CHEM1034 - Week 30 Lecture - Polar, cylindrical and spherical coordinates

Chapter 16 of Monk and Munro, "Maths for Chemistry", 2nd edition.
Section 3.5 and Chapter 10 of Steiner, "The Chemistry Maths Book", 2nd edition.

Many problems in physics have rotational symmetry – hydrodynamics in cylindrical pipes, electromagnetism of point charges and charged spheres, quantum mechanics of single atoms and diatomic molecules, *etc.* Describing such problems using Cartesian coordinates, although formally correct, may be inconvenient. As an example, consider the equation for a unit sphere. In Cartesian coordinates, it is

$$x^2 + y^2 + z^2 = 1$$

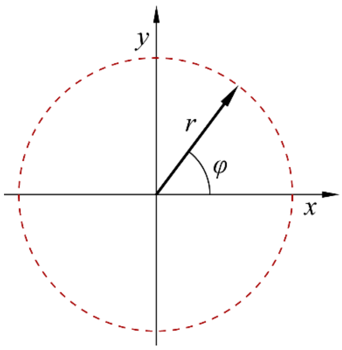
This equation is cumbersome – solving it for any of the three variables requires us to keep track of the positive and the negative solution, any processes (for example, diffusion) happening on the surface of this sphere would have to be described by non-linear equations and so on. This lecture focuses on coordinate systems that are more natural for systems with cylindrical and spherical symmetry.

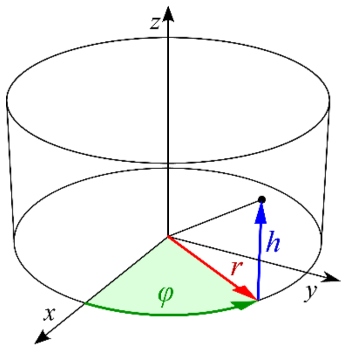
Definitions

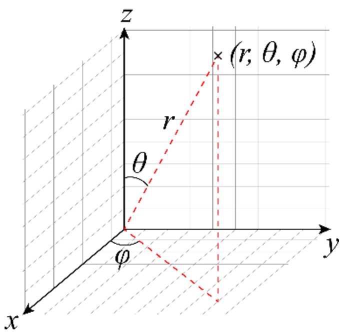
Polar coordinates (2D): $x = r\cos\varphi,\ y = r\sin\varphi$

Cylindrical coordinates (3D): $x = r\cos\varphi,\ y = r\sin\varphi,\ z = h$

Spherical coordinates (3D): $x = r\sin\theta\cos\varphi,\ y = r\sin\theta\sin\varphi,\ z = r\cos\theta$







The conventions above are the ISO 31-11 standard definitions normally used in physical sciences. The ranges for the angular variables are as follows: $0 \le \varphi < 2\pi$ for the polar coordinates and $0 \le \varphi < 2\pi,\ 0 \le \theta \le \pi$ for the spherical coordinates.

Example 1: rewrite the equation of a unit sphere $x^2 + y^2 + z^2 = 1$ in spherical coordinates.

Solution:

$$\begin{aligned} & x^2 + y^2 + z^2 = r^2\sin^2\theta\cos^2\varphi + r^2\sin^2\theta\sin^2\varphi + r^2\cos^2\theta = \\ & = r^2\sin^2\theta\left(\cos^2\varphi + \sin^2\varphi\right) + r^2\cos^2\theta = r^2\left(\sin^2\theta + \cos^2\theta\right) = r^2 \quad \Rightarrow \quad r^2 = 1 \end{aligned}$$

Example 2: differentiate the function $f(x, y) = x^2 - y^2$ with respect to the polar coordinates radius-vector r and convert the result into polar coordinates.

Solution:

$$\frac{\partial f}{\partial r} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial r} = 2x\cos\varphi - 2y\sin\varphi = 2r\cos^2\varphi - 2r\sin^2\varphi = 2r\cos 2\varphi$$

The inverse relationships that convert polar, cylindrical and spherical coordinates back to Cartesian coordinates are (not examinable):

$$\begin{cases} r=\sqrt{x^2+y^2} \\ \varphi=\arctan\left(y/x\right) \end{cases} \qquad \begin{cases} r=\sqrt{x^2+y^2} \\ \varphi=\arctan\left(y/x\right) \\ h=z \end{cases} \qquad \begin{cases} r=\sqrt{x^2+y^2+z^2} \\ \theta=\arccos\left(z/r\right) \\ \varphi=\arctan\left(y/x\right) \end{cases}$$

As the two examples given above illustrate, the transformation of algebraic expressions from one coordinate system into another is accomplished by a simple variable substitution followed by simplification.

Transformation of differential operators

In situations when differential equations must be transformed from one coordinate system into another the transformation must be applied to the derivative operators. Such transformations are accomplished using the generalized chain rule that we have derived in Week 23:

$$\begin{gathered} \frac{\partial}{\partial\alpha} f\left(x\left(\alpha,\beta,\ldots\right),y\left(\alpha,\beta,\ldots\right),\ldots\right)=\frac{\partial f}{\partial x}\frac{\partial x}{\partial\alpha}+\frac{\partial f}{\partial y}\frac{\partial y}{\partial\alpha}+\ldots \\ \Downarrow \\ \frac{\partial}{\partial\alpha}=\frac{\partial x}{\partial\alpha}\frac{\partial}{\partial x}+\frac{\partial y}{\partial\alpha}\frac{\partial}{\partial y}+\ldots \end{gathered} \tag{1}$$

For example, the partial derivative operator with respect to the azimuthal angle θ, written in Cartesian coordinates, would be:

$$\frac{\partial}{\partial\theta}=\frac{\partial x}{\partial\theta}\frac{\partial}{\partial x}+\frac{\partial y}{\partial\theta}\frac{\partial}{\partial y}+\frac{\partial z}{\partial\theta}\frac{\partial}{\partial z}=\left(r\cos\theta\cos\varphi\right)\frac{\partial}{\partial x}+\left(r\cos\theta\sin\varphi\right)\frac{\partial}{\partial y}+\left(-r\sin\theta\right)\frac{\partial}{\partial z}=$$

$$=r\left[\frac{z}{r}\frac{x}{\sqrt{x^2+y^2}}\frac{\partial}{\partial x}+\frac{z}{r}\frac{y}{\sqrt{x^2+y^2}}\frac{\partial}{\partial y}-\frac{\sqrt{x^2+y^2}}{r}\frac{\partial}{\partial z}\right]=\frac{zx}{\sqrt{x^2+y^2}}\frac{\partial}{\partial x}+\frac{zy}{\sqrt{x^2+y^2}}\frac{\partial}{\partial y}-\sqrt{x^2+y^2}\frac{\partial}{\partial z}$$

A particularly famous example that you would encounter multiple times in your subsequent courses is the transformation of the Laplacian operator

$$\Delta=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2} \tag{2}$$

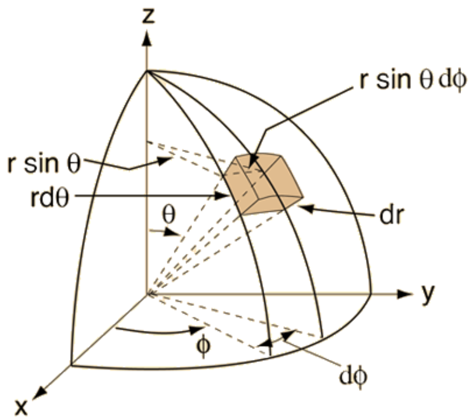
into spherical coordinates. The most straightforward way to proceed is to transform individual first derivatives and then put the result together. After a very long derivation (do it as an exercise), we get

$$\Delta=\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}+\frac{\cos\theta}{r^2\sin\theta}\frac{\partial}{\partial\theta}+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}$$

The angular part of this operator is responsible for the shapes of atomic orbitals and the structure of the Periodic Table. The radial part determines, in particular, the $1/r$ distance dependence of electrostatic and gravitational potentials from point charges and masses.

Note that multiple conventions exist for the definitions of spherical angles and different sources would therefore have different expressions for the differential operators in what each of them calls "spherical coordinates". The ISO 31-11 standard definitions given above are strongly recommended.

Integration in curvilinear coordinates



It is easy to see that simply switching the integration variables and updating integration limits is insufficient because, unlike the volume element $dV = dxdydz$ that is the same everywhere in Cartesian coordinates, the volume element $drd\theta d\varphi$ is different in different locations. The same applies to the area element $dS = dxdy$ and its polar equivalent $drd\varphi$. We must therefore find a way to correctly transform integrals from one coordinate system into another.

We do not have sufficient time in this course to formally prove this statement (google *Jacobian determinants* if you are interested), but the following relations hold for polar, cylindrical and spherical coordinates respectively:

$$dxdy = rdrd\varphi, \qquad dxdydz = rdrd\varphi dh, \qquad dxdydz = r^2 \sin\theta drd\theta d\varphi \tag{3}$$

<u>Example 1</u>: integrate $f(x,y) = 1/(1+x^2+y^2)$ over the disk of radius 1 with the centre at the origin.

<u>Solution</u>: an attempt to take this integral in Cartesian coordinates is unlikely to succeed

$$\iint_{\text{disk}} \frac{1}{1+x^2+y^2} dxdy = \int_{-1}^{1} dx \int_{-\sqrt{1-x^2}}^{+\sqrt{1-x^2}} \frac{dy}{1+x^2+y^2} = \ldots$$

we can, however, notice that the disk has rotational symmetry and that x^2+y^2 has a particularly simple form in polar coordinates: $x^2+y^2 = r^2(\cos^2\varphi + \sin^2\varphi) = r^2$. The integration limits also become rather simple in polar coordinates:

$$\iint_{\text{disk}} \frac{1}{1+x^2+y^2} dxdy = \int_0^1 dr \int_0^{2\pi} \frac{r}{1+r^2} d\varphi$$

where the extra r appeared in the outer integral because of the relationship between $dxdy$ and $drd\varphi$ given in Equation (3). That integral is easy to take:

$$\int_0^1 dr \int_0^{2\pi} \frac{r}{1+r^2} d\varphi = 2\pi \int_0^1 \frac{rdr}{1+r^2} = \begin{Bmatrix} \text{subst:} \\ x = r^2 \end{Bmatrix} = \pi \int_0^1 \frac{dx}{1+x} = \pi \ln 2$$

<u>Example 2</u>: integrate $f(x,y,z) = 4z$ over the upper half of the sphere defined by $x^2+y^2+z^2=1$.

<u>Solution</u>: we would not attempt to write this integral in its Cartesian form and move straight into spherical coordinates, not forgetting the Jacobian

$$\int_0^{2\pi} d\varphi \int_0^{\pi/2} \sin\theta d\theta \int_0^1 (4r\cos\theta) r^2 dr = 2\pi \int_0^{\pi/2} \cos\theta \sin\theta d\theta \int_0^1 4r^3 dr =$$

$$= 2\pi \int_0^{\pi/2} \cos\theta \sin\theta d\theta \left[1^4 - 0^4\right] = 2\pi \int_0^{\pi/2} \cos\theta \sin\theta d\theta =$$

$$= \begin{Bmatrix} \text{subst:} \\ x = \sin\theta \end{Bmatrix} = 2\pi \int_0^1 xdx = \pi$$

Week 31 workshop exercises

Steiner, 2nd edition: section 10.7, problems 1-24.

Extra difficulty exercises for the brave

1. Sketch the solids described by the following inequalities:

   (a) $r^2 \le h \le 2 - r^2$ (b) $r \le 2,\ 0 \le \theta \le \pi/2,\ 0 \le \varphi \le \pi/2$

2. A cylindrical shell is 20 cm long, with inner radius 6 cm and outer radius 7 cm. Write inequalities that describe the shell in an appropriate coordinate system. Explain how you have positioned the coordinate system with respect to the shell.

3. A solid lies above the cone $z = \sqrt{x^2 + y^2}$ and below the sphere $x^2 + y^2 + z^2 = z$. Write a description of the solid in terms of inequalities involving spherical coordinates.

Minimal difficulty exercises for the terrified

1. Convert the following Cartesian coordinates $[x, y]$ to polar coordinates:

   (a) $[8,10]$ (b) $[-1,8]$ (c) $[-5,-9]$ (d) $[\zeta,\xi]$

2. Convert the following polar coordinates $[r,\varphi]$ to Cartesian coordinates:

   (a) $[7,\pi]$ (b) $[6,3\pi/4]$ (c) $[-3,3\pi/2]$ (d) $[\rho,\beta]$

3. Convert the following Cartesian equations to equivalent polar equations:

   (a) $x^2 + y^2 = 15$ (b) $x^2 + y^2 = 7y$ (c) $y = 6$ (d) $xy = 1$

4. Convert the following polar equations to equivalent Cartesian equations:

   (a) $r = 10$ (b) $r = 10\sin\varphi$ (c) $r = 5/\cos\varphi$ (d) $\cos\varphi = 1$

5. Sketch the graphs of the following polar equations:

   (a) $r = 5$ (b) $r = \varphi$ (c) $r = \cos\varphi$ (d) $\varphi = 0$

6. Convert the following Cartesian coordinates $[x, y, z]$ to spherical coordinates:

   (a) $[1,-1,1]$ (b) $[0,1,0]$ (c) $[0,\sqrt{2},\sqrt{2}]$ (d) $[\zeta,\xi,\eta]$

7. Convert the following spherical coordinates $[r,\theta,\varphi]$ to Cartesian coordinates:

   (a) $[1,0,0]$ (b) $[1,\pi/3,0]$ (c) $[1,\pi/2,\pi/3]$ (d) $[0,\theta,\varphi]$

8. Convert the following Cartesian equations to (i) equivalent cylindrical equations and (ii) equivalent spherical equations:

   (a) $x^2 - y^2 - z^2 = 1$ (b) $z = x^2 - y^2$ (c) $x^2 + y^2 = y$ (d) $x = 3$

9. Convert the following equations to equivalent Cartesian equations ("c" and "d" are spherical):

   (a) $h = r^2$ (b) $r = \sin\theta\cos\varphi$ (c) $r^2 - 6r + 8 = 0$ (d) $r^2 = r$