_0^{(n)} \sin(\sqrt{-\lambda_y^{(n)}}\, y)$ with $\lambda_y^{(n)} = -\frac{n^2 \pi^2}{B^2}$

We need to solve now

$$Z'' = \lambda_z Z , \qquad (*)$$

with $\lambda_z = \dfrac{m^2 \pi^2}{A^2} + \dfrac{n^2 \pi^2}{B^2}$

and boundary conditions $\phi(z=0) = 0,$

$$\phi(x,y, z=0) = V(x,y) .$$

Because $\lambda_z > 0$, the solutions to the eigenvalue equation $(*)$ are

$$Z = e^{\pm kz} , \qquad \text{with} \qquad \lambda_z = k^2$$

The appropriate linear combination that satisfies the b.c $Z(z=0) = 0$ is

$$Z(z) = \alpha_{mn} \sinh(\gamma_{mn} z) , \qquad \text{with}$$

$$\gamma_{mn} = \pi \sqrt{\frac{m^2}{A^2} + \frac{n^2}{B^2}}$$

Therefore, the set of functions

$$\phi_{mn}(x,y,z) = \alpha_{mn} \sin\left(\frac{m\pi x}{A}\right) \sin\left(\frac{n\pi y}{B}\right) \sinh(\gamma_{mn} z)$$

solves the linear, homogeneous equation

$$\vec{\nabla}^2 \phi = 0.$$

The general solution is thus the linear combination

$$\phi(x,y,z) = \sum_{m,n} \alpha_{mn} \sin\left(\frac{m\pi x}{A}\right) \sin\left(\frac{n\pi y}{B}\right) \sinh(\gamma_{mn} z),$$

with α_{mn} determined by the remaining bc:

$$V(x,y) = \phi(x,y,z=C) \overset{!}{=} \sum_{m,n} \alpha_{mn} \sin\left(\frac{m\pi x}{A}\right) \sin\left(\frac{n\pi y}{B}\right) \sinh(\gamma_{mn} C)$$

To determine these coefficients, we note that the functions $\sin\left(\frac{n\pi x}{L}\right)$ $n = 0, 1, \ldots$ form a normal set on the interval $[0, L]$:

$$\int_0^L dx \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) = \frac{L}{2}\delta_{mn}$$

In fact because on the interval $[0, L]$

the operator $p_x^2 = -\partial_x^2$ is <u>self-adjoint</u>

(acting on functions with $f(0) = f(L) = 0$)

(which are eigenvectors of p_x^2)

these functions form a <u>complete set</u>:

$$\sum_m \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{n\pi y}{L}\right) = \frac{L}{2}\,\delta(x-y)$$

In any case, using the normality condition

we find

$$\alpha_{mn} = \frac{1}{\sinh(\gamma_{mn} C)}\,\frac{4}{AB}\int_0^A dx \int_0^B dy\; V(x,y)\,\sin\left(\frac{m\pi x}{A}\right)\sin\left(\frac{n\pi y}{B}\right)$$

The sin functions are specific examples of

sets of complete orthonormal systems

of functions $u_n(x)$, which satisfy

$$\int_a^b u_n^*(x)\,u_m(x) = \delta_{mn}\,, \qquad \sum_n u_n(x)\,u_n^*(y) = \delta(x-y)$$

orthonormality $\qquad\qquad$ completeness

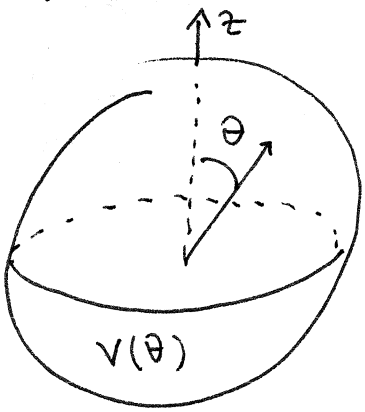
These relations are the analogues of

$$\langle n | m \rangle = \delta_{mn} \quad , \quad \sum_n |n\rangle\langle n| = \mathbb{1}$$

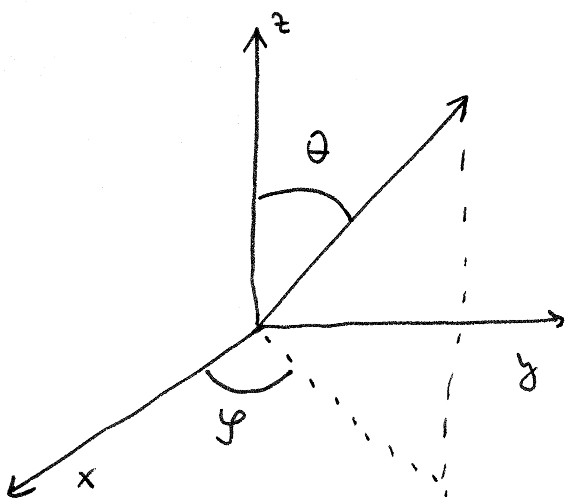
in quantum mechanics.

4.2 Spherical Coordinates

Suppose now we are asked to calculate the potential outside a sphere kept at a potential $V = V(\theta)$



Because of the geometry of the problem, it turns out to be convenient to work in spherical coordinates:



$$x = r \sin\theta \cos$$

$$y = r \sin\theta \sin\varphi$$

$$z = r \cos\theta$$

In spherical coordinates, the Laplace operator is

$$\vec{\nabla}^2 \phi = \frac{1}{r} \frac{\partial^2 (r\phi)}{\partial r^2} - \frac{1}{r^2} L^2 \phi , \quad \text{where}$$

the operator L^2 is

$$-L^2 \phi = \frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial \phi}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2 \phi}{\partial \varphi^2} .$$

To solve the Laplace equation with the given bc we try the separation ansatz

$$\phi = R(r)\, Y(\theta, \varphi)$$

(we shall see that Y can be written as $\Theta(\theta) \cdot \Phi(\varphi)$)

The ansatz leads to

$$\frac{1}{rR} \frac{d^2 (rR)}{dr^2} - \frac{1}{r^2} \frac{L^2 Y}{Y} = 0.$$

As before, we can satisfy this eq if

$$L^2 Y = \lambda Y , \quad \text{with } \lambda \text{ a constant.}$$

We already know the solutions of the eigenvalue equation: the <u>spherical harmonics</u>.

$$Y_{\ell m}(\theta, \varphi) = (-1)^m \; N_{\ell m} \; P_\ell^m(\cos\theta) \, e^{im\phi} \quad , \quad \text{with}$$

associated Legendre functions

$$N_{\ell m} = \sqrt{\frac{2\ell+1}{4\pi} \; \frac{(\ell-m)!}{(\ell+m)!}}$$

$$m = -\ell, -\ell+1, \ldots, \ell \qquad \text{and} \qquad \ell = 0, 1, 2, \ldots$$

They satisfy $\quad L^2 Y_{\ell m} = \ell(\ell+1) Y_{\ell m}$

and form an orthonormal complete set on the sphere:

$$\int d\Omega \;\; Y^*_{\ell_1 m_1}(\theta, \varphi) \, Y_{\ell_2 m_2}(\theta, \varphi) = \delta_{\ell_1 \ell_2} \, \delta_{m_1 m_2} \, ,$$

$$\sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\theta', \varphi') \, Y_{\ell m}(\theta, \varphi) = \delta(\varphi' - \varphi) \, \delta(\cos\theta' - \cos\theta)$$

With $\quad \dfrac{L^2 Y_{\ell m}}{Y_{\ell m}} = \ell(\ell+1) \quad$ we just need to solve

$$\frac{1}{rR} \qquad\qquad - \frac{\ell(\ell+1)}{r^2} = 0$$

Because of the structure of the ~~solutions~~ equation,

we try the power-law ansatz

$R = r^q$, which leads to

$$q(q+1) - \ell(\ell+1) = 0 \quad , \quad \text{with solutions}$$

$$q_1 = +\ell \qquad \text{and} \qquad q_2 = -(\ell+1)$$

A solution with $q_1 = \ell$ blows up at infinity and is unphysical.

Therefore, the general solution of $\vec{\nabla}^2 \phi = 0$ is

$$\phi = \sum_{\ell m} \frac{a_{\ell m}}{r^{\ell+1}} Y_{\ell m}(\theta, \varphi)$$

The coefficients $a_{\ell m}$ are determined by the boundary conditions:

$$\phi(r=R, \theta, \varphi) = \sum_{\ell m} \frac{a_{\ell m}}{R^{\ell+1}} Y_{\ell m}(\theta, \varphi) \stackrel{!}{=} V(\theta, \varphi)$$

Using the orthonormality relation,

$$a_{\ell m} = R^{\ell+1} \int d\Omega \; V(\theta, \varphi) \, Y^*_{\ell m}(\theta, \varphi) \, .$$

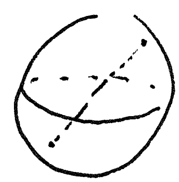
The expansion $\phi = \sum_{lm} \frac{a_{lm}}{r^{l+1}} Y_{lm}(\theta, \varphi)$ is a multipole expansion (more about it later)

In problems with azimuthal symmetry (e.g. $V = V(\theta)$) only harmonics with $m=0$ enter the expansion. In this case the spherical harmonics reduce to the <u>Legendre polynomials</u>: $Y_{l\,m=0} = \frac{1}{\sqrt{4\pi}} P_l(\cos\theta)$

4.2.5 Spherical harmonics

Spherical harmonics satisfy a number of useful relations and identities. Among others

- Parity (spatial inversion)



$$Y_{lm}(\pi - \theta, \phi + \pi) = (-1)^l \, Y_{lm}(\theta, \varphi)$$

- $$Y_{l\,-m}(\theta, \varphi) = (-1)^m \, Y^*_{lm}(\theta, \varphi)$$

• Addition Theorem :

i) Let (θ_1, φ_1) and (θ_1', φ_1') be the coordinates of two points on the sphere

ii) Let (θ_2, φ_2) and (θ_2', φ_2') be the coordinates of the same points after a (passive) rotation.

Then,

$$\sum_m Y_{\ell m}(\theta_1, \varphi_1)\, Y^*_{\ell m}(\theta_1', \varphi_1') = \sum_m Y_{\ell m}(\theta_2, \varphi_2)\, Y^*_{\ell m}(\theta_2', \varphi_2')$$

This is just an expression of the fact that

$\sum_m |\ell m\rangle\langle \ell m|$ is a <u>scalar</u> under rotations.

If we choose $\theta_2 = 0$, then $Y_{\ell m}(\theta_2 = 0, \varphi_2) = 0$ $m \neq 0$

and the addition theorem reduces to

$$\sum_m Y_{\ell m}(\theta, \varphi)\, Y^*_{\ell m}(\theta', \varphi') = \frac{2\ell+1}{4\pi} P_\ell(\cos\gamma)$$

where γ is the angle