INTRODUCTION TO VECTORS

1st Year Physical Chemistry

1 Introductory Notes

Geometry is one of the oldest fields of Mathematics. Vector algebra, however, is relatively new, formalised by *Hermann Grassmann* and *William Rowan Hamilton* in the middle of the 19th century.

Vectors are central to the mathematical description of nature in physics and chemistry. They appear in classical mechanics as position, velocity, force and momentum or describe rotational motions through vector quantities like rotational axis, torque, or angular momentum. Electric and magnetic fields are vector fields, vector-valued functions of the three-dimensional space, which are used to describe electric and magnetic effects and hence the behaviour of light.

Also microscopic quantities are expressed through vectors. Examples are electric and magnetic dipole moments, but also more abstract quantities such as the wavevector or the orientation of a electronic or nuclear spin.

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2 Definitions

Scalar – a physical quantity completely specified by it's magnitude
Examples: temperature, density, mass.

Vector – describes a physical quantity with magnitude and direction in space
Examples: velocity, force, electric- and magnetic field

Notation – arrow above: $\overrightarrow{a}, \overrightarrow{r}, \overrightarrow{x}$; bold font: $\mathbf{a}, \mathbf{r}, \mathbf{x}$; underlined $\underline{r}, \underline{a}, \underline{x}$ (handwriting); Fraktur font: $\mathfrak{a}, \mathfrak{r}, \mathfrak{x}$ (ancient), or none at all a, r, x (when obvious or lazy).

In this manuscript I will use the bold typeface for vectors, as in most printed works nowadays, simply because it offers highest clarity and best readability.

2.1 Operations

Addition

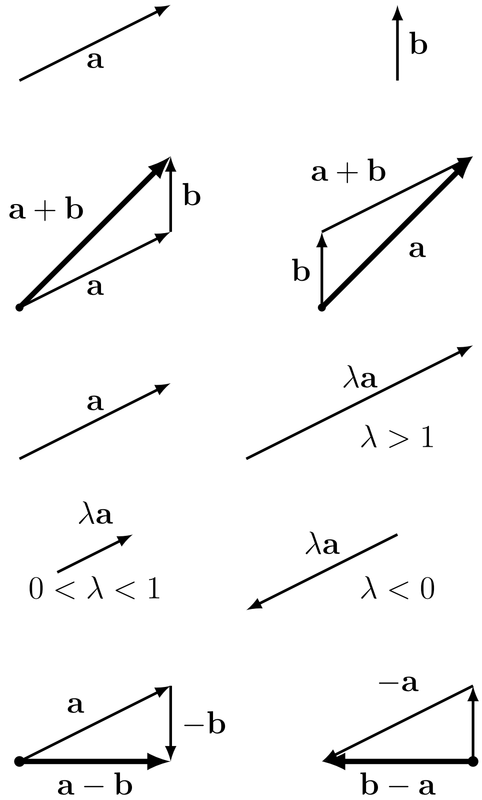
$\overrightarrow{a} + \overrightarrow{b} = \overrightarrow{b} + \overrightarrow{a}$
$\mathbf{a} + \mathbf{b} = \mathbf{b} + \mathbf{a}$

Multiplication by Scalars

$\lambda \overrightarrow{a} \qquad \lambda \mathbf{a}$

Subtraction

$\overrightarrow{a} - \overrightarrow{b} = \overrightarrow{a} + (-1)\overrightarrow{b}$
$\mathbf{a} - \mathbf{b} = \mathbf{a} + (-1)\mathbf{b}$



Vector operations represented by arrows.

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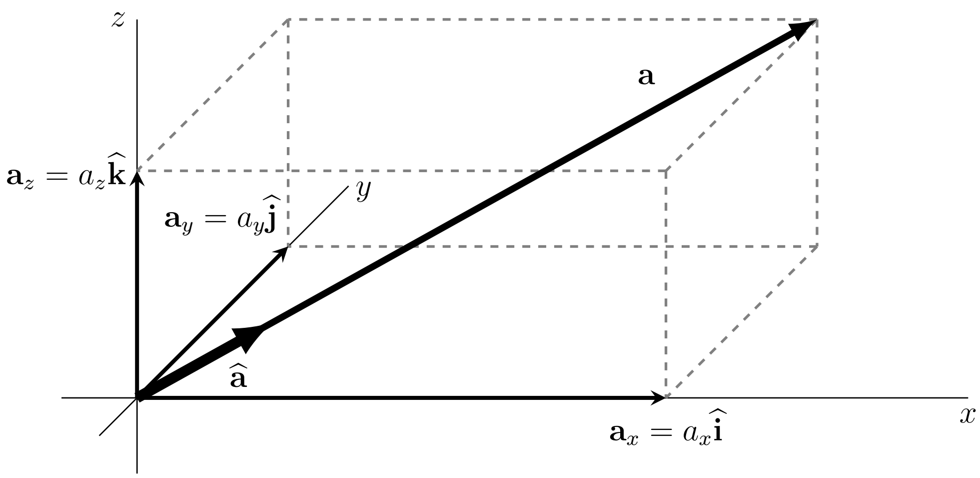
2.2 Basis Vectors, Components, Magnitude

A vector in three-dimensional (3d) space can be written as a set of components:

$$\mathbf{a} = a_x\widehat{\mathbf{i}} + a_y\widehat{\mathbf{j}} + a_z\widehat{\mathbf{k}} = (a_x, a_y, a_z) = \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix}$$

The **components** of the vector $\mathbf{a}$ are a_x, a_y, a_z along x, y, and z direction respectively. Here $\widehat{\mathbf{i}}$, $\widehat{\mathbf{j}}$, and $\widehat{\mathbf{k}}$ are the **unit vectors** or **basis vectors** of the cartesian coordinate system (orthogonal x,y, and z-axis), with $|\widehat{\mathbf{i}}| = |\widehat{\mathbf{j}}| = |\widehat{\mathbf{k}}| = 1$. They form one possible basis vector set of three-dimensional space.



Vector components represented in a coordinate systems.

The **magnitude** of a vector $\mathbf{a}$ is defined as

$$|\mathbf{a}| = a = \sqrt{a_x^2 + a_y^2 + a_z^2}$$

The direction of a vector is given by the unit vector

$$\widehat{\mathbf{a}} = \frac{\mathbf{a}}{|\mathbf{a}|} = \frac{\mathbf{a}}{a}$$

.

Addition and scalar multiplication, as defined before, can be computed by each component

$$\mathbf{a} + \mathbf{b} = (a_x + b_x)\widehat{\mathbf{i}} + (a_y + b_y)\widehat{\mathbf{j}} + (a_z + b_z)\widehat{\mathbf{k}}$$

$$\lambda\mathbf{a} = (\lambda a_x)\widehat{\mathbf{i}} + (\lambda a_y)\widehat{\mathbf{j}} + (\lambda a_z)\widehat{\mathbf{k}}$$

Note: Often basis sets other than the cartesian are used because the right choice of the basis can simplify a problem significantly, for instance cylindrical coordinates for a current flowing in a wire or spherical coordinates for electrons around a nucleus.

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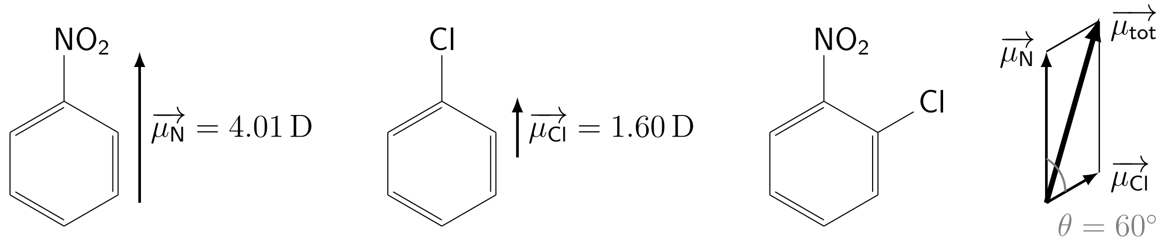
2.3 Example: Dipole Moments

Estimate the dipole moments of the isomers of chloro-nitro-benzene from the dipole moment of chloro-benzene $\mu_{\mathrm{Cl}} = 1.60\,\mathrm{D}$ and nitro-benzene $\mu_{\mathrm{N}} = 4.01\,\mathrm{D}$ (unit: $1\,\mathrm{D} = 1\,\mathrm{Debye} = 3.38{\cdot}10^{-30}\,\mathrm{Cm}$).



Dipole moments of nitro-benzene, chloro-benzene and of the 1-2 nitro-chloro-benzene.

If both dipole moments are present in the same molecule, we can approximate the total dipole as the sum of the two components, considering the angles between the different isomers.

The nitro-benzene dipole is assumed to be aligned with the y-direction (w.l.o.g.[i]):
$\overrightarrow{\mu_{\mathsf{N}}} = \mu_{\mathsf{N}}\,\widehat{\mathbf{j}}$.

Then the chloro-benzene dipole is oriented relative to it at an angle θ, depending on the isomer:

$\overrightarrow{\mu_{\mathsf{Cl}}} = \mu_{\mathsf{Cl}}\,(\widehat{\mathbf{i}}\,\sin\theta + \widehat{\mathbf{j}}\,\cos\theta)$.

Componentwise adding yields

$\overrightarrow{\mu_{\mathsf{tot}}} = \widehat{\mathbf{i}}\,\mu_{\mathsf{Cl}}\,\sin\theta + \widehat{\mathbf{j}}\,(\mu_{\mathsf{N}} + \mu_{\mathsf{Cl}}\,\cos\theta)$.

The magnitude of the dipole moment is the length of $\mu_{\mathsf{tot}} = |\overrightarrow{\mu_{\mathsf{tot}}}|$

$\mu_{\mathsf{tot}} = \sqrt{\mu_{\mathsf{Cl}}^2\,\sin^2\theta + (\mu_{\mathsf{N}} + \mu_{\mathsf{Cl}}\,\cos\theta)^2}$.

1,2 -isomer $\theta = 60^\circ$: $\sin 60^\circ = \frac{\sqrt{3}}{2}, \quad \cos 60^\circ = \frac{1}{2}$

$\mu_{1,2} = \sqrt{\frac{3}{4}\,(1.6\,\mathrm{D})^2 + (4.01\,\mathrm{D} + \frac{1}{2}\,1.6\,\mathrm{D})^2} = 5.01\,\mathrm{D}$

1,3 -isomer $\theta = 120^\circ$: $\sin 120^\circ = \frac{\sqrt{3}}{2}, \quad \cos 120^\circ = -\frac{1}{2}$

$\mu_{1,3} = \sqrt{\frac{3}{4}\,(1.6\,\mathrm{D})^2 + (4.01\,\mathrm{D} - \frac{1}{2}\,1.6\,\mathrm{D})^2} = 3.50\,\mathrm{D}$

1,4 -isomer $\theta = 180^\circ$: $\sin 180^\circ = 0, \quad \cos 180^\circ = -1$

$\mu_{1,4} = \sqrt{0\,(1.6\,\mathrm{D})^2 + (4.01\,\mathrm{D} - 1\,\cdot\,1.6\,\mathrm{D})^2} = 2.41\,\mathrm{D}$

[i] w.l.o.g. = without loss of generality

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2.4 Generalisation: Vector Space

Vectors can be 2d (plane), 3d (space), or 4d (spacetime). But also many other objects can be considered as vectors, most importantly functions and linear equations.

Definition: A set of vector elements V, a field $\mathbb{K}$ with the operations $V \oplus V \longrightarrow V$ (called vector addition) and $\mathbb{K} \odot V \longrightarrow V$ (called scalar multiplication) form a **vector space** when they have the following eight properties for all $u, v, w \in V$ and $\alpha, \beta \in \mathbb{K}$

V1: $u \oplus (v \oplus w) = (u \oplus v) \oplus w$ (associativity of addition)

V2: $v \oplus u = u \oplus v$ (commutativity of addition)

V3: Existence of an identity element $0_V \in V$ of addition, with $v \oplus 0_V = 0_V \oplus v = v$

V4: Existence of an inverse element $-v \in V$ for each $v \in V$ with $v \oplus (-v) = (-v) \oplus v = 0_V$

S1: Compatibility of scalar multiplication with field multiplication: $(\alpha \cdot \beta) \odot v = \alpha \odot (\beta \odot v)$

S2: Identity element $1 \in \mathbb{K}$ of scalar multiplication $1 \odot v = v$.

S3: Distributivity of scalar multiplication with respect to vector addition $\alpha \odot (u \oplus v) = (\alpha \odot u) \oplus (\alpha \odot v)$

S4: Distributivity of scalar multiplication with respect to field addition $(\alpha + \beta) \odot v = (\alpha \odot v) \oplus (\beta \odot v)$

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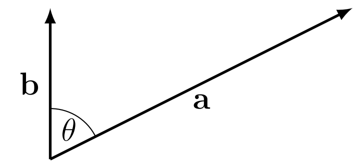
3 Multiplication of Vectors – Scalar (Dot) Product

Definition for two vectors $\mathbf{a}$ and $\mathbf{b}$ $(0 \leq \theta \leq 180°)$

Geometric definition: $\mathbf{a} \cdot \mathbf{b} = |a||b|\cos(\theta)$.

Algebraic definition: $\mathbf{a} \cdot \mathbf{b} = a_x b_x + a_y b_y + a_z b_z$



Vectors $\mathbf{a}$ and $\mathbf{b}$ and the enclosing angle θ.

Properties

(i) orthogonal vectors: $\mathbf{a} \cdot \mathbf{b} = 0 \quad \Longrightarrow \quad \theta = 90°$

(ii) magnitude: $\mathbf{a} \cdot \mathbf{a} = a^2 \cos(0) = a^2 \quad \Longrightarrow \quad a = \sqrt{\mathbf{a} \cdot \mathbf{a}}$

(iii) commutative: $\mathbf{a} \cdot \mathbf{b} = \mathbf{b} \cdot \mathbf{a}$

(iv) distributive: $\mathbf{a} \cdot (\mathbf{b} + \mathbf{c}) = \mathbf{a} \cdot \mathbf{b} + \mathbf{a} \cdot \mathbf{c}$

(v) Basis vectors are orthonormal:

normalised $\widehat{\mathbf{i}} \cdot \widehat{\mathbf{i}} = \widehat{\mathbf{j}} \cdot \widehat{\mathbf{j}} = \widehat{\mathbf{k}} \cdot \widehat{\mathbf{k}} = 1$;

orthogonal $\widehat{\mathbf{i}} \cdot \widehat{\mathbf{j}} = \widehat{\mathbf{j}} \cdot \widehat{\mathbf{k}} = \widehat{\mathbf{k}} \cdot \widehat{\mathbf{i}} = 0$

(vi) $\mathbf{a} \cdot \mathbf{b} = (a_x\widehat{\mathbf{i}} + a_y\widehat{\mathbf{j}} + a_z\widehat{\mathbf{k}}) \cdot (b_x\widehat{\mathbf{i}} + b_y\widehat{\mathbf{j}} + b_z\widehat{\mathbf{k}}) = a_x b_x \widehat{\mathbf{i}} \cdot \widehat{\mathbf{i}} + a_x b_y \widehat{\mathbf{i}} \cdot \widehat{\mathbf{j}} + a_x b_z \widehat{\mathbf{i}} \cdot \widehat{\mathbf{k}} + \ldots + a_z b_z \widehat{\mathbf{k}} \cdot \widehat{\mathbf{k}} =$
$= a_x b_x + a_y b_y + a_z b_z$

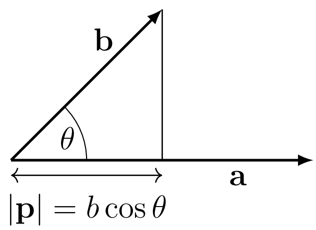
Note: The dot product is sometimes referred to as an *inner product*. It allows the definition of geometric properties such as length and angles. Often other notations such as $(\mathbf{a}, \mathbf{b})$ or $\langle \mathbf{a}, \mathbf{b} \rangle$ are found.

3.1 Orthogonal Projection.

With two vectors defining a plane in $\mathbb{R}^3$, the projection component of vector $\mathbf{b}$ on another vector $\mathbf{a}$ is $|\mathbf{p}| = b\cos\theta$.

This can be related to the scalar product by dividing the definition by the magnitude of $\mathbf{a}$:

$$\mathbf{a} \cdot \mathbf{b} = ab\cos(\theta) \quad \Longrightarrow \quad \frac{1}{|a|}\mathbf{a} \cdot \mathbf{b} = \widehat{\mathbf{a}} \cdot \mathbf{b} = b\cos\theta = |\mathbf{p}|$$



Orthogonal projections: The component of $\mathbf{b}$ in the direction of $\mathbf{a}$ is $b\cos(\theta)$.

We can then write the projection vector $\mathbf{p}$ as

$$\mathbf{p} = (\widehat{\mathbf{a}} \cdot \mathbf{b})\,\widehat{\mathbf{a}} \quad .$$

hence $\widehat{\mathbf{a}} \cdot \mathbf{b}$ is the component of $\mathbf{b}$ along $\mathbf{a}$.

Example 1: Determine the projection of $\mathbf{b}$ onto $\mathbf{a}$.

$\mathbf{a} = (1, 1, 1) = \widehat{\mathbf{i}} + \widehat{\mathbf{j}} + \widehat{\mathbf{k}}$

$\mathbf{b} = (1, 2, 1) = \widehat{\mathbf{i}} + 2\widehat{\mathbf{j}} + \widehat{\mathbf{k}}$

magnitude: $a = |\mathbf{a}| = \sqrt{a_x^2 + a_y^2 + a_z^2} = \sqrt{1^2 + 1^2 + 1^2} = \sqrt{3}$

unit vector: $\widehat{\mathbf{a}} = \frac{\mathbf{a}}{a} = \frac{1}{\sqrt{3}}(\widehat{\mathbf{i}} + \widehat{\mathbf{j}} + \widehat{\mathbf{k}}) = \frac{1}{\sqrt{3}}(1, 1, 1) = \frac{1}{\sqrt{3}}\mathbf{a}$

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projected length: $\widehat{\mathbf{a}} \cdot \mathbf{b} = \frac{1}{\sqrt{3}}(\widehat{\mathbf{i}} + \widehat{\mathbf{j}} + \widehat{\mathbf{k}})(\widehat{\mathbf{i}} + 2\widehat{\mathbf{j}} + \widehat{\mathbf{k}}) = \dots$
$= \frac{1}{\sqrt{3}}(1 \cdot 1 + 1 \cdot 2 + 1 \cdot 1) = \frac{4}{\sqrt{3}} = \frac{4}{3}\sqrt{3} \approx 2.31$
projection vector: $\mathbf{p} = (\widehat{\mathbf{a}} \cdot \mathbf{b})\widehat{\mathbf{a}} = \frac{4}{\sqrt{3}} \cdot \frac{1}{\sqrt{3}}(\widehat{\mathbf{i}} + \widehat{\mathbf{j}} + \widehat{\mathbf{k}}) = \frac{4}{3}(\widehat{\mathbf{i}} + \widehat{\mathbf{j}} + \widehat{\mathbf{k}}) = \frac{4}{3}\mathbf{a}$

Example 2: Find the angle θ between three points A, B, and C given by the position vectors:

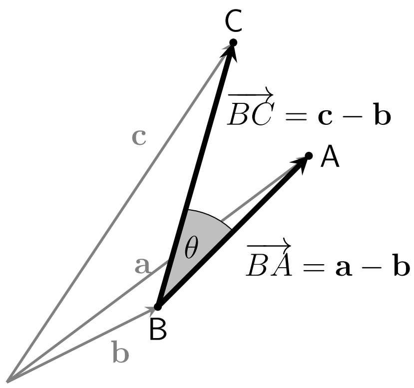
$\mathbf{a} = \begin{pmatrix} 2 \\ 3\sqrt{2} \\ 0 \end{pmatrix}$, $\mathbf{b} = \begin{pmatrix} 2 \\ \sqrt{2} \\ 0 \end{pmatrix}$, and $\mathbf{c} = \begin{pmatrix} 2+\sqrt{3} \\ 2\sqrt{2} \\ \sqrt{3} \end{pmatrix}$.

$$\overrightarrow{BA} = \mathbf{a} - \mathbf{b} = \begin{pmatrix} 0 \\ 2\sqrt{2} \\ 0 \end{pmatrix}, \quad \overrightarrow{BC} = \mathbf{c} - \mathbf{b} = \begin{pmatrix} \sqrt{3} \\ \sqrt{2} \\ \sqrt{3} \end{pmatrix}$$

$$|\overrightarrow{BA}| = 2\sqrt{2}, \quad |\overrightarrow{BC}| = \sqrt{3+2+3} = \sqrt{8} = 2\sqrt{2}$$

$$|\overrightarrow{BA}| \cdot |\overrightarrow{BC}| = \begin{pmatrix} 0 \\ 2\sqrt{2} \\ 0 \end{pmatrix} \cdot \begin{pmatrix} \sqrt{3} \\ \sqrt{2} \\ \sqrt{3} \end{pmatrix} = 2\sqrt{2} \cdot \sqrt{2} = 4$$

$$\cos\theta = \frac{\overrightarrow{BA} \cdot \overrightarrow{BC}}{|\overrightarrow{BA}| \cdot |\overrightarrow{BC}|} = \frac{4}{(2\sqrt{2})(2\sqrt{2})} = \frac{1}{2} \qquad \Longrightarrow \qquad \theta = \cos^{-1}\left(\frac{1}{2}\right) = 60^\circ = \frac{\pi}{3}$$



Sketch of the three points A, B, and C, the vectors $\mathbf{a}$, $\mathbf{b}$, *and* $\mathbf{c}$ *pointing to them, and the angle* θ.

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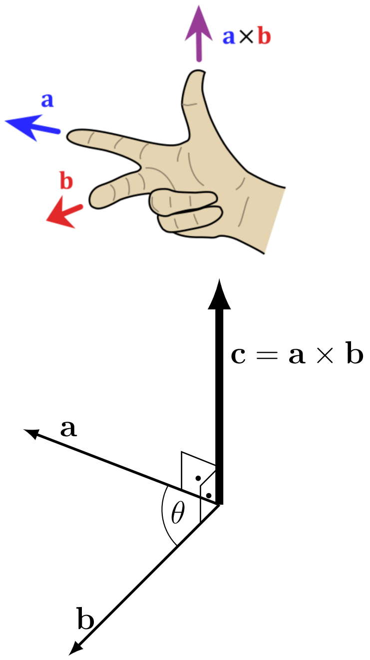
4 Multiplication of Vectors: Vector / Cross Product



Right hand rule. The coordinate system formed by three fingers (thumb, index, middle finger) of the right hand form a right handed coordinate system, which also defines the direction of the result of the vector product.

Definition: The vector product of two vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^3$, denoted by $\mathbf{a} \times \mathbf{b}$, is a vector $\mathbf{c} \in \mathbb{R}^3$, which is perpendicular to both $\mathbf{a}$ and $\mathbf{b}$ and has the magnitude $ab\sin(\theta)$:

$$|\mathbf{a} \times \mathbf{b}| = ab\sin(\theta) \quad ,$$

with θ the angle between $\mathbf{a}$ and $\mathbf{b}$.

Properties:

1. linear dependence:
   $\mathbf{a} = \lambda\mathbf{b} \quad \Longleftrightarrow \quad \mathbf{a} \times \mathbf{b} = 0$
   as this implies $sin(\theta) = 0$ hence $\mathbf{a}$ and $\mathbf{b}$ are parallel or antiparallel.
2. anticommutative: $\mathbf{a} \times \mathbf{b} = -\mathbf{b} \times \mathbf{a}$
3. distributive: $(\mathbf{a} + \mathbf{b}) \times \mathbf{c} = \mathbf{a} \times \mathbf{c} + \mathbf{b} \times \mathbf{c}$
4. non-associative: $(\mathbf{a} \times \mathbf{b}) \times \mathbf{c} \neq \mathbf{a} \times (\mathbf{b} \times \mathbf{c})$
   (instead: $\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = \mathbf{b}(\mathbf{a} \cdot \mathbf{c}) - \mathbf{c}(\mathbf{a} \cdot \mathbf{b})$)
5. applied to orthonormal vectors $\widehat{\mathbf{i}}$, $\widehat{\mathbf{j}}$, $\widehat{\mathbf{k}}$:
   $\widehat{\mathbf{i}} \times \widehat{\mathbf{i}} = \widehat{\mathbf{j}} \times \widehat{\mathbf{j}} = \widehat{\mathbf{k}} \times \widehat{\mathbf{k}} = 0$
   $\widehat{\mathbf{i}} \times \widehat{\mathbf{j}} = \widehat{\mathbf{k}}; \quad \widehat{\mathbf{j}} \times \widehat{\mathbf{k}} = \widehat{\mathbf{i}}; \quad \widehat{\mathbf{k}} \times \widehat{\mathbf{i}} = \widehat{\mathbf{j}}.$
   note: each exchange changes the sign.

4.1 Calculation of the Cross Product

Written in cartesian basis vectors:

$$\begin{aligned}
\mathbf{a} \times \mathbf{b} &= (a_x\widehat{\mathbf{i}} + a_y\widehat{\mathbf{j}} + a_z\widehat{\mathbf{k}}) \times (b_x\widehat{\mathbf{i}} + b_y\widehat{\mathbf{j}} + b_z\widehat{\mathbf{k}}) \\
&= a_yb_z\,\widehat{\mathbf{j}} \times \widehat{\mathbf{k}} + a_zb_y\,\widehat{\mathbf{k}} \times \widehat{\mathbf{j}} + \\
&\quad\; a_xb_z\,\widehat{\mathbf{i}} \times \widehat{\mathbf{k}} + a_zb_x\,\widehat{\mathbf{k}} \times \widehat{\mathbf{i}} + \\
&\quad\; a_xb_y\,\widehat{\mathbf{i}} \times \widehat{\mathbf{j}} + a_yb_x\,\widehat{\mathbf{j}} \times \widehat{\mathbf{i}} \\
&= (a_yb_z - a_zb_y)\widehat{\mathbf{i}} + (a_zb_x - a_xb_z)\widehat{\mathbf{j}} + (a_xb_y - a_yb_x)\widehat{\mathbf{k}}
\end{aligned}$$

Calculation via a determinant: The cross product can be calculated as the determinant of the 3×3 matrix, containing the unit vectors in the first row and the vectors $\mathbf{a}$ and $\mathbf{b}$ in second and third row respectively.

$$\mathbf{a} \times \mathbf{b} = \begin{vmatrix} \widehat{\mathbf{i}} & \widehat{\mathbf{j}} & \widehat{\mathbf{k}} \\ a_x & a_y & a_z \\ b_x & b_y & b_z \end{vmatrix} = \det\begin{pmatrix} \widehat{\mathbf{i}} & \widehat{\mathbf{j}} & \widehat{\mathbf{k}} \\ a_x & a_y & a_z \\ b_x & b_y & b_z \end{pmatrix}$$

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A determinant can be evaluated with several methods.

Example 1: Method of Sub-Determinants. One column or row is chosen to iterate along its elements and sum up sub-determinants, thereby alternating signs and multiplying by each the element. The 2×2 sub-determinants is found by deleting row and column of the present element and is computed as

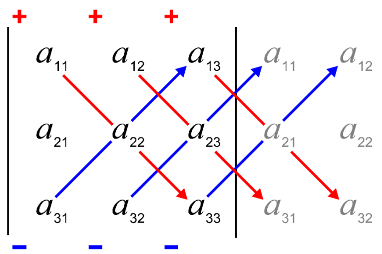
$$\det \begin{pmatrix} p & q \\ r & s \end{pmatrix} = pq - rs \quad .$$

For the vectors $\mathbf{a} = (0, 1, 1)$; $\mathbf{b} = (1, 1, 0)$:

$$\begin{aligned} \mathbf{a} \times \mathbf{b} &= \begin{vmatrix} \widehat{\mathbf{i}} & \widehat{\mathbf{j}} & \widehat{\mathbf{k}} \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{vmatrix} = \widehat{\mathbf{i}} \begin{vmatrix} 1 & 1 \\ 1 & 0 \end{vmatrix} - \widehat{\mathbf{j}} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} + \widehat{\mathbf{k}} \begin{vmatrix} 0 & 1 \\ 1 & 1 \end{vmatrix} \\ &= \widehat{\mathbf{i}}(0-1) - \widehat{\mathbf{j}}(0-1) + \widehat{\mathbf{k}}(0-1) = -\widehat{\mathbf{i}} + \widehat{\mathbf{j}} - \widehat{\mathbf{k}} = (-1, 1, -1) \end{aligned}$$

Test: Because $\mathbf{a} \times \mathbf{b}$ must be orthogonal to both $\mathbf{a}$ and $\mathbf{b}$, it follows that
$0 \stackrel{!}{=} \mathbf{a} \cdot (\mathbf{a} \times \mathbf{b}) = (0, 1, 1) \cdot (-1, 1, -1) = 0 \cdot (-1) + 1 \cdot 1 + 1 \cdot (-1) = 1 - 1 = 0$
$0 \stackrel{!}{=} \mathbf{b} \cdot (\mathbf{a} \times \mathbf{b}) = (1, 1, 0) \cdot (-1, 1, -1) = 1 \cdot (-1) + 1 \cdot 1 + 0 \cdot (-1) = -1 + 1 = 0$

Sarrus Scheme is a general method to calculate determinants. The determinant is extended as illustrated. The values along each of the arrows are multiplied and added up with the respective sign.



Sarrus Scheme for calculating determinantes.

For the above example:

$$\left|\begin{array}{ccc|cc} \widehat{\mathbf{i}} & \widehat{\mathbf{j}} & \widehat{\mathbf{k}} & \widehat{\mathbf{i}} & \widehat{\mathbf{j}} \\ 0 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 \end{array}\right. =$$

$$= \widehat{\mathbf{i}} \cdot 0 \cdot 1 + \widehat{\mathbf{j}} \cdot 1 \cdot 1 + \widehat{\mathbf{k}} \cdot 0 \cdot 1 - \widehat{\mathbf{k}} \cdot 1 \cdot 1 - \widehat{\mathbf{i}} \cdot 1 \cdot 1 - \widehat{\mathbf{j}} \cdot 0 \cdot 0$$
$$= -\widehat{\mathbf{i}} + \widehat{\mathbf{j}} - \widehat{\mathbf{k}}$$

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5 Vector Differentiation

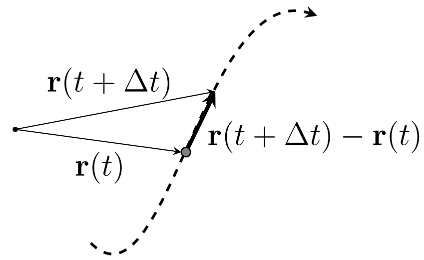
Functions can be vector valued, implying dependencies on time as on position, for which derivatives can be defined.

Here we only consider the differentiation of a time-dependent vector valued function

$$\mathbf{r}(t) = x(t)\,\widehat{\mathbf{i}} + y(t)\,\widehat{\mathbf{j}} + z(t)\,\widehat{\mathbf{k}}$$

with the derivative in time defined as

$$\dot{\mathbf{r}} = \frac{d\mathbf{r}}{dt} = \lim_{\Delta t \to 0}\left[\frac{\mathbf{r}(t+\Delta t) - \mathbf{r}(t)}{\Delta t}\right] \quad .$$



Vector differentiation.

Differential can be done by component

$$\frac{d}{dt}\mathbf{a}(t) = \frac{dx(t)}{dt}\,\widehat{\mathbf{i}} + \frac{dy(t)}{dt}\,\widehat{\mathbf{j}} + \frac{dz(t)}{dt}\,\widehat{\mathbf{k}}$$

$$\dot{\mathbf{r}}(t) = \dot{x}(t)\,\widehat{\mathbf{i}} + \dot{y}(t)\,\widehat{\mathbf{j}} + \dot{z}(t)\,\widehat{\mathbf{k}}$$

Note on notation: derivatives in time are typically denoted by a dot above the quantity $\dot{x}$. You might, however, also encounter the prime x', although it is rather used for spatial derivatives of scalar quantities.

Example: position, velocity, acceleration.

The trajectory of an object is given by the vector $\mathbf{r}(t)$, denoting its position as a function of time.

The first derivative in time is the velocity $\mathbf{v}$, the second derivative in time is the acceleration, i.e. the first derivative of the velocity in time:

$$\mathbf{v} = \dot{\mathbf{r}} = \frac{d\mathbf{r}}{dt} \qquad\qquad \mathbf{a} = \dot{\mathbf{v}} = \frac{d\mathbf{v}}{dt} = \frac{d^2}{dt^2}\mathbf{r} = \frac{d}{dt}\left(\frac{d}{dt}\mathbf{r}\right)$$

Properties for $\mathbf{a}(t)$ and $\mathbf{b}(t)$ two vector valued, time-dependent functions and λ a time independent scalar ($\lambda(t) = \mathrm{const.}$)

$$\frac{d}{dt}(\lambda\mathbf{a}) = \lambda\frac{d}{dt}\mathbf{a} \tag{1}$$

$$\frac{d}{dt}(\mathbf{a}+\mathbf{b}) = \frac{d}{dt}\mathbf{a} + \frac{d}{dt}\mathbf{b} \tag{2}$$

$$\frac{d}{dt}(\mathbf{a}\cdot\mathbf{b}) = \frac{d}{dt}\mathbf{a}\cdot\mathbf{b} + \mathbf{a}\cdot\frac{d}{dt}\mathbf{b} \tag{3}$$

$$\frac{d}{dt}(\mathbf{a}\times\mathbf{b}) = \frac{d}{dt}\mathbf{a}\times\mathbf{b} + \mathbf{a}\times\frac{d}{dt}\mathbf{b} \tag{4}$$

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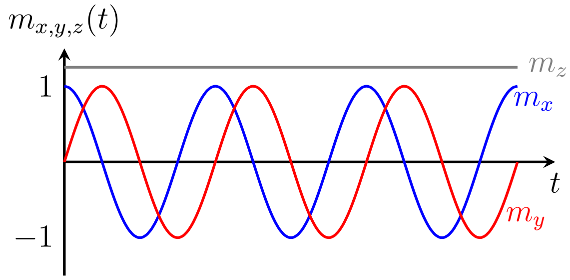
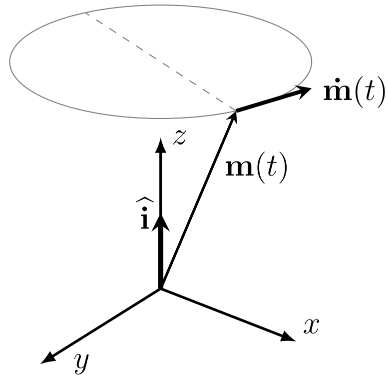
Example: circular motion $\mathbf{m}(t)$ given by

$$\begin{aligned} m_x(t) &= \sin \omega t \\ m_y(t) &= \cos \omega t \\ m_z(t) &= \text{const.} \end{aligned}$$



Both x- and y- component of this vector oscillate with the same frequency ω, while the z-component is constant.

$$\begin{aligned} \mathbf{m}(t) &= \widehat{\mathbf{i}} \sin \omega t + \widehat{\mathbf{j}} \cos \omega t + \widehat{\mathbf{k}}\, m_z \\ \dot{\mathbf{m}}(t) &= \widehat{\mathbf{i}}\, \omega \cos \omega t - \widehat{\mathbf{j}}\, \omega \sin \omega t \\ &= \widehat{\mathbf{i}}\, \omega m_y(t) - \widehat{\mathbf{j}}\, \omega m_x(t) \\ &= \omega \begin{vmatrix} \widehat{\mathbf{i}} & \widehat{\mathbf{j}} & \widehat{\mathbf{k}} \\ m_x & m_y & m_z \\ 0 & 0 & 1 \end{vmatrix} \\ &= \omega\, \mathbf{m} \times \widehat{\mathbf{k}} \end{aligned}$$



Precession around the $\widehat{\mathbf{k}}$ basis vector.

Because the derivate of the magnetisation vector can be expressed as a vector product of $\mathbf{m}$ and the basis vector $\widehat{\mathbf{k}}$, $\dot{\mathbf{m}}$ is always perpendicular to $\mathbf{m}$ and $\widehat{\mathbf{k}}$.

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