CHEM2024 - Week 23 Lecture 1 - 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, quantum mechanics of atoms and diatomic molecules, *etc.* Solving 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. The version of the same equation that uses the distance from the origin is much simpler:

$$r^2 = 1$$

This lecture introduces coordinate systems that are natural for problems with rotational symmetry.

1. Definitions of polar, cylindrical, and spherical coordinates

The following are ISO 31-11 standard definitions normally used in physical sciences:

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

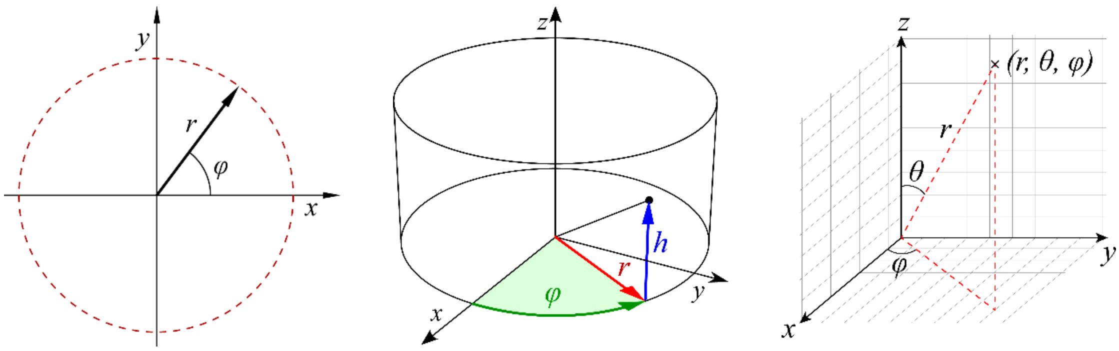

Figure 1. *Schematic diagrams of the polar (left), cylindrical (middle), and spherical (right) coordinates.*

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. Positive φ rotation is counter-clockwise from the X axis. Note that other definitions and conventions exist, particularly in the engineering literature.

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

Solution:

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

2. Inverse relationships

The equations that produce polar, cylindrical and spherical coordinates from Cartesian coordinates are less straightforward. The length of the radius vector is obtained from the definition: $\sqrt{x^2+y^2}$ in polar and cylindrical coordinates, and $\sqrt{x^2+y^2+z^2}$ in spherical coordinates. Multiple trigonometric expressions are possible for the φ angle (*via* arccos, arcsin, or arctan, depending on the choice of the Cartesian variables), but arctan is preferred in practice for numerical stability reasons. The θ angle in spherical coordinates is always positive, and so an arccos is fine:

$$\begin{cases} r=\sqrt{x^2+y^2} \\ \varphi=\arctan\left(y/x\right) \end{cases} \qquad \begin{cases} r=\sqrt{x^2+y^2} \\ \varphi=\arctan\left(y/x\right) \\ h=z \end{cases} \qquad \begin{cases} r=\sqrt{x^2+y^2+z^2} \\ \theta=\arccos\left(z/r\right) \\ \varphi=\arctan\left(y/x\right) \end{cases} \tag{1}$$

<u>Example 2</u>: rewrite the equation describing a logarithmic spiral $r=ae^{b\varphi}$ in Cartesian coordinates.

<u>Solution</u>: a direct substitution followed by a logarithm yields:

$$\ln\frac{\sqrt{x^2+y^2}}{a}=b\arctan\left(y/x\right)$$

This is an implicit equation satisfied by all points of the spiral.

3. Transformation of derivatives

In situations when differential equations are transformed from one coordinate system into another, the transformation must be applied to the derivative operators as well as coordinates. Such transformations are accomplished using the multivariate chain rule:

$$\frac{\partial}{\partial\alpha}f\left[x\left(\alpha,\beta,...\right),y\left(\alpha,\beta,...\right),...\right]=\frac{\partial f}{\partial x}\frac{\partial x}{\partial\alpha}+\frac{\partial f}{\partial y}\frac{\partial y}{\partial\alpha}+... \tag{2}$$

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

<u>Solution</u>:

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

4. Spherical Laplacian

A particularly common differential operator in chemical physics is Laplace operator:

$$\Delta=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2} \tag{3}$$

which occurs, for example, in Schrödinger's equation for the hydrogen atom:

$$\left[-\frac{\hbar^2}{2\mu}\Delta-\frac{e^2}{4\pi\varepsilon_0 r}\right]\psi\left(x,y,z\right)=E\psi\left(x,y,z\right) \tag{4}$$

where μ is the reduced mass of the electron-proton system, and all other symbols have their usual meaning. In preparation for the lecture in which we will solve this equation, we need find the expression for Laplace operator in spherical coordinates.

Derivative operators may be transformed using the chain rule, for example:

$$\begin{aligned}&\frac{\partial f}{\partial r}=\frac{\partial f}{\partial x}\frac{\partial x}{\partial r}+\frac{\partial f}{\partial y}\frac{\partial y}{\partial r}+\frac{\partial f}{\partial z}\frac{\partial z}{\partial r}=\\&=\sin\theta\cos\varphi\frac{\partial f}{\partial x}+\sin\theta\sin\varphi\frac{\partial f}{\partial y}+\cos\theta\frac{\partial f}{\partial z}\end{aligned}\tag{5}$$

In the matrix form, the relation between derivative operators is:

$$\begin{pmatrix}\partial/\partial r\\ \partial/\partial\theta\\ \partial/\partial\varphi\end{pmatrix}=\begin{pmatrix}\sin\theta\cos\varphi & \sin\theta\sin\varphi & \cos\theta\\ r\cos\theta\cos\varphi & r\cos\theta\sin\varphi & -r\sin\theta\\ -r\sin\theta\sin\varphi & r\sin\theta\cos\varphi & 0\end{pmatrix}\begin{pmatrix}\partial/\partial x\\ \partial/\partial y\\ \partial/\partial z\end{pmatrix}\quad\Leftrightarrow\quad\nabla_{r\theta\varphi}=\mathbf{R}\nabla_{xyz}\tag{6}$$

The Laplacian in Equation (3) then has the following form:

$$\Delta=\nabla_{xyz}^{\mathrm{T}}\cdot\nabla_{xyz},\qquad\nabla_{xyz}=\mathbf{R}^{-1}\nabla_{r\theta\varphi}\tag{7}$$

Substitution and simplification yields:

$$\Delta=\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{1}{r^2}\hat{L}^2\tag{8}$$

where $\hat{L}^2$ arises in physical problems that deal with angular momenta:

$$\hat{L}^2=\frac{\partial^2}{\partial\theta^2}+\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\tag{9}$$