Graz University of Technology
Institute of Analysis and Number Theory
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Winter term 2023
Graz, 07.12.2023

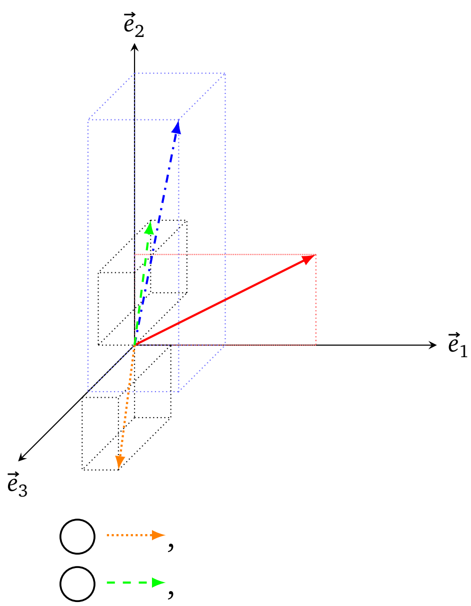
8. exercise sheet for Mathematics for Advanced Materials Science

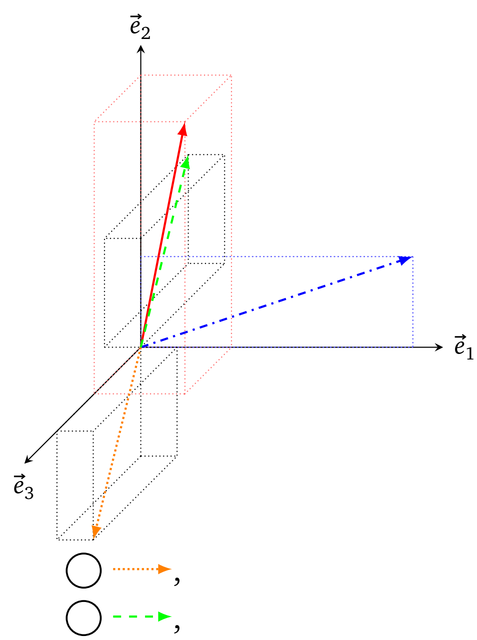
(first name) (last name)

(student id number)

8.1. *(Cross products and orientation)* (4 credits)

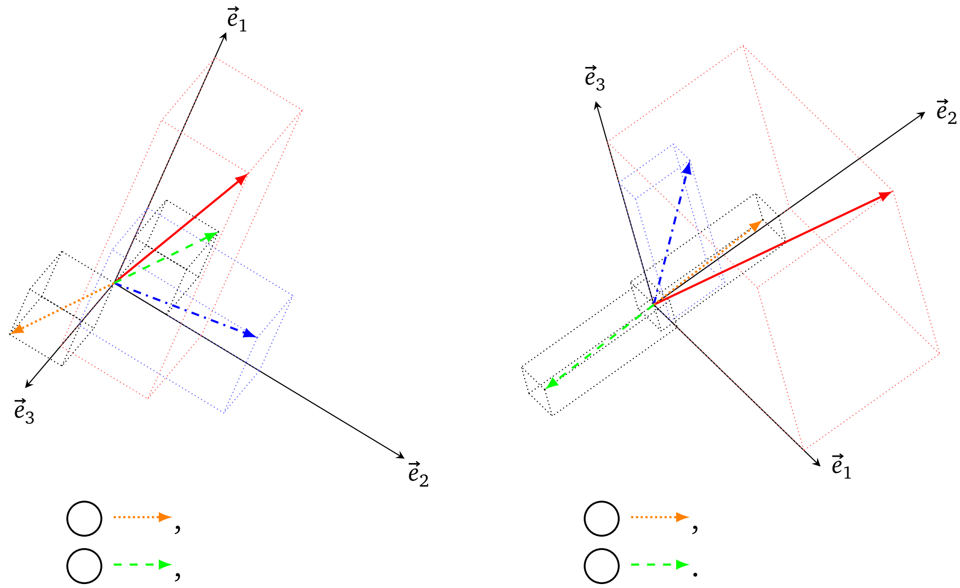
In each of the figures below you see a vector $\vec{v}$ drawn as ⟶ and a vector $\vec{w}$ drawn as -·-·→. Discern for each figure whether the vector $\vec{v} \times \vec{w}$ is ········→ or - - - →.





Please submit your solutions during the next lecture (14.12.2023).

https://www.math.tugraz.at/~mtechnau/teaching/2023-w-mams.html



(Hint: pay very close attention to the direction of the three standard unit vectors $\vec{e}_1$, $\vec{e}_2$ and $\vec{e}_3$ for every figure separately.)

8.2. *(Computing the dot and cross product)* (4 credits)
Consider the three vectors

$$\vec{v}_1 = (0,0,1), \quad \vec{v}_2 = (1,0,2), \quad \vec{v}_3 = (-1,0,2).$$

Compute $\vec{v}_i \bullet \vec{v}_j$ and $\vec{v}_i \times \vec{v}_j$ for all pairs (i,j) of indices with $1 \leq i,j \leq 3$.
(Hint: *a-priori* there are $2 \cdot 3 \cdot 3 = 18$ things to compute, but by exploiting various symmetries you can reduce your work siginificantly. For instance, $\vec{v}_i \bullet \vec{v}_j = \vec{v}_j \bullet \vec{v}_i$. How do the left and right hand side of this relate when one replaced $\bullet$ by $\times$? Check your answer on $\vec{v}_1 \times \vec{v}_2$ and $\vec{v}_2 \times \vec{v}_1$.)

$$\begin{pmatrix} \vec{v}_1 \bullet \vec{v}_1 & \vec{v}_1 \bullet \vec{v}_2 & \vec{v}_1 \bullet \vec{v}_3 \\ \vec{v}_2 \bullet \vec{v}_1 & \vec{v}_2 \bullet \vec{v}_2 & \vec{v}_2 \bullet \vec{v}_3 \\ \vec{v}_3 \bullet \vec{v}_1 & \vec{v}_3 \bullet \vec{v}_2 & \vec{v}_3 \bullet \vec{v}_3 \end{pmatrix} = \begin{pmatrix} \square & \square & \square \\ \square & \square & \square \\ \square & \square & \square \end{pmatrix},$$

$$\begin{pmatrix} \vec{v}_1 \times \vec{v}_1 & \vec{v}_1 \times \vec{v}_2 & \vec{v}_1 \times \vec{v}_3 \\ \vec{v}_2 \times \vec{v}_1 & \vec{v}_2 \times \vec{v}_2 & \vec{v}_2 \times \vec{v}_3 \\ \vec{v}_3 \times \vec{v}_1 & \vec{v}_3 \times \vec{v}_2 & \vec{v}_3 \times \vec{v}_3 \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} \square \\ \square \\ \square \end{pmatrix} & \begin{pmatrix} \square \\ \square \\ \square \end{pmatrix} & \begin{pmatrix} \square \\ \square \\ \square \end{pmatrix} \\ \begin{pmatrix} \square \\ \square \\ \square \end{pmatrix} & \begin{pmatrix} \square \\ \square \\ \square \end{pmatrix} & \begin{pmatrix} \square \\ \square \\ \square \end{pmatrix} \\ \begin{pmatrix} \square \\ \square \\ \square \end{pmatrix} & \begin{pmatrix} \square \\ \square \\ \square \end{pmatrix} & \begin{pmatrix} \square \\ \square \\ \square \end{pmatrix} \end{pmatrix}.$$

8.3. *(Vectors and angles)* (4 credits)

Consider the linear map $f\colon \mathbb{R}^2 \to \mathbb{R}^2$, $(v_1, v_2) \mapsto (-v_2, v_1)$.

(a) Check which of the following statements are true. (None, one or multiple of them may be true. Wrong answers also count negatively, so do not get tempted to check too much.)

- ◯ Geometrically, f describes a rotation by 90° in clockwise direction.
- ◯ Geometrically, f describes a rotation by 90° in anti-clockwise direction.
- ◯ Geometrically, f describes a reflection across the line $\mathbb{R}\binom{0}{1}$.
- ◯ $\operatorname{area} f(\Omega) = \operatorname{area} \Omega$, where Ω is the set $[1,2] \times [0,1]$.
- ◯ $\operatorname{area} f(\Omega) = 2 \operatorname{area} \Omega$, where Ω is the set $[1,8] \times [1,8]$.
- ◯ There is a non-zero vector $\vec{b}$ such that $f(\vec{b}) = \vec{0}$.
- ◯ f has an eigenvector $\vec{b} \in \mathbb{R}^2$.

(b) For vectors $\vec{v} = (v_1, v_2)$ and $\vec{w} = (w_1, w_2)$, compute

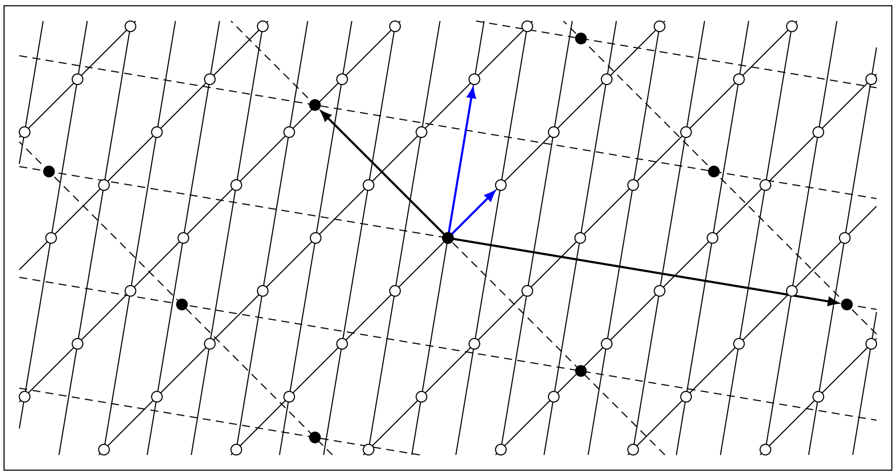
$$\begin{pmatrix} | & | \\ -f(\vec{w}) & f(\vec{v}) \\ | & | \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} | & | \\ \vec{v} & \vec{w} \\ | & | \end{pmatrix} = \begin{pmatrix} \square & \square \\ \square & \square \end{pmatrix}.$$

8.4. *(Reciprocal lattice)* (4 credits)

In your solid state physics course, you will have looked at the lattices $\{ n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 : n_1, n_2, n_3 \in \mathbb{Z} \}$ spanned by vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3 \in \mathbb{R}^3$ (which are usually called ***primitive lattice vectors*** in this context). We assume throughout that $\operatorname{vol} \varnothing(\vec{a}_1, \vec{a}_2, \vec{a}_3) > 0$. For reasons related to the discussion in § 4.4 of the lecture notes (see, in particular, Example 4.10), one is interested in computing so-called ***reciprocal lattice vectors*** $\vec{b}_1, \vec{b}_2, \vec{b}_3 \in \mathbb{R}^3$, given by

$$\vec{b}_1 = c\,(\vec{a}_2 \times \vec{a}_3), \quad \vec{b}_2 = -c\,(\vec{a}_1 \times \vec{a}_3), \quad \vec{b}_3 = c\,(\vec{a}_1 \times \vec{a}_2),$$

where $c = 2\pi/(a_1 \cdot (a_2 \times a_3))$. (The factor 2π is customary in many physics texts; a mathematician may prefer to omit it.) The following picture illustrates a two-dimensional version of this:



The following tasks require some space. Use a separate sheet.

(a) Justify that $a_1 \cdot (a_2 \times a_3) = \det \begin{pmatrix} | & | & | \\ \vec{a}_1 & \vec{a}_2 & \vec{a}_3 \\ | & | & | \end{pmatrix} = \pm \operatorname{vol} \varnothing(\vec{a}_1, \vec{a}_2, \vec{a}_3) \neq 0$ for an appropriate choice of sign $\pm$, so that the constant c is actually well-defined (no division by zero). (Hint: your should already know this from our discussion of the cross product.)

(b) Verify that computing reciprocal lattice vectors is essentially nothing else than matrix inversion:

$$\begin{pmatrix} | & | & | \\ \vec{a}_1 & \vec{a}_2 & \vec{a}_3 \\ | & | & | \end{pmatrix}^{-1} = \frac{1}{2\pi} \begin{pmatrix} | & | & | \\ \vec{b}_1 & \vec{b}_2 & \vec{b}_3 \\ | & | & | \end{pmatrix}^{\mathrm{T}}. \qquad (\dagger)$$

(Hint: this is, up to the 2π factor, Theorem 3.13 which, in turn, is claimed to be nothing but Proposition 3.2 in disguise. To solve this exercise, either give more details to show that the asserted equation indeed follows from Proposition 3.2, or—mimicking the proof of Proposition 3.2—multiply A to the right hand side of (†) [from the right, say] and check that the resulting matrix–matrix product yields the 3×3 identity matrix $\mathbf{1}_3$.)