Linear Algebra

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Axel Maas

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Chapter 1

Introduction

Linear algebra, as a generalization of geometry, is the mathematical description of space (in a very general sense). I. e., it describes positions in space in an abstract sense. More importantly, linear algebra can be used to describe also relations between different positions, and especially classes of relations. It is this feature, which makes linear algebra so important to physics, as physical statements, in a very general sense, are just descriptions of how relations between different positions, or generally events, look like. As a consequence, linear algebra is the language of all of physics, much more important than e. g. analysis or even more complex mathematical concepts. Linear algebra is required in the most simple examples of classical mechanics from the antiques, and is the basic elements on which quantum physics, general relativity and any other modern theory of physics is build. Thus linear algebra is the most essential mathematical tool for a physicist, no matter whether they are theoreticians or experimentalists. Also many mathematical problems from other fields, e. g. analysis, can be sufficiently approximated by linear algebra to obtain all relevant information. Thus, also from a practical point of view linear algebra is indispensable.

This importance has led to an enormous development of the underlying concepts of linear algebra. Thus, much more is known about its topic than can be covered in a single lecture. The aim is thus to introduce all the necessary basic concepts, such that extensions can be acquired as needed. This is particularly important as linear algebra transcends in its more abstract forms easily any intuitive access by everyday experience. Though much of this may seem esoteric at first, many of these levels of abstraction play a role in modern physics. The question to be posed must therefore always be: "What are the structures?" rather than "What are the numerical values?".

Chapter 2

Vectors in space

Though linear algebra can become quickly quite abstract, it is best to use an intuitively accessible example wherever possible to understand the concepts. The most useful example is actually ordinary space, i. e. the ordinary three-dimensional space with length, width, and height. This space will therefore often be used to present examples, but it is equally important to also understand the generalization to more abstract spaces.

The aim of this chapter is to introduce many concepts of linear algebra using this space, before generalizing them in the following chapters. This approach will also be rehearsed repeatedly for many other concepts in later chapters.

2.1 Vectors in the 3-dimensional real space

So, start with a three-dimensional space. This space has three directions, the x-direction, the y-direction, and the z-direction. Thus, to identify a position in this space, we need three numbers signifying the position in each direction. To make these numbers meaningful, they need to be relative to a starting point, the so-called origin. They then define how far[1] the point in every direction is away from the origin. Conventionally, positive numbers will be to the right of the origin, and negative numbers to the left of the origin for every direction. Since the space is continuous, these numbers should be elements of the real numbers $\mathbb{R}$.

Hence, an ordered tuple

$$\vec{v} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{2.1}$$

identifies uniquely a point in space, and is called a vector. Such a vector will be signified by the $\vec{}$ above its designation v, to separate it from normal numbers.

The full space, i. e. the set of all possible vectors, is therefore called the (vector) space $\mathbb{R}^3$. The exponent gives the number of directions, and the $\mathbb{R}$ stands for the type of distance-measuring numbers. The ordering is conventional, but widespread. To refer to an element also an index notation is used, $(\vec{v})_1 = v_1 = x$, $(\vec{v})_2 = v_2 = y$, and $(\vec{v})_3 = v_3 = z$. The

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[1]Note that no units, like meters, will be attached in this lecture, but they could be used if wished for. From the mathematical point of view (human-made) units are irrelevant.

elements v_i of a vector are also called its components. Writing a vector instead of as a column vector as a row vector, (x, y, z), is also possible. To distinguish both versions, the row vector is called the transpose of the column vector and indicated by an upper-placed T after the vector, and vice versa. Thus for (2.1) $\vec{v} = (x, y, z)^T$ and $\vec{v}^T = (x, y, z)$. This will have much more significance later on.

However, so far this is not sufficient to really identify the point, since this just gives three values. It is therefore necessary to explicitly specify a point of reference, the origin of the space, which is given by $v_i = 0$, or $\vec{v} = \vec{0}$, the zero vector. Then, the numbers give the distance in the three possible directions x, y, and z.

These values are then called coordinates with respect to the origin, though usually only coordinates. It is possible to think of the space filled up by a grid, a coordinate system, such that every point becomes a unique set of values. Especially, a vector

$$\vec{v} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \tag{2.2}$$

would then be interpreted as a connection from the origin along the x-direction of the coordinate system to the point with the given coordinates. Likewise a vector $(2, -3, 4)^T$ denotes some point in this space.

Vectors like (2.2), where the ith vector has only an element in the ith component of size 1, and all other components being zero, are somewhat special, as they point along a particular direction only. They are therefore called base vectors, and are denoted as $\vec{e}_i$ Thus (2.2) is also written as $\vec{e}_1$. The others are $\vec{e}_2 = (0, 1, 0)^T$ and $\vec{e}_3 = (0, 0, 1)^T$.

When put into a coordinate system, a vector can hence be visualized as a straight arrow pointing from the origin to the described point. The vectors of type (2.2) can then be thought of as pointing along the coordinate axis, or even defining the coordinate axis.

2.2 Paths

The most elementary object to be described by vectors are paths, i. e. a possibility to describe how to get from one point described by the vector $\vec{a}$ to another point described by a vector $\vec{b}$. Every point in between the two vectors will also be described by a vector, and differing paths between the starting vector and end vector will have a different sequence of points.

This requires to somehow make statements where along the path a position is. The most convenient description is that of a vector $\vec{p}$ which is parameterized by a parameter t such that

$$\begin{aligned} \vec{p}(0) &= \vec{a} \\ \vec{p}(1) &= \vec{b} \end{aligned}$$

then moving in the interval $t = [0, 1]$ describes the path. While a pretty standard choice, the parameter could also vary over some other interval, including $[-\infty, \infty]$, depending on context.

Of course, this requires all components to be functions of the parameter t, $\vec{p}(t) = (p_1(t), p_2(t), p_3(t))^T$. Properties of these component function determine whether the path is smooth or has edges and so on. Any kind of function would be possible, provided it is defined in the interval. Note that mathematically there may be jumps in the path, though in the context of physics this is rarely useful.

Examples for such paths for $t \in [0, 1]$ are

$$
\begin{aligned}
\vec{p}_1(t) &= \begin{pmatrix} t \\ 0 \\ 0 \end{pmatrix} \\
\vec{p}_2(t) &= \begin{pmatrix} \cos(2\pi t) \\ \sin(2\pi t) \\ 0 \end{pmatrix} \\
\vec{p}_3(t) &= \begin{pmatrix} \cos(2\pi t) \\ \sin(2\pi t) \\ t \end{pmatrix} \\
\vec{p}_4(t) &= \begin{pmatrix} (1 - 2t)\theta\left(\frac{1}{2} - t\right) \\ (2t - 1)\theta\left(t - \frac{1}{2}\right) \\ 0 \end{pmatrix} \\
\theta(t) &= \begin{cases} 1 \text{ if } t \geq 0 \\ 0 \text{ if } t < 0 \end{cases}
\end{aligned}
\tag{2.3}
$$

where $\theta(t)$ is called the step function or Heaviside function[2]. The path $\vec{p}_1$ describes a movement from the origin to the point $(1, 0, 0)^T$ along the x-axis. The path $\vec{p}_2$ describes a path along the complete unit circle in the x-y-plane, starting and ending in the same point $(1, 0, 0)^T$, and centered on the origin $\vec{0}$. Such a path, where start and end coincide, is called a closed path. The path $\vec{p}_3$ describes a single winding of a screw along the z-axis, where the winding extends over one unit along the z-axis. The path $\vec{p}_4$ starts at $(1, 0, 0)^T$, moves then along the x-axis to the origin, and after making a sharp turn by $\pi/2$ to $(0, 1, 0)^T$.

In general, a path is given by a vector with components $f_i(t)$, where the f_i are arbitrary functions. Paths are called continuous (and differentiable), if all component functions are continuous (and differentiable).

The idea of paths is thus to replace components with fixed values by functions. This generalizes. Whenever there are components in the following they can be upgraded to describe paths by replacing them with functions of a parameter varying in some interval. It is sometimes also useful to consider a path as a set of the vectors along the path, and the same is also possible for its components.

2.3   Scalar multiplication and length of a vector

Coordinate axes are usually extended from negative infinity to positive infinity. To create them from the vectors pointing in their direction, (2.2), it is necessary to somehow have

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[2]There are cases, in which it is defined that $\theta(0) = 1/2$, instead of 1.

vectors of arbitrary length. Of course, this could be implemented by an (infinite) set of vectors. More natural is to permit to scale a vector to give it a particular length. This can be achieved by defining the so-called scalar multiplication of a vector by a real number. This real number is called a scalar for reasons which will become clear in chapter 8.

The definition of a multiplication of a scalar a and a vector $\vec{v}$ is

$$a\vec{v} = a \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} av_1 \\ av_2 \\ av_3 \end{pmatrix},$$

i. e. every component is multiplied by the same real number a, $(a\vec{v})_i = av_i$. In the same way, division by a scalar $a \neq 0$ is defined as a multiplication with the real number $1/a$.

Thus, by having a scaling factor it is now possible to address every point along a line just by tuning a prefactor. This implies that the direction of the vector has been separated from the length of a vector. The length can be thought of as just the usual distance from the origin. Thus, the length of a vector can be defined as

$$|\vec{v}| = +\sqrt{x^2 + y^2 + z^2}, \tag{2.4}$$

where the notation on the left-hand side implies calculating the length. Hence, e. g. all $\vec{e}_i$ have length 1. Sometimes the length of a vector is denoted by the same symbol, but without the $\rightarrow$, i. e. the length of $\vec{v}$ is $v = |\vec{v}|$. This is distinguished from the components of the vector by the absence of an index.

Note that the square of the length of a vector often appears, and is therefore often abbreviated as $|\vec{v}|^2 = \vec{v}^2 = v^2$. In an abuse of language $\vec{v}^2$ is often called the square of the vector $\vec{v}$. But this is not a square, nor a multiplication at all.

The direction of a vector and its length can now be separated. Take any vector which has a non-vanishing length. Then it is possible to write

$$\vec{v} = |\vec{v}|\vec{e}_{\vec{v}}$$
$$\vec{e}_{\vec{v}} = \frac{1}{|\vec{v}|}\vec{v}.$$

The vector $\vec{e}_{\vec{v}}$ has by definition unit length, and is therefore called a unit vector in direction of $\vec{v}$. The concept that now every point along this direction can be accessed by just scalar multiplication of $\vec{e}_{\vec{v}}$ is formulated by talking of a vector $\vec{w} = a\vec{e}_{\vec{v}}$ obtained by scalar multiplication with a number a from $\vec{e}_{\vec{v}}$ as being a representative of a ray. I. e. a ray is defined as the set $\{\vec{e}_{\vec{v}}, \mathbb{R}\}$, and thus a direction and any possible length.

As an example, the three coordinate axes are given by the three rays $\{\vec{e}_i, \mathbb{R}\}$.

2.4 Vector addition

A quite often appearing problem is that one needs to go first to a given point and then from there on to a second point, and finally to obtain the vector to this new point. Mathematically, this could be described by first describing a point, the first aim. Then,

describe the second point relative to the first point, i. e. create the vector for this second part of the path. Finally, one should get back to a description with the original origin. Geometrically, this corresponds to a parallel displacement of the vector, by putting its start at the end of the first vector, and then draw a vector connecting the beginning of the first vector with the end of the second vector.

To obtain a suitable formulation, it is best to first have a look at a much simpler space, $\mathbb{R}^1 = \mathbb{R}$. In this case, all vectors are just simple real numbers. Then the problem boils down to first go to a value x, and then onward an amount x'. The total distance from the origin is then $x + x'$, thus the coordinates have just been added. The three coordinates in $\mathbb{R}^3$ are independent. The same could be repeated by just doing the same, piece by piece, independently for all three coordinates. Thus, the process of adding two vectors is performed by adding the individual components

$$\vec{v} = \vec{x} + \vec{y} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} x_1 + y_1 \\ x_2 + y_2 \\ x_3 + y_3 \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix},$$

or $v_i = x_i + y_i$. A good test is to see what happens if the goal is to first go to a point, and then go back to the origin. Then, both vectors should have the same, but negative, components, and thus $x_i - x_i = 0$, as required.

If one now uses the three base vectors $\vec{e}_i$, any vector can thus be written as

$$\vec{v} = v_1\vec{e}_1 + v_2\vec{e}_2 + v_3\vec{e}_3 = \sum_{i=1}^{3} v_i\vec{e}_i = \sum_i v_i\vec{e}_i. \tag{2.5}$$

Thus, using scalar multiplication and vector addition every vector can be decomposed into the base vectors, emphasizing the reason for their name, and its components.

The fact that every vector can be written as in (2.5) is summarized by calling the set $\{\vec{e}_i\}$, usually abbreviated as just $\vec{e}_i$ if the context is unambiguous, a basis for the vectors, and, by extension to the set of all vectors, for the space $\mathbb{R}^3$. These vectors have, by construction, unit length, and are therefore unit vectors along the three directions.

Since vector addition has now been mapped to the addition of the individual components, the subtraction of vectors can be introduced immediately as the subtraction of the individual components, i. e.

$$\vec{a} - \vec{b} = \sum_{i=1}^{3} (a_i\vec{e}_i - b_i\vec{e}_i) = \sum_{i=1}^{3} (a_i - b_i)\vec{e}_i.$$

Thus, geometrically subtraction corresponds to traversing one of the vectors backwards. Especially, $\vec{a} - \vec{a} = \vec{0}$, i. e. traversing a vector first forward and then backwards returns to the origin $\vec{0}$.

2.5   Compactified notation

Since expressions like (2.5) appear very often often, it is useful to introduce an abbreviation,

$$\sum_{i=1}^{3} x_i \vec{e}_i \equiv x_i \vec{e}_i,$$

the so-called Einstein summation convention. In this case, if the limits of the summation are clear from the context, any doubly repeated indices, and only those, are summed over the range given by the context. Single indices, or indices appearing more than twice, are never summed automatically. Thus, e. g., neither a_i nor $a_i b_i c_i d_i$ implies summation. It also only applies to products, and thus a statement like, e. g., $a_i + b_i$ does not imply summation over i. However, for $a_i b_i + c_i d_i$ both terms will be summed individually, and thus correspond to

$$a_i b_i + c_i d_i = \sum_{i=1}^{3} a_i b_i + \sum_{i=1}^{3} c_i d_i.$$

Furthermore, a statement like a_i^2 is thus interpreted as $\sum_{i=1}^{3} a_i a_i$. Thus, in particular,

$$v_i^2 = v_i v_i = \sum_{i=1}^{3} v_i v_i = \sum_{i=1}^{3} v_i^2.$$

This needs to be looked at quite carefully. Consider, e. g.,

$$(v_1^2 + v_2^2 + v_3^2)(w_1^2 + w_2^2 + w_3^2) = \left(\sum_{i=1}^{3} v_i^2\right)\left(\sum_{j=1}^{3} w_j^2\right) = \sum_{i=1,j=1}^{3} v_i v_i w_j w_j = v_i v_i w_j w_j,$$

where the summation convention has only been applied in the last step. Thus, when introducing indices to keep track of the component formulation of, e. g., $\vec{v}^2$ it is necessary to introduce always an independent pair of indices - this can be summarized in the statement that such, so-called dummy, indices are only created and removed pairwise.

This Einstein summation convention is essentially ubiquitous in (theoretical) physics, and will be used from now on throughout, except when noted otherwise.

A useful quantity in this context is the so-called Kronecker δ-function, which is defined as

$$\delta_{ij} = \delta_{ji} = \begin{cases} 1 \text{ for } i = j \\ 0 \text{ otherwise} \end{cases} \tag{2.6}$$

Thus, the Kronecker δ-function has two arguments, two integer indices, and it is only nonvanishing if both coincide. It is also symmetric in both indices, i. e. when exchanging both indices, its value does not change.

With it, it is e. g. possible to write the components of the vectors $\vec{e}_i$ conveniently as

$$(\vec{e}_i)_j = \delta_{ij}.$$

where the index j on the parentheses requires to take the jth component of the vector inside the parentheses, and i denotes which vector. This notation is common, and will reappear often.

Another context, in which the Kronecker-δ will often appear, is that it collapses double sums. E. g.

$$\sum_{i,j} a_i b_j \delta_{ij} = \sum_i a_i b_i,$$

or, with using the summation convention

$$a_i b_j \delta_{ij} = a_i b_i.$$

Thus, a Kronecker-δ allows to remove one summation, if it is summed over both its indices. It is often convenient to express squares with the summation convention, and introduce and remove sums using the Kronecker-δ

$$a_i a_i = a_i^2 = a_i a_j \delta_{ij}.$$

All of this are the same expression, just written in different ways.

Other useful properties of the δ functions are, e. g.

$$\begin{aligned}
\delta_{ii} &= \sum_{i=1}^{N} \delta_{ii} = N \\
\delta_{i,i\pm 1} &= 0 \\
\delta_{i+1,i-1} &= 0,
\end{aligned}$$

where the additional "," in the last two expressions was inserted to separate the operations on the two indices clearly.

2.6   Scalar and vector product in three dimensions

While addition and multiplication are straightforward extensions of their counterparts in one dimension, there is no a-priori obvious extension of how to multiply two vectors. Of course, since addition and subtraction have been defined component-wise, it appears tempting to just define multiplication and division also by just multiplying or dividing the components. Though this is possible, the result has no simple geometrical interpretation like the addition and subtraction of vectors. It also turns out to be not useful for anything than being mere mathematical constructions.

Instead, it turns out to be better to construct geometrical operations on vectors which can be viewed as generalized multiplications. They are quite different from the usual notation of multiplication, but will coincide with the ordinary one in one dimension, that is with the usual numbers.

However, there are two paths how to generalize multiplication. At first it may seem more natural to generalize multiplication such that the product of two vectors is again a vector, but it turns out that the more natural generalization is yielding again a real number, just like ordinary multiplication does.

2.6.1 Scalar product

This first product is called scalar product, because it yields a scalar, i. e. an ordinary number. It is also sometimes called dot product or, for more fundamental reasons to be skipped here, inner product.

To introduce it, reduce for the moment the number of dimensions to two rather than three. This will not affect in any way anything of the topics discussed beforehand in any qualitative way, except for counting everywhere only up to two instead of three.

Now consider two vectors $\vec{a}$ and $\vec{b}$. A geometrical question, which can be posed is what is the angle γ between the two vectors. Since they are just two lines in a plane, they can be extended by a third line to yield a triangle, where the third vector should be called $\vec{c}$. It is given by the difference of both vectors, $\vec{c} = \vec{a} - \vec{b}$, where the relative sign will turn out to be irrelevant. Then, elementary geometry yields

$$\vec{c}^2 = \vec{a}^2 + \vec{b}^2 - 2|\vec{a}||\vec{b}|\cos\gamma.$$

Rewriting this in components, using the expression for the length of a vector from section 2.3, yields

$$c_i^2 = (a_i - b_i)^2 = a_i^2 + b_i^2 - 2a_ib_i = a_i^2 + b_i^2 - 2|\vec{a}||\vec{b}|\cos\gamma.$$

Simplifying this equation yields

$$a_ib_i = |\vec{a}||\vec{b}|\cos\gamma.$$

This implies that the sum of the product of the components of two vectors equals the length of two vectors multiplied with the enclosed angle. Moreover, this implies for the corresponding unit vectors

$$(\vec{e}_{\vec{a}})_i(\vec{e}_{\vec{b}})_i = \cos\gamma,$$

and thus the (cosine of the) desired angle is just given by this product-sum of the components of the unit vectors in the direction of the two original vectors.

This fact motivates to introduce the scalar product $\cdot$, defined as

$$\vec{a} \cdot \vec{b} = \vec{a}\vec{b} = a_ib_i = |\vec{a}||\vec{b}|\cos\gamma, \tag{2.7}$$

where the second equality is a common abbreviation of the $\cdot$ operation. This prescription is a map of two vectors to a real number, i. e. a scalar. It is zero, if both vectors are orthogonal to each other, and equals the product of their lengths if they are parallel to each other. Thus, it reduces to the ordinary product of two real numbers in the special case of a one-dimensional space.

This product is also intimately linked to the length of a vector, since

$$\vec{a} \cdot \vec{a} = a_ia_i = |\vec{a}|^2. \tag{2.8}$$

Hence, taking the scalar product of a vector with itself yields the length squared of the vector, since the vector is parallel to itself. Moreover, by construction, the scalar product of a vector with itself is zero if and only if the vector is the zero vector, and positive

otherwise. It is hence a positive semi-definite operation. This does not imply that the scalar product of two vectors is always positive, but only for a vector with itself. E. g. the product of the two vectors $(1,0)^T$ and $(-1,0)^T$ is -1.

Since two vectors are necessarily always in a plane, also in three dimensions an enclosed angle can be determined in the same way. In fact, the whole construction done for two dimensions is valid identically in three dimensions, and thus the definition of the scalar product (2.7) can be transferred to three dimensions identically using elementary geometry. Just sum the indices up to three, instead of two.

E. g. the scalar product of the two vectors $\vec{a} = (1,2,3)^T$ and $\vec{b} = (-1,0,\pi)^T$ is

$$\vec{a}\vec{b} = 1(-1) + 2(0) + 3(\pi) = 3\pi - 1.$$

Since their respective lengths are $\sqrt{14} \approx 3.74$ and $\sqrt{1+\pi^2} \approx 3.30$, the enclosed angle is

$$\cos\gamma = \frac{3\pi - 1}{\sqrt{14}\sqrt{1+\pi^2}} \approx 0.683 \rightarrow \gamma \approx 0.819 \approx 46.9° \qquad (2.9)$$

2.6.2 Vector product

Having now a product at hand which maps two vectors into a scalar, the obvious question is, whether there is also a product which maps two vectors into a vector. This question turns out to be surprisingly non-trivial, and is best first answered in three dimensions.

To obtain such a map, two properties of the resultant vector must be determined: Its direction and length. The direction should be uniquely defined. Since two vectors always are within a plane, the most natural choice is a vector which is perpendicular to the plane. It is a matter of convention, in which direction with respect to the plane, as the two possibilities only differ by an overall sign. The usual convention is the right-hand-rule, where the vectors form a right-hand screw.

For the length, consider the following. In three dimensions, three non-parallel vectors define a volume. The case of two vectors parallel is special, and can be signaled by the resultant vector to have length zero, to avoid an ambiguity for its direction. Since this is signaled by the sine of the enclosed angle, the length of the resultant vector should therefore be proportional to $\sin\alpha$, where α is again the enclosed angle. Similarly, if either vector is the zero vector, also the resultant vector should have zero length. This suggests to construct a resultant vector of the vector product of the vectors $\vec{a}$ and $\vec{b}$ of length $|\vec{a}||\vec{b}|\sin\alpha$.

It remains to obtain a vector which is orthogonal to both other vectors and has this length. This is best done by introducing a very useful object, the so-called Levi-Civita tensor[3] ϵ. What the name tensor signifies will be discussed later in chapter 9. For now, this is just a name. The Levi-Civita tensor is, like the Kronecker-δ, an object which maps a set of indices to a number. While the Kronecker-δ maps two indices, the Levi-Civita tensor maps three indices, ϵ_{ijk}. It is defined such that $\epsilon_{123} = 1$. All other values are derived from it by the following two rules: If two indices coincide, the value is zero, e. g.

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[3]To be precise, of rank three

$\epsilon_{112} = 0$, but also $\epsilon_{iik} = 0$, no matter whether the indices are summed over or a single pair. The second rule is that if two adjacent indices are exchanged, the sign is flipped. E. g. $\epsilon_{123} = -\epsilon_{132}$ or $\epsilon_{ijk} = -\epsilon_{jik}$. If the indices are not adjacent, it can always be reduced to multiple exchanges, e. g.

$$\epsilon_{ijk} = -\epsilon_{jik} = \epsilon_{jki} = -\epsilon_{kji},$$

and so on. Thus

$$\epsilon_{ijk} = \begin{cases} 1 \text{ for } \{ijk\} = \{123\}, \{231\}, \{312\} \\ -1 \text{ for } \{ijk\} = \{132\}, \{213\}, \{321\} \\ \qquad 0 \text{ otherwise} \end{cases}$$

are all possible values.

Using the Levi-Civita tensor, it is possible to construct a vector $\vec{c}$ orthogonal to both vectors $\vec{a}$ and $\vec{b}$ defined as

$$(\vec{c})_i = (\vec{a} \times \vec{b})_i = \epsilon_{ijk} a_j b_k. \tag{2.10}$$

This defines the vector product of $\vec{a}$ and $\vec{b}$, which yields the vector $\vec{c}$. The symbol $\times$ is used to distinguish the vector product explicitly from the scalar product $\cdot$. It is sometimes also called the outer product, in contrast to the scalar (inner) product. Because of the symbol, the vector product is sometimes also called the cross product. The individual components of the resulting vector are

$$\vec{c} = \vec{a} \times \vec{b} = \begin{pmatrix} a_2 b_3 - a_3 b_2 \\ a_3 b_1 - a_1 b_3 \\ a_1 b_2 - a_2 b_1 \end{pmatrix},$$

as can be seen by direct calculation.

Interestingly, this product is not commutative, as $\vec{a} \times \vec{b} = -\vec{b} \times \vec{a}$, as can be seen directly from the definition. Such an anti-commutativity is impossible for ordinary numbers, and explicitly demonstrates that the resulting object is certainly not a number. Such a behavior, i. e. an operation changing sign under exchange of its arguments but is otherwise unaltered, is called anti-linearity.

It needs to be shown that (2.10) has indeed the required properties. To show this, note first that the following holds true

$$\epsilon_{12k} a_1 a_2 + \epsilon_{21k} a_2 a_1 = \epsilon_{12k} a_1 a_2 - \epsilon_{12k} a_1 a_2 = 0.$$

Thus

$$\vec{c}\vec{a} = \epsilon_{ijk} a_j b_k a_i = \frac{1}{2} \left(\epsilon_{ijk} a_j b_k a_i - \epsilon_{jik} a_j b_k a_i \right) = \frac{1}{2} \left(\epsilon_{ijk} a_j b_k a_i - \epsilon_{ijk} a_i b_k a_j \right) = 0, \tag{2.11}$$

where in the second-to-last step the names of the dummy indices in the second term have been changed. For a multiplication with $\vec{b}$ the same result follows in the same way. Thus, $\vec{a} \times \vec{b}$ is indeed orthogonal to both $\vec{a}$ and $\vec{b}$.

It remains to show that the length of $\vec{a} \times \vec{b}$ is $|\vec{a}||\vec{b}| \sin \alpha$. This can be seen in the following way,

$$\begin{aligned} \vec{c}^2 &= \epsilon_{ijk} a_j b_k \epsilon_{ilm} a_l b_m = (\delta_{jl} \delta_{km} - \delta_{jm} \delta_{kl}) a_j a_l b_k b_m \\ &= \vec{a}^2 \vec{b}^2 - (\vec{a} \cdot \vec{b})^2 = |\vec{a}|^2 |\vec{b}|^2 (1 - \cos^2 \alpha) = |\vec{a}|^2 |\vec{b}|^2 \sin^2 \alpha. \end{aligned}$$

Thus, the length is indeed correct.

Herein, an important relation was used

$$\epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}. \tag{2.12}$$

Such a relation is also called a (tensor) contraction, as a common index is summed over. In that sense also the scalar product is a contraction. That the right-hand side of (2.12) is correct is not obvious, and the simplest way of establishing it is by explicit calculation of one set of indices, and obtaining the rest by using the properties of both symbols. More general contractions appear very often. They play a fundamental role in physics and will reappear numerous times throughout the lecture.

Consider now an explicit example, with again $\vec{a} = (1, 2, 3)^T$ and $\vec{b} = (-1, 0, \pi)^T$. Based on (2.9), the length of their vector product should be ≈ 9.01. The vector product yields

$$\begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \times \begin{pmatrix} -1 \\ 0 \\ \pi \end{pmatrix} = \begin{pmatrix} 2\pi \\ -3 - \pi \\ -2 \end{pmatrix},$$

which has indeed length $\sqrt{13 + 6\pi + 5\pi^2} \approx 9.01$.

In contrast to the scalar product, the vector product has no non-trivial behavior in lower dimensions, as it always vanishes. This can be seen from the definition (2.10), as in lower dimensions it is never possible to obtain three different indices. Geometrically, this makes also sense. In one dimension, any vector (i. e. numbers) are either parallel or anti-parallel. In two dimensions, any vector different from the two original ones will be inside the same plane, and any objects dependent on the two initial vectors can then be constructed using addition and/or scalar multiplication of the two vectors, and thus the vector product could not create anything independent.

It is useful to collect a few more properties of the vector product. Very interesting is that the vector product is not only non-commutative, but also non-associative. Perform

$$(\vec{a} \times (\vec{b} \times \vec{c}))_i = \epsilon_{ijk}\epsilon_{klm}a_j b_l c_m = b_i a_j c_j - c_i a_j b_j \neq ((\vec{a} \times \vec{b}) \times \vec{c})_i, \tag{2.13}$$

where the last identity is obtained using (2.12). If $\vec{a}$ is perpendicular to $\vec{b}$ and $\vec{c}$ then the first cross-product cannot lie in the same plane as the last, and therefore the cross-product cannot be associative. However, it satisfies the important so-called Jacobi identity

$$(\vec{a} \times (\vec{b} \times \vec{c}))_i + (\vec{b} \times (\vec{c} \times \vec{a}))_i + (\vec{c} \times (\vec{a} \times \vec{b}))_i = 0,$$

which can be seen from inserting (2.13), as then every term appears twice with opposite signs.

2.7 Generalization to n dimensions

In physics applications, it is very often necessary to perform linear algebra in spaces with more or less than three dimensions, even in infinite-dimensional spaces. It is therefore

necessary to formulate all that has been said so far for an arbitrary number of dimensions n, the so-called $\mathbb{R}^n$.

The generalization of the vector concept is straightforward. Instead of three numbers/coordinates, there are now n, and the vector has n components. Addition/subtraction as well as multiplication with a scalar can also be immediately generalized, as well as the geometric definitions of length and direction.

Since the scalar product is entirely a statement w. r. t. the plane which is created by the two vectors, also the scalar product is extended to be just the sum of the products of the components. Since the angle is also defined inside this plane, there is no ambiguity in its definition. However, in contrast to three dimensions, there is much more freedom in how a plane can be positioned in a higher-dimensional space. Especially, there can be two vectors, which are both perpendicular to a plane, but not parallel to each other, like they would be in three dimensions. An example in four dimensions is $(1,0,0,0)^T$, $(0,1,0,0)^T$, $(0,0,1,0)^T$, and $(0,0,0,1)^T$, which are all non-zero vectors, orthogonal to each other, and none parallel to any of the others.

This immediately indicates that there is a problem with the vector product. Its geometric construction required a vector which has a unique direction (up to a scalar factor of -1) with respect to two other, non-parallel vectors. In more than three dimensions, this requirement becomes ambiguous. Since coplanar vectors, i. e. vectors within the same plane as the two original vectors, can be described by addition, there is no unique way of extending the vector product with the same geometric meaning to higher dimensions.

It is, however, possible to abandon the simple geometric definitions, and define a higher-dimensional vector product formally by (2.10). The Levi-Civita tensor is then defined such that if all three indices are different, and in increasing order, it is unity. The other rules are just kept like they are in the three-dimensional case. The so-defined quantity is still orthogonal to the two original vectors, as (2.11) goes through unchanged, but its length and relative direction in the other dimensions are not necessarily as expected from three dimensions. The use of this generalization is much more limited than that of the scalar product, but it is occasionally encountered in physics. A much more powerful generalization will be discussed in section 8.5.2, but this will require some more concepts.

2.8 Hypersurfaces

To provide an example for the geometrical usefulness of the scalar product also in more than three dimensions, consider the following.

Since two non-parallel vectors $\vec{f_1}$ and $\vec{f_2}$ lie always in a plane, they can be used to define a surface. If the surface is through the origin, it is described by the vector-valued function $\vec{s}$ defined as

$$\vec{s}(a,b) = a\vec{f_1} + b\vec{f_2}.$$

I. e., the two real numbers a and b are used to define all points in the plane. They are essentially the coordinates of all points of the plane. This is very similar to the parameter t used to describe every point along a path in section 2.2.

If the plane does not contain the origin, it is sufficient to have a single point, described by a vector $\vec{c}$, on the surface, to obtain a new parametrization

$$\vec{s}(a,b) = \vec{c} + a\vec{f_1} + b\vec{f_2}, \tag{2.14}$$

where a different choice of $\vec{c}$ yields different meanings for the parameters a and b, as $a = b = 0$ always reduce to the point $\vec{c}$ on the surface. This is true in any number of dimensions.

Now introduce the scalar product. An alternative to characterize a surface is then Hess' normal form. First note that a straight line in $\mathbb{R}^2$ can be characterized as a ray. But alternatively, it could also be characterized by the fact that, given a vector of unit length $\vec{n}$ orthogonal to a line and oriented outwards with respect to the origin,

$$\vec{n}\vec{x} = d,$$

where d is the distance of closest approach to the origin, and may also be zero for a line going through the origin. Then any vector $\vec{x}$ fulfilling this equation describes a point on the line. This is true, as the scalar product gives the projection of $\vec{x}$ in the direction of $\vec{n}$. Since $\vec{n}$ is orthogonal to the line, it has the direction from the origin to the line at the point of closest approach, and thus the projection for any line element must be d.

This can be generalized. Consider the equation

$$\vec{n}\vec{x} = d$$

in $\mathbb{R}^3$ with $\vec{n}$ again of unit length. Then every vector $\vec{x}$ satisfying this condition has projected upon $\vec{n}$ a component of size d, but is otherwise free. This describes a surface, where the two free components describe the movement in the surface. Thus, this is an equivalent way of describing a surface as (2.14), which is already visible since there are two degrees of freedom left. In fact

$$\vec{n}\vec{s}(a,b) = \vec{n}\vec{c} + a\vec{n}\vec{f_1} + b\vec{n}\vec{f_2} = d + 0 + 0$$

and both statements are equivalent.

Considering the $\mathbb{R}^n$, an $n - 1$-dimensional hypersurface can then be defined then in either of the two forms

$$\vec{s}(a_1, ..., a_{n-1}) = \vec{c} + \sum_i^{n-1} a_i\vec{f_i}$$

as an explicit form or by

$$\vec{n}\vec{x} = d$$

in the implicit Hess' normal form.

As an example, consider $\mathbb{R}^4$. Then the vector $(0,0,0,1)^T$ can be used to describe the hypersurface characterized by

$$\vec{s} = \begin{pmatrix} a \\ b \\ c \\ 0 \end{pmatrix} = \vec{0} + a\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + b\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} + c\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \vec{0} + a\vec{f_1} + b\vec{f_2} + c\vec{f_3}$$

which is a three-dimensional volume, though still called a hypersurface.

Describing objects with less than $n - 1$ dimensions, this is best performed by the corresponding generalization of (2.14). This form is also more suitable for a generalization, as the geometrical interpretation of d is otherwise lost, since d can then become something conceptually different.

Chapter 3

Vector spaces

The previous chapter has mostly dealt with a well-known situation, the three-dimensional space. Only at the end it generalized this concept to more than three dimensions. Except for the vector-product, this was possible in a straightforward way without modifying the geometrical concepts behind the structures.

These geometrical concepts are very useful, and in the following often the comparatively simply visualized three-dimensional space will be used to illustrate concepts. The true power of linear algebra, however, lies elsewhere, especially when it comes to quantum physics. While length, breadth, and depth are concepts of special familiarity, the concepts of linear algebra can operate on much more abstract entities. This generalization will be performed here.

Thus, from here on, it will be necessary to let go of the idea that vectors (always) describe points in the space around one. Vectors will become arbitrary entities, like functions or the ominous wave-functions of quantum physics. Vector addition will become a composition rule, and a scalar product can be something like integration. On the other hand, this will show that there are very few mathematical concepts actually underlying a rich multitude of physical structures. This will be essential to find the common laws describing natural phenomena. But it is challenging to becoming used to such abstract thinking. Especially in the beginning it requires to break one's association of vectors with actual space.

3.1   Definition

To distill the basic properties of what will become a vector space, it is foremost necessary to consider what are the concepts we would like to hold most important from the ordinary three-dimensional space $\mathbb{R}^3$.

The concept of vectors is something of fundamental importance. Thus, a vector space, should be a set of vectors. To retain some resemblance of geometry, there should be defined some type of operation which joins two vectors to give another vector. This will be defined as vector addition.

It would certainly be helpful to endow a vector space with a group structure, as this

would provide many powerful features. As a reminder, a group is a set $\mathcal{S}$ of arbitrary objects and a composition rule $\circ$ such that for any elements a, b, and c from the set hold

i) $a \circ b \in \mathcal{S}$, this is called closure

ii) $(a \circ b) \circ c = a \circ (b \circ c)$, this is called associativity

iii) There exists $e \in \mathcal{S}$ such that for any a $e \circ a = a \circ e = a$, which is called the neutral or identity element e

iv) For any a there exists an element, called[1] $\bar{a}$, such that $a \circ \bar{a} = \bar{a} \circ a = e$, which is called the inverse

v) If $a \circ b = b \circ a$, the group is called Abelian, otherwise it is called non-Abelian

The group generalizes the usually multiplication or addition of real numbers.

Thus, to create a vector space, first require that there exists some set of objects $\mathcal{V}$. The elements of $\mathcal{V}$ will be called vectors $\vec{v}$. There can be a finite or enumerable or denumerable infinite number of elements. There should exist an Abelian composition rule $\oplus$, called vector addition, such that the set is closed under it. Thus, $\vec{v} \oplus \vec{w} \in \mathcal{V}$ for all $\vec{v}, \vec{w} \in \mathcal{V}$. The details must be given for any application, of course, but at the current level only these abstract features are relevant.

To obtain a group, there needs to exist a neutral vector $\vec{0} \in \mathcal{V}$, called the zero vector, such that

$$\vec{v} \oplus \vec{0} = \vec{0} \oplus \vec{v} = \vec{v}$$

for any $\vec{v} \in \mathcal{V}$. There must exist also an inverse element for any $\vec{v}$, which will be called $\bar{\bar{v}}$, such that

$$\vec{v} \oplus \bar{\bar{v}} = \vec{0}.$$

Note that this does not have any geometric implications, nor is $\bar{\bar{v}}$ defined as any mathematical operation acting on $\vec{v}$.

The last property is associativity for any $\vec{v}_i \in \mathcal{V}$

$$\vec{v}_1 \oplus (\vec{v}_2 \oplus \vec{v}_3) = (\vec{v}_1 \oplus \vec{v}_2) \oplus \vec{v}_3,$$

which is also intuitive from a geometrical point of view: Following the path of three vectors should not depend on how the path elements are traversed. Likewise, the geometrical interpretation of the sum of two vectors being the endpoint of the path described by following first the first vector and then the second vector is maintained by the Abelian nature of $\oplus$,

$$\vec{v} \oplus \vec{w} = \vec{w} \oplus \vec{v},$$

and thus telling us the geometrical feature that the endpoint of a vector addition is unique. These are the reasons to require an Abelian group structure for the vectors and vector addition.

---

[1]Note that $\bar{a}$ is often denoted by a^{-1}. To avoid confusion of and prevent any attempt to divide by a vector later, this different notation will be used.

So far, even if a geometric idea is behind the vectors, the structure is yet just that of an Abelian group. But there is an important geometrical feature not yet included in the definition of a vector space, the concept of direction. More precisely, the statement that different vectors can have the same direction. This is encoded in the geometrical important concept of rays, which is uniquely connected with some vector and some factor. However, to be more precise, it will not be required to have a specific set of numbers for the factors. Rather, the factors are requested to form a field.

As a reminder, a field (or body) is a set of elements $\mathcal{B}$ with two operations $\circ$ and $\bullet$. It requires that

i) it is an Abelian group under $\circ$ with neutral element e. e does not need to have an inverse with respect to $\bullet$

ii) it is an Abelian group under $\bullet$ with a neutral element E. E does not need to have an inverse with respect to $\circ$. E and e can be different

iii) and a composition of $\circ$ and $\bullet$ obeys $a \bullet (b \circ c) = (a \bullet b) \circ (a \bullet c)$ and $(b \circ c) \bullet a = (b \bullet a) \circ (c \bullet a)$ for all elements of the group, which is called distributivity

This generalizes the real numbers under addition and multiplication.

Now, everything is available to define a vector space: A vector space V is defined as a combination of two elements: An Abelian group of vectors $\{\mathcal{V}, \oplus\}$ and a field $\{\mathcal{B}, \circ, \bullet\}$. The latter are called scalars.

In addition, a third property is required to create a connection between the vectors and the scalars, and to obtain rays. This is an operation called scalar multiplication $\odot$. It combines a scalar a and a vector $\vec{v}$ and yields again a vector $a \odot \vec{v}$. It is furthermore required that

$$(a \bullet b) \odot \vec{v} \;=\; a \odot (b \odot \vec{v}) \tag{3.1}$$
$$a \odot (\vec{v} \oplus \vec{w}) \;=\; (a \odot \vec{v}) \oplus (a \odot \vec{w}) \tag{3.2}$$
$$(a \circ b) \odot \vec{v} \;=\; (a \odot \vec{v}) \oplus (b \odot \vec{v}) \tag{3.3}$$
$$E \odot \vec{v} \;=\; \vec{v}$$
$$e \odot \vec{v} \;=\; \vec{0}. \tag{3.4}$$

This completes the list of properties for a vector space. Note that $\odot$ is given a higher precedence than $\oplus$, such that $(a \odot \vec{v}) \oplus \vec{w} = a \odot \vec{v} \oplus \vec{w}$.

The conventional situation in chapter 2 with the $\mathbb{R}^n$ satisfies all these requirements, e is 0 and E is 1, and thus is a vector space. But vector spaces can be much more, as will be encountered throughout physics. In particular, while it looked like there are only two different operations at play in chapter 2, there are actually four, $\bullet$, $\circ$, $\oplus$ and $\odot$. They can act very differently.

To see, how this plays out for non-conventional building blocks consider the following example. Start with the Abelian group Z_2, which contains just the two elements $\{1, -1\}$, and which is a group under conventional multiplication, with the element 1 being the neutral element. This can be then used to form the vectors of the vector space, while the

fields can remain to be the real numbers. It is then important to note that $a \odot 1$ is a vector, while a is a real number. Also, $a \odot 1$ is not the same as the vector 1, and a vector a does not exist.

This makes some of the rules (3.1-3.4) strange. Consider e. g. (3.2) for $\vec{v}_1 = 1$ and $\vec{v}_2 = -1$. Then $\vec{v}_1 \oplus \vec{v}_2 = -1 = \vec{v}_2$ and

$$a \odot (\vec{v}_1 \oplus \vec{v}_2) = a \odot \vec{v}_2 = (a \odot \vec{v}_1) \oplus (a \odot \vec{v}_2),$$

where it is important to note that $\vec{v}_1 \oplus \vec{v}_2 = 1(-1) = -1 = \vec{v}_2$! Thus, it is necessary to be wary what the symbols mean.

It is conventional in physics to use the symbol + to mean both $\oplus$ and $\circ$,

$$\begin{aligned} \vec{v} + \vec{w} &\equiv \vec{v} \oplus \vec{w} \\ a + b &\equiv a \circ b \end{aligned}$$

and to suppress $\bullet$ and $\odot$ altogether

$$\begin{aligned} a\vec{v} &\equiv a \odot \vec{v} \\ ab &\equiv a \bullet b. \end{aligned}$$

Also, subtraction of vectors is defined as vector addition with the inverse vector

$$\vec{v} - \vec{w} \equiv= \vec{v} \oplus \overline{\vec{w}}$$

and likewise subtraction and division of scalars

$$\begin{aligned} a - b &\equiv a \circ \overline{b} \\ \frac{a}{b} &\equiv a \bullet \overline{b}. \end{aligned}$$

The rest of the lecture will often switch back to this simplified notation. But if confusion arises, it is very helpful to always return back to these basic distinctions and definitions.

Note that at no point angles, a scalar product, a tool to calculate the length of a vector, let alone a vector product, has been used. In fact, even though we introduced scalar multiplication, there is no possibility to state that $a \odot \vec{v}$ should be parallel to $\vec{v}$. Thus, though geometrical features have inspired a vector space, such vector spaces can be quite strange. Endowing a vector space with further operations will yield more specialized spaces, which will be more familiar, and also more useful in physics. However, from a mathematical point of view, the definitions listed here are sufficient to construct vector spaces with interesting properties.

3.2 Complex vector spaces

A very useful example of the general construction of vector spaces are complex vector spaces. These are in some parts of physics, e. g. quantum physics, even more common than the real vector spaces of chapter 2.

3.2.1   Complex numbers as sets or fields of vector spaces

So far, all vector spaces where over the field of real numbers. Also, all examples where based on the real vector space $\mathbb{R}^n$. It is, however, possible to use as field the complex numbers $\mathbb{C}$ as well. Note that this does not necessitates that the set of vectors is not the $\mathbb{R}^n$, though this requires pedantic distinction between scalars and components, and is almost never encountered.

On the other hand, it is possible to consider a vector space with vectors having components in $\mathbb{C}^n$ as well. The simplest example is $\mathbb{C}$, the one-dimensional complex vector space. Since only addition needs to be defined, this is a vector space. It is important to note that so far no multiplication of complex numbers as vectors in $\mathbb{C}$ is defined, and therefore a complex number as a vector in $\mathbb{C}$ is not having a multiplication operation attached to it. It is, however, necessary, to attach a field to it. This can be, e. g. both, the real numbers and the complex numbers. Again, care has to be taken, especially if the set and the field are just $\mathbb{C}$ what is what. This distinction is better seen when taking $n > 1$, since then the vectors are n-dimensional with coordinates being in $\mathbb{C}^n$, just as with the real numbers in $\mathbb{R}^n$ before, with so far no multiplication operation defined.

In fact, if the field is again $\mathbb{C}$, the multiplication with an element of the field becomes, e. g. for $\mathbb{C}^2$,

$$z \begin{pmatrix} z_x \\ z_y \end{pmatrix} = \begin{pmatrix} zz_x \\ zz_y \end{pmatrix}, \tag{3.5}$$

where the products zz_i are again performed as for ordinary complex numbers.

3.2.2   Mapping complex vector spaces to real vector spaces

An interesting question is the relation between complex vector spaces and real vector spaces. Formally, a complex number $z = a + ib$ consists out of two real numbers, a and b. Moreover, the addition of two complex numbers yields

$$z_1 + z_2 = (a_1 + ib_1) + (a_2 + ib_2) = (a_1 + a_2) + i(b_1 + b_2),$$

i. e. the components are not mixed under addition. This suggests to map the complex vector space $\mathbb{C}$ to a two-dimensional real vector space $\mathbb{R}^2$, by just defining the real and imaginary part of the complex number as the two directions of the real vector space, i. e.

$$z = a + ib \rightarrow \begin{pmatrix} a \\ b \end{pmatrix}.$$

Based on section 3.1, this fulfills under the usual addition of the complex numbers all requirements to be a vector space. The zero of the complex numbers, 0, is then just the vector $\vec{0} = (0,0)^T$.

This requires then to add a field. An important point is that the product of two complex numbers,

$$z_1 z_2 = (a_1 + ib_1)(a_2 + ib_2) = (a_1 a_2 - b_1 b_2) + i(a_1 b_2 + b_1 a_2) \tag{3.6}$$

is not trivially mapped, as this would mix the components of the space $\mathbb{R}^2$. Indeed, only the multiplication with real numbers would behave as expected.

Also, when considering the scalar product in $\mathbb{R}^2$ of section (2.3), this has nothing to do with the multiplication in $\mathbb{C}$ (3.6). Rather, it would yield

$$z_1 z_2 = \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = a_1 a_2 + b_1 b_2$$

which is a real number, and different from either real or imaginary part of (3.6). In fact, this definition of the scalar product for complex numbers is usually not useful, and a better version will be introduced in chapter 4.

Thus, a mapping is possible, but only the addition behaves as expected. Any other structure requires a different approach. Nonetheless, there are connections, which will become more transparent, once the more general ideas have been introduced.

3.3 Basis

The first interesting question is a seemingly innocuous one: What is the dimension of a vector space? For the $\mathbb{R}^n$, this was simple enough: By definition n, and thus the number of independent directions. But to define directions, it was necessary to have a sense of direction, and to be able to tell apart when vectors are parallel or not. Since the latter is a question which cannot even be posed in a vector space so far, it is less obvious what dimension a given vector space has. Or even what a dimension is.

To identify a more general concept of dimension, it is best to return and ask what characterizes a dimension (or direction) geometrically in $\mathbb{R}^n$? The answer to this has to do with the number of independent directions. Independent in the sense that if there are some vectors, none of them pointing in this direction, it is not possible to construct using vector addition a vector in this direction from those vectors. It is independent.

This notion of independence can be generalized in the following way. A vector $\vec{v}$ is said to be (linearly) independent from a set of vectors $\{\vec{w}_i\}$ if the only solution for the equation

$$a \odot \vec{v} \oplus b_i \odot \vec{w}_i = \vec{0}$$

is $a = b_i = e$. In the context of $\mathbb{R}^n$, this translates to $a = b_i = 0$. Otherwise, it is said to be (linearly) dependent on the vectors $\vec{w}_i$. Note that we do not yet pose the question of how to calculate the scalars a and b_i in practice. For the definition, it does not matter. Especially, the definition of a vector space just guarantees the well-definiteness, but by no means any computation rules, as there are no coordinates or anything yet. They come now.

This concept can now be used to define the dimensionality of a vector space. The dimension of a vector space n is the minimum number of vectors $\vec{e}_i$ necessary such that every other vector $\vec{v}$ of the vector space is linearly dependent, i. e. there is always a solution to the equation

$$\oplus_i b_i \odot \vec{e}_i = b_i \odot \vec{e}_i = \vec{v} \tag{3.7}$$

with at least one $b_i \neq 0$, including the option that only for $b_j = E$, if $\vec{v} = \vec{e}_j$. Herein the notation $\oplus_i$ (and later $\circ_i$) generalizes the concept of a sum, and for it also the Einstein convention is applied.

This generalizes the idea of dimension in the sense that the dimension gives the number of independent directions $\vec{e}_i$ in a given vector space. The set $\{\vec{e}_i\}$ is then called a basis of the vector space. The values b_i are then called the coordinates of the vector $\vec{v}$ in the basis $\{\vec{e}_i\}$. The requirement of the minimal number is essential to give a unique number of dimensions, as otherwise it would also be possible to add another vector to the equation, which is linearly dependent on the set $\{\vec{e}_i\}$, and thus obtain a larger number of involved vectors. The scalars b_i used to describe a vector in a basis are also called the components of the vector in this basis, and

$$\vec{v} = \oplus_i(b_i \odot \vec{e}_i) \tag{3.8}$$

holds.

It should be noted that at no point it is required that the basis is unique. Thus, it is perfectly possible, but not necessary, that there are different sets of vectors $\{\vec{e}_i\}$ and $\{\vec{f}_i\}$ which both form a minimal set, and thus a basis. These may be created in several ways. Either by scalar multiplying any (or all) vectors with scalars. This, in a trivial sense, creates a new basis. This is called also a rescaling of the basis. Any such operation will rescale also the coordinates by the inverse of these factors. The other option is to replace any or all of the vectors $\vec{e}_i$ by other vectors. However, since every vector is by definition linearly dependent on the old basis, these new vectors will also be linearly dependent on the old basis. Thus, there is always a solution to the set of n equations

$$\vec{e}_i = c_{ij} \odot \vec{f}_j$$

giving n^2 coefficients c_{ij}. This is called a base transformation, a concept which will be discussed in much more detail later in section 8.9.1. Of course, vectors will have in this basis new coordinates,

$$\vec{v} = b_i \odot \vec{e}_i = (b_i \bullet c_{ij}) \odot \vec{f}_j = \oplus_j(\circ_i b_i \bullet c_{ij}) \odot \vec{f}_j$$

where the two sets of pairs of indices requires double summation as indicated. The new coordinates are then the n scalars $\circ_j b_j \bullet c_{ji}$.

Thus, the choice of a basis is arbitrary, and every vector can be rewritten in any basis. Choosing a basis is therefore not more than a convenience. The vectors $(\vec{e}_i)_j = \delta_{ij}$ encountered in the $\mathbb{R}^n$ in section 2.4 are, e. g., an explicit example of a basis, the so-called Cartesian or, since it is the standard choice, canonical (usual) basis.

3.4   Curvilinear coordinates

To show that bases can be quite different from the canonical basis of $\mathbb{R}^n$, it is useful to consider the following examples.

The following bases play also an important role in practical calculations in physics, and can alternatively be used to discuss the $\mathbb{R}^n$. They are adapted to certain geometrical features of problems, for which Cartesian coordinates are often impractical.

For these examples again all the features of the $\mathbb{R}^n$ of chapter 2 will be used, even if not all of them have yet been generalized.

3.4.1 Circle

Consider for example a circle of radius r in two dimensions. It can be described using either a vector

$$
\begin{aligned}
\vec{r} &= \begin{pmatrix} x \\ y \end{pmatrix} \\
\vec{r}^2 &= r^2,
\end{aligned}
$$

where r is a fixed number, and thus involves a second condition, or by

$$
\vec{r} = \begin{pmatrix} r\cos\alpha \\ r\sin\alpha \end{pmatrix},
$$

where the angle α runs from 0 to 2π. This appears to be a rather useful concept.

However, the decomposition

$$
\vec{r} = r\cos\alpha\,\vec{e}_x + r\sin\alpha\,\vec{e}_y
$$

with the conventional orthonormal Cartesian unit vectors appears somewhat clumsy.

Consider instead the two following vectors

$$
\begin{aligned}
\vec{e}_r &= \begin{pmatrix} \cos\alpha \\ \sin\alpha \end{pmatrix} \\
\vec{e}_\alpha &= \begin{pmatrix} -\sin\alpha \\ \cos\alpha \end{pmatrix}.
\end{aligned}
$$

which are both normal vectors, and orthogonal for any value of α. The circle is then described by the vector

$$
\vec{r} = r\vec{e}_r
$$

and thus in a much more natural form. Furthermore, since both vectors are linearly independent, they must form a basis in two dimensions, and therefore any vector can be described by them as well,

$$
\begin{aligned}
\vec{x} &= (x\cos\alpha + y\sin\alpha)\vec{e}_r + (y\cos\alpha - x\sin\alpha)\vec{e}_\alpha \\
&= \begin{pmatrix} x\cos^2\alpha - (-x)\sin^2\alpha + y\cos\alpha\sin\alpha - y\cos\alpha\sin\alpha \\ y\sin^2\alpha + y\cos^2\alpha + x\cos\alpha\sin\alpha - x\sin\alpha\cos\alpha \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix},
\end{aligned}
$$

and they do indeed form a basis.

These new base vectors are better suited to describe a circle, but are ill-equipped for usual Cartesian problems. Such coordinates are therefore called curvilinear coordinates, as they are adapted to problems involving curves.

The important difference compared to ordinary Cartesian coordinates is that the new unit vectors are no longer pointing at every point in the same direction, but at different points in different directions. This yields one problem, for the zero vector. For it, the angle α is not well-defined, as the zero vector does not have a direction. Thus, this change of basis is not well-defined at this point. This can also be seen in the following way. The new unit vectors are obtained from the ordinary ones by a rotation. Acting with this rotation on the zero vector, creates again the zero vector, so this vector is invariant, while all other vectors are rotated. Thus, in these coordinates special care has to be taken when discussing the origin.

This result is also related to the paths of section 2.2. Consider a path along the circle. Then at every point the vector $\vec{e}_\alpha$ points in the direction of the path, and describes thus the path in the same way as in section 2.2. The vector $\vec{e}_r$ is everywhere orthogonal to $\vec{e}_\alpha$, and thus describes therefore an orthogonal direction off the path.

These coordinates are not the only ones adapted to particular problems, and a few more will be discussed in the following.

3.4.2 Cylinder

Another typical example are cylinders. A cylinder is an extension of the circle into three dimensions. Therefore, a suitable set of unit vectors, the so-called cylinder coordinates, is given by

$$\vec{e}_r = \begin{pmatrix} \cos\alpha \\ \sin\alpha \\ 0 \end{pmatrix}, \qquad \vec{e}_\alpha = \begin{pmatrix} -\sin\alpha \\ \cos\alpha \\ 0 \end{pmatrix}, \qquad \vec{e}_z = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

which is therefore a mixture of a Cartesian base vector and curvilinear coordinates. However, any point on (or in) the cylinder can now be addressed by $r\vec{e}_r + z\vec{e}_z$, where r just gives the distance from the origin, and z the height along the cylinder, while $\vec{e}_\alpha$ is not a relevant direction for the cylinder: It describes a movement around the cylinder.

It may look at first sight that somehow a three-dimensional object would now be described by only two variables, r and z. This is not the case, and the third information is encoded in the fact that the vector $\vec{e}_r$ has a changing direction.

Note that the whole z-axis now becomes a singular point, as there the unit vectors $\vec{e}_r$ and $\vec{e}_\alpha$ have no longer a well-defined direction.

3.4.3 Sphere

In a very similar manner, it is useful to construct coordinates describing a sphere, so-called spherical coordinates, as

$$\vec{e}_r = \begin{pmatrix} \cos\phi\cos\theta \\ \sin\phi\cos\theta \\ -\sin\theta \end{pmatrix}, \qquad \vec{e}_\theta = \begin{pmatrix} \cos\phi\sin\theta \\ \sin\phi\sin\theta \\ \cos\theta \end{pmatrix}, \qquad \vec{e}_\phi = \begin{pmatrix} -\sin\phi \\ \cos\phi \\ 0 \end{pmatrix}$$

where the angle ϕ varies between 0 and 2π and θ between 0 and π. The case $\theta = 0$ recreates again a circle in the x-y plane described by the vectors $\vec{e}_\phi$ and $\vec{e}_r$. The vector $\vec{e}_r$

describes the direction from the center of the sphere outwards, while the vectors $\vec{e}_\theta$ and $\vec{e}_\phi$ create a surface orthogonal to $\vec{e}_r$. Of course, for the two vectors spanning this surface there is an ambiguity, as any rotated basis in this surface works equally well.

The second angle only needs to span half a period, as this describes a half-circle, which by rotation around the z-axis by the full period of ϕ already creates a sphere. The latter is described by the second angle.

In contrast to the case of cylindrical coordinates, for spherical coordinates again only the origin is ill-defined, and everywhere else the unit vectors have a well-defined direction.

3.4.4 Hypersphere

Comparing the cases for the sphere in three dimensions and the circle in two dimensions immediately suggests to generalize the concept to arbitrary dimensions, so-called hyperspheres and hyperspherical coordinates. There is a constructive way of creating the unit vectors. To see how it works, consider the case of four dimensions

Start first with the generalization of $\vec{e}_\phi$, yielding

$$\vec{e}_\phi = \begin{pmatrix} -\sin\phi \\ \cos\phi \\ 0 \\ 0 \end{pmatrix}.$$

The next vector must be orthogonal, and linearly independent. This requires to add one more angle, and one more component, yielding

$$\vec{e}_\theta = \begin{pmatrix} \cos\phi\sin\theta \\ \sin\phi\sin\theta \\ -\cos\theta \\ 0 \end{pmatrix}$$

and continue onward with another angle

$$\vec{e}_\eta = \begin{pmatrix} \cos\phi\cos\theta\sin\eta \\ \sin\phi\cos\theta\sin\eta \\ \sin\theta\sin\eta \\ -\cos\eta \end{pmatrix}.$$

The final ingredient cannot have another additional component, and therefore needs to be orthogonal to the previous one, yielding finally the radial vector

$$\vec{e}_r = \begin{pmatrix} \cos\phi\cos\theta\cos\eta \\ \sin\phi\cos\theta\cos\eta \\ \sin\theta\cos\eta \\ \sin\eta \end{pmatrix}.$$

As before, only the angle ϕ goes from 0 to 2π, while θ and η are between 0 and π only.

The process is thus that for every vector one component and one new angle appears, suitably normalized and orthogonalized to the previous vectors, adding as new component the negative cosine of the new angle. Only the last vector, the radial one, is special, as here no new component can be added, and thus only all sines of the previously added angles are flipped to cosines, and the cosine to a negative sine. Constructions in higher dimensions then follow these rules. It should be noted that setting angles to 0 reduces the hyperspherical unit vectors to the unit vector of a hypersphere of one dimensions less (suitable embedded in the higher-dimensional space).

Again, only the origin is ill-defined.

3.5 Subspaces

If the dimension of a vector space is larger than 1, it is possible to define subspaces of it. A genuine subspace of a vector space is any subset of the original vector space which is also a vector space, but has a number of dimensions less than the original vector space. A vector space can be split also into many subspaces. In the extreme case, a vector space of n dimensions can be split into n genuine subspaces, which have only the vector $\vec{0}$ in common. However, formally also the whole vector space can be considered as a subspace, and there is the trivial subspace containing only the vector $\vec{0}$, which has formally dimension 0. Note that sometimes such subspaces are also called hypersurfaces, like in section 2.8 , in analogy to a surface which is a subspace of a volume.

Such a subspace is then spanned by a subset of basis vectors. If the subspace has dimension n_1, the remainder of the original vector space of dimension $n_2 = n - n_1$ is considered to be its complement. The only common vector of these subspaces is the vector $\vec{0}$. If the subspace of V is called S, then the complement is denoted as $S^\perp$. It is often convenient to define a basis of the vector space such that a subspace of interest will be described by the first n_1 basis vectors, and its complement by the remaining n_2 vectors.

As an example, consider $\mathbb{R}^3$ in the Cartesian basis. A subspace would be, e. g., the vector space $\mathbb{R}^2$ spanned by the base vectors $\{\vec{e}_1, \vec{e}_2\}$. The complement is spanned by $\{\vec{e}_3\}$. Note that from this point of view, vectors which have non-zero components in directions 1 or 2 and 3 are no longer living in either sub-space. The union of both sub-spaces is not the full original sub-space, except when including all sums and rays, called the linear hull or linear span. However, the complement of the complement is again the original subspace, $S = (S^\perp)^\perp$.

Subspaces play an important role in physics, e. g. when movement of an object is reduced to a restricted part of space, e. g. an object moving on a plane. In this context the linear span or linear hull plays also an important, though often implicit, role.

More formally, a linear hull is defined to be the intersection of all subspaces of a given vector space, which includes a defined subset S of vectors. By construction, it is therefore a vector space. E. g., the set $S = \{(1,0,0)^T, (1,1,0)^T\}$ in $\mathbb{R}^3$ has as linear hull the $\mathbb{R}^2$ subspace spanned by the basis $\{\vec{e}_1, \vec{e}_2\}$. Especially, any linear hull contains all vectors reachable by addition of the vectors in S as well as by multiplication with scalars of vectors in S. As a consequence, the linear hull of a basis is the vector space they describe.

3.6 Tangential basis

Another relevant concept in the context of bases is the following. Consider a path parametrized by a vector $\vec{F}(t)$. Normalizing this vector by its length, yielding $\vec{f}(t)$ is a vector of constant length. Because every component is an ordinary function, it follows that

$$0 = \frac{d(\vec{f})^2}{dt} = 2\vec{f}\frac{d\vec{f}}{dt}.$$

This is the tangential vector, pointing into the direction of change of the path. Thus, the temporal change of the normalized vector pointing to the path is orthogonal to the normalized vector itself. This can be extended to an orthogonal basis in three dimensions by

$$\vec{f}' = \vec{f} \times \frac{d\vec{f}}{dt}.$$

In two dimensions this is already a basis, in more dimensions the other orthogonal vectors need a convention to construct.

his basis is generated by the original curve at every point. Since $\vec{f}(t)$ changes at every point, this base will change in general at every point. Thus, this base can be considered as a comoving basis.

Alternatively, the ray generated by the tangent vector can also be considered to be a one-dimensional vector space. This vector space is then called the tangent space to the curve. This can be generalized to arbitrary (hyper-)surfaces. Since hyper-surfaces of dimensionality n need at every point n vectors depending on n parameters to characterize them, there are n, not necessarily linearly independent, tangent vectors, which span again a tangent space.

These concepts can be generalized, and lead to the concept of differential geometry, which is beyond the scope of this lecture.

Chapter 4

Structures on vector spaces

4.1 Normed and Banach spaces

So far, the abstract vector space has only vector addition and multiplication by scalars. Thus, not even a notion of the length of a vector (and thus that scalar multiplication in a sense 'rescales' a vector) has been introduced, much less that of a distance. However, especially in physics, such concepts are necessary in almost all cases to describe physical quantities. But, from a purely mathematical point of view, vector spaces do not need such a structure. Hence, such vector spaces which have an implementation of a distance and length measurement are special cases of vector spaces, and thus have an own name, so-called normed vector spaces.

First of all, what will be necessary are two operations. The first maps a vector $\vec{v}$ into the real numbers $\mathbb{R}$, $\|\vec{v}\| \to \mathbb{R}$. The second does the same for the scalars, $|a| \to \mathbb{R}$.

The relevant properties, from a geometrical or physical point of view, to create a length or a norm of a vector by $\|\vec{v}\|$ are then threefold:

i) $\|\vec{v}\| \geq 0$ with $\|\vec{v}\| = 0$ if and only if $\vec{v} = \vec{0}$

ii) $\|a\vec{v}\| = |a|\|\vec{v}\|$. This implies that also the operation $|a|$ needs to yield a positive number, or zero if and only if $a = e$.

iii) The equation

$$\|\vec{a} \oplus \vec{b}\| \leq \|\vec{a}\| + \|\vec{b}\| \tag{4.1}$$

should hold. This requirement is less obvious. It is called the triangle inequality. It expresses the requirement that the length of the sum of two vectors should never exceed the sum of the length of the two vectors.

Note that it is possible to construct operations on vectors, which only fulfill the first two conditions. If so, much less stringent consequences follow. Such cases are called seminorms, and thus the vector space is then only seminormed. Since these play very little role in physics, they will not be considered in this lecture further.

For the length defined in section 2.3, generalized straightforwardly to $\mathbb{R}^n$, these three conditions hold. The first two can be seen directly from the definition (2.4). The third

is not directly evident. However, as the maximum length of the sum is reached if both vectors are parallel, and this saturates the inequality. An alternative in the $\mathbb{R}^n$ is the so-called maximum norm, which identifies the length of a vector with the absolute value of its largest component,

$$\|\vec{v}\| = \max_i |v_i|.$$

This satisfies certainly the first two conditions. The third follows as that the addition of two positive or negative largest components cannot be larger than the sum of their absolute values, and if both have opposite sign it will only decrease the length.

An interesting special case of normed vector spaces are Banach spaces, also called complete normed spaces. Banach spaces are normed vector spaces with the additional constraint that the field is either $\mathbb{R}$ or $\mathbb{C}$ and that the norm is complete in the sense that all Cauchy sequences converge. This is the statement that for any (infinite) set of vectors $\vec{v}$ the sum

$$\sum_n \|\vec{v}_n\| < \infty,$$

converges, and it then follows that the vector $\vec{v}$, defined as

$$\vec{v} = \sum_n \vec{v}_n,$$

and called the limit of the Cauchy sequence, is part of the vector space. That is not trivial. The standard counter example is an n-dimensional sphere in $\mathbb{R}^{n+1}$ without its boundary. Though being certainly a normed vector space, there are sequences where the limit would be on the boundary, and therefore the norm is not complete, and thus it is not a Banach space. Whether a space is a Banach space or not plays an important role in physics, as often the existence of limits is crucial.

4.2 Scalar product and Hilbert spaces

In the $\mathbb{R}^n$ the norm was found to be equivalent to the square-root of the scalar product of a vector with itself. The norm constructed, either in (2.4) or in the section 4.1, both did not refer to any scalar product. Scalar products are therefore an additional structure for a vector space. As it will turn out, a scalar product will automatically introduce a norm, and therefore every vector space with a scalar product will automatically also be a normed vector space.

On an abstract level, the one thing the scalar product did was mapping two vectors into a real number. To generalize it, the basic definition is hence that it is some map of two vectors $\vec{v}$ and $\vec{w}$ to a scalar, denoted as

$$\langle \vec{v} | \vec{w} \rangle = a$$

where a is some scalar, and the notation should for now emphasize that this is a different operation than the usually experienced scalar product. It is a map $\langle \cdot | \cdot \rangle$, which maps two vectors to an element of the field. An example is the one of $\mathbb{R}^3$ in (2.7).

To proceed further, it is necessary to restrict the field to either $\mathbb{R}$ or $\mathbb{C}$. If this restriction is not done, it is still possible to continue, but all other cases play essentially no role in physics. But since restricting to either fields will open up many powerful, and for physics essentially necessary, consequences, the restriction is very valuable. So, this will hold true for the rest of the lecture, except if otherwise noted. This immediately reduces $\circ$ and $\bullet$ to the usual addition and multiplication of real or complex numbers.

With this restriction, the scalar product is required to have a number of further properties, all fulfilled by (2.7),

$$
\begin{array}{rcll}
\langle \vec{v}|\vec{w}\rangle & = & \langle \vec{w}|\vec{v}\rangle^* & (4.2)\\
\langle \vec{v}|a\odot\vec{w}\rangle & = & a\langle \vec{v}|\vec{w}\rangle & (4.3)\\
\langle \vec{v}|\vec{u}\oplus\vec{w}\rangle & = & \langle \vec{v}|\vec{u}\rangle + \langle \vec{v}|\vec{w}\rangle & (4.4)\\
\langle \vec{v}|\vec{v}\rangle & \geq & 0 & (4.5)\\
\langle \vec{v}|\vec{v}\rangle & = & 0 \Leftrightarrow \vec{v} = \vec{0}. & (4.6)
\end{array}
$$

Actually, in section 4.5 the last two conditions will be dropped, but for now they will be part of the following. If they are not included, the scalar product is called a semi-scalar product.

Generalizing from the usual case in $\mathbb{R}^n$, two vectors are then said to be orthogonal if their scalar product vanishes. Two vectors in a normed vector space are said to be parallel, if the absolute value of their scalar product has the same size as the product of their lengths, and anti-parallel if it is of the same size, but negative. Note that this does not necessarily imply the usual geometrical picture.

The last two requirements (4.5-4.6) are then realizing the idea that a scalar product should also make a statement about relative orientation. Especially, the property (4.5) states that no vector is orthogonal to itself, except for the vector $\vec{0}$. It also guarantees that the scalar product maps twice the same vector to a positive number, which will be essential in recovering the relation to the norm in the sense of (2.8).

The conditions (4.3-4.4) guarantee that the scalar product is linear in its arguments, i. e. it is a linear function of its two arguments. It is therefore also called a linear form, a linear map, or a linear operator. The latter concept will be made more precise in chapter 10. Especially, it is possible to think of the scalar product as a linear operator $L_{\vec{v}}$ which yields for every vector $\vec{w}$ the scalar product of $\vec{w}$ with $\vec{v}$. This very abstract way of thinking about the scalar product will be quite useful in quantum physics.

Finally, the condition (4.2) is relevant only for complex vector spaces. It ensures that the scalar product of a vector with itself is a real number, and can therefore be interpreted later as a length. Note that the combination of (4.2) and (4.3) implies

$$
\langle \vec{v}|a\odot\vec{w}\rangle = a\langle \vec{v}|\vec{w}\rangle = (a^*\langle \vec{w}|\vec{v}\rangle)^* = \langle \vec{w}|a^*\odot\vec{v}\rangle^* = \langle a^*\odot\vec{v}|\vec{w}\rangle,
$$

i. e. moving a scalar from the second to the first argument complex conjugates it.

The way of writing a scalar product has lead to the simplification of notation that the vector arrow is often dropped, i. e.

$$
\langle \vec{v}|\vec{w}\rangle \equiv \langle v|w\rangle,
$$

a notation often encountered in quantum physics. In this context, the object $|w\rangle$ is taken to be equivalent to a vector, and is called 'ket'. At the same time, the object $\langle v|$, called 'bra', cannot be really also a vector, as the fact that a is conjugated during scalar multiplication shows. The complex conjugation indicates that the bra is also changed, therefore also called (complex) conjugated. Furthermore, it will be seen later that it is also the transposed vector, and thus, in a loose language, $\langle w| \sim \vec{w}^\dagger$, the bra is the so-called Hermitian conjugate, i. e. transposed and complex conjugated and indicated by the sign $\dagger$, called dagger, of the vector $\vec{w}$. While this distinction will be of very limited importance in the following, this fine distinction is of central importance is many aspects of modern physics, especially general relativity and quantum physics. In the following, this so-called bra-ket notation will not be used for the vectors themselves, to avoid confusion. The notation for the scalar product is kept, nonetheless, to make clear that it can be quite general.

A vector space with scalar product is upgraded to a so-called Hilbert space[1] by relating the length function of section 4.1 with the scalar product by

$$
\begin{aligned}
\|\vec{v}\| &= +\sqrt{\langle \vec{v}|\vec{v}\rangle} \\
\|\vec{a} \oplus \vec{b}\| &= +\sqrt{\langle \vec{a} \oplus \vec{b}|\vec{a} \oplus \vec{b}\rangle}.
\end{aligned}
\tag{4.7}
$$

Note that the triangle inequality (4.1) can then only be fulfilled if the scalar product obeys (4.5-4.6). If the vector space in question should only be normed but not complete, it is called a pre-Hilbert space

Almost all vector spaces encountered in physics are either Hilbert spaces or indefinite-norm Hilbert spaces, i. e. Hilbert spaces without the condition (4.5-4.6).

To emphasize, consider again the example at the end of section 3.1 of Z_2 for the vectors of the space. Define for the two vectors 1 and -1 the scalar product as $\langle 1|1\rangle = 0$, $\langle -1|-1\rangle = 1$ and $\langle 1|-1\rangle = \langle -1|1\rangle = 0$. This satisfies the conditions (4.2-4.3) and (4.5-4.6) trivially. Only (4.4) requires some more consideration:

$$
\begin{aligned}
\langle 1|1 \oplus 1\rangle &= \langle 1|1\rangle = & \langle 1|1\rangle + \langle 1|1\rangle \\
\langle 1|1 \oplus -1\rangle &= \langle 1|-1\rangle = & \langle 1|1\rangle + \langle 1|-1\rangle \\
\langle 1|-1 \oplus -1\rangle &= \langle 1|1\rangle = & \langle 1|-1\rangle + \langle 1|-1\rangle \\
\langle -1|1 \oplus 1\rangle &= \langle -1|1\rangle = & \langle -1|1\rangle + \langle -1|1\rangle \\
\langle -1|1 \oplus -1\rangle &= \langle -1|-1\rangle = & \langle -1|1\rangle + \langle -1|-1\rangle \\
\langle -1|-1 \oplus -1\rangle &= \langle -1|1\rangle = & \langle -1|-1\rangle + \langle -1|-1\rangle
\end{aligned}
$$

This system of equations cannot be solved, except if the scalar product is always zero. Thus, on this vector space it is only possible to define a scalar product fulfilling (4.2-4.5), but not at the same time (4.6). Thus, this vector space can become at most an indefinite Hilbert space using this definition of a scalar product.

---

[1]There are fine subtleties in the following. Especially, from a correct mathematical perspective, a Hilbert space will require (4.5-4.6) to be fulfilled. In most physics contexts, the name of Hilbert space is often also used if these are not fulfilled, though this is a strict mathematical sense not correct.

4.3 Orthonormal basis

Once a scalar product is defined, it can be used to define the two important concepts of orthogonality and normality, provided (4.5-4.6) hold for it, and the norm is introduced as (4.7). A vector $\vec{a}$ is then said to be normal, if its length is $\|\vec{a}\| = \langle \vec{a}|\vec{a}\rangle = 1$. Any vector can be made normal by multiplying it with its inverse length. As noted, two vectors $\vec{a}$ and $\vec{b}$ are said to be orthogonal, if their scalar product vanishes $\langle \vec{a}|\vec{b}\rangle = 0$. If two normal vectors are orthogonal, they are said to be orthonormal.

It is especially convenient to apply these concepts to a basis. So far, a basis $\{\vec{e}_i\}$ was just a minimal set of linearly independent vectors. If the elements of this basis are orthogonal to each other $\langle \vec{e}_i|\vec{e}_j\rangle \sim \delta_{ij}$, this basis is called an orthogonal basis. If, in addition, every base vector is normal, $\langle \vec{e}_i|\vec{e}_j\rangle = \delta_{ij}$, it is called an orthonormal basis.

Such bases have particular advantages. Especially the components of a vector $\vec{v}$ in this basis

$$\vec{v} = v_i \odot \vec{e}_i$$

can be calculated by taking the scalar product with a base vector $\vec{e}_i$,

$$\langle \vec{e}_i|\vec{v}\rangle = v_j\langle \vec{e}_i|\vec{e}_j\rangle = v_j\delta_{ij} = v_i,$$

i. e. the components are just the scalar products of the base vectors with the vector.

Especially, given any, often normal[2], basis $\{\vec{a}_i\}$, it is possible to construct an orthonormal basis, provided the scalar product satisfies (4.5-4.6). This is the so-called Gram-Schmidt orthogonalization procedure. To start, take an arbitrary base vector $\vec{a}_1$. This will be the first vector $\vec{b}_1 = \vec{a}_1/|\vec{a}_1|$ of the new base. Then construct a second vector by

$$\vec{c}_2 = \vec{a}_2 \oplus \overline{\langle \vec{b}_1|\vec{a}_2\rangle \odot \vec{b}_1}. \tag{4.8}$$

For the vector space $\mathbb{C}^n$, this reads

$$\vec{c}_2 = \vec{a}_2 - \langle \vec{b}_1|\vec{a}_2\rangle\vec{b}_1.$$

This vector is, by construction, orthogonal to the vector $\vec{b}_1$,

$$\langle \vec{b}_1|\vec{c}_2\rangle = \langle \vec{b}_1|\vec{a}_2\rangle - \langle \vec{b}_1|\vec{a}_2\rangle\langle \vec{b}_1|\vec{b}_1\rangle = 0,$$

since $\vec{b}_1$ is normalized, $\langle \vec{b}_1|\vec{b}_1\rangle = 1$. The purpose of the operation (4.8) was therefore to remove the component of $\vec{a}_2$ which is parallel to $\vec{b}_1$. Normalizing $\vec{c}_2$ then yields the new base vector $\vec{b}_2 = \vec{c}_2/\|\vec{c}_2\|$.

The orthogonalization procedure now proceeds in the same manner for all the other base vectors. Given another vector of the original set, the components parallel to the already orthogonalized base vectors are projected out

$$\vec{c}_i = \vec{a}_i \oplus \left(\oplus_{j=1}^{i-1} \overline{\langle b_j|a_i\rangle \odot \vec{b}_j} \right)$$

---

[2]Any basis can be immediately normalized by dividing each base vector by its length,

or in $\mathbb{C}^n$

$$\vec{c}_i = \vec{a}_i - \sum_{j=1}^{i-1} \langle b_j | a_i \rangle \vec{b}_j.$$

After normalization this yields the next base vector $\vec{b}_i$. Since the vectors of the original basis are mutually linearly independent, the base vector $\vec{a}_i$ have to be linearly independent from the created base vectors $\vec{b}_j$ with $j = 1, ..., i-1$ as these are, by construction, linear combinations of only the subset $\vec{a}_1, ..., \vec{a}_{i-1}$ of the original base vectors. Since they are linearly independent of $\vec{a}_i$, no linear combination of them can yield a vector which can cancel $\vec{a}_i$. Thus, the new vector is non-zero, and still linearly independent of the previously obtained $\vec{b}_1, ..., \vec{b}_{i-1}$. By repeating this procedure, always an orthonormal basis $\{\vec{b}_i\}$ is obtained. Note that this basis will depend on the order of choosing the $\vec{a}_i$ in the process.

As an example, consider the ordinary $\mathbb{R}^3$ with the basis $\{\vec{a}_1, \vec{a}_2, \vec{a}_3\}$ $= \{(1,1,1)^T, (1,-1,1)^T, (-1,-1,1)^T\}$. The first new vector is the normalized first vector, and thus $\vec{b}_1 = (1,1,1)^T/\sqrt{3}$. The second vector is

$$\vec{c}_2 = \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} - \frac{1}{3} \left\langle \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \middle| \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} \right\rangle \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{2}{3} \\ -\frac{4}{3} \\ \frac{2}{3} \end{pmatrix}$$

and thus $\vec{b}_2 = 1/(\sqrt{6})(1,-2,1)^T$. The third vector then is obtained as

$$\vec{c}_3 = \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix} - \frac{1}{3} \left\langle \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \middle| \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix} \right\rangle \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} - \frac{1}{6} \left\langle \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \middle| \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix} \right\rangle \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}$$

and thus $\vec{b}_3 = (-1,0,1)^T/\sqrt{2}$.

4.4 Metric

To finally obtain even more non-trivial examples of scalar products (and finally recover the situation of section 2.6.1), consider now an n-dimensional Hilbert space. The condition (4.4) requires that a scalar product is a linear function in its second argument. Together with condition (4.2) this also requires it to be linear in its first argument,

$$\langle \vec{a} \oplus \vec{b} | \vec{c} \rangle = \langle \vec{c} | \vec{a} \oplus \vec{b} \rangle^* = \langle \vec{c} | \vec{a} \rangle^* + \langle \vec{c} | \vec{b} \rangle^* = \langle \vec{a} | \vec{c} \rangle + \langle \vec{b} | \vec{c} \rangle.$$

Furthermore, the condition (4.3) requires it to be a homogeneous function, i. e. there cannot be any linear term.

The most general function which has the required properties is given by

$$\langle \vec{v} | \vec{w} \rangle = g_{ij} v_i^* w_j = (g_{ij}^* v_i w_j^*)^* = \langle \vec{w} | \vec{v} \rangle^*, \tag{4.9}$$

where the $n \times n$ numbers g_{ij} are called the metric coefficients, or briefly the set $g = \{g_{ij}\}$ is called the metric, and the v_i and w_j are the components with respect to a given basis. They are thus either real or complex numbers.

There are a few general statements which can be made about the metric. However, it is better to introduce them latter, when more powerful techniques to discuss them are available. For now, it must be sufficient that not every choice of g is possible to maintain (4.2-4.6). the simplest example is that $g_{ij} = 0$ would immediately violate (4.6). Also, if for any fixed index the value of the metric coefficients for all values of the other indices vanishes, then there are vectors which are non-zero but have zero scalar product with themselves, violating (4.6).

The situation of the $\mathbb{R}^3$ is recovered by selecting as metric the Kronecker-δ, $g_{ij} = \delta_{ij}$,

$$\langle \vec{v} | \vec{w} \rangle = \delta_{ij} v_i w_j = v_i w_i = \vec{v}^T \vec{w}.$$

This is called an Euclidean metric. Including the statements about how the length of a vector was defined in section 2.3, the $\mathbb{R}^3$ with the geometrically introduced scalar product is indeed a Hilbert space. The last line now also uses the notation of what the bra vectors are to define what the multiplication of a transposed vector with a vector means: This is the true definition of the scalar product in $\mathbb{R}^3$. This kind of metric is called an Euclidean metric.

In section 3.2 it was not simple to give a meaning to how the scalar product in $\mathbb{C}^n$ should be defined. Here, it now follows immediately as a generalization from the case of the $\mathbb{R}^n$: Use the definition (4.9) again with $g_{ij} = \delta_{ij}$ for two complex vectors v and w,

$$\langle \vec{v} | \vec{w} \rangle = v_i^* w_i = (\Re v_i - i \Im v_i)(\Re w_i + i \Im w_i) = \vec{v}^\dagger \vec{w}.$$

Especially, this implies that the squared length of a complex vector is just the sum of the absolute values of the components,

$$\langle \vec{v} | \vec{v} \rangle = v_i^* v_i = (\Re v_i)^2 + (\Im v_i)^2 = |v_i|^2,$$

a rather natural generalization of the squared length of an ordinary real vector, which is also given by the squared absolute values of its arguments. This shows also that the requirement (4.2) makes sense, as it permits a generalization of the length to complex vector spaces in an intuitive way. Still, the resulting vector product is even in one dimension not the ordinary product of two complex numbers, as one of the numbers is complex conjugated.

It should be noted that it is by no means necessary to use the Kronecker-δ as the metric. An equally possible choice is, e. g., $g_{11} = 2$, $g_{22} = 1/2$ and $g_{12} = g_{21} = 0$. Though the result has no obvious geometrical interpretation (e. g. in $\mathbb{R}^2$ the vector $(1,0)^T$ is four times a as long as $(0,1)^T$), it is a valid choice. Relativity, in particular, is a theory in which a non-trivial metric is central.

4.5   Indefinite metric spaces

When the conditions (4.5-4.6) are dropped, it is possible to have metrics which are different. The arguably best known example is the so-called Minkowski metric in a four-dimensional

real space, of which there are two (equivalent) versions: $g_{11} = -1$ and $g_{22} = g_{33} = g_{44} = 1$ or $g_{11} = 1$ and $g_{22} = g_{33} = g_{44} = -1$ and in both cases $g_{ij} = 0$ for $i \neq i$.

Such a metric is indeed not compatible with (4.5-4.6), as e. g. the vector $(1, 0, 0, 1)^T$ has zero length and the vector $(1, 0, 0, 0)^T$ (for the first case) has indeed a negative scalar product with itself. Thus, interpreting the scalar product as a length or distance is a non-trivial issue. Length and distance can then be even for non-zero vectors zero, positive or even negative.

A negative length or distance appears at first sight something unreasonable from the point of view of geometry. But here experience fools us, as our intuitive understanding is based on the three-dimensional Euclidean space. Indeed, it can be shown that this vector space has a geometry quite different from the Euclidean space we are used to. In physics, this metric appears in the theory of special relativity and also general relativity. In these theories it will turn out that the question of positive length or negative length will be statements about causal connection: Distances of one sign (which depends on convention) can causally influence each other, while those with the other sign cannot. In general, in physics of indefinite metric spaces, different signs indicate different kinds of physical relations between the physical objects represented by the vectors. Hence, despite their counter-intuitive properties, they are fundamentally important. Thus, this topic will be taken up again in due course in the lectures on theoretical physics.

4.6   Infinite-dimensional vector spaces

So far, the vector spaces discussed had some arbitrary, but finite dimensions. Especially due to the intended geometrical meaning, this was important. However, none of the structures introduced so far requires a finite umber of dimensions, but only a denumerable one. This is best seen when considering an example. This will also show that the geometrical idea of vectors is a far too limited concept, and vector spaces can be much more complex, but also much richer.

A rather important vector space in physics can be build up from functions which are polynomials,

$$f(x) = \sum_i f_i x^i.$$

I. e., a vector is a polynomial, $\vec{f} = f(x)$, as strange as this seems. Vector addition $\oplus$ will then be the addition of two polynomials,

$$\vec{f} \oplus \vec{g} = f(x) + g(x) = \sum_i (f_i + g_i)x^i. \tag{4.10}$$

With this definition, the set of polynomials forms a group under addition, with 0 being the neutral element and $-f(x)$ the inverse. As a body, the real numbers will be used with the usual addition and multiplication. Scalar multiplication is then defined as

$$\alpha \odot \vec{f} = \alpha \sum_i f_i x^i = \sum (\alpha f_i)x^i,$$

which immediately implements all other rules for vector spaces, since

$$
\begin{aligned}
(\alpha \bullet \beta) \odot \vec{f} &= (\alpha\beta)\sum_i f_i x^i = \alpha\sum_i(\beta f_i)x^i = \alpha\odot(\beta\odot\vec{f}) \\
\alpha\odot(\vec{f}\oplus\vec{g}) &= \alpha\sum_i(f_i+g_i)x^i = \alpha\sum_i f_i x^i + \alpha\sum_i g_i x^i = \alpha\odot\vec{f}\oplus\alpha\odot\vec{g} \\
(\alpha\circ\beta)\odot\vec{f}v &= (\alpha+\beta)\sum_i f_i x^i = \alpha\sum_i f_i x^i + \beta\sum_i f_i x^i = \alpha\odot\vec{f}\oplus\beta\odot\vec{f} \quad (4.11) \\
E\odot\vec{f} &= 1\sum_i f_i x^i = \vec{f} \\
e\odot\vec{v} &= 0\sum_i f_i x^i = \vec{0}.
\end{aligned}
$$

It is thus a vector space. Note that while ordinary polynomials can be multiplied, this is not a valid operation in this vector space.

To obtain a suitable Hilbert space later, it will be necessary to require that only functions are included with the following two properties:

- The sum exists, i. e. $|f(x)| < \infty$ for every finite x. Since this remains true for any sum of functions and for all multiples of functions, this is a closed set under the necessary operations. It also ensures that the vector space is complete

- The function should be bounded in the sense that $-\infty < f(x)e^{-|x|} < \infty$ for all x and that $f(x)$ grows slower than exponential for $x \to \pm\infty$. This will be necessary for the norm and the scalar product chosen in this example. Again, this is a constraint which cannot be broken by either addition or multiplication, and therefore is a sensible statement about a set of functions to form the vector space

These two conditions may seem to be somewhat ad-hoc, but they are typical properties of functions encountered in physics. It is at this stage not obvious why this is the case, and it will become clear only in physics lectures.

The functions $f(x) = \vec{f}$ play the role of vectors in the vector space to be defined. When doing so, the monomials $x^i = \vec{e}_i$ will become the basis, which is now denumerable infinite, as i can run from 0 to infinity, but only in integer steps. That this is indeed a basis can be seen by the fact that, say, x^2 cannot be written by a sum which does not contain x^2. The field are now the real numbers making up the α. Note that the coefficients f_i are from the same field, but this is not necessary in general. The addition is then the addition of monomials, with the neutral element being zero. A possible sequence of base vectors is then $\{1, x, x^2, ...\}$.

A possibility to obtain a normed vector space would be the norm

$$
||f|| = \int_0^\infty dx\, e^{-x}|f(x)| \tag{4.12}
$$

That this is a norm can be seen by checking the requirements of a norm. Since the absolute value appears, only $f(x) = 0$ can have norm zero, since otherwise a non-vanishing, positive function is integrated, which will yield a non-zero positive result. A multiplication by a

field element is no problem, since $\|\alpha f(x)\| = |\alpha|\|f(x)\|$ as any constant can be moved outside the integral. Finally, since

$$\|\vec{f_1} + \vec{f_2}\| = |f_1(x) + f_2(x)| \leq |f_1(x)| + |f_2(x)| = \|\vec{f_1}\| + \|\vec{f_2}\|$$

for any two functions at the same positions x can be derived from the triangle inequality for ordinary numbers, this would be a norm, and would upgrade the vector space to a normed space.

As an alternative to the normed vector space an interesting knack appears when the vector space should be upgraded to a Hilbert space by implementing a scalar product. The multiplication $f(x)g(x)$ will not be a possibility, as this actually produces again a vector, i. e. a new function $h(x)$. Though this could be considered as some different kind of vector product, though it is not anti-linear and therefore quite a different object as the previously considered one, it is certainly not an element of the field, i. e. a real number.

There are, in fact, several possibilities how to define a suitable inner product. Here, for the sake of variety, a scalar product leading to a different norm than (4.12) will be chosen,

$$\langle \vec{f}|\vec{g} \rangle = \int_{-\infty}^{\infty} dx e^{-x^2} f(x)g(x).$$

This definition is certainly mapping the two functions to a real number. The appearance of the factor $\exp{-x^2}$, the so-called integral measure, has the only purpose of ensuring that the integral is finite. This also explains the condition for the functions to vanish sufficiently fast at in infinity. It has also all the properties (4.2-4.4). Also, only the zero vector $f(x) = 0$ will have a vanishing inner product, as in all other cases only the positive semi-definite square of a function is integrated. Since the integral measure is positive, this does not change the result.

It should be noted that for two different vectors, i. e. functions, the integral can become both positive or negative or zero. In this sense, two functions can be orthogonal with respect to each other. However, taking the monomials as basis, this basis is no longer orthogonal, nor normal, since neither the inner product of two monomials vanishes, nor is the norm of a monomial one.

This already concludes all the necessary steps to create an infinite-dimensional Hilbert space. Note that no real vector product has been discussed, and there is indeed no obvious generalization of a vector product on this space, but this is also not necessary for the purpose of constructing a Hilbert space. As is seen, the vectors are quite different from the usual idea of points in space. Hence, it is also said that the vectors here are elements in a function space. Function spaces are the fundamental building blocks of quantum physics.

A typical property of infinite-dimensional vector spaces is the appearance of infinite sums. This is the root of where most differences between finite-dimensional vector spaces and infinite-dimensional vector spaces are located. A finite sum of finite elements is always finite. An infinite sum of finite elements is not necessarily so. This is the reason why there are subtle differences between both cases, and why not necessarily every statement made about finite-dimensional vector spaces automatically carries over to infinite-dimensional

vector spaces. However, if not stated explicitly otherwise, this will be true for results in this lecture.

4.7   Vector product

The scalar product as a map of two vectors to the field could be generalized in a rather straightforward way. The vector product, mapping two vectors to a vector, is an entirely different problem. As already noted in section 2.7, even the generalization to higher dimensions is far from obvious. The resulting operation suggested there is not really a vector product, as one of its geometric features, the orthogonality with respect to the two vectors it is formed from, is no longer unambiguous. Its extension in this form is therefore subtle.

The situation becomes even worse when attempting to generalize the concept further, if one insists on having a mapping from two vectors to one vector: There is no unique geometrical generalization. Rather, the key to generalize it is not to insist on the orthogonality as a guiding principle, but the anti-linearity. With this in mind, it is possible to extend the idea, and also to show why in the end three dimensions is so special. This will be done in section 8.5.2. But this requires another concept first: Matrices.

Chapter 5

Matrices

5.1 An example: Rotation

5.1.1 Rotations of vectors

To start the discussion of the extremely important topic of matrices, it is best to start once more with a geometrical example. Consider a vector space $\mathbb{R}^2$ over the field of real numbers, with an orthonormal basis $\{(1,0)^T, (0,1)^T\}$, where the upper component plays the role of the x-axis and the lower component that of the y-axis. This is just a plane.

Start with some point on the plane, say $(1,0)^T$. Rotate the point in the plane around the origin by $\pi/2$ counter-clockwise. It will then have the new coordinates $(0,1)^T$. In general, if the vector would be rotated by an angle α between the original and the new vector (counter-clockwise), the new vector would be $(\cos\alpha, \sin\alpha)^T$.

The question to be posed now is: Is there some map $M : \vec{v} \to \vec{v}'$ which realizes the rotation of the vector $\vec{v}$ into the vector $\vec{v}'$? Or, in a more formal way, in

$$M \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\alpha \\ \sin\alpha \end{pmatrix}, \tag{5.1}$$

what is the map, or operator, M?

Since a rotation should not change the length of a vector, this operator M must be linear:

$$Ma\vec{v} = aM\vec{v},$$

i. e. any multiplicative factor must commute with the operator.

5.1.2 Definition of matrices and matrix-vector multiplications

To achieve this, it is useful to introduce the concept of a matrix. A matrix M is a rectangular scheme of $n \times j$ entries M_{ij} with the indices running from 1 to n and 1 to k, respectively. These entries are elements of the field. Here, they will be most often numbers. Thus, a 2×2 matrix M will be given by

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}.$$

A matrix for which $n = k$ is called a square matrix. This type of matrices is actually the by far most prevalent type encountered in physics. Special matrices are the unit matrix with matrix elements given by $M_{ij} = \delta_{ij}$ and the zero matrix with $M_{ij} = 0$. Matrices with non-zero elements only for $i = j$ are called diagonal matrices, and often abbreviated as $M = \text{diag}(M_1, ..., M_{\min(n,k)})$, dropping the second index[1].

Now, it is possible to define the action of an $n \times k$ matrix M on a k-dimensional vector $\vec{v}$, such that this yields a n-dimensional vector $\vec{v}'$ by

$$\vec{v}'_i = (M\vec{v})_i = M_{ij} v_j \tag{5.2}$$

This is called matrix-vector multiplication. The v_i are the components of the vector in a fixed basis. What a change of basis implies for matrix-vector multiplication will be explored later.

As an example, consider

$$\begin{pmatrix} 2 & 3 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} -2 \\ 5 \end{pmatrix} = \begin{pmatrix} -2 \cdot 2 + 3 \cdot 5 \\ (-1) \cdot (-2) + 1 \cdot 5 \end{pmatrix} = \begin{pmatrix} 11 \\ 7 \end{pmatrix}.$$

Analyzing this statement in detail, it is helpful to consider each row of the matrix as a transposed, k-dimensional vector:

$$M = \begin{pmatrix} \vec{M}_1^T \\ ... \\ \vec{M}_n^T \end{pmatrix}.$$

The vectors $\vec{M}_i$ are called row vectors. Then the definition (5.2) requires to build a new vector with each entry of its n entries being the ordinary $\mathbb{R}^n$ scalar product of the ith row vector of the matrix with the vector:

$$M\vec{v} = \begin{pmatrix} \vec{M}_1^T \cdot \vec{v} \\ ... \\ \vec{M}_N^T \cdot \vec{v} \end{pmatrix},$$

which, by construction, is an n-dimensional vector. However, this is only an analogy. The scalar product on the vector space in question may actually be defined entirely differently, or non-existent, and both the field and the vector space may be made up from entirely different objects. Still, the definition (5.2) holds always. It uses only features necessary to define a vector space at all.

Since in this case the vector $\vec{w}$ has been positioned on the right of the matrix, it is also called a right-multiplication. It is useful to define also a left-multiplication. In this case, an n-dimensional, transposed and, if complex, conjugated vector is multiplied from the left using the definition

$$(\vec{w}^\dagger M)_j = w_i^* M_{ij}. \tag{5.3}$$

---

[1]Diagonal matrices with $n \neq k$ are sometimes not considered to be properly diagonal.

This yields a k-dimensional transposed vector in the same way as before. This can be considered as a vector with entries obtained from scalar products of the column vectors $\vec{M}'$ of the matrix M

$$M = \begin{pmatrix} \vec{M}'_1 & ... & \vec{M}'_K \end{pmatrix}$$

with the original vector $\vec{w}$

$$\vec{w}^\dagger M = (\vec{w}^\dagger \cdot \vec{M}'_1, ..., \vec{w}^\dagger \cdot \vec{M}'_K)$$

and thus in a very similar fashion as before. An example is

$$\begin{pmatrix} 1 \\ i \end{pmatrix}^\dagger \begin{pmatrix} 1 & i \\ 0 & -i \end{pmatrix} = (1, -i) \begin{pmatrix} 1 & i \\ 0 & -i \end{pmatrix} = (1, -1+i) = \begin{pmatrix} 1 \\ -1-i \end{pmatrix}^\dagger,$$

where the complex entries were conjugated explicitly.

This implies also that it is possible to simultaneously multiply a matrix from the left and the right by vectors to obtain a scalar

$$\vec{w}^\dagger M \vec{v} = w_i^* M_{ij} v_j = w_i^*(M_{ij}v_j) = w_i^* v_i' = (w_i^* M_{ij})v_j = w_i'^* v_i$$

where the primed vectors are obtained by the action of the matrix on the vector. An explicit example is

$$(2,1) \begin{pmatrix} 1 & 1 \\ -1 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ -2 \end{pmatrix} = (2,1) \begin{pmatrix} -1 \\ -5 \end{pmatrix} = -7,$$

showing one possible path for the two-step process.

For the matrix-vector product it is not necessary that the matrix is square. Using the definition (5.2) an $n \times k$ matrix maps k-dimensional column vectors to n-dimensional column vectors and (5.3) n-dimensional row vectors to k-dimensional row vectors, respectively.

This also shows that the ordinary scalar product of $\mathbb{R}^n$ and $\mathbb{C}^n$ can be interpreted as matrix-vector left-multiplication, interpreting the second vector as an $1 \times n$ matrix. This view will be analyzed further in section 5.2.

5.1.3   Rotation using a matrix

With this scheme, it is possible to return back to the example of rotation of section 5.1.1. Given the desired properties, the linear map implementing a rotation can now be chosen to be the matrix

$$R = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix}. \tag{5.4}$$

Acting with this matrix on a vector $(1,0)^T$ using the definition of the matrix multiplication will indeed yield (5.1). Likewise

$$R \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -\sin\alpha \\ \cos\alpha \end{pmatrix},$$

as would be expected. Thus, a matrix can be used to implement a rotation.

There are many other features of matrices which implement rotations, and this topic will be taken up again in section 8.9.1.2. Before this, it is useful to first collect general properties of matrices.

One thing one should be wary about is, however, the following. While every rotation in a two-dimensional vector space can be mapped to a matrix, not every matrix can be mapped to a rotation. Thus, matrices are a much more general concept. In physics, this is made explicit by saying that certain special sets of matrices are tensors, i. e. matrices with certain special properties which are well-defined in a given context. But very often in physics essentially all matrices appearing are belonging to some set of tensors. Therefore, sloppily, often the names matrix and tensors are used interchangeably though this is, strictly speaking, not correct. This will be discussed more in chapter 9.

5.2 General matrices and vectors

One of the first things to notice is that the definition of matrices actually also encompasses vectors. A normal vector in an n-dimensional vector space is a $1 \times n$ matrix. Thus, a vector is just a special case of a matrix. For real vectors, the transposed vector is then an $n \times 1$ matrix. Moreover, the usual scalar product is a special case of the matrix-vector product for these two particular kinds of matrices. For complex vectors, the definition has to be enlarged, as the Hermitian conjugate vector is a $n \times 1$ matrix of the complex conjugated elements of the original vector.

As has already been done, matrices and vectors, as well as the associated operations, can be directly enlarged to arbitrary vector spaces, by using the components of the vectors with respect to a given basis as defined in (3.8) and then applying (5.2),

$$(M\vec{v})_i = \circ_j M_{ij} \bullet v_j = \vec{v}_i',$$

which requires the matrix elements to be in the same field as the scalars, i. e. usually $\mathbb{R}$ or $\mathbb{C}$. In the case of the standard vector spaces $\mathbb{R}^n$ and $\mathbb{C}^n$, this reads

$$(M\vec{v})_i = M_{ij} v_j = \vec{v}_i'$$

and is thus a conventional sum of products.

Given that also vectors are matrices, the fact that both the scalar product and the rotation are linear maps proves to be a portent. In fact, any linear map on a (finite-dimensional) vector space can be represented by a matrix and can be written as a matrix product with the vectors and this matrices. To see this requires to check that the properties of a linear map are implemented by matrix-vector products.

These are by, definition, linearity, additivity, and the existence of a zero element

$$
\begin{aligned}
M \cdot (\alpha \odot \vec{v}) &= \alpha \odot (M \cdot \vec{v}) \\
M \cdot (\vec{a} \oplus \vec{b}) &= M \cdot \vec{a} \oplus M \cdot \vec{b} \\
M \cdot \vec{0} &= \vec{0} = 0 \odot (M \cdot \vec{v}),
\end{aligned}
$$

where $\cdot$ is the application of the linear map to a vector, in case the linear operator is more abstract than a matrix, as will be the case in chapter 10. These are trivially fulfilled by matrix vector multiplication, and therefore matrix multiplication is a linear map or linear operator.

The proof to the opposite is more complicated. It requires to show that any map which has these properties can be represented as a matrix. For linear operators mapping into the same Hilbert space, this can be shown using the fact that there exists an orthonormal basis. Any linear operation M acts necessarily as

$$M \cdot (\oplus_i a_i \odot \vec{e}_i) = \oplus_i a_i \odot M \cdot \vec{e}_i.$$

The $M \cdot \vec{e}^i$ are again vectors, as the linear map is again into the same vector space. In addition, there is always an orthonormal base. Assume that the given base is orthonormal. This gives the matrix elements

$$M_{ij} = \langle \vec{e}_j | M \cdot \vec{e}_i \rangle,$$

and thereby constructively proofs the assertion.

5.3   Operations on matrices

Before moving on, it is useful to establish a number of computational rules for matrices. In the following, this will only be used in cases where the matrix elements are either from $\mathbb{R}$ or $\mathbb{C}$. If the matrix elements are from a more general body, this has to be taken into account. Also, the body of the vector space is taken to be the same body.

First, matrices can have complex entries. It is therefore useful to define complex conjugated matrices as

$$(M^*)_{ij} = (M_{ij})^*,$$

i. e. complex conjugation complex conjugates every element. It is also useful to extend the concept of transposition from vectors also to matrices, by defining

$$\left(M^T\right)_{ij} = M_{ji}$$

i. e. the matrix is mirrored at its diagonal. Rectangular matrices are thus changed from a $n \times m$ matrices to $m \times n$ matrices. This generalizes the concept from vectors, where transposition maps $1 \times n$ vectors to $m \times 1$ vectors, and vice versa. In physics, it occurs very frequently that a matrix must be both transposed and complex conjugated. This lead to the introduction of the so-called Hermitian conjugation, which is just the combination of both[2],

$$\left(M^\dagger\right)_{ij} = M_{ji}^*$$

and which therefore generalizes from the vector case of section 4.2.

---

[2]Actually, on very general vector spaces which will be encountered later, there is a subtle difference, but this is rarely of relevance in physics.

When regarding vectors as special cases of matrices, it appears reasonable that matrices are also affected by similar calculational rules as vectors. Especially, the addition of two matrices is defined as
$$(M + N)_{ij} = M_{ij} + N_{ij},$$
i. e. components are added, and likewise subtracted. This also implies that the addition of matrices is only well-defined, if both have the same size and shape, i. e. both are $n \times k$ matrices with the same n and k. In this context the zero matrix, $0_{ij} = 0$, is the neutral element of addition.

It is also useful to define multiplication with a field element as
$$(aM)_{ij} = aM_{ij},$$
i. e. every element of the matrix is multiplied by the field element. This is, like for vectors, called scalar multiplication.

When multiplying a vector with a matrix, the situation was such that multiplying an $n \times m$ matrix with an $m \times 1$ matrix yielded an $n \times 1$ matrix/vector, or a $1 \times m$ matrix/vector multiplied by an $m \times n$ matrix yielded a $1 \times n$ vector. Especially, the corresponding sides had to match. This suggests to also define multiplications between two general matrices of which the two prior cases are special cases. Comparing the situation, this would require that it is only possible to multiply $n \times m$ matrices with $m \times k$ ones, yielding an $n \times k$ one. The correct rules such that the special cases emerge is
$$(NM)_{ij} = N_{ik}M_{kj},$$
i. e. a scalar product is formed between the rows of the first matrix and the columns of the second matrix, a so-called row-column product, to obtain as a result the entries for the product matrix.

As an example, consider
$$\begin{pmatrix} 1 & 0 \\ -1 & -2 \end{pmatrix} \begin{pmatrix} 2 & -1 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 2 & -1 \\ -2 & -1 \end{pmatrix},$$
showing that the product of two 2×2 matrices is again a 2×2 matrix.

It should be noted that the first matrix is not complex conjugated, different from the scalar product on complex vector spaces. The reason is that the product of two matrices is in general again a matrix, and not a number as with the scalar product. Therefore, a multiplication of, e. g., three matrices is well-defined, while this is not the case for the scalar product of three vectors. Thus, matrix multiplication is only similar to the usual scalar product, but by far not the same!

It is in this context useful to note that the square unit matrix $1_{ij} = \delta_{ij}$, i. e. a diagonal matrix $1 = \text{diag}(1, ..., 1)$ which has 1s on the diagonal and zero everywhere else, is the neutral element of the matrix multiplication. By definition
$$(1M)_{ij} = \delta_{ik}M_{kj} = M_{ij} = (M1)_{ij}$$
and therefore a multiplication with the unit matrix leaves a matrix untouched.

Note that both matrix addition and multiplication are, by definition, associative. They inherit this feature from the associativity of the elements.

There is special care to be taken for matrix multiplication, as it is different in a particular way from ordinary multiplication: It is not commutative, i. e.

$$AB \neq BA$$

which can be seen by explicit calculation of a counter example, e. g. for a 2×2 matrix,

$$
\begin{aligned}
AB &= \begin{pmatrix} A_{11}B_{11} + A_{12}B_{21} & A_{11}B_{12} + A_{12}B_{22} \\ A_{21}B_{11} + A_{22}B_{21} & A_{21}B_{12} + A_{22}B_{22} \end{pmatrix} \\
&\neq \begin{pmatrix} A_{11}B_{11} + A_{21}B_{12} & A_{12}B_{11} + A_{22}B_{12} \\ A_{11}B_{21} + A_{21}B_{22} & A_{12}B_{21} + A_{22}B_{22} \end{pmatrix} = BA
\end{aligned}
$$

and thus care has to be taken. This leads to the definition of the commutator

$$[A, B] = AB - BA,$$

which is the zero matrix if and only if the order of multiplication of A and B does not matter. If the commutator is vanishing, it is said that the two specific matrices A and B commute. This test plays a major role in quantum physics.

This has also consequences on taking the Hermitian conjugate of a product of matrices,

$$\left((MN)^{\dagger}\right)_{ij} = (MN)^*_{ji} = M^*_{jk}N^*_{ki} = \left(N^{\dagger}\right)_{ik}\left(M^{\dagger}\right)_{kj} = \left(N^{\dagger}M^{\dagger}\right)_{ij},$$

which is thus the product of the Hermitian conjugate matrices in reverse order. This can be extended to a longer product, which is then completely reversed.

Matrices are abundant in physics. As a first example, they play an interesting role in the context of linear equations.

Chapter 6

Systems of linear equations

6.1   Matrices and linear systems of equations

So far, matrices played an important role for rotations. However, matrices appear ubiquitously. Arguably one of the most important situations is the one within the context of sets of linear equations. Such equations arise in an enormous number of contexts in physics, from elementary mechanics, astrophysics to quantum physics to particle physics, but also in numerics.

A single linear equation has the form

$$mx + b = 0,$$

which has the solution $-b/m$ if $m \neq 0$. It is a comparatively simple equation, as the independent variable x appears only linearly, and it can therefore be solved with elementary operations in terms of the two constants m and b.

A set of two linear equations for two unknowns x_1 and x_2

$$
\begin{aligned}
m_1 x_1 + m_2 x_2 + b_1 &= 0 \\
m_3 x_1 + m_4 x_2 + b_2 &= 0
\end{aligned}
$$

is more complicated, as now two equations are coupled, and in total six constants $m_{1\ldots4}$ and $b_{1,2}$ appear. Its solution

$$x_1 = \frac{b_2 m_2 - b_1 m_4}{m_1 m_4 - m_2 m_3} \tag{6.1}$$

$$x_2 = \frac{b_1 m_3 - b_2 m_1}{m_1 m_4 - m_2 m_3} \tag{6.2}$$

can still be obtained by elementary operations, but is much less straightforward. Especially, there can only be a solution if $m_1 m_4 - m_2 m_3 \neq 0$, a fact which is not obvious from the original set of equations.

The situation deteriorates quickly with more and more independent variables. For n variables, there are $n(n+1)$ constants of which the solutions are functions.

A first step to improve the situation is by recognizing that the set of linear equations is actually a set of equations for the components of a vector $\vec{x}$. This can be seen by noticing that the ith equation can be rewritten as

$$M_{i1}x_1 + ... + M_{in}x_n + b_i = 0$$

which are precisely the coordinates of the vector-valued equation

$$M\vec{x} + \vec{b} = \vec{0}. \tag{6.3}$$

Thus, a set of linear equations can be written in so-called matrix-vector form.

Usually, there are as many equations as there are unknowns, and thus the matrix M is square. But this is not always the case. If M is not square, the number of equations does not match the number of unknowns. If there are more variables than there are equations, the system is said to be underdetermined. An example is

$$M_{11}x_1 + M_{12}x_2 = b,$$

with both $M_{ij} \neq 0$, that is a single equation with two variables. In this case, the solutions are, e. g.,

$$x_1 = \frac{b - M_{12}x_2}{M_{11}},$$

i. e. there are infinitely many solutions, as there is a solution for x_1 for every x_2, given by the above relation and if $M_{11} \neq 0$. However, also underdetermined systems may have only a finite number of solutions, or none at all.

The other extreme is if there are more equations than independent variables. Such a system is called overdetermined or overconstrained. E. g.

$$\begin{aligned} M_{11}x_1 &= b_1 \\ M_{21}x_1 &= b_2 \end{aligned}$$

would be such a system. If $b_1/M_{11} = b_2/M_{12}$, this system still has a solution, but in general it will not be possible to find a solution.

6.2 Solving a set of linear equations

Solving a set of linear equations can be done in various ways, most of them involving the matrix M. Before moving on to these rather powerful possibilities, it is very useful, and also in some practical applications helpful, to also get acquainted with possibilities to solve a system of linear equations without explicitly involving the matrix-vector form.

Arguably the best known approach is the Gauss' elimination procedure. The basic idea is to use the knowledge provided by the equations to solve them.

For just one equation, the approach is straightforward. Given the equation

$$Mx = b$$

divide it on both sides by m to obtain the solution

$$x = \frac{b}{M},$$

which therefore does not involve any particular insight into the properties of the system.

The basic principles of the approach can already be seen from a system of two equations

$$M_{11}x_1 + M_{12}x_2 = b_1 \tag{6.4}$$
$$M_{21}x_1 + M_{22}x_2 = b_2 \tag{6.5}$$

To start, multiply the second equation by M_{12}/M_{22}, assuming that M_{22} is non-zero. If not, the second equation does not involve M_{22}, and can therefore be solved like in the one-equation case for x_1, giving x_1 and thus turning the first equation again into a single equation for x_2. If not, the result is

$$M_{11}x_1 + M_{12}x_2 = b_1$$
$$\frac{M_{21}M_{12}}{M_{22}}x_1 + M_{12}x_2 = \frac{M_{12}}{M_{22}}b_2.$$

Since if the equations can be solved, both equations must be true, it is permissible to subtract the first from the second, yielding

$$M_{11}x_1 + M_{12}x_2 = b_1$$
$$\frac{M_{21}M_{12} - M_{11}M_{22}}{M_{22}}x_1 = \frac{M_{12}}{M_{22}}b_2 - b_1.$$

The second equation no longer involves x_2, and can therefore be solved for x_1 yielding

$$x_1 = \frac{M_{12}b_2 - M_{22}b_1}{M_{11}M_{22} - M_{21}M_{12}},$$

reproducing (6.1). Knowing x_1, the first equation becomes again an equation for a single variable, which can immediately be solved, and will yield (6.2). Thus, the basic idea is to transform the system of equations such that it finally has the form

$$M'_{11}x_1 + ... + M'_{1n}x_n = b'_1$$
$$M'_{22}x_2 + ... + M'_{2n}x_n = b'_2$$
$$\vdots$$
$$x_n = b'_n,$$

where the M'_{ij} and b'_i are some functions of the original M_{ij} and b_i. This is called a tridiagonal form. Of course, in many practical calculations it may be simpler to not have the exact ordering, but a relabeling will always bring the result into this form, if desired.

This already provides the gist of the Gauss' procedure. By suitably adding and subtracting multiples of equations together, eliminate from one equation all but one variable.

This is then an ordinary equation for a single variable, which can be immediately solved. Knowing the result, the original system of equations is reduced to a system of one variable less. To this reduced system the Gauss' algorithm can then again be applied, and so on, until only one equation for a single variable is left, which can then be solved immediately, completing the solution. If during the procedure either any way to eliminate a variable involves a division by zero or yields otherwise an insolvable single equation, the system does not have a solution.

There are several extensions of this procedure for practical applications, e. g. the Gauss-Jordan algorithm, which tries to accelerate the procedure by manipulating all equations simultaneously. Though more efficient in detail, any approach is ultimately based on the same concept as the Gauss' algorithm.

6.3 Inverse matrices

An interesting simplification of the system of linear equations in matrix-vector form (6.3) could be obtained if some matrix N would exist with

$$NM = 1, \tag{6.6}$$

where 1 signifies again the unit matrix, $1_{ij} = \delta_{ij}$. If this matrix N exists, which is usually written as $M^{-1} \equiv N$, it would be possible to multiply (6.3) by it, yielding

$$\left(M^{-1}M\vec{x}\right)_i = \left(M^{-1}\right)_{ij} M_{jk}x_k = \delta_{ik}x_k = \vec{x}_i = \left(M^{-1}\vec{b}\right)_i$$

and therefore the solution would be given by $M^{-1}\vec{b}$, and hence by a matrix-vector multiplication, which is much simpler than, e. g. the algorithm of Gauss. This is not restricted to square matrices, but works as well for rectangular matrices, in which case the inverse of an $m \times n$ matrix is a $n \times m$ matrix such that their multiplication can yield the $n \times n$ or $m \times m$ unit matrix when multiplying from the left or right, respectively.

Hence, this also works with underdetermined or overdetermined systems of equations. In particular, this reduces the question of the existence of a solution to the question of the existence of this so-called inverse of the matrix M. Note that if for a square matrix such a matrix exists then

$$M^{-1}M = 1 = MM^{-1}, \tag{6.7}$$

which can be obtained from (6.6) by multiplying from the left by M and from the right by M^{-1}. Thus, if there exists a so-called left-inverse satisfying (6.6), then there also exists a right-inverse satisfying (6.7), which is the same[1].

The inverse has the interesting feature that necessarily the inverse of a product of matrices is the reverse product of the individual inverse matrices,

$$(AB)^{-1}AB = B^{-1}A^{-1}AB = B^{-1}B = 1.$$

---

[1]Again, there exist subtleties if the number of dimensions is not finite

This originates from the fact that the matrix product is non-commutative. For ordinary numbers, which commute under multiplication, it would be possible to reverse the order.

Of course, if the solution to a system of linear equations is known, the inverse matrix can be reconstructed. E. g., for the two-equations case (6.4-6.5), it can explicitly be derived from the solution, and is given by

$$M^{-1} = \frac{1}{M_{11}M_{22} - M_{12}M_{21}} \begin{pmatrix} M_{22} & -M_{12} \\ -M_{21} & M_{11} \end{pmatrix},$$

since

$$\begin{aligned} M^{-1}M &= \frac{1}{M_{11}M_{22} - M_{12}M_{21}} \begin{pmatrix} M_{22} & -M_{12} \\ -M_{21} & M_{11} \end{pmatrix} \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \\ &= \frac{1}{M_{11}M_{22} - M_{12}M_{21}} \begin{pmatrix} M_{11}M_{22} - M_{12}M_{21} & 0 \\ 0 & M_{11}M_{22} - M_{12}M_{21} \end{pmatrix}, \end{aligned}$$

and therefore having indeed the required property.

However, this also illustrates an important restriction. If

$$M_{11}M_{22} - M_{12}M_{21} = 0, \tag{6.8}$$

then the inverse matrix does not exist, since the pre-factor diverges. Thus, not every matrix has an inverse. This is a quite different situation than for numbers. Here, every number r, except zero generalizing to the non-invertible zero matrix, has an inverse $1/r$. This again shows that matrices are quite distinct from numbers.

To discuss criteria for the invertibility of matrices, it is useful to define first some more functions on matrices.

6.4   Trace and determinant

So far, it is has been discussed how matrices act on both vectors and other matrices. It is furthermore useful to introduce special functions, which map a square matrix to the field, i. e. usually to the real numbers or complex numbers.

6.4.1   Trace

The first such function is called the trace of a matrix. It is defined as

$$\mathrm{tr}M = M_{ii},$$

i. e. it is the sum of the diagonal elements of a matrix. If the matrix is not a square matrix, the sum extends to the shorter of both sides. E. g., for a 2×2 matrix

$$\mathrm{tr} \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = M_{11} + M_{22}.$$

Especially, the trace is independent of the off-diagonal part of the matrix, and is the sum of the diagonal elements of the matrix.

There are a number of further properties of the trace which are very useful. First, it is cyclic for products of matrices,

$$
\begin{aligned}
\mathrm{tr}AB \quad &= A_{ij}B_{ji} = B_{ji}A_{ij} = \quad \mathrm{tr}BA \\
\mathrm{tr}ABC \quad &= A_{ij}B_{jk}C_{ki} = C_{ki}A_{ij}B_{jk} = \quad \mathrm{tr}CAB = \mathrm{tr}BCA,
\end{aligned}
$$

and so on.

It is furthermore the same under transposition

$$
\mathrm{tr}A^T = (A^T)_{ii} = A_{ii} = \mathrm{tr}A
$$

and is complex conjugated for a complex conjugated matrix

$$
\mathrm{tr}A^* = (A^*)_{ii} = (\mathrm{tr}A)^*.
$$

Thus the trace of the Hermitian conjugate of a matrix is the conjugate of the trace of the original matrix

$$
\mathrm{tr}A^\dagger = (\mathrm{tr}A)^*,
$$

which are properties which are useful in actual calculations. Finally, for linear combinations of matrices

$$
\mathrm{tr}k(A + B) = (k(A + B))_{ii} = kA_{ii} + kB_{ii} = k\mathrm{tr}A + k\mathrm{tr}B,
$$

and thus the trace is a linear operation[2].

6.4.2   Determinant

The second is the so-called determinant, which is only defined for square matrices. This operation is best defined in a recursive way. Start by defining the determinant of a one-dimensional square matrix M as the matrix element itself,

$$
\det M = \det(M_{11}) = M_{11}.
$$

Next, define the determinant of a 2×2 matrix as

$$
\det \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = M_{11}M_{22} - M_{12}M_{21}
$$

That this is the same as appearing in the expression relevant to determine the invertibility of a 2×2 matrix in (6.8) is auspicious, and will be returned to.

---

[2]Note that it is no represented by a matrix, as it does not map a vector into a vector, but a matrix into a number.

But first, define now the determinant of an $n \times n$ matrix in the following way. First define for a matrix A a reduced matrix in which the 1st row and the ith column is deleted, A^{1i}. Then the determinant is given by

$$\det A = \sum_i (-1)^{i+1} A_{1i} \det A^{1i}. \tag{6.9}$$

This works for the 2×2 case

$$\det A = A_{11} \det A^{11} - A_{12} \det A^{12} = A_{11}A_{22} - A_{12}A_{21}$$

and yields for a 3×3 matrix

$$\begin{aligned} \det A &= A_{11} \det A^{11} - A_{12} \det A^{12} + A_{13} \det A^{13} \\ &= A_{11}(A_{22}A_{33} - A_{23}A_{32}) - A_{12}(A_{21}A_{33} - A_{31}A_{23}) + A_{13}(A_{21}A_{32} - A_{31}A_{22}), \end{aligned}$$

and so on. For the calculation of the determinants of reduced matrices the recursive algorithm can be used until a known expression is encountered.

There are a number of observations which can be made on the result. The first is that every element appears in the expressions always the same number of times. This suggests that rather than giving the first row a special role, it should be possible to use rather some arbitrary row j, yielding

$$\det A = \sum_i (-1)^{i+j} A_{ji} \det A^{ji}$$

or, alternatively, a column

$$\det A = \sum_i (-1)^{i+j} A_{ij} \det A^{ij}.$$

It is straightforward that this always yields the same results. It is also said that the determinant is developed with respect to the chosen row or column, which is made special in these formulas. These forms imply that whenever a line or column vanishes, the determinant vanishes, as it is always possible to use the formulation utilizing specifically this line or column.

The simplest way to see that all these formulas are equivalent is by noting that the determinant can also be written without recursion for an $n \times n$ matrix as[3]

$$\det A = \sum_{i_k} \epsilon_{i_1 \ldots i_n} \Pi_j A_{j i_j} = \frac{1}{n!} \sum_{i_k} \sum_{j_m} \epsilon_{i_1 \ldots i_n} \epsilon_{j_1 \ldots j_n} \Pi_l A_{i_l j_l}, \tag{6.10}$$

where the second equality is a combinatorial rewriting. Note again that the ϵ are anti-symmetric. Thus $\epsilon_{123 \ldots n} = 1$, cyclic permutations have the same value and anticyclic a negative, and if two indices coincide it vanishes. This form does not depend on any singled out row or column.

---

[3]The notation $\sum_{i_k}$ is the same as $\sum_{i_1} \sum_{i_2} \ldots \sum_{i_n}$, and thus a shorthand for n summations.

That this is equivalent can be seen by induction. For $n = 1$

$$\det A = \sum_{1_1=1}^{1} \epsilon_{i_1} \Pi_{j=1}^{1} A_{1i_1} = A_{11}$$

and for $n = 2$

$$\det A = \sum_{i_1} \sum_{i_2} \epsilon_{i_1 i_2} A_{1i_1} A_{2i_2} = \epsilon_{12} A_{11} A_{22} + \epsilon_{21} A_{12} A_{21} = A_{11} A_{22} - A_{12} A_{21}.$$

Hence, this agrees. Now

$$
\begin{aligned}
\det A &= \sum_{i} (-1)^{i+1} A_{1i} \det A^i = \sum_{i} (-1)^{i+1} A_{1i} \sum_{i_k, i_k \neq i} \epsilon_{i_2 \dots i_n} \Pi_{j, j \neq i} A_{j i_j} \\
&= \sum_{i_1} \sum_{i_k, i_k \neq i_1} (-1)^{i_1+1} \epsilon_{i_2 \dots i_n} \Pi_j A_{j i_j}
\end{aligned}
\tag{6.11}
$$

The remaining step requires to consider the combination of the ϵ and the pre-factor. By construction, there is no contribution where any of the indices of the ϵ coincides with the index i. Furthermore, consider the case of ϵ with the desired index attached as the first one. If it is odd, and the sequence is cyclic, then this has the same sign as the existing expression (e. g. $+1\epsilon_{23} = 1$ is the same as $\epsilon_{123} = 1$). Alterations in the order of the remaining indices are already contained in the behavior of the ϵ with one index less. If it is even and the remaining indices are cyclic, then it has to be negative compared to the case with one index more (e. g. $-\epsilon_{13} = -1$ is the same as $\epsilon_{213} = -1$.). Thus, indeed both are possible ways to evaluate a determinant.

The expressions (6.9) and (6.10) are very useful to establish properties of the determinant.

One is that if a matrix is diagonal then the determinant is the product of the diagonal elements,

$$
\begin{aligned}
\det \text{diag}(A_{ii}) &= \sum_{i} (-1)^{i+1} A_{1i} \det A^{1i} = \sum_{i} (-1)^{i+1} A_{11} \delta_{i1} \det A^{1i} \\
&= A_{11} \det A^1 = \dots = \Pi_i A_{ii},
\end{aligned}
$$

where no summation is implied in the first step. This was achieved by reusing the same formulas repeatedly, and that only one non-zero element exists per column and row to collapse the sums. Especially, this implies $\det 1 = 1$, i. e. the determinant of any unit matrix is one. In fact, for any matrix which has triangle form, i. e. non-zero elements only on the diagonal and exclusively above or below the diagonal, the determinant is a product of its diagonal elements. This follows by developing the matrix always with respect to a row or column in which there is only one non-vanishing entry (left), the one on the diagonal.

Also useful is

$$\det A^T = \frac{1}{n!} \sum_{i_k} \sum_{j_l} \epsilon_{i_1 \dots i_n} \epsilon_{j_1 \dots j_n} \Pi_l A_{j_l i_l} = \frac{1}{n!} \sum_{j_l} \sum_{i_k} \epsilon_{j_1 \dots j_n} \epsilon_{i_1 \dots i_n} \Pi_l A_{i_l j_l} = \det A,$$

where in the second step the indices have just be renamed. Thus, transposition does not alter the value of a matrix.

It is also useful that

$$\det A^\dagger = (\det A)^*$$

since transposition does not change the determinant, and by the explicit form the product of the matrix elements of the complex conjugate matrix elements is just the complex conjugated of the product of the matrix elements, as the ϵ-tensors are real.

The arguably most important property of determinants is that about the determinant of products of matrices,

$$
\begin{aligned}
\det(AB) &= \frac{1}{n!} \sum_r \sum_{i_k} \sum_{j_m} \epsilon_{i_1...i_n} \epsilon_{j_1...j_n} \Pi_l A_{i_l r} B_{r j_l} = \sum_{i_k} \sum_{j_m} \epsilon_{i_1...i_n} \epsilon_{j_1...j_n} \Pi_l A_{i_l l} B_{l j_l} \\
&= \sum_{i_k} \sum_{j_m} \epsilon_{i_1...i_n} \epsilon_{j_1...j_n} \Pi_l A_{i_l l} \Pi_m B_{m j_m} \\
&= \left(\sum_{i_k} \epsilon_{i_1...i_n} \Pi_l A_{i_l l} \right) \left(\sum_{j_m} \epsilon_{j_1...j_n} \Pi_m B_{m j_m} \right) = \det A \det B^T = \det A \det B
\end{aligned}
$$

where it has been used in the second step that the sum over the product is just giving all possible rearrangements, and thus cancels the factor $n!$. The splitting of the product is then always possible, as it is also just a rewriting. This formula will be very useful in many instances.

Note that while the determinant is well-defined only for its argument being a quadratic matrix, the individual components A and B of the product AB may not be so. In this case the above proof fails, as the number of possibilities differ.

If a $n \times n$ matrix is multiplied by a constant factor, then the form (6.11) immediately shows that

$$\det kA = k^n \det A$$

and thus the determinant is, in contrast to the trace, not a linear operation. On the other hand, if only a single column or row is multiplied by a constant then the formula (6.9) and its generalization shows that this implies that then the determinant is only multiplied by this factor, as it is always possible to develop in this particular line or column. Finally, exchanging two adjacent rows or columns multiplies the determinant by a factor of -1, as this is the same as by developing for one row number/or column number less or more, which increase the exponent of the -1 by one, and therefore yields the prefactor.

Another important fact about matrices is that if any two columns (or rows) are linearly dependent, the determinant vanishes. To see this, note that the determinant of a matrix with a zero row or column vanishes, since it is always possible to develop the determinant with respect to this row or column. Furthermore, adding one row of a matrix to another can be achieved by multiplying a matrix with another matrix of form

$$T_{ij}^{kl} = \delta_{ij} + \delta_{ik} \delta_{lj}, \tag{6.12}$$

from the left, where k is the row to which the column l should be added,

$$(T^{kl}A)_{ij} = T^{kl}_{im}A_{mj} = (\delta_{im} + \delta_{ik}\delta_{lm})A_{mj} = A_{ij} + \delta_{ik}A_{lj}.$$

E. g.

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a+c & b+d \\ c & d \end{pmatrix}$$

Multiplication from the right does the same to a column,

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} a & a+b \\ c & c+d \end{pmatrix}$$

The matrix T^{kl} has unit determinant, as it has triangle form. Thus

$$\det A = \det T^{kl} \det A = \det(T^{kl}A).$$

This can now be repeated as often as necessary to reduce the linearly dependent column or row to zero, and then the determinant is zero, proving the claim.

6.5 Invertibility of matrices

The determinant will now be very useful to determine if a square matrix is invertible.

Assume that an inverse exist, then

$$1 = \det 1 = \det AA^{-1} = \det A \det A^{-1}, \tag{6.13}$$

and therefore for an invertible matrix the determinant of the inverse matrix has to be the inverse of the determinant of the original matrix. Since it is impossible to divide by zero, this implies that an invertible matrix has a non-vanishing determinant. The question is now whether the reverse is also true, and that a non-invertible matrix has determinant zero.

To show this, it is useful to return to systems of linear equations. First assume once more that a matrix A is invertible. Consider the set of linear equations

$$A\vec{x} = \vec{0}. \tag{6.14}$$

Such a system, where the right-hand side vanishes, is called a homogeneous (set of) linear equation(s). Otherwise it is called inhomogeneous. Multiply this by A^{-1} which, by assumption, exists, Then $A^{-1}A\vec{x} = \vec{x} = \vec{0}$. Thus, if A is invertible then the only solution to (6.14) is the trivial one, $\vec{x} = \vec{0}$.

The next step is to recognize that Gauss's elimination procedure can be viewed as a sequence of matrix multiplications. Consider again the 2×2 case.

$$\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}\vec{x} = \vec{b}$$

Multiplying a line with a constant is multiplying the matrix-vector equation by a diagonal matrix E where only in the desired line there appears the constant, and otherwise 1,

$$\begin{pmatrix} 1 & 0 \\ 0 & \frac{M_{12}}{M_{22}} \end{pmatrix} \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \vec{x} = \begin{pmatrix} 1 & 0 \\ 0 & \frac{M_{12}}{M_{22}} \end{pmatrix} \vec{b}$$

$$\begin{pmatrix} M_{11} & M_{12} \\ \frac{M_{21}M_{12}}{M_{22}} & M_{12} \end{pmatrix} \vec{x} = \begin{pmatrix} b_1 \\ \frac{M_{12}}{M_{22}}b_2 \end{pmatrix}$$

Removing now the term in the second line, i. e. subtracting the first and second line to create a new second line, is achieved by a tridiagonal matrix T, just like in (6.12),

$$\begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} M_{11} & M_{12} \\ \frac{M_{21}M_{12}}{M_{22}} & M_{12} \end{pmatrix} \vec{x} = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} b_1 \\ \frac{M_{11}}{M_{22}}b_2 \end{pmatrix}$$

$$\begin{pmatrix} M_{11} & M_{12} \\ \frac{M_{21}M_{12}-M_{11}M_{22}}{M_{22}} & 0 \end{pmatrix} \vec{x} = \begin{pmatrix} b_1 \\ \frac{M_{11}}{M_{22}}b_2 - b_1 \end{pmatrix}$$

Thus, Gauss's elimination procedure is thus equivalent to multiplying the matrix A by a string of either tridiagonal matrices T or diagonal matrices E, especially

$$TEA = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & 0 \end{pmatrix},$$

and thus the resulting matrix is tridiagonal, or of upper/lower (depending on choice) triangular form. Note that this construction shows that this always possible for any matrix. Of course, by redoing in a different order, it is as well possible to obtain

$$f(T_k, E_r)A = C = \begin{pmatrix} C_{11} & C_{12} & ... & C_{1n} \\ 0 & C_{22} & ... & C_{2n} \\ 0 & 0 & \ddots & \vdots \\ 0 & 0 & 0 & C_{nn} \end{pmatrix}.$$

where m and r depend on the matrix in question, and f is a product of these matrices, as needed for the system in question. Once this form has been reached, further adding or subtracting scaled lines will finally bring this matrix to a diagonal form $C' = \mathrm{diag}(C'_{11}, ..., C'_{nn})$ if there are no non-vanishing lines. Otherwise, the form will remain tridiagonal. The maximally reduced form C' of A is also called its reduced step form. If no line vanishes, this can be continued until a unit matrix is reached.

For the present case, the solution to $A\vec{x} = 0$ is $\vec{x} = 0$, this implies necessarily that there is such a string of E and T matrices such that $C' = 1$.

To make progress, note that all matrices E are trivially invertible, since they are diagonal,

$$\mathrm{diag}(E_{11}, ..., E_{nn})^{-1} = \mathrm{diag}\left(\frac{1}{E_{11}}, ..., \frac{1}{E_{nn}}\right),$$

since by construction none of the elements are zero. For the T matrices, this is a little less obvious. It follows from the fact that subtraction is an invertible process. If the first line

is added to the second line in the example, the original status is recovered, i. e. the matrix

$$T^{-1} = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \tag{6.15}$$

is indeed the inverse of T, as can be seen immediately by calculation. The generalization is given by the fact that the matrix elements for a general subtraction/addition matrix of rows a and b is given by $T_{ij} = \delta_{ij} \pm \delta_{ia}\delta_{bj}$ and thus

$$(T^{-1})_{ij}T_{jk} = (\delta_{ik} + \delta_{ib}\delta_{ja})(\delta_{jk} - \delta_{ka}\delta_{jb}) = \delta_{ij} + \delta_{ib}\delta_{ka} - \delta_{ka}\delta_{ib} - \delta_{ib}\delta_{ka}\delta_{ab} = \delta_{ik},$$

and the last term vanishes, because by assumption $a \neq b$.

This also implies that

$$A = f(T_k, E_r)^{-1}1,$$

since the inverse of f, being a product of T and E matrices, exists. However, if A can be written in this form, then it is necessarily invertible, as the right-hand-side, by construction, is. Since the invertibility has only be used by concluding that an invertible matrix has as a solution to (6.14) only the trivial solution, but not otherwise, this creates a ring of implications: If any of the conditions

- A is invertible

- $A\vec{x} = \vec{0}$ has only the trivial solution $\vec{x} = \vec{0}$

- There is some $f(T, E)$ such that $f(T, E)A = 1$

- A can be written as some $A = f(T, E)^{-1}1$

is true all other ones follow.

The only remaining step is now to show that if $\det A \neq 0$ but A cannot be written only as a string of T and E matrices, then it is still invertible, using that E is (tridiagonal) and T are diagonal, and their determinants are non-vanishing. Now, if $\det A \neq 0$, this implies that its reduced step form has a non-vanishing determinant, since

$$\det A = \det f(T, R)B = \det f(T, R) \det B,$$

and the determinant of f is non-zero, because it is a product of matrices with non-vanishing determinants. Thus, $\det B$ must be non-vanishing. But, as shown, either one or more rows of B vanish, or B is the unit matrix, and thus A invertible. But if a row of B vanishes, then its determinant vanishes, in contradiction to the fact that $\det A$ does not vanish. Thus, B must be the unit matrix, and thus by virtue of the previous statement A must be invertible. Thus for any invertible matrix A the determinant is non-vanishing, and it can always be reduced to the unit matrix.

Since the last statement is actually an equivalence, the statement (6.13) is actually no longer necessary. This permits to provide an independent proof of $\det AB = \det A \det B$. If A is not invertible, then neither is AB, even if B is, since

$$X^{-1}AB = 1 \rightarrow X^{-1}A = B^{-1} \rightarrow A = XB^{-1} = (B^{-1}X)^{-1},$$

which contradicts the assumption. But then $\det AB = 0 = \det A \det B$ because $\det A$ is zero as well. If neither A nor B is invertible, then neither is AB, as the inverse of AB is necessarily $B^{-1}A^{-1}$. Then this reduces to $0 = 0$.

If both matrices are invertible, then either can be written as a product of E and T matrices,

$$\det AB = \det f(T, E)B,$$

However, multiplication of B by an E matrix just multiplies a single column by a factor, which therefore can be outside the determinant. A matrix T however is tridiagonal with ones on the diagonal, and therefore has determinant 1. Especially $\det A = \det f(T, E) = E_1...E_m$ for some value of m, and thus

$$\det AB = \det f(T, E)B = E_1...E_m \det B = \det A \det B,$$

completing the proof.

6.6 Similarity transformations

Many of the previous manipulations of matrix-vector equations can now be put into a larger perspective. Consider a matrix A. A similarity transformation of a matrix is then defined in the following way. For any given invertible matrix S, form

$$A' = SAS^{-1}$$

where A' is then called the similarly transformed matrix. Note that the unit matrix does not change under a similarity transformation. In fact, this is true for any matrix proportional to the unit matrix, $D = \mathrm{diag}\, d = d1$, as such matrices commute with any other matrix B, $DB = BD$, and thus

$$SDS^{-1} = SS^{-1}D = D.$$

Whether the inverse matrix is on the right or left does not matter. Since the matrix is invertible, it is possible to choose the inverse and obtain the other version. It is hence a matter of convention. The only important thing is that once a convention has been chosen, it is kept.

A similarity transformation is invertible, as

$$A = 1A1 = S^{-1}SAS^{-1}S = S^{-1}A'S.$$

However, the inversion has the opposite order of inverse matrix and matrix. This once more emphasizes that any convention chosen must be kept. If the alternative convention would have been chosen, the order in the inverse similarity transformation would also be reversed.

It is noteworthy that both the trace and the determinant are invariant under similarity transformations. For the trace this follows from the cyclicity under matrix multiplication,

$$\mathrm{tr} SAS^{-1} = \mathrm{tr} S^{-1}SA = \mathrm{tr} AS^{-1}S = \mathrm{tr} A.$$

For the determinant it follows from the factorization of products of matrices and the fact that the determinant of an inverse of a matrix is the inverse determinant,

$$\det SAS^{-1} = \det S \det A \det S^{-1} = \frac{\det S}{\det S} \det A = \det A,$$

where $\det S \neq 0$ because S is invertible.

Coming back to matrix-vector equations, similarity transformations can be used to rephrase the manipulations done beforehand. Consider

$$A\vec{x} = \vec{b} \rightarrow SAS^{-1}S\vec{x} = S\vec{b}.$$

Thus, the system of equation is transformed by a similarity transformation. But since S is known, this can be reversed.

The interesting question arising is, whether there exist similarity transformations which make the system of equations particularly simple. This may seem like a superfluous question, as it has been seen that, at least for invertible matrices A, it is just necessary to invert A to find the solution by

$$\vec{x} = A^{-1}\vec{b}.$$

There are two reasons why this is not sufficient. One is that for non-invertible matrices this will not help. The other is that in practice inverting a matrix is not a simple exercise. Especially, so far the only procedure how to do this is finding the sequence of E and T matrices required to solve the system, but then the quest for the inverse of A has become irrelevant. Thus, the question remains, whether there is a simpler way. Sometimes there is. To understand how requires first to learn more about matrices, especially square matrices.

Chapter 7

Eigenvalues and eigenvectors

7.1 The eigenproblem

So far, matrices have mainly been regarded as a convenient way to describe a system of linear equations. But this is not necessary. Matrices can also be considered as stand-alone entities. They are then $n \times m$ schemes of numbers. They can therefore be considered also as linear operators mapping a vector from an m-dimensional space to an n-dimensional space,

$$A : \mathbb{R}^m \to \mathbb{R}^n,$$

or, of course, also for complex spaces.

But then, linear operations usually have objects on which they trivially act. For matrices, this can only be the case for square matrices. It is hence a meaningful question whether there are vectors $\vec{v}_i^A$ and numbers λ_i^A for some $n \times n$ matrix A with the property

$$A\vec{v}_i^A = \lambda_i^A \vec{v}_i^A,$$

where no summation is implied. Of course, different matrices will have different such vectors. If such vectors exist, they are called eigenvectors. The constant of proportionality is called the corresponding eigenvalue. Geometrically, this implies that A acts on its eigenvectors as if it would be the unit matrix multiplied by the corresponding eigenvalue. In the ordinary $\mathbb{R}^n$, this is then an elongation or a shortening of the eigenvector, depending on whether the eigenvalue is larger than one or smaller than one, respectively.

As an example, consider the matrix

$$A = \begin{pmatrix} 2 & 1 \\ 1 & \frac{1}{2} \end{pmatrix}. \tag{7.1}$$

Explicit calculation shows

$$\begin{pmatrix} 2 & 1 \\ 1 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 2 \\ 1 \end{pmatrix} = \begin{pmatrix} 5 \\ \frac{5}{2} \end{pmatrix} = \frac{5}{2} \begin{pmatrix} 2 \\ 1 \end{pmatrix},$$

and thus the eigenvalue to the eigenvector $(2,1)^T$ of this matrix is $5/2$. In addition

$$\begin{pmatrix} 2 & 1 \\ 1 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} -\frac{1}{2} \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} = 0 \begin{pmatrix} -\frac{1}{2} \\ 1 \end{pmatrix},$$

and thus the matrix has a second eigenvalue 0 with eigenvector $(-1/2, 1)^T$. This exhausts the possibilities.

Systems of eigenvectors retain the property,

$$A(a\vec{v}_i^A + b\vec{v}_j^A) = \lambda_i^A a\vec{v}_i^A + \lambda_j^S b\vec{v}_j^A. \tag{7.2}$$

Thus, if in a linear system of equations it would be possible to decompose the vector $\vec{b}$ on the right-hand side into eigenvectors, and the eigenvalues are known, this could be immediately used to calculate the solution. Since if

$$\vec{b} = \sum_i a_i \vec{v}_i^A$$

then

$$A \sum_i \frac{a_i}{\lambda_i^A} \vec{v}_i^A = \sum_i a_i \vec{v}_i^A,$$

and therefore knowledge of $\vec{b}$ in this form yields knowledge of $\vec{x}$. This type of manipulations is actually one of the mainstays of tools in quantum physics. In fact, eventually the eigenvalues and eigenvectors will become much more important than either the matrix or any kind of system of linear equations. However, for it to work it requires to answer the following questions: How many eigenvectors are there and which kind of vectors can be decomposed into them? What are the eigenvalues? Are there zero eigenvalues? This is the so-called eigenproblem. Finding the answers to these questions will be done in the following, and it will turn out that the operation of determinant will again play a central role.

Note that trivially $\vec{0}$ appears to be an eigenvector to any eigenvalue, but to be precise an eigenvector is a vector for a fixed eigenvalue, and therefore $\vec{0}$ is not an eigenvector.

7.2 Characteristic equation and the eigenvalue problem

The first thing to note is that the maximum number of eigenvectors cannot be larger than n, since this is the maximum number of linearly independent vectors in the vector space. If there are n linearly independent eigenvectors, this would form a basis of the vector space in question, and any further eigenvector could be decomposed into it, along the lines of (7.2).

It turns out that to proceed it is actually easier to first determine the eigenvalues, and the eigenvectors then only in a second step. For brevity, from now on the superscript A will be suppressed on both the eigenvector and the eigenvalue, as it will always be clear from context to which matrix they belong.

Assume that λ is an eigenvalue and $\vec{v}_\lambda \neq \vec{0}$ the associated eigenvector for some fixed matrix A. Then

$$A\vec{v}_\lambda = \lambda\vec{v}_\lambda \rightarrow (A - \lambda\mathbb{1})\vec{v}_\lambda = 0.$$

Thus the eigenvector $\vec{v}$ is the solution to this linear equation. However, if $A - \lambda 1$ is invertible, then, according to section 6.5, the only solution to this equation is $\vec{v}_\lambda = \vec{0}$, in contradiction to the requirement that $\vec{v}_\lambda$ is an eigenvector. Thus, $A - \lambda 1$ may not be invertible. If it is for all values of λ, this matrix has no eigenvalues and no eigenvectors, which is the case, e. g., for the zero matrix, as $\lambda 1$ is invertible for any value $\lambda \neq 0$.

Looking for non-trivial solutions thus requires $A - \lambda 1$ to be not invertible. As shown in section 6.5, this implies

$$\det(A - \lambda 1) = 0. \tag{7.3}$$

Hence, finding the eigenvalues corresponds to finding the solution to this equation. It is therefore called the characteristic equation of the matrix A.

The next step is to obtain the explicit form of the characteristic equation. This requires to determine

$$\det \begin{pmatrix} A_{11} - \lambda & A_{12} & ... & A_{1n} \\ A_{21} & A_{22} - \lambda & ... & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & ... & A_{nn} - \lambda \end{pmatrix}. \tag{7.4}$$

Using the form (6.9) to calculate the determinant, it is helpful to always develop with respect to the first row. Then in every reduced determinant the element with the subtracted eigenvalue appears exactly once. Therefore, the characteristic equation is a polynomial of order n in λ. E. g. for $n = 2$ the characteristic equation takes the form

$$\begin{aligned} \det \begin{pmatrix} A_{11} - \lambda & A_{12} \\ A_{21} & A_{22} - \lambda \end{pmatrix} &= (A_{11} - \lambda)(A_{22} - \lambda) - A_{12}A_{21} \\ &= \lambda^2 - \lambda(A_{11} + A_{22}) + A_{11}A_{22} - A_{12}A_{21} = 0, \end{aligned} \tag{7.5}$$

and thus is a polynomial equation of order 2 in λ.

The solutions to this equation are

$$\lambda_{1,2} = -\frac{1}{2}\left(A_{11} + A_{22} \pm \sqrt{(A_{11} + A_{22})^2 - 4(A_{11}A_{22} - A_{12}A_{21})} \right)$$

This result has a number of immediate implications.

If the field of the vector space is real, the eigenvalues must also be real. Thus, there are 2, 1 or no solution to the characteristic equation (7.5). Correspondingly, there are 0 or 2 eigenvalues. There is also the special case of apparently one eigenvalue, if the square-root is zero. However, this is only the case that the eigenvalue appears twice. Because, provided there are solutions to (7.3), the equation can be rewritten as

$$\det \begin{pmatrix} A_{11} - \lambda & A_{12} \\ A_{21} & A_{22} - \lambda \end{pmatrix} = (\lambda - \lambda_1)(\lambda - \lambda_2) = 0$$

as this is precisely the form which an order 2 polynomial can have, for suitable choices of $\lambda_{1,2}$. In the degenerate case, this becomes $(\lambda - \lambda_1)^2$, thus showing that the eigenvalue appears twice. This is also called a degenerate eigenvalue or that the eigenvalue has degeneracy two.

The situation is radically different if the field is complex. As then the square-root of any number exists, there are always two eigenvalues. There can be either two different real eigenvalues, two degenerate real eigenvalues, or, if all coefficients in the polynomial are real, two conjugate complex eigenvalues. That they need to be complex conjugated can be seen for this case by explicit calculation and decomposing the matrix entries into their real and imaginary part, though this is tedious. Otherwise, i. e. already if any coefficients are complex, the result can be any two complex numbers, not necessarily complex conjugated to each other.

In the general case, this will be a polynomial of order n. There is a theorem in algebra, proven in the lecture on advanced mathematics, that states that such a polynomial equation for complex numbers has exactly n solutions, or roots, of which the complex ones appear pairwise as complex conjugated pairs if the coefficients are all real. Note that if n is odd, this implies necessarily that there is one real root, and thus one real eigenvalue, if the coefficients are real. If they are complex, not even this is guaranteed.

Thus, if there exists at least one eigenvalue, the characteristic polynomial can always be rewritten as

$$P(\lambda) = (\lambda - \lambda_1)^{\mu_1}...(\lambda - \lambda_m)^{\mu_m} \tag{7.6}$$

for the m distinct eigenvalues λ_i, which are of algebraic multiplicities $1 \leq \mu_i \leq n$ such that

$$\sum_i \mu_i = n$$

for a complex vector space and

$$0 < \sum_i \mu_i \leq n$$

for a real vector space. Though this implies that there are always n, not necessarily distinct, eigenvalues for the complex case, in the real case there may be anything from 0 to n eigenvalues. Actually calculating them is a problem of algebra, and not necessarily entirely trivial, but can be algorithmitized. This will not be detailed further here. Of course, since only zeros are searched for, any overall factor of the characteristic polynomial is irrelevant.

If in the real case less real roots than possible exists, it is possible to show that the characteristic polynomial can be decomposed as

$$P(\lambda) = ...(\lambda - \lambda_i)^{\mu_i}...(\lambda^2 + a_j\lambda + b_j)^{\mu_j}...$$

and thus it is at least possible to break it down into factors of implicit quadratic equations, which do not have real solutions. That is a consequence of (7.6): It is always possible to still find all complex roots, but any pair of complex conjugate roots can be combined to yield such a quadratic factor. The algebraic multiplicities of these factors is hence always even. Since for this case the coefficients are always real, the complex solutions are always conjugate pairs.

As an example, consider the matrix (7.1). Its characteristic polynomial is

$$\det \begin{pmatrix} 2 - \lambda & 1 \\ 1 & \frac{1}{2} - \lambda \end{pmatrix} = (2 - \lambda)\left(\frac{1}{2} - \lambda\right) - 1 = \lambda^2 - \frac{5}{2}\lambda = \lambda\left(\lambda - \frac{5}{2}\right) = 0$$

and the two eigenvalues 0 and 5/2 can be read off directly in the last step. Both are of algebraic multiplicity one.

7.3   Eigenvectors

Once the eigenvalues are known, the next question is how to determine the eigenvectors $\vec{v}_i$ of

$$A\vec{v}_i = \lambda_i \vec{v}_i. \tag{7.7}$$

These are again systems of linear equations, and the problem can therefore be tackled with the methods described in section 6.2. For an arbitrary matrix, there is no general procedure how these eigenvectors can be computed, and therefore in general indeed the corresponding set of linear equations has to be solved for every eigenvalue separately.

Note that because the eigenvector equation is invariant under multiplication by a constant, the norm of the eigenvectors, as far as defined in the vector space at hand, is not determined by the eigenvector equation. Therefore, the results are often conventionally normalized to one, but this is not necessary. This also implies that the equation (7.7) is necessarily an underdetermined set of linear equations.

Consider again the matrix (7.1). The eigenvector equation for the eigenvalue 0 is

$$\begin{pmatrix} 2 & 1 \\ 1 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 2x + y \\ x + \frac{y}{2} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Both coefficient equations are proportional to each other, which stems from the arbitrary normalization. The solution is thus $y = -2x$, yielding for $x = -1/2$ $y = 1$, and thus the known solution. Likewise

$$\begin{pmatrix} 2x + y \\ x + \frac{y}{2} \end{pmatrix} = \begin{pmatrix} \frac{5x}{2} \\ \frac{5y}{2} \end{pmatrix}$$

gives two equations proportional to each other, and which read $y = x/2$. Selecting $x = 2$ yields $y = 1$, and thus the solution found above.

While eigenvectors play an important role in physics, mathematically they are rather straightforward. An interesting concept derived from them is the classification of the eigenvectors in form of the so-called eigenspaces.

7.4   Subspaces created by a matrix

The effect a matrix has on the vectors in a vector space is classified by the (sub)spaces the matrix generates. These are the eigenspaces, image, kernel, and cohomology of a matrix. Later also other such spaces may arise. Note that while there is some connection between these spaces, they are independently defined concepts, which do not rely on each other.

7.4.1 Eigenspace

An eigenspace is the space which is spanned by the eigenvectors to a fixed eigenvalue. Given a fixed eigenvalue, there are two basic possibilities. Either its algebraic multiplicity is one. Then there is one eigenvector, and the corresponding eigenspace is one-dimensional. If the algebraic multiplicity is larger than one, there can be more eigenvectors, but there do not need to be more than one. This will manifest itself by finding as solution to (7.7) less (linearly independent) solutions than the algebraic multiplicity of the eigenvalue.

Take as an (almost trivial) example the matrix

$$M = \begin{pmatrix} 2 & 0 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{7.8}$$

This matrix has eigenvalue 1 with algebraic multiplicity one and 2 with algebraic multiplicity two. The eigenvector to the eigenvalue 1 is $(0,0,1)^T$. However, there is only one solution the eigenvector equation for $\lambda = 2$, $(0,1,0)^T$. Thus, also the eigenspace to the eigenvalue 2 is also an one-dimensional space.

To characterize the situation, the concept of geometric multiplicity γ_i is introduced, which denotes the dimensionality of the eigenspace of a fixed eigenvalue λ_i. In this case, the geometric multiplicities for both eigenvalues are one. It is surprisingly non-trivial to show that $\gamma_i \leq \mu_i$, i. e. for every eigenvalue there can be no more linearly different eigenvectors than its algebraic multiplicity. Also, by construction, the eigenspaces to different eigenvalues are different, and thus eigenvectors to a fixed eigenvalue are always linearly independent from all eigenvectors to different eigenvalues. The proof will be skipped here.

The sum of the geometric multiplicities obeys

$$\sum_{i=1}^{m} \gamma_i = n' \leq \sum_{i=1}^{m} \mu_i \leq n, \tag{7.9}$$

where m is the number of distinct eigenvalues. This implies that if $n' = n$ the eigenvectors of the matrix are n linearly independent vectors, and therefore form a (not necessarily orthonormal) basis of the vector space. It is important to note that this is a necessary and sufficient condition.

Of course, if the sum of algebraic multiplicities is smaller than n, i. e. for a real vector space there are not n eigenvalues, always $n' < n$. The concept of eigenspaces gives rise to a number of different definitions.

If an eigenspace to an eigenvalue λ_j has dimension greater than one, any linear combination of eigenvectors $\vec{v}_j^i$ inside this eigenspace is again an eigenvector. Here, the index i of $\vec{v}_j^i$ counts the number of dimensions of the eigenspace, and thus runs from 1 to γ_j. This follows as

$$A \sum_i \left(a_i \vec{v}_j^i \right) = \sum_i \left(a_i A \vec{v}_j^i \right) = \sum_i \left(a_i \lambda_j \vec{v}_j^i \right) = \lambda_j \left(\sum_i a_i \vec{v}_j^i \right),$$

where no summation is implied. From this follows that any choice of basis within an eigenspace is made up from eigenvectors. This can be frequently used to simplify calculations.

7.4.2 Image

The image $\mathcal{I}$ of a matrix A is the set of vectors $\{\vec{b}\}$ obtained by acting on all vectors $\vec{a}$ of the vector space by the matrix,

$$\mathcal{I} = \left\{\vec{b} \,\middle|\, A\vec{a} = \vec{b} \forall \vec{a}\right\}.$$

This space can be much smaller than the vector space, and at most be identical to the vector space. The dimension of the image is called the rank of the matrix.

The extreme case is the zero matrix, for which the image is just the zero-vector, and thus is zero-dimensional. If the eigenvectors form a full basis of the vector space, the image is automatically the full vector space. This is hence a sufficient, but not necessary, condition. E. g., the unit matrix, or any matrix proportional to it, has the full vector space as image. The example (7.1) has also the full vector space as image. But for the example (7.8) this would a separate investigation, as the sum of geometric multiplicities is smaller than the dimensionality of the vector space.

Note that the image of the transposed matrix is the same as for the original matrix, since

$$(A\vec{a})^T = \vec{a}^T A^T = \vec{b}^T,$$

and if the $\vec{b}$ are linearly independent, then so are the $\vec{b}^T$. Likewise, the entire eigenproblem for the transposed matrix is trivially connected to the one of the original matrix.

It should be noted that the rank may be different from the number of linearly independent eigenvectors, and thus the sum of the geometric multiplicities (7.9). E. g. if the matrix has one or more vanishing eigenvalues, the corresponding eigenvectors are mapped to the zero vector, and therefore cannot contribute to the dimensionality of the image. The same is, of course, true if there are less eigenvalues (for real spaces) than there are dimensions.

7.4.3 Kernel

A matrix can map some vectors to the zero vector,

$$A\vec{a} = \vec{0}, \tag{7.10}$$

even if it is not the zero matrix. An example is given by $m = \text{diag}(1,0)$, which maps the vectors $(0,c)^T$ for any c to the zero matrix. This is quite different from scalar/matrix multiplication, were this can only happen if either of the involved quantities is zero.

This situation plays an important role in many cases in physics, and the set of vectors $\vec{v}$ satisfying (7.10) is called the kernel $\mathcal{K}$ of the matrix,

$$\mathcal{K} = \left\{\vec{a} \,\middle|\, A\vec{a} = \vec{0}\right\}.$$

Its dimension is sometimes called the defect of the matrix.

There is an important relation between the rank and the defect of the matrix: The sum of rank and defect is n, the number of dimensions of the space. This can be seen as follows. The kernel condition (7.10) is a homogeneous system of linear equations. As discussed in section 6.5, a system of linear equations can be manipulated by matrix multiplications. But the zero vector is invariant under matrix multiplications. Thus, at some point, the equations have been transformed such that there must be the same number of trivial equations of type $0 = 0$ as the defect of the matrix - in a suitable basis the kernel will be spanned by a set of vectors with only entries in a number of dimensions equal to the defect.

But then the remainder of the equations are just parameterized by the components v_i, and therefore parameterize a defect-dimensional set of solutions, as by assumption the remaining equations are no longer trivial. Thus, the remaining equations are mapped to an (n-defect)-dimensional system of inhomogeneous equations. But by assumption, this reduced set is not part of the kernel, and therefore cannot have a non-trivial solution to (7.10). Thus, this reduced matrix is by construction invertible, and there is thus a non-trivial solution for any base-vector of the remaining space, and therefore this is just the image of the matrix of dimension rank, completing the statement.

Note that for non-square matrices, the number of independent vectors which can be produced and on which it can act can be not larger than the smaller of its dimension. Thus, the sum of defect and rank will in this case always yield the smaller of the two numbers.

It is noteworthy that because an invertible matrix has only trivial solutions to (7.10), according to section 6.5, its defect is always zero, and its rank always n. Furthermore, this implies that a matrix with non-zero defect has a determinant of zero. Note, however, that a matrix with determinant zero does not need to have a non-zero defect. E. g. (7.1) has determinant zero, but has defect zero.

7.4.4 Cohomology

An interesting construction, though of no immediate use in this lecture, is the so-called cohomology $\mathcal{C}$ of a matrix. It is defined as the sub-space of the kernel of the matrix from which the image is removed

$$\mathcal{C} = \left\{ \vec{c} \,\middle|\, A\vec{c} = \vec{0} \text{ and } A\vec{a} \neq \vec{c} \,\forall\, \vec{a} \right\}. \tag{7.11}$$

This implies that only non-invertible matrices can have a non-trivial cohomology, as a non-zero defect is required.

An example is given by the matrix

$$M = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

It acts like

$$M(a\vec{e}_1 + b\vec{e}_2 + c\vec{e}_3) = b\vec{e}_1$$

Its kernel is thus given by

$$\mathcal{K} = \{a\vec{e}_1 + c\vec{e}_3\}$$

and its image by

$$\mathcal{I} = \{b\vec{e}_1\}.$$

Thus, its cohomology is

$$\mathcal{C} = \{a\vec{e}_3\},$$

as the $\vec{e}_1$ ray is both in the kernel and the image. So its need to be removed from the kernel, leaving only the $\vec{e}_3$ ray.

7.4.5 Injective, surjective, and onto

These concepts can also be used to define certain properties of general operators, or maps, which are exemplified by matrices.

A map $f : x \to y$ is defined to be injective, if $x_1 \neq x_2$ implies $f(x_1) \neq f(x_2)$. It maps different sources to different targets. Many matrices can be not injective. E. g. a matrix with non-trivial kernel is not injective, as multiple source vectors are mapped to the same target vector, $\vec{0}$.

A map $f : x \to y$ is defined to be surjective, or onto, if for every y there exists some x such that $f(x) = y$. E. g. any diagonal matrix with non-zero entries is surjective. Also the non-rectangular matrix (1 0) is surjective, as there is for all of the one-dimensional target vectors there is one (actually infinitely many) two-dimensional source vectors.

A map $f : x \to y$ is bijective, if it is both injective and surjective, that is every element of the domain is mapped to one and only one element in the image, and there is hence a one-to-one correspondence. In particular, this implies there is an inverse map. Square, invertible matrices with rank equal the dimension, which therefore maps the whole vector space invertible into itself, are of this type. Note that this requires that the same number of source objects and target objects exists, and thus only invertible, square matrices can be bijective.

7.5 Diagonalization

The eigenvectors permit some rather strong statements about matrices. Especially, if the there are as many linearly independent eigenvectors as there are dimensions, i. e. if in (7.9) it is equality and the eigenvectors form a basis.

The first is about whether a matrix can be made diagonal by a similarity transformation, a process called diagonalization. Diagonalization is a two-step process, starting out from the concept of a similarity transformation, as discussed in section 6.6. Then the diagonalization of a matrix M is defined to be a similarity transformation using a matrix S such that the result is a diagonal matrix,

$$SMS^{-1} = \text{diag}(m'_{11}...m'_{nn}) = M'.$$

At this time, it is not yet clear, whether this is possible. To see why this is important, note that for any eigenvector $\vec{v}$

$$SMS^{-1}S\vec{v} = \lambda S\vec{v} = \text{diag}(m'_{11}...m'_{nn})\vec{v}' = \lambda\vec{v}' = \lambda S\vec{v}.$$

Thus, the diagonal form of the matrix has much simpler relations to its eigenvalues: The Cartesian basis forms now necessarily the set of transformed eigenvectors $\vec{v}'$ with eigenvalues the diagonal entries m_{ii}, and thus λ necessarily equals one of those. It is therefore desirable to get information about when such a diagonalization is possible. This would allow to circumvent the necessity to find the roots of a polynomial. It will then be seen that there are even more properties, which can be deduced from diagonalizability, some of which are quite powerful statements.

For now, consider only matrices with a full set of linearly independent eigenvectors. The case of matrices where the sum of the geometric multiplicities is less than the dimension of the vector space will be considered in the section 7.6. Then the eigenvectors are all linearly independent. Define a matrix S^{-1} as[1]

$$S^{-1}_{ij} = (\vec{v}_i)_j,$$

where $\vec{v}_i$ is the eigenvector to a the eigenvalue λ_i. If some geometric multiplicities are non-zero, the different eigenvectors would need a further index to enumerate them. This is left implicit, but could be understood to be part of the index i. Assume further that the eigenvectors are normalized to unity, though this is not necessary, but convenient.

This matrix has the property to be invertible. This follows from the fact that the homogeneous system

$$(S^{-1}\vec{x})_i = (\vec{v}_i)^T\vec{x} = (\vec{0})_i$$

can have only the trivial solution, since the vectors $\vec{v}_i$ are linearly independent by assumption, and this is just a linear combination of them. As shown in section 6.5 this implies that S^{-1} is invertible.

This implies

$$(MS^{-1})_{ik} = \sum_j M_{ij}(\vec{v}_j)_k = \lambda_k(\vec{v}_i)_k, \tag{7.12}$$

where no summation is implied. This is the matrix S^{-1} with every column multiplied by its eigenvalue. When multiplying with the inverse, the presence of a common factor in a column does not matter. If

$$(S)_{ij}S^{-1}_{jk} = \delta_{ik}$$

then

$$(SMS^{-1})_{ik} = \sum_j (S)_{ij}\lambda_k S^{-1}_{jk} = \lambda_k\delta_{ik},$$

---

[1]That here the inverse of S appears is due to the chosen convention, and that first the matrix to the right should be determined. At the moment, this is just a label, and not yet it is implied that the so constructed matrix is indeed invertible.

where again no summation is implied. Thus, the similarity transformation yields a diagonal matrix with the eigenvalue of the original matrix as diagonal elements

$$SMS^{-1} = \mathrm{diag}(\lambda_1, ..., \lambda_n).$$

The result for this particular similarity transformation is hence especially simple. This also implies that $S\vec{v}^i$ is necessarily a vector with only an element in the ith component to remain an eigenvector to the same eigenvalue. Thus, this particular similarity transformation also transforms the system of eigenvectors into an orthonormal basis of the same form as the Cartesian basis.

   This new basis is also called the eigendecomposition of the matrix at hand. Note that it was not necessary that the matrix M itself is invertible, and thus to have only non-zero eigenvalues. Diaganolizability and invertibility are two distinct concepts, and should not be mixed. Many physically relevant systems in 8quantum) physics in involve diagonalizable but not invertible matrices. An important aside of this result is that this implies that the determinant of such a matrix is the product of the eigenvalues while the trace is the sum of it, as both are invariant under similarity transformations. This feature is exploited in physics, as sometimes only this sum or product is needed. It is then not necessary to determine the actual eigenvalues.

   As an example, consider the matrix

$$M = \begin{pmatrix} 1 & -1 \\ 0 & 0 \end{pmatrix},$$

which has determinant zero and eigenvalues zero and one. It has determinant zero and is thus not invertible. Its eigenvectors are $(1,0)^T$ and $(1,1)^T/\sqrt{2}$. Thus, the sum of geometric multiplicities is 2, the dimension of the vector space. The matrix is thus diagonalizable. These eigenvectors which can be used to diagonalize the matrix:

$$
\begin{aligned}
S^{-1} &= \begin{pmatrix} 1 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \\
S &= \begin{pmatrix} 1 & -1 \\ 0 & \sqrt{2} \end{pmatrix} \\
SMS^{-1} &= S \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.
\end{aligned}
$$

The eigenvalues can be read off, and are 0 and 1, each with algebraic multiplicity one.

7.6   Jordan normal form

If a matrix has a true lesser in (7.9) it is not possible to bring it into diagonal form. However, it is possible to bring a $N \times N$ matrix still into a simpler form, the so-called Jordan normal form.

This form is defined to be block-diagonal, i. e.

$$
S^{-1}AS = J = \begin{pmatrix} J_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & J_M \end{pmatrix} \tag{7.13}
$$

where only the $M < N$ Jordan blocks J_i have non-zero entries. Note that if $N = M$, the matrix would be diagonal. Of course, if $M = 1$, then the Jordan normal form is just the original matrix. Furthermore, the Jordan blocks J_i for complex spaces have the form

$$
J_i = \begin{pmatrix} \lambda_i & 1 & 0 & \dots & 0 \\ 0 & \lambda_i & 1 & \dots & 0 \\ 0 & 0 & \ddots & \ddots & 1 \\ 0 & 0 & \dots & 0 & \lambda_i \end{pmatrix} \tag{7.14}
$$

I. e. it has the eigenvalue on the diagonal, and the next diagonal above has ones (or below, this does not matter and is a choice of convention).

If for real vector-spaces also the algebraic multiplicities do not add up to the dimension of the space, it is still possible to form blocks

$$
J_i = \begin{pmatrix} a_i & b_i & 0 & 0 & \dots \\ -b_i & a_i & 1 & 0 & \dots \\ 0 & 0 & a_i & b_i & \dots \\ 0 & 0 & \ddots & \ddots & \vdots \end{pmatrix}.
$$

where the 2×2 blocks are repeated correspondingly often. Though suggestive, it is not necessary that every block belongs to different eigenvalues. But it is possible.

At any rate, to determine the Jordan normal form, and the corresponding similarity transformation, it is first required, as in case of the diagonalization, to determine all eigenvalues and eigenvectors. Also, for every Jordan block it will be necessary to determine its respective kernel and image. So, assume that all eigenvalues and eigenvectors of A are known.

Since the following is quite involved, it is useful to track every step with an explicit example. Consider to this end the matrix

$$
A = \begin{pmatrix} \frac{5}{3} & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{18}} \\ \frac{1}{\sqrt{6}} & \frac{1}{2} & \frac{1}{2\sqrt{3}} \\ -\frac{1}{\sqrt{18}} & -\frac{1}{\sqrt{12}} & \frac{11}{6} \end{pmatrix}. \tag{7.15}
$$

This matrix has eigenvalues 1 and 2 with algebraic multiplicities 2 and 1, respectively. Its (normalized) eigenvalues areas

$$
\vec{v}_2 = \begin{pmatrix} -\frac{1}{\sqrt{3}} \\ 0 \\ \sqrt{\frac{2}{3}} \end{pmatrix} \qquad \vec{v}_1 = \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{pmatrix}, \tag{7.16}
$$

showing that each eigenvector has geometric multiplicity one. Thus, the matrix is not diagonalizable, and thus a candidate for the Jordan normal form. Note that its determinant is 2, and it remains thus an invertible matrix.

It can now be shown that there are exactly as many Jordan blocks as there are linearly independent eigenvectors. To see this, it is best to construct explicitly the required matrix S to perform the similarity transformation to the Jordan normal form. Thus, assume the Jordan normal form J is known. Then, for a base vectors $\vec{e}_i$ holds

$$AS\vec{e}_i = SJ\vec{e}_i$$

Because of the block-diagonal form, $J\vec{e}_i$ will have only components within the subspace of the Jordan block in which $\vec{e}_i$ is.

In the example, the Jordan block form will be necessarily

$$J = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

In the end, the matrix

$$S = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\frac{\sqrt{2}}{\sqrt{3}} \end{pmatrix} \tag{7.17}$$

will do the transformation. Choosing a Cartesian basis, this yields, e. g.

$$AS\vec{e}_1 = \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{pmatrix} = SJ\vec{e}_1,$$

as asserted.

The trick to determine S is now to see that for S to be invertible, it is necessary that all its row/columns are linearly independent. This is visible in (7.17). It is therefore necessary to somehow upgrade the single eigenvector associated with each block in a unique way to a full subspace which is orthogonal to all subspaces created by the other Jordan blocks.

Assume that there is such a matrix S which needs to have linearly independent rows. Then because $AS = SJ = T$, the action of a Jordan block i of size k induces a set of column vectors in T of type

$$\lambda\vec{s}_a$$
$$\vec{s}_a + \lambda\vec{s}_{a+1}$$
$$\vec{s}_{a+1} + \lambda\vec{s}_{a+2}$$
$$...,$$

a so-called Jordan chain.

In the example, this yields

$$AS = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{3}} & \frac{2}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{6}} & \sqrt{\frac{2}{3}} & -\sqrt{\frac{8}{3}} \end{pmatrix}.$$

In this case the Jordan chain has only two elements,

$$\lambda \vec{s}_1 \;=\; 1 \times \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{pmatrix} \tag{7.18}$$

$$\vec{s}_1 + \lambda \vec{s}_2 \;=\; \begin{pmatrix} \frac{2}{\sqrt{3}} \\ 0 \\ \sqrt{\frac{2}{3}} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{pmatrix} + 1 \times \begin{pmatrix} \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{pmatrix} \tag{7.19}$$

At the same time, this is identical to the action of A on the rows of S. This implies when considering $AS - SJ$ column by column,

$$\begin{aligned} (A - \lambda 1)\vec{s}_a &= 0 \\ (A - \lambda 1)\vec{s}_{a+1} &= \vec{s}_a \\ (A - \lambda 1)\vec{s}_{a+2} &= \vec{s}_{a+1}, \end{aligned}$$

which necessarily implies

$$\begin{aligned} (A - \lambda 1)^2 \vec{s}_{a+1} &= (A - \lambda 1)\vec{s}_a = 0 \\ (A - \lambda 1)^3 \vec{s}_{a+2} &= (A - \lambda 1)^2 \vec{s}_{a+1} = (A - \lambda 1)\vec{s}_a = 0. \end{aligned}$$

Vectors satisfying this properties are called generalized eigenvectors.

For the example, it follows that

$$(A - 1 \times \mathbf{1})\vec{s}_1 \;=\; \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$(A - 1 \times \mathbf{1})\vec{s}_2 \;=\; \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} \end{pmatrix}$$

as required. Thus, (7.18-7.19) are indeed the generalized eigenvectors to eigenvalue 1 of the matrix (7.15).

Hence, to show the existence of an invertible S requires to show that the $\vec{s}_a$ form a complete basis, and therefore S can be inverted. For Jordan blocks of size 1, this is trivial, as this is true for the single eigenvector. To show that this is true in general, perform a proof by induction. For a 1×1 matrix, this is trivial if there is a single eigenvalue, so the

seed is trivial. If there are zero eigenvalues, these form a trivial kernel, for which any base vectors will do, as the base of the kernel of the matrix, so this is also trivial.

Assume that a Jordan normal form has been constructed for everything up to a certain row/column. If the newly added column does not extend an existing block, the new block is a 1×1-block, for which the corresponding base vector will serve the purpose. If it does extend an existing Jordan block, it extends a Jordan chain. Then, by assumption, the intersection of the kernel of $A - \lambda 1$ and the image of the reduced matrix is not empty, and therefore there must exist a vector such that

$$(A - \lambda 1)\vec{q} = \vec{p},$$

where $\vec{p}$ is the lead-element of one of the Jordan chains of the reduced matrix. The vector $\vec{q}$ is not part of the kernel $(A - \lambda 1)$, as it would otherwise vanish. But they must also be linearly independent of the existing vectors, as otherwise they would be in the kernel, a contradiction. Therefore they are linearly independent.

Since in this form all vectors are linearly independent, the $\vec{p}$ by induction assumption, the kernel vector since they are an arbitrary basis, and the new $\vec{q}$ as they are not linearly dependent on the former, this proves the existence of the Jordan normal form in the complex case. Since this gives now a constructive way to determine an invertible S such that (7.13) holds for any matrix A, the general proof has been obtained.

In the real case, this can be reconstructed from the solution in the complex case. Then every set of two complex conjugate eigenvalues is expanded into a 2×2 matrix, which precisely yields the real form of the Jordan normal form.

That this is true can now be seen from the example, since

$$S = \begin{pmatrix} \vec{s}_1 & \vec{s}_2 & \vec{v}_2 \end{pmatrix} \tag{7.20}$$

as can be seen from explicit comparison between (7.17) and (7.16), (7.18), and (7.19). The constructive procedure to determine S is then

1. Determine the eigenvalues and eigenvectors

2. Construct for any eigenvalues with geometric multiplicity less then algebraic multiplicity the generalized eigenvectors, by creating a chain from each linearly independent eigenvector

3. Combine the vectors to form S, which will deliver J.

As J could equally be obtained after step 1 already, the other steps will only be necessary if S is needed. Whether this is the case depends on the problem.

7.7 Matrix powers, roots and exponentials

It is an interesting observation that invertible matrices form a non-Abelian group under the associative matrix multiplication. This follows, as the product of two invertible matrices

A and B is itself invertible, $(AB)^{-1}(AB) = B^{-1}A^{-1}AB = 1 = AB(AB)^{-1}$ and the unit matrix is invertible and acts as the neutral element. This will be discussed in more detail in section 8.8.

As this makes (invertible, square) matrices similar to other groups, like the ordinary real numbers, it is a very interesting question, whether it is possible to also construct further mathematical operations on them. It turns out that the answer to this is positive, and shows interesting relations to the eigenvalue problem.

7.7.1 Matrix roots

The simplest operation is, of course, to construct higher integer powers of matrices, in a straightforward way by performing sequential multiplications.

A much more involved question is whether there is a solution to

$$A^2 = B$$

with B a fixed matrix, i. e. whether there is a square-root of a matrix. Since the 1×1 matrices are just the ordinary numbers, it is clear that there are exceptions if the matrices are real, but what is if it is complex? If such a matrix exist, it is called the root of the matrix B.

The situation is highly involved. Consider the unit matrix. Then

$$\begin{pmatrix} 1 & a \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & a \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & a - a \\ 0 & 1 \end{pmatrix} = 1$$

for any value of a. Thus, in contrast to real or complex numbers a matrix can have an infinite number of roots, even for a real matrix and real roots. In fact, it can be shown that even the zero matrix has non-trivial roots, in great distinction to ordinary numbers. An example is, e. g.

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

This will lead to an interesting concept later in section 8.3.

For diagonal matrices, the situation is comparatively simple, as there at least some solutions are given by taking the roots of the diagonal elements. Especially

$$V^{-1}A^2V = V^{-1}AVV^{-1}AV = V^{-1}BV$$

implies that diagonalizing a matrix, performing the square-root, and then returning to the original version will yield the square root. Specifically, if the diagonal elements are distinct, there is no choice, except for the sign. However, if there are degenerate eigenvalues, there is an arbitrariness in the diagonalization procedure, since the transformation can order the diagonal elements arbitrarily by a further base transformation. Hence, there are additional possible ambiguities in comparison to the one-dimensional case.

Hence, a square root of a matrix can be defined, but just like with numbers, this is a multi-valued operations, which can have an infinite number of solutions. Accepting this,

a square root is a meaningful operation. In the same way, it is possible to define higher roots, and calculate them using diagonalization methods.

The calculation of arbitrary powers can then be again constructed as a limiting procedure of integer powers and integer roots, and therefore power-laws of matrices can be calculated, and are meaningful to the same extent this is true for numbers, but can in general yield again an infinite number of possible results.

Non-diagonalizable matrices could still have no square roots. In fact, it turns out that it is non-trivial to show whether a general matrix can have a square root. For 2×2 matrices M, a general sufficient criterion can be constructed: A (possibly complex) square root exists, if

$$\left(\text{tr} M + 2\sqrt{\det M} \right)^2 \neq 0.$$

Of course, there can be more than one. However, if a matrix does not fulfill this condition, it can still have square roots. Thus, taking the root of a non-diagonalizable matrix is a non-trivial problem.

7.7.2 Matrix exponentials

Thus, a power of a matrix is a difficult issue. The situation changes when taking the matrix to be the power, especially in form of the matrix exponential, i. e. exponentiating e by a matrix. The result of this operation will again be a matrix. However, this requires to define what this operation should actually mean.

For this, it is useful that the exponential function can be defined in various ways. Two particular useful definitions valid for numbers, real or complex, are

$$\begin{aligned} \exp(x) &= \lim_{n \to \infty} \left(1 + \frac{x}{n} \right)^n \\ \exp(x) &= \sum_{n=0}^{\infty} \frac{x^n}{n!}, \end{aligned}$$

which will be shown in other lectures.

Both definitions only require to take a positive, integer power and perform addition and multiplication. They can therefore be straightforwardly generalized to matrices, and both provide a definition of a matrix exponential. Especially, since for a diagonal matrix

$$\text{diag}(a_1, ..., a_n)^n = \text{diag}(a_1^n, ..., a_n^n)$$

the definitions imply that the exponential of a diagonal matrix is a diagonal matrix with the entries exponentiated.

This definition can then also be used to define the logarithm of a matrix as the inversion of the exponentiation, if necessary. However, as is the case for real and complex numbers, the existence of a logarithm of a matrix is not guaranteed, and if it exists can be multivalued.

A particular useful consequence of the definition of the exponential is a direct way to evaluate the determinant of an exponentiated matrix where the sum of the algebraic

multiplicities gives the size of the matrix, so that for an $n \times n$ matrix there are n, not necessarily distinct, eigenvalues λ_i. Then

$$e^{\mathrm{tr}A} = e^{\sum_i \lambda_i} = \Pi_i e^{\lambda_i} = \det e^A,$$

where it has been used twice that such a matrix has a Jordan normal form J, but that the necessary similarity transformation S does neither change the trace nor the determinant. This follows because

$$\mathrm{tr}A = \mathrm{tr}SS^{-1}A = \mathrm{tr}S^{-1}AS = \mathrm{tr}J = \sum_i \lambda_i$$

$$\det A = \frac{\det S}{\det S} \det A = \det S \det A \det S^{-1} = \det S^{-1}AS = \det J = \Pi_i \lambda_i$$

and for any Jordan block J_i

$$\mathrm{tr}J_i = \mathrm{tr}\begin{pmatrix} \lambda_i & 1 & 0 & \dots & 0 \\ 0 & \lambda_i & 1 & \dots & 0 \\ 0 & 0 & \ddots & \ddots & 1 \\ 0 & 0 & \dots & 0 & \lambda_i \end{pmatrix} = \lambda_i + \dots + \lambda_i$$

$$\det J_i = \det\begin{pmatrix} \lambda_i & 1 & 0 & \dots & 0 \\ 0 & \lambda_i & 1 & \dots & 0 \\ 0 & 0 & \ddots & \ddots & 1 \\ 0 & 0 & \dots & 0 & \lambda_i \end{pmatrix} = \lambda_i \cdot \dots \cdot \lambda_i,$$

where the determinant has been developed always in the first line.

Chapter 8

Matrix types

As has been seen, matrices have a host of interesting properties. It can be expected that many consequences arise from these properties. Especially, there are particular subtypes of matrices, which are of great relevance in physics, which exhibit combinations of very particular consequences. These form the so-called matrix groups.

8.1 Permutation matrices

The first subclass of matrices are so-called permutation matrices. They are constructed such as to exchange two rows (or columns) k and l of a matrix they are multiplied to. They take the form

$$(P^{kl})_{ij} = \delta_{ij}(1 - \delta_{ik})(1 - \delta_{jl}) + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} + \delta_{ij}\delta_{kl},$$

where no summation is implied. E. g. for $n = 3$ and exchanging the first and second row,

$$P^{12} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{8.1}$$

Thus, this is a unit matrix, where the kth and lth row (or, equivalently columns) are exchanged.

When acting as $P^{kl}M$, the result is a matrix where the lth and kth row of M are interchanged, but otherwise it is M. Likewise, MP^{kl} gives a result where the columns are exchanged.

Such a matrix has the property

$$P^{kl}P^{kl} = 1,$$

i. e. it squares to one. Conversely, any permutation matrices are thus (some of the) roots of the unit matrix. This is intuitively clear, as swapping twice the same rows or columns reproduces the original matrix.

The trace of a permutation matrix of dimension n is $n - 2$, as there are two diagonal elements with entry zero. The determinant of P can only be ± 1, as $(\det P)^2 = \det P^2 = \det 1 = 1$. It has actually determinant -1. This follows, as it is always possible to develop the determinant after the rows and columns such that the reduced matrix is ultimately just

$$P' = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{8.2}$$

which has determinant -1. The other factors are all from a unit matrix, so the total result is -1.

The eigenvalues are also all one, except for one which is minus -1. This can be seen by noting that (8.2) has eigenvalues 1 and -1, but the rest of the matrix is just a unit matrix, which has eigenvalues 1. Similar, the eigenvectors are for all eigenvectors just the base vectors, except for those associated with the submatrix (8.2). For it, the eigenvectors are $(1, -1)^T$ and $(1, 1)^T$. However, these are linearly independent vectors, and therefore the eigenvectors form a full system. The permutation matrix can therefore be diagonalized.

Implicitly, the permutation matrix has been used before when reordering in a system of linear equations the equations, which can be obtained by multiplying the system in matrix-vector form by a suitable permutation matrix.

8.2 Projection matrices

Another important class of matrices are so-called projection matrices. Projection matrices are defined by the fact that their image is a sub-space of the original vector space of lesser dimensions. E. g. the projection matrix

$$P = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \tag{8.3}$$

projects every two-dimensional vector on its x-component, and therefore on a one-dimensional sub-space.

The defining property of projection matrices is that they leave a once-projected vector invariant, i. e.

$$PP\vec{v} = P\vec{v}$$

for any vector $\vec{v}$, or more succinctly as a matrix equation

$$PP = P.$$

Matrices satisfying this property are called idempotent, and projection matrices are examples of such matrices.

Furthermore, there is a second projection matrix

$$P' = 1 - P.$$

which by construction is also idempotent and sums with the original projection matrix to one,

$$
\begin{aligned}
P'P' &= (1-P)(1-P) = 1 - 2P + PP = 1 - 2P + P = 1 - P = P' \\
P' + P &= 1 - P + P = 1.
\end{aligned}
$$

For the example (8.3) it is given by

$$
P' = 1 - P = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.
$$

The subspace into which P' projects is also called the complement of the space into which P projects, since

$$
P'P = (1-P)P = P - PP = 0 = P(1-P) = PP'
$$

and thus a projection by the one and then by the other one results in a zero vector. Hence, the vector $P\vec{v}$ needs to be in the kernel of $P' = (1-P)$.

Projection matrices have necessarily vanishing determinant, since

$$
0 = \det 0 = \det P \det(1-P) = (\det P)^2 (\det(1-P))^2. \tag{8.4}
$$

But the only number squaring to zero is zero itself. This implies that projection matrices cannot be inverted, which is geometrically intuitive: information is lost, and cannot be regained. This implies that there is a non-trivial kernel, which is formed by the vectors belonging to the complement of the projector.

However, the eigenvectors form a full base system, and therefore the projectors can be diagonalized, like in the example (8.3).

The trace of P is not necessarily zero, but it is necessarily positive

$$
\mathrm{tr} P = \mathrm{tr} PP = (P_{ii})^2 \geq 0,
$$

and the sum of the traces of the projector and its orthogonal complement is

$$
\mathrm{tr}(P + (1-P)) = \mathrm{tr} 1 = d,
$$

the number of dimensions. Note that both the unit matrix and the zero matrix are formally also projection matrices, and project to the full space and the null space, and are therefore complements of each other[1].

Note that if $P = P^\dagger$ then the vectors from the projected sub-space and its complement are actually orthogonal to each other, because

$$
((1-P)\vec{v})^\dagger P\vec{v} = (\vec{v})^\dagger (1-P^\dagger) P\vec{v} = 0.
$$

---

[1]The unit matrix has determinant one, but here the associated second matrix $P' = 1 - 1$ is the zero matrix, ensuring (8.4). Thus, in a sense, projection matrices where both the matrix and the associated one have zero determinant can be considered as the proper projection matrices.

The complement is then called an orthogonal complement.

This is not necessary, however. If this is not the case, the space is still separated into two sub-spaces, but the vectors in both sub-spaces still retain a part of the old one. E. g. a possible projection matrix is

$$P = \begin{pmatrix} 1 & i \\ 0 & 0 \end{pmatrix}.$$

It still projects the (complex) vectors only on their first component, and thus on a one-dimensional sub-space. Its orthogonal complement is

$$1 - P = \begin{pmatrix} 0 & -i \\ 0 & 1 \end{pmatrix} \tag{8.5}$$

and projects vectors into another sub-space, and sums by construction to one, but the vectors created are not orthogonal to the previous ones. E. g.

$$\left(\begin{pmatrix} 0 & -i \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right)^{\dagger} \begin{pmatrix} 1 & i \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} -i \\ 1 \end{pmatrix}^{\dagger} \begin{pmatrix} 1+i \\ 0 \end{pmatrix} = i - 1.$$

8.3 Nilpotent matrices

Another subclass of matrices has the strange property

$$SS = 0,$$

but are not the zero-matrix itself. This has already been seen for roots of the zero matrix in section 7.7.

That is a rather strange thing, and requires at least two dimensions. A two-dimensional example is

$$S = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

Matrices with this property are said to be nilpotent. This implies that their determinant vanishes, since $(\det S)^2 = 0$, which again can only be fulfilled by having $\det S = 0$. This implies that they cannot be inverted. Furthermore

$$0 = \text{tr}SS = (s_{ii})^2$$

and therefore for real nilpotent matrices all diagonal elements vanish. For complex ones, this may not be the case.

Note that by construction any vector $\vec{v}$ which is in the image of S creates a vector $\vec{w}$ which is in the kernel of S,

$$S\vec{w} = SS\vec{v} = 0.$$

Thus, the cohomology of nilpotent matrices can be a non-empty set. This is also one of the main consequences relevant in physics applications of nilpotent matrices.

8.4   Symmetric and hermitian matrices

A very important class of matrices in physics are hermitian matrices, which have the defining property

$$H^\dagger = H. \tag{8.6}$$

This property is also called self-adjointness[2]. In finite-dimensional vector space $(H^\dagger)^\dagger = H$ holds.

An example are the famous Pauli matrices,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{8.7}$$

which play an extremely important role throughout quantum physics, and also an important role in some branches of mathematics, especially the general theory of groups. These examples also show that Hermitian matrices can be real, and may or may not have diagonal form.

Furthermore, hermiticity implies

$$(\det H)^* = \det H^\dagger = \det H,$$

Therefore Hermitiean matrices have a real determinant. They also have a real trace, since to fulfill (8.6) the elements on the diagonal have to be real.

The main reason for their importance follows from the fact that the eigenvalues of a Hermitian matrix are real. To see this, note first that for any matrix for any eigenvalue

$$(M\vec{v})^\dagger = \vec{v}^\dagger M^\dagger = (\lambda\vec{v})^\dagger = \lambda^*\vec{v}^\dagger.$$

Multiply this equation again with the eigenvector. For a Hermitian matrix

$$\lambda^*\vec{v}^\dagger\vec{v} = (\vec{v}^\dagger H^\dagger)\vec{v} = \vec{v}^\dagger H\vec{v} = \vec{v}^\dagger \lambda\vec{v} = \lambda\vec{v}^\dagger\vec{v}.$$

Now, either the eigenvalue needs to be zero for this to be true. Or, since at least one eigenvector for any non-zero eigenvalue has non-zero length, is real. Thus, all eigenvalues are real.

Eigenvectors $\vec{v}$ and $\vec{w}$ to different, non-zero eigenvalues $\lambda_{1,2}$ of hermitian matrices are mutually orthogonal, since

$$|\lambda_1|^2(\vec{v}\vec{v} - \vec{v}\vec{w}) = \vec{v}H^\dagger H(\vec{v} - \vec{w}) = \vec{v}(|\lambda_1|^2\vec{v} - |\lambda_2|^2\vec{w}) = |\lambda_1|^2\vec{v}\vec{v} - |\lambda_2|^2\vec{v}\vec{w}$$

which implies

$$(|\lambda_1|^2 - |\lambda_2|^2)\vec{v}\vec{w} = 0$$

---

[2]There is a small difference between both concepts for infinite-dimensional vector spaces. The proper definition requires $(\vec{v}^\dagger H^\dagger)\vec{v} = \vec{v}^\dagger(H\vec{v})$ for every vector of the vector space. Especially $(H^\dagger)^\dagger = H$, which is true for arbitrary matrices for a finite number of dimensions may no longer hold for an infinite number of dimensions.

which requires $\vec{v}$ to be orthogonal to $\vec{w}$. Note that for orthogonality of the eigenvectors it was actually only necessary that $H^\dagger H = H H^\dagger$, which is a weaker statement than hermiticity. Matrices satisfying this condition are called normal.

E. g. the first Pauli matrix (8.7) has the two eigenvalues ± 1 and eigenvectors

$$0 = \det \begin{pmatrix} -\lambda & 1 \\ 1 & -\lambda \end{pmatrix} = \lambda^2 - 1 = (\lambda + 1)(\lambda - 1)$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} = +1 \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} -1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} = -1 \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} -1 \\ 1 \end{pmatrix} = 1 - 1 = 0,$$

exhibiting all the properties listed above. This is also almost trivial for the third Pauli matrix.

Thus eigenspaces to different eigenvalues are orthogonal[3]. This would imply that the eigensystem forms a complete basis, if for every eigenspace the geometric multiplicity equals the arithmetic multiplicity, to also include zero eigenvalues. This can actual be shown by the fact that any Hermitian matrix is diagonalizable, and therefore according to section 7.5 the eigenvectors must form a full basis. For that use the fact that any matrix can be brought into upper triangular form following the procedures in section 6.5. For any upper triangular matrix T, $T^\dagger$ is lower triangular. This implies

$$T^\dagger = (U^{-1}HU)^\dagger = U^\dagger H^\dagger U^{\dagger -1} = U^{-1}HU = T$$

where its has been used that the for every matrix in the sequence build in section 6.5 $U^\dagger = U^{-1}$ applies[4], as can be directly read off. But then an upper and lower triangular matrix should be equal, which is only possible if they are diagonal matrices, which completes the proof.

The combination of properties of Hermitiean matrices of the reality of eigenvalues and that the eigenvectors form an orthonormal basis is also called the spectral theorem. This theorem will be essential for the description of quantum physics.

Note that if the vector space is real, a hermitian matrix just satisfies

$$H = H^T,$$

which is called symmetric. Since in the derivation of the various properties nothing changes when exchanging a complex vector space with a real vector space, the spectral theorem also applies to symmetric matrices. This is remarkable, as this implies that the characteristic

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[3]In case of degenerate eigenvalues and thus multiple eigenvectors, it is always possible to find an orthonormal basis in the corresponding eigenspace. All vectors of this basis are also eigenvectors, as discussed in section 7.4.1.

[4]Note that no pure rescaling is involved to bring a matrix to upper triangular form, only adding and subtracting multiples of some columns and rows.

polynomial of a symmetric matrix has indeed as many real solutions as possible. This is not entirely trivial, since a real matrix can have also complex eigenvalues.

Note that the number of independent, real or complex, matrix elements of a hermitian or symmetric matrix is smaller than the $n \times n$ elements of an ordinary matrix. First, the real case. There are n diagonal elements, which are free. There are also $(n^2 - n)/2$ elements above (or below) the diagonal, which are unconstrained, while the other ones are uniquely determined by them. Thus, the total number of independent matrix elements are $n^2/2 - n/2 + n = n(n+1)/2$. For the hermitian case, the situation is a bit different. Because of the hermiticity, the diagonal elements need to be real, while either the part above or below the diagonal are complex and unrestricted, while the other part is fixed. Thus, there are $n^2 - n + n = n^2$ real parameters independent.

8.5   Antisymmetric and antihermitian matrices

8.5.1   Properties

A variation on the topic of symmetric/hermitian matrices are antisymmetric/antihermitian matrices, which satisfy

$$A^\dagger = -A$$

For any antihermitian matrix A, the matrix iA is hermitian. Thus, all eigenvalues of an anti-hermitian matrix are either zero or purely imaginary. The same is thus also true for an antisymmetric matrix. Because this is just a multiplicative factor, the eigenvectors still form an orthonormal system, with all consequences.

Note for real $d \times d$ matrices that because

$$\det A = \det -A^T = (-1)^d \det A^T = (-1)^d \det A$$

the determinant is zero in odd dimensions, since the imaginary eigenvalues come in pairs, and the surplus eigenvalue has therefore to be zero to ensure this. In even dimensions, this is not necessary, as here two imaginary eigenvalues can, by squaring, compensate each other.

The number of independent entries is smaller than in the symmetric/hermitian case. For real matrices, the diagonal elements have to vanish, and therefore there are $n(n-1)/2$ free elements. In the complex case, the diagonal elements need to be purely imaginary, but the off-diagonal elements are not constrained. Thus, there they have the same number of independent entries as the hermitian ones above the diagonal. Hence, in total there are $n(n-1)$ real parameters.

8.5.2   Vector product and anti-symmetric matrices

Anti-symmetric matrices also permit to think about the vector product in an entirely different way. Consider two vectors $\vec{v}$ and $\vec{w}$ in $\mathbb{R}^3$ and construct the following object

$$m_{ij} = v_i w_j - v_j w_i, \tag{8.8}$$

which is an antisymmetric matrix. However, upon closer inspection, this matrix has the form

$$M = \begin{pmatrix} 0 & v_1 w_2 - v_2 w_1 & v_1 w_3 - v_3 w_1 \\ v_2 w_1 - v_1 w_2 & 0 & v_2 w_3 - v_3 w_2 \\ v_3 w_1 - v_1 w_3 & v_2 w_3 - v_3 w_2 & 0 \end{pmatrix} = -M^T, \qquad (8.9)$$

and thus has as elements the components of the vector product of two vectors in $\mathbb{R}^3$. This is possible, as an anti-symmetric matrix has in $\mathbb{R}^3$ the same number of independent components as a vector.

Thus, the vector product could also be considered not to be a map of two vectors into a vector, but of two vectors into an antisymmetric matrix. In fact, the definition (8.8) will generate always an anti-symmetric matrix, and therefore is in addition to (2.10) an alternative way to generalize the vector product, then usually called outer product, to a different number of dimensions than three. Indeed, in this case there is also a non-trivial result for a vector product in two dimensions, a two-dimensional antisymmetric matrix,

$$M = \begin{pmatrix} 0 & v_1 w_2 - v_2 w_1 \\ v_2 w_1 - v_1 w_2 & 0 \end{pmatrix},$$

which then has only one non-trivial entry. In dimensions larger than three, the number of independent entries in an antisymmetric matrix is larger than for a vector. Thus, in this case three dimensions is very special. This is also true in the sense that the entries of the matrix (8.9) can be assembled into a vector and then behave as a vector.

It is in fact this generalization of the vector product, which is most useful, and plays also a certain role in physics. This feature is generalized in differential geometry, which appears in many contexts in theoretical physics.

8.6 Orthogonal and unitary matrices

Another important class of matrices has the property

$$U^\dagger = U^{-1},$$

i. e. the inverse of the matrix is the same as its hermitian adjoint. Such matrices of dimension n are called unitary matrices of dimension n. This definition implies that only invertible matrices can be unitary matrices, and therefore any unitary matrix has non-zero determinant. Actually, the norm of their determinant is necessarily one,

$$1 = \det 1 = \det U U^{-1} = \det U (\det U)^* = |\det U|^2$$

If the determinant itself, rather than its norm, is one, the matrix is called special unitary of dimension n.

One of the central properties of unitary matrices is that they act as transformations on vectors which are norm-preserving and angle-preserving. If every vector is transformed by U, $\vec{v}' = U\vec{v}$, then for any two vector $\vec{v}$ and $\vec{w}$

$$\vec{v}'^\dagger \vec{w}' = \vec{v}^\dagger U^\dagger U \vec{w} = \vec{v}^\dagger U^{-1} U \vec{w} = \vec{v}^\dagger \vec{w},$$

and therefore scalar products are preserved. Also any decomposition of the vector space in subspaces is preserved under the action of a unitary matrix, in the sense that the number and dimensionality of subspaces are preserved. This is seen by considering the action on a projection matrix,

$$U^{-1}P'U = U^{-1}UPU^{-1}U = P = P^2 = PU^{-1}UP = U^{-1}UPU^{-1}UPU^{-1}U = U^{-1}P'^2U,$$

and therefore $UPU^{-1} = P'$ is again a projection matrix. Since this implies $PU = U^{-1}P'$, the transformed vectors are still forming as a decomposition of the same type.

This norm preservation implies especially that all eigenvalues of a unitary matrix are of norm one. If $\vec{v}$ is a (normalized) eigenvector of U then

$$1 = \vec{v}^{\dagger}\vec{v} = \vec{v}^{\dagger}1\vec{v} = \vec{v}^{\dagger}U^{\dagger}U\vec{v} = \lambda^*\lambda\vec{v}^{\dagger}\vec{v} = |\lambda|^2.$$

This is an independent proof that the determinant has norm one.

A particular important example of such matrices are those used to modify systems of linear equations in section 6.5, since there the inverse of these matrices were indeed their hermitian conjugate.

Unitarity has an immediate consequence for the column and row vectors: The column/row vectors of unitary matrices need to be orthonormal to each other, since

$$\delta_{ij} = (U^{-1})_{ik}U_{kj} = (U^*_{ki})U_{kj} = (\vec{U}^i)^{\dagger}\vec{U}^j, \tag{8.10}$$

where $\vec{U}^i$ are the ith row vectors. Thus the columns and rows of a unitary matrix form an orthonormal base system for the vector space. Because hermitian conjugating the statement yields the same equations, the orthonormality of the rows automatically ensures the orthonormality of the columns. This can be used to show that they are furthermore diagonalizable.

As an example, consider

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$$

$$\det U = \frac{1}{2}\left(1 - i^2\right) = 1$$

$$U^{\dagger}U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 - i^2 & i - i \\ -i + i & -i^2 + 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

and which has eigenvalues $\exp(\pm i\pi/4)$. Since the determinant is one, it is actually special unitary.

If the vector space is real, then matrices satisfying

$$O^T = O^{-1}$$

are the analogue to unitary matrices, and are called orthogonal. For them, the eigenvalues can thus be only ± 1, and also the determinant can only be ± 1. However, an orthogonal

matrix may neither be diagonalizable, nor does it need to have eigenvalues. They are also called special if the determinant is 1.

Note that the number of independent entries for a unitary or orthogonal matrix is reduced due to the condition (8.10). This yields n conditions in the real case and $2n$ real or n complex conditions in the complex case. Thus, there are $n^2 - n = n(n - 1)$ independent real or complex entries.

In section 8.9.1 the properties of unitary matrices will be used to construct base transformations.

8.7 Summary of matrix types

In total, the following matrix types have been identified, and characterized, with d being the dimensionality

- Invertible matrices I: Matrices for which $\det I \neq= 0$, and thus I^{-1} exists.

- Diagonalizable matrices D: Matrices for which $\sum \gamma_i = \sum \mu_i = d$ holds, and thus can be brought into diagonal form, with eigenvalues on the diagonal, by a similarity transformation using a matrix build from their eigenvectors. The eigenvectors form a basis of the vector space.

- Permutation matrices P: Invertible and diagonalizable matrices obeying $P^2 = 1$, with $\text{tr} P = d - 2$, $\det P = -1$, eigenvalues are 1 with algebraic multiplicity $d - 1$ and -1 with algebraic multiplicity 1.

- Projection matrices P: Non-invertible and diagonalizable matrices obeying $P^2 = P$, with $\text{tr} P > 0$ and $\det P = 0$.

- Nilpotent matrices S: Non-invertible matrices obeying $S^2 = 0$, with $\det S = 0$.

- Symmetric matrices S: Diagonalizable matrices obeying $S^T = S$, whose eigenvectors form an orthogonal basis (after orthogonalization in subspaces with degenerate eigenvalues)

- Hermitiean matrices H: Diagonalizable matrices obeying $H^\dagger = H$, with real eigenvalues and eigenvectors form an orthogonal basis (after orthogonalization in subspaces with degenerate eigenvalues)

- Antisymmetric matrices A: Matrices obeying $A^T = -A$, which do not have eigenvalues in a real vectorspace, and purely imaginary ones in a complex vector space. In the latter case, the eigenvectors form an orthogonal basis (after orthogonalization in subspaces with degenerate eigenvalues), and the matrix is diagonalizable. The diagonal is always zero.

- Antihermitian matrices A: Diagonalizable matrices obeying $A^\dagger = -A$, with all eigenvalues purely imaginary and eigenvectors form an orthogonal basis (after orthogonalization in subspaces with degenerate eigenvalues). The diagonal elements are always purely imaginary.

- Orthogonal matrices O: Invertible matrices obeying $O^T = O^{-1}$. If eigenvalues exist, they are ± 1, and $\det O = \pm 1$.

- Unitary matrices U: Invertible and diagonalizable matrices obeying $U^\dagger = U^{-1}$. Eigenvalues have the form $e^{i\lambda}$ and $\det U = e^{i\phi}$.

- Special matrices S obey $\det S = 1$.

Properties, which are not specifically mentioned, may or may not apply, e. g. often diagonalizability.

8.8   Matrix groups

The presence of so many particular sets of matrices is not a coincidence. It rather shows that matrices also have an abstract superstructure: Matrices form groups. Especially, there are two possible group structures, one with respect to matrix addition and one for matrix multiplication.

The one corresponding to matrix addition is closed, as the sum of two matrices is a matrix, has with the zero matrix a unit element, and with the negative of a matrix also the inverse element. It is hence an Abelian group.

A very important subgroup of this group is the group of Hermitian matrices. Since

$$(A + B)^\dagger = A^\dagger + B^\dagger = A + B,$$

if A and B are both Hermitian, the group of Hermitian matrices is closed under addition. Since the zero matrix is also Hermitian, these matrices indeed form a subgroup, the group of hermitian matrices. Also the symmetric matrices form for real vector spaces such a subgroup. Note that the antihermitian/antisymmetric matrices do not, as the zero matrix cannot act as a neutral element as it is neither antihermitian nor antisymmetric.

Another interesting one is the so-called general linear group $\mathrm{GL}(F,d)$, where F denotes the field and d the dimension. It is a group under matrix multiplication, and therefore contains only the invertible matrices, and thus not all matrices, since, e. g., projection matrices are not part. The unit element is here the unit matrix. Since the matrix product is by construction associative, the last of the group axioms is also fulfilled. This group is for $d > 1$ non-Abelian.

The special linear group $\mathrm{SL}(F,d)$ is the subgroup of all invertible matrices with unit determinant, since

$$1 = \det U \det W = \det UW = 1$$

this is actually meaningful: If two matrices have each unit determinant, then so has its product, and thus the group is closed. Since furthermore

$$1 = \det U^{-1} = \frac{1}{\det U} = 1$$

also the inverse element belongs to the group. The unit matrix has also unit determinant, and therefore also belongs to the group, providing the identity under matrix multiplications.

The reason why the general linear group is so relevant is that there are important subgroups, i. e. subsets of matrices which also fulfill the group axioms among only themselves.

Especially important are the unitary matrices, since

$$(AB)^{-1} = B^{-1}A^{-1} = B^\dagger A^\dagger = (AB)^\dagger,$$

and thus this subgroup is closed under matrix multiplication. Moreover, the unit matrix is also unitary, and therefore the unit element is part of this group. Since they will play a very important role in the following, this group of matrices have also a special name, they are called the unitary matrices of dimension d, or briefly U(d).

Similar to the SL subgroup of GL, there is another subgroup, those of unitary matrices of determinant 1, for the same reason as before. These are called the special unitary matrices of dimensionality d, or SU(d).

Consequently, there is for real matrices the subgroup of orthogonal matrices, called O(d) and of orthogonal matrices of determinant 1, the special orthogonal matrices SO(d). The groups (S)U(d) and (S)O(d) are also particular examples of so-called Lie groups, a certain class of matrix groups which play a central role in modern physics.

Also the permutation matrices form a subgroup of the group SL, as any product of permutation matrices is again a permutation matrix, with the unit matrix a trivial permutation.

Note that enforcing additional conditions on the determinant will reduce the number of independent entries by one for any case.

These are just a few of the many more subgroups of the group GL. These are subject of group theory, which is covered in a different lecture. For many parts of physics, the groups discussed here play the central role, while the other groups are relevant only in special circumstances. Thus, they will not be discussed here.

8.9 Applications of matrix groups

8.9.1 Base transformation

8.9.1.1 General concepts

The particular importance of (special) unitary matrices becomes evident when considering the following problem. As noted in sections 3.3 and 4.3, there are many different possibilities how to construct a basis. In section 4.3 it was shown how to construct from a given set

of basis vectors an orthonormal basis. Since any basis is as good (though not necessarily as practically useful) as any other, the natural question is therefore to ask whether there is somehow a connection between two given bases. The answer is yes, and the connection will be in form of a unitary or orthogonal matrix. Since this is true with trivial changes in both cases, in the following only the case of unitary matrices in complex vector spaces will be considered.

Note first that unitary matrices, according to section 8.6, preserve scalar products, if they act on two vectors. Given any two base vectors $\vec{e}_i$ of an orthonormal basis, the transformed vectors $U\vec{e}_i$ have the property

$$\vec{e}_i^{\dagger} U^{\dagger} U \vec{e}_j = \vec{e}_i^{\dagger} \vec{e}_j = \delta_{ij}$$

and thus the set of transformed vectors are again an orthonormal basis. Thus, application of a unitary matrix to an orthonormal basis creates a new orthonormal basis. Note that the same is true for an orthogonal basis. Since by the Gram-Schmidt orthogonalization procedure any basis is equivalent to an orthogonal basis this implies that all bases can be transformed into other bases by a multiplication with a unitary matrix, or, as it is also called, a unitary transformation.

Secondly, if there is some basis, not necessarily orthonormal, any vector $\vec{a}$ can be decomposed into this basis. The components of the vector $\vec{a}$ in the new basis are then given by

$$a_i' = \vec{e}_i^{\dagger} U^{\dagger} \vec{a} = \vec{e}_i^{\dagger} U^{\dagger} \vec{e}_j = U_{ij}^{\dagger} a_j = (U^{\dagger} \vec{a})_i,$$

where the U_{ij} are defined to be the components of the U in the old basis. This implies that while the base transforms with U, the other vectors transform as $U^{-1} = U^{\dagger}$. Alternatively, the basis could have been transformed by $U^{\dagger}$ and the vectors by U. This is sometimes used to distinguish between active and passive base transformations, with active if the base is transformed by U.

A natural question is, of course, if every basis can be reached from every other basis. It is sufficient to show that any basis can be reached from the normal Cartesian one. For any other pairing, it is otherwise just sufficient to first transform back to the Cartesian one it originates from. Since unitary matrices are invertible this is always possible. Afterwards it then needs to transform forward to the desired basis. The full transformation is then obtained by a combination of the two unitary transformations.

Consider, e. g. the two bases

$$B_1 \quad = \quad \left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \end{pmatrix} \right\} \tag{8.11}$$

$$B_2 \quad = \quad \left\{ \frac{1}{2} \begin{pmatrix} \sqrt{3} \\ 1 \end{pmatrix}, \frac{1}{2} \begin{pmatrix} -1 \\ \sqrt{3} \end{pmatrix} \right\}. \tag{8.12}$$

The first one can be transformed to the Cartesian basis with the special unitary matrix

$$U_1^{\dagger} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}, \tag{8.13}$$

which can then be transformed to the second basis by

$$U_2 = \frac{1}{2} \begin{pmatrix} \sqrt{3} & -1 \\ 1 & \sqrt{3} \end{pmatrix}. \tag{8.14}$$

It is noteworthy that the new base vectors appear in the columns of the transformation basis. This is true for any base transformation starting from the Cartesian basis, as will be seen below.

Alternatively, the inverse matrices $U_2^\dagger$ and U_1 do it in the opposite order. A direct transformation is obtained using

$$U = U_2 U_1^\dagger = \frac{1}{2\sqrt{2}} \begin{pmatrix} i + \sqrt{3} & -1 - i\sqrt{3} \\ 1 - i\sqrt{3} & \sqrt{3} - i \end{pmatrix}, \tag{8.15}$$

which would probably not seem obvious.

It still needs to be shown in general. This is best done in a constructive way. First, consider some other orthonormal basis. Arranging the base vectors $\vec{u}^i$ as the columns of a matrix, this matrix will be unitary, by virtue of (8.10). Then

$$(U\vec{e}^i)_j = U_{jk}e_k^i = U_{jk}\delta_{ik} = U_{ji} = (\vec{u}^j)_i$$

and therefore indeed in general the image of the Cartesian basis is written in the columns of the transformation matrix.

This is indeed the case in the example also for the first basis. Comparing (8.12) to (8.14) and noting for (8.13)

$$U_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$$

and comparing this to (8.11) shows this explicitly. Note, however, that (8.15) shows that this is not true for a transformation between two orthonormal bases different from the Cartesian basis.

If the base $\vec{v}^i$ is not orthonormal, then it can always be expanded in another suitable orthonormal basis $\vec{f}^i$, e. g. constructed using the Gram-Schmidt orthogonalization procedure of section 3.3. This basis can again be reached from the standard Cartesian basis. Thus

$$\vec{v}^i = a_{ij}\vec{f}^j = a_{ij}(U\vec{e}^j) = (AU\vec{e})^i.$$

The matrix AU is necessarily invertible, and thus $(AU)^{-1} = U^{-1}A^{-1}$ exists. However, it cannot be unitary, since it does not preserve the angles between the vectors, since the input vectors are orthonormal, and the output vectors are, by assumption, not. It is, however, an upper triangular matrix with non-zero eigenvalues, and can therefore also be diagonalized. Thus, the property of angle-preservation of unitary matrices does not permit to transform an orthogonal to a non-orthogonal base, as well as the norm-preservation forbids to transform a normal to a non-normal basis. This requires the multiplication with a suitable additional matrix. However, a unitary transformation transforms a non-orthonormal basis in another non-orthonormal basis, where the base vectors keep the relative angles and lengths.

A base transformation can also be considered to be actually a similarity transformation on matrices instead. Consider a Cartesian basis and any matrix A. Its matrix elements are

$$A_{ij} = \vec{e}_i^{\dagger} A \vec{e}_j.$$

Performing a base transformation with U yields

$$\vec{e}_i^{\dagger} U^{\dagger} A U \vec{e}_j.$$

Thus, rather than to transform the base vectors, this can also be considered as a similarity transformation

$$A' = U^{-1} A U = U^{\dagger} A U$$

of the matrix. Put it differently, any similarity transformation with a unitary matrix is reexpressing a matrix in a new base. This preserves the action of a matrix on an arbitrary vector in the following sense,

$$\vec{b}' = A' \vec{a}' = U^{\dagger} A U U^{\dagger} \vec{a} = U^{\dagger} A \vec{a} = U^{\dagger} \vec{b}.$$

Thus, a base transformation does not change the image, kernel etc. of a matrix. Especially, a base transformation does not change the eigenvalues of a matrix,

$$\lambda' = \lambda' \vec{v}'^{\dagger} \vec{v}' = \vec{v}'^{\dagger} A' \vec{v}' = \vec{v}^{\dagger} U U^{\dagger} A U U^{\dagger} \vec{v} = \lambda \vec{v} \vec{v} = \lambda,$$

where for simplicity it was assumed that the eigenvectors $\vec{v}$ were normalized, and which is not changed by the unitary transformation due to the norm preservation.

Note that the determinant of a matrix and the trace of a matrix are invariant under base transformations, as they are particular similarity transformations.

8.9.1.2   Once again, rotations

Now, finally, is the time to return to the rotations of section 5.1. The matrix defined in section 5.1.3

$$R = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix}.$$

can now be identified to be a special orthogonal matrix, as

$$\begin{aligned} R^T R &= \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \\ &= \begin{pmatrix} \cos^2\alpha + \sin^2\alpha & \cos\alpha\sin\alpha - \cos\alpha\sin\alpha \\ \cos\alpha\sin\alpha - \cos\alpha\sin\alpha & \cos^2\alpha + \sin^2\alpha \end{pmatrix} = 1 \end{aligned}$$

and

$$\det R = \cos^2\alpha + \sin^2\alpha = 1.$$

Hence, the rotation is a special type of base transformation, mediated by an SO(2) matrix: The coordinate axes become rotated by the angle α.

In fact, since the number of independent entries for an SO(2) matrix is one, all SO(2) matrices can be written in the above form, and are parameterized by the rotation angle α. The only type of base transformations not covered in two dimensions are those with $\det P = -1$, the mirroring or parity transformation, which by a similarity transformation always can be brought into the form

$$P = \begin{pmatrix} \pm 1 & 0 \\ 0 & \mp 1 \end{pmatrix},$$

which correspond to mirroring of the x-axis and y-axis. Together with R, they form the matrix group of O(2).

The situation becomes more involved for higher dimensions. Again, all base transformations between orthonormal base systems are mediated by matrices of the group O(N). E. g. an arbitrary SO(3) matrix can be written as

$$D(\alpha_1, \alpha_2, \alpha_3) = \begin{pmatrix} \cos\alpha_1 & \sin\alpha_1 & 0 \\ -\sin\alpha_1 & \cos\alpha_1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\alpha_2 & 0 & \sin\alpha_2 \\ 0 & 1 & 0 \\ -\sin\alpha_2 & 0 & \cos\alpha_2 \end{pmatrix} \times$$
$$\times \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha_3 & \sin\alpha_3 \\ 0 & -\sin\alpha_3 & \cos\alpha_3 \end{pmatrix},$$

and likewise a number of mirroring matrices. However, there is no unique way to write these matrices, as now there is the possibility to select different rotation axes. However, a suitable similarity transformation can always bring any element of SO(3) to this form. Moreover, rotations in three dimensions are no longer commutative, so things are more complicated.

The generalization to higher dimensions becomes correspondingly more unpleasant, but the main result remains: (Real) Rotations between orthonormal base systems are mediated by elements of O(d).

8.9.2 Generalized ellipsoids

A very important particular geometric problem is the description of ellipsoids in $\mathbb{R}^3$, i. e. the geometric objects whose surface is described by the equation

$$a^2 x^2 + b^2 y^2 + c^2 z^2 = r^2$$

with a, b, c, and r constants. If r is varied between zero and a fixed maximum value, this equation describes the volume of the ellipsoid. For $a = b = c$, this describes the surface of a sphere of radius r, and otherwise of an ellipsoid with main axes r/a, r/b, and r/c. This equation can be rewritten in matrix vector form as

$$\vec{x}^T M \vec{x} = \vec{x}^T \begin{pmatrix} a^2 & 0 & 0 \\ 0 & b^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix} \vec{x} = r^2,$$

and is therefore characterized by a diagonal matrix M.

On the other hand, rewrite M as $S^T M S$, then

$$\vec{x}^T S^T M S \vec{x} = r^2 > 0.$$

Then $M' = S^T M S$ is a symmetric matrix and $S\vec{x}$ can be considered as the vectors of a new basis. Thus, in general, any three-dimensional diagonalizable matrix describes an ellipsoid in some coordinate system. In this context, diagonalization is therefore also called main axis transformation, as it brings the main axes of the ellipsoid on the coordinate axes. This also shows that, like unitary/orthogonal matrices have a geometrical interpretation in terms of rotation, symmetric matrices, which are diagonalizable by the spectral theorem, have a geometric interpretation in terms of ellipsoids[5].

The conditions for the the diagonal elements can also be relaxed, and only require that

$$\vec{x}^T \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix} \vec{x} \geq 0.$$

The objects described by this situation are quite different, and it is useful to first consider the two-dimensional projections, so called cone projections, of these, i. e. equations of type

$$ax^2 + by^2 = r.$$

Then there are three possibilities. One is that either a and b have negative sign, but r is positive. This describes hyperbolas, starting out from $\pm r$. Reversing the signs of a and b just flips this by $\pi/2$. In three dimensions, these are then saddles, or two separated hyperboloids, depending on the relative sign of the z-axis.

Together, this implies that the equation

$$\vec{x}^T M \vec{x} \geq 0,$$

can be classified according to the eigenvalues of the matrix M. Note that it is sufficient to actually consider only the case that the right-hand side is equal to one, as it is always possible to rescale the matrix by a corresponding factor

If the matrix M can be brought into diagonal form, it depends on the values of the eigenvalues. If they are all positive, it describes an ellipsoid. If one is negative, it becomes a saddle, if two are negative, it becomes two separated hyperboloids. All three negative cannot be, as then the inequality cannot be fulfilled. If one is zero, this degenerates into the equation of a cylinder, and if two are zero to a plane. If the matrix does not have three eigenvalues, it is not describing such a body.

It is interesting to consider also the case of

$$(\vec{x}^T + \vec{b}^T) M (\vec{x} + \vec{b}) = r,$$

---

[5]There is a generalization for hermitian matrices in complex vector spaces, but this has less geometrical appeal.

with $\vec{b}^T M \vec{b} = r$. This compensates the right-hand side. E. g. in two dimensions, this yields

$$ax^2 + by + cx + dy^2 = 0.$$

In a suitable basis, this reduces to

$$ax^2 + by = 0.$$

It therefore describes a parabola, positive or negative depending on prefactors. This combines then with the various possibilities for z.

An alternative to classify all possible such forms is by considering

$$\vec{x}^T M \vec{x} + \vec{b}^T \vec{x} + r = 0. \tag{8.16}$$

Thus, all previous cases are just special cases of this so-called quadratic form. In a sense, this is a generalization of the concept of the Hessian normal form of section 2.8.

All of this, especially equation (8.16) can be generalized to arbitrary dimensions, describing the n-dimensional generalizations of these bodies.

8.9.3 Solving linear systems of equations

Also the solution of linear equations discussed in section 6.2 takes now a new perspective. Given a system of linear equations in matrix-vector form

$$A\vec{x} = \vec{b}, \tag{8.17}$$

there are now multiple ways to reinterpret it.

One is that if A is diagonalizable, there is always a base transformation with a unitary matrix such that

$$UAU^\dagger U \vec{v} = U \vec{b}$$

such that in this basis the solution becomes trivial. Alternatively, if A is invertible, i. .e $\det A \neq 0$,

$$\vec{x} = A^{-1} \vec{b}$$

and the solution can be mapped to a matrix inversion.

Conversely, the absence of a solution is now signaled by $\det A = 0$.

Multiple solutions appear if the kernel of A is non-trivial. Take a vector $\vec{k}$ from the kernel $\mathcal{K}$, then

$$\vec{b} = A\vec{x} = A\vec{x} + \vec{0} = A\vec{x} + A\vec{k} = A(\vec{x} + \vec{k}),$$

and hence adding to a solution any vector from the kernel creates a new solution to the system of equations. Alternatively, this can be read that the solution to the inhomogeneous system (8.17) is a combination of a particular solution to (8.17) to which an arbitrary solution of the homogeneous system

$$A\vec{x} = 0$$

can be added, which just defines the kernel.

Hence, the solvability of a system of linear equations can now be classified by the matrix A and its properties.

If the system of linear equations has indeed a single solution, it is possible to use the determinants to construct it explicitly. This is known as Cramer's rule. Consider a system of linear equations in matrix vector form (8.17) with exactly one solution, as assured with the above methods. The result is

$$x_i = \frac{\det A_i}{\det A}$$

where A_i is the same matrix as A, but with the ith column replaced by the vector $\vec{b}$. The proof uses the calculational scheme (6.9) for determinants, which gives a determinant based on the determinants in terms of subdeterminants with a certain row and column eliminated, denoted by $\det A^i$.

Now sum the equations weighted with the corresponding subdeterminant $\det A^i$. The coefficient of x_i will then be $\det A$, while the coefficient of all other x vanishes, since these are the determinant of a matrix with twice the same column. The right-hand side is then precisely the determinant $\det A_i$, thus completing the proof.

Chapter 9

Tensors

Tensors are a particular subclass of matrices. They have the property that they transform under a base transformation in a very particular way. In fact, all physics theories are formulated using tensors, i. e. they are tensor equations: Both sides transform in the same way under base transformations, both sides are tensors. Vectors are in this case special cases of such tensors (as vectors are special cases of matrices), as they have a definite transformation property under base transformations, as shown in section 8.9.1. Thus, e. g. Newton's second law is a tensor equation, as the force and the acceleration, which are equated with a scalar factor of mass, are vectors.

9.1 Tensors and base transformation

With the construction of basis transformations, it is possible to introduce the notion of tensors. Given a basis transformation U, a tensor of rank n is defined to be an object with n indices which transforms under a basis transformation as

$$v'_{i_1...i_n} = U_{i_1 j_1}...U_{i_n j_n} v_{j_1...j_n}, \tag{9.1}$$

and thus every index is transformed by a separate transformation matrix.

This implies that a vector[1] is a tensor of rank 1. However, an arbitrary matrix transforms not with twice the same transformation matrix U, but on one index with U and one with U^{-1}, i. e.

$$M'_{ij} = (UMU^{-1})_{ij} = U_{ik}M_{km}U^{-1}_{mj} = U_{ik}U^{-1}_{mj}M_{km}. \tag{9.2}$$

A tensor of rank two would transform as

$$m'_{ij} = U_{ik}U_{jm}m_{km},$$

which is distinctively different.

However, the matrix still has a definite transformation property under a basis transformation. To account for this, it is useful to introduce the concept of covariant tensors and contravariant tensors.

---

[1]Sometimes rather a row vector is defined to be a tensor of rank 1, rather than the column vector.

A covariant tensor is a tensor which transforms like (co) a vector under a basis transformation, and thus like (9.1). A contravariant tensor is defined to transform like

$$v'_{i_1...i_n} = U^{-1}_{j_1 i_1}...U^{-1}_{j_n i_n} v_{j_1...j_n}$$

and therefore in the opposite (contra) way as a vector. A tensor is said to be mixed, if it transforms as

$$v'_{i_1...i_n j_1...j_m} = U_{i_1 l_1}...U_{i_n l_n} U^{-1}_{k_1 j_1}...U^{-1}_{k_m j_m} v_{l_1...l_n k_1...k_m},$$

having n covariant indices and m contravariant indices. The consequence is that a scalar product of a covariant tensor v and a contravariant tensor r remains unchanged under the transformation, e. g. at rank 1

$$v_i r_i = U_{ij} U^{-1}_{ki} v_i r_k = v_i r_i \tag{9.3}$$

It is important to notice the ordering of the indices. A normal matrix under a similarity transformation does transform with a left multiplication like a covariant tensor, and a right multiplication light a contravariant tensor. A normal matrix transforming like (9.2) would therefore be a mixed tensor of rank 2.

It is often useful to keep track of the nature of a tensor by using the index position to signal how it transforms under a basis transformation, e. g. by putting covariant indices in a lower position and contravariant indices in an upper position. In the simplest case, the transformation matrix with reversed index positions will then necessarily be the inverse of the one with indices oppositely placed, to maintain (9.3),

$$v_i r^i = U^j_i v_j U^i_k r^k = (U^j_i U^i_k) v_j r^k = \delta^j_k v_j r^k = v_j r^j.$$

This will be encountered often in physics, especially in theories involving relativity, starting from special relativity and extending to quantum gravity. However, ultimately physics, and thus empirical information, will decide which physical quantities will be represented by which type and rank of tensors. This cannot be determined from mathematics alone.

Note that in real spaces for a symmetric transformation the distinction is irrelevant, since

$$U^{-1}_{ij} = U^T_{ij} = U_{ji}$$

and therefore all tensors of any rank transform in the same way.

It should be noted that, depending on the application and context, the transformation may differ from the inverse, covariant can be used to denote the transformation properties of a row vector rather than a column vector, whether covariant transformations are by convention always from the left and contravariant ones from the right and many other details. The general guideline is that tensors have a definite transformation property under basis transformation, and covariant and contravariant can be used to distinguish different behaviors, which cancel eventually to ensure that scalar products remain invariant.

9.2   Tensor compositions

9.2.1   Vector spaces

It is interesting to extend the concepts of matrices further. This can be done using tensor compositions.

Tensor compositions are, overly simply speaking, a way how to get from two lower-dimensional spaces into a single higher-dimensional space. The name of tensor originates from the fact that this is most useful when applied to tensors.

The simplest way of a tensor composition is by appending two vectors to each other, called a tensor addition. E. g. combing an n-dimensional vector space and an m-dimensional vector space, this yields

$$\vec{v}^{n+m} = \vec{v}^n \oplus \vec{w}^m = \begin{pmatrix} v_1 \\ \vdots \\ v_n \\ w_1 \\ \vdots \\ w_m \end{pmatrix}.$$

creating a space of higher dimensionality $n+m$. Of course, this requires to have compatible vector spaces, such that e. g. scalar multiplication is still well-defined. Thus, in most cases tensor addition occurs for vector spaces of the same type.

Matrices are in this case composed in a block diagonal form,

$$M \oplus N = \begin{pmatrix} M & 0 \\ 0 & N \end{pmatrix}, \tag{9.4}$$

and thus continue to act only on vectors in the corresponding subspaces. Note that this implies that in the new vector space there are additional matrices, which are not in this sense block-diagonal, which can now mix the different subspaces. Tensors of the same rank created in this way under tensor addition remain tensors of the same rank. But they may become mixed if they were not so before, e. g. if M transforms covariantly and N transforms contravariantly in (9.4).

A second option originates from the question, if it would be possible to have vectors of vectors, i. e. the component of a vector is not, e. g., some number, but again a vector. Of course, if this would be the case, these subvectors could be expanded, such that again an ordinary vector would be obtained, just with instead of n components now with nm components, where m would be the dimensionality of the embedded vectors. If this is done, this is called a tensor product of two vector spaces, $V^n \otimes W^m$, with vectors written as

$$\vec{a}^{nm} = \begin{pmatrix} \vec{v}_1^n \\ \vdots \\ \vec{v}_m^n \end{pmatrix}, \tag{9.5}$$

and thus forming a new vector space of dimension nm. Of course, if the vector spaces would have different types of vectors and/or different fields, things would become very

complicated, thus neglect this possibility for a moment. However, this will happen in physics systems, especially quantum physics.

A consequence of (9.5) is that vectors could be regarded as having now two indices. An 'outer' index, which addresses the original component, and an inner index, which addresses the component in the 'inner' vector,

$$\vec{v}_{jm+i} = \vec{v}_i^{\,j} = \vec{w}_j,$$

where $\vec{w}$ are vectors of the space V^m. This already shows that in this way not all components become independent if only a single vector in one vector space is used to create one in the tensor-product space. Hence, the simple tensorization will not create all vectors of V^{nm}.

9.2.2 Tensors

There is also another possibility how to tensorize two objects. It is possible to tensorize two vectors as

$$(\vec{v} \otimes \vec{w})_{ij} = v_i w_j,$$

and therefore construct a matrix out of them. In particular, this constructs a matrix, a rank two tensors, out of two vectors, two rank one tensors. In the same way, it is possible to construct higher-rank tensors out of lower-rank tensors. It is possible that this creates mixed objects. At the same time, this does not change the vector space, in contrast to the possibilities of section 9.2.1. This kind of tensorization also appears repeatedly in all areas of physics.

An interesting application for tensor products is the spectral decomposition of a diagonalizable matrix. Then, the (normalized) eigenvectors $\vec{v}_i$ form a basis, and it is possible to spectrally decompose a matrix as

$$M = \sum_i \lambda_i \vec{v}_i \otimes \vec{v}_i^{\dagger},$$

where the sum runs over all eigenvectors and λ_i are the corresponding eigenvectors. To see that this is correct, decompose an arbitrary vector in the eigenbasis of the matrix, and act with both versions on it

$$M\vec{a} \qquad = M \sum_i a_i \vec{v}_i = \sum_i a_i M \vec{v}_i = \qquad \sum_i a_i \lambda_i \vec{v}_i$$

$$\sum_i \lambda_i \vec{v}_i \otimes \vec{v}_i^{\dagger} \vec{a} \; = \sum_{ij} a_j \lambda_i \vec{v}_i \otimes \vec{v}_i^{\dagger} \vec{v}_j = \sum_{ij} a_j \lambda_i \vec{v}_i \otimes \delta_{ij} = \qquad \sum_i a_i \lambda_i \vec{v}_i,$$

proving the correctness of the spectral decomposition.

Chapter 10

Linear operators

Matrices have so far been $n \times k$ sets of numbers. But just as with vectors and vector spaces, it is possible, and indeed useful, to generalize them. In fact, there are many useful examples of this.

10.1 Matrices as a (normed) vector space

In section 8.8 it has been noted that the matrices form an Abelian group under matrix addition.

This property can be upgraded to have a vector space of matrices under addition. Add a field to the set of matrices, being either the real or complex numbers. Then scalar multiplication can be defined as

$$(aM)_{ij} = am_{ij}.$$

This fulfills all the usual rules of scalar multiplication as enumerated in section 3.1, since

$$
\begin{aligned}
(a(M+N))_{ij} &= am_{ij} + an_{ij} = (aM + aN)_{ij} \\
((ab)M)_{ij} &= abm_{ij} = (a(bM))_{ij} \\
(a(M+N))_{ij} &= (a(m_{ij} + an_{ij})) = (aM)_{ij} + (aN)_{ij} \\
((a+b)M)_{ij} &= (a+b)m_{ij} = (aM)_{ij} + (bM)_{ij} \\
(0M)_{ij} &= 0m_{ij} = 0.
\end{aligned}
$$

Thus, matrices themselves form a vector space. Note that the above did not require the matrices to be square, and it thus also applies to rectangular matrices.

This does not imply that any of the matrix groups introduce in section 8.8 form a vector space, and in fact most do not. The notable exception are the hermitian (symmetric) matrices of section 8.4. Since

$$(H + M)^\dagger = H^\dagger + M^\dagger = H + M$$

if both H and M are hermitian, the hermitian (or symmetric) matrices are closed under addition. Since

$$(aH)^\dagger = a^* H^\dagger = a^* H$$

it is possible to construct a vector space over the field of real numbers. That has a number of very useful application in quantum physics, especially in the context of group theory.

A question following from the construction of a vector space of matrices is, whether it is possible to upgrade it to a normed vector space, or even a Hilbert space.

Consider first the case of a normed vector space. It requires just to define a proper norm. There are many possibilities. One is, e. g.

$$||A|| = \left(\sum_{ij} |A_{ij}|^2 \right)^{\frac{1}{2}}$$

but this is only one out of many. This definition guarantees only the zero matrix to have a zero norm. Since it is based on properties of the norm of the elements of the field, it also ensures the triangle inequality, and the scaling of scalar multiplication is also automatically ensured.

Probably the most interesting property is that for a square matrix A with eigenvalues λ_i and eigenvectors $\vec{v}_i$ with the above norm and the usual norm for $\mathbb{R}^n$ or $\mathbb{C}^n$

$$|\lambda_i||\vec{v}_i| = |\lambda_i \vec{v}_i| = |A\vec{v}_i| \leq ||A|| |\vec{v}_i|,$$

where no summation is implied. The last inequality holds because it can be reduced to inequalities of the real or complex numbers. Thus, $|\lambda_i| \leq ||A||$, and hence the matrix norm provides an upper limit to the size of the eigenvalues.

The condition

$$|A\vec{v}| \leq ||A|| |\vec{v}|$$

or more general

$$||AB|| \leq ||A|| ||B||,$$

is not automatically guaranteed, but depends on the norms in question. It applies for the usual norms encountered in physics. This property of matrix norms is called submultiplicativity.

What has been said about norms is also true for scalar products. It is possible to define also scalar products of matrices. However, it is more useful to introduce this as a more abstract concept, once matrices have been generalized to linear operators in section 10.2.

10.2   Definitions of linear operators

So far, the generalizations still used the concept of the matrices as rectangular schemes of numbers. This is not necessary, and will be removed now. The new concept is called linear operator. It is based, as for all generalizations, on the most useful properties of the inspiring object, in this case the matrices.

The basic definition of an arbitrary linear operator M is that it acts on vectors and maps them to another vector, but possibly in a different vector space. This is also called the target of the linear operator, and the set of all targets the target space.

The only requirements are that a linear operator M fulfills the following properties when acting on vectors $\vec{a}$ and $\vec{b}$, which could be scaled by some factor α from the field,

$$
\begin{aligned}
M(\vec{a} + \vec{b}) &= M\vec{a} + M\vec{b} & (10.1) \\
M(\alpha\vec{a}) &= \alpha M\vec{a} & (10.2) \\
M\vec{0} &= \vec{0}. & (10.3)
\end{aligned}
$$

This definition applies to matrices, and for finite-dimensional vector spaces, it was shown in section 5.2 that it is always possible to write a linear operator as a matrix. However, linear operators can take very different forms.

As a non-trivial example, consider some fixed vector $\vec{v}$ in a complex Hilbert space. Then the scalar product with this vector is also a linear operator $M_{\vec{v}}$, since for any other vectors $\vec{w}$ and $\vec{x}$ and field element a

$$
\begin{aligned}
M_{\vec{v}}(\vec{w} + \vec{x}) &= \vec{v}^{\dagger}(\vec{w} + \vec{x}) = \vec{v}^{\dagger}\vec{w} + \vec{v}^{\dagger}\vec{x} = M_{\vec{v}}\vec{w} + M_{\vec{v}}\vec{x} \\
M_{\vec{v}}(a\vec{w}) &= a\vec{v}^{\dagger}\vec{w} = aM_{\vec{v}}\vec{w} \\
M_{\vec{v}}\vec{0} &= \vec{v}^{\dagger}\vec{0} = 0,
\end{aligned}
$$

and thus fulfills the requirements of a linear operator. Since it maps a vector into a number, it is not realized by a square matrix, but rather by the matrix given by the vector itself. Thus, it shows that a linear operator maps elements of one vector space into another, in this case from the $\mathbb{C}^n$ into the $\mathbb{C}^1$. Hence, a linear operator does not need to have an inverse, and it usually does not have. As noted before, any linear operator can be rewritten as a matrix, but not necessarily a square one. However, if the corresponding matrix is invertible, so is the linear operator.

There are also antilinear operators, which differ from linear operators by the fact that

$$
M(\alpha\vec{v}) = \alpha^* M\vec{v}.
$$

An example for such an anti-linear operator would be, e. g. the scalar product where the fixed vector is the second vector, rather than the first.

In general, for any linear operator it is possible to define

$$
\vec{y}^{\dagger} M \vec{x},
$$

provided $\vec{x}$ and $\vec{y}$ are from suitable vector spaces. Linear operators which map a vector to the same vector space are then classified by their action on the same vector,

$$
\vec{x}^{\dagger} M \vec{x} = a,
$$

which is necessarily a scalar. Such an operator is called positive definite if $a > 0$, positive semi-definite if $a \geq 0$, negative definite if $a < 0$, and negative semi-definite if $a \leq 0$ for all $\vec{x} \neq \vec{0}$, and indefinite otherwise.

E. g., the linear operator M

$$
M = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}
$$

yields

$$\vec{x}^{\dagger} M \vec{x} = a|x_1|^2 + b|x_2|^2. \tag{10.4}$$

For $a = b = 1$ it is positive definite, for $a = 1$ and $b = 0$ it is positive semi-definite, and likewise for $a = b = -1$ negative definite and for $a = -1$ and $b = 0$ negative semi-definite. It is indefinite for $a = 1$ and $b = -1$, as it depends then on the vector whether the result is positive or negative.

Provided the vector space in question is at least a Banach space, there is another important classification. Given that the vector $\vec{x}$ on which M is acting is from a bounded subspace, i. e. in practice usually its components are finite, then the operator M is called compact if it maps these vectors to a subspace which is also bounded.

In any finite-dimensional vector space any matrix with finite entries will provide a compact operator. However, in an infinite-dimensional vector space, this is no longer necessarily the case.

10.3   Differential operators as linear operators

The true power of linear operators becomes more apparent when considering again infinite-dimensional functional spaces. Consider a space build from real or complex arbitrarily often differentiable functions with real or complex numbers as the field. The differentiable functions form an Abelian group with addition, as the sum of two differentiable functions is again differentiable, and the neutral element, zero, yields that the negative function is the inverse. Since multiplication by a number does not change differentiable, the proof that it is a vector space is complete.

Then the differential operator d/dx is a linear operator, since

$$\begin{aligned} \frac{d}{dx}(f(x) + g(x)) &= \frac{df(x)}{dx} + \frac{dg(x)}{dx} \\ \frac{d}{dx}(af(x)) &= a\frac{df(x)}{dx} \\ \frac{d}{dx}0 &= 0 \end{aligned}$$

and it maps the vector space of (arbitrarily often differentiable) functions into itself. Of course, the corresponding matrix is not a finite-dimensional matrix, but rather an infinite-dimensional one, just like the vector space itself.

In the same sense also integration can be considered as a linear operator, as long as the function space contains only integrable functions. That this is a vector space with the group constructed from the addition of the functions proceeds as for the differentiable functions. However, it is necessary that the functions are either integrable over the whole range of arguments, or the integration range is only over an interval where all functions

included are integrable. Then

$$\int_a^b dx(f(x) + g(x)) = \int_a^b dxf(x) + \int_a^b dxg(x)$$

$$\int_a^b dx(cf(x)) = c\int_a^b dxf(x)$$

$$\int_a^b dx0 = 0.$$

However, it is important that these are definite integrals, as a non-zero integration constant would spoil multiplicativity. It would be necessary to negotiate to have always this constant set to zero to have the indefinite integral being a linear operator. Again, an infinite-dimensional matrix would be necessary for a matrix representation of this operator. Note that integration as a linear operator does not map the vector space into itself, but rather the vector space to the (vector space of) real or complex numbers.

It should be noted that in neither case the operators can be expected to be positive semi-definite, i. e. ≥ 0. However, to check this would require to test (10.4). This is problematic for two reasons. First, this is not multiplying by the same function. This operation is not defined. Rather, it would be necessary to expand the functions in a suitable basis, which is a non-trivial problem in itself, which will not be solved here, and then provide an explicit matrix representation[1]. The second is that integration is not mapping the vector space into itself. If for differentiation the vector space is enlarged to only differentiable functions, also then the vector space is not mapped into itself. Then the compactness itself cannot be tested, as the criterion is not applicable. Thus, care has to be taken when making statements about compactness.

This shows that a wide range of operations are actually linear operators, and that the space they operate on can be rather abstract.

10.4 Images, kernels and eigenspaces

Just like for matrices, it is useful to introduce the concepts of images and kernels also for linear operators. Given some vector space of vectors $\vec{x}$, the space

$$M\vec{x} = \vec{y}$$

spanned by the vectors $\vec{y}$ is called the image of the linear operator M. Note that the image may not be in the same vector space as the vectors $\vec{x}$.

Likewise, the vector space, or subspace, of vectors $\vec{x}$ such that

$$M\vec{x} = \vec{0}$$

is called the kernel of the linear operator M.

---

[1]For some finite-dimensional function spaces this is/was discussed in the exercises to this lecture.

Note that these vector spaces can both be infinite-dimensional, but still be smaller than the original vector space. Such is the subtlety of infinite-dimensional vector spaces.

If M maps a vector space in itself and has the property

$$MM\vec{x} = \vec{0}$$

for any $\vec{x}$, it is called a nilpotent operator.

If a linear operator maps a vector space in itself, it is possible to define eigenvectors $\vec{v}_i$ and eigenvalues λ_i as

$$M\vec{v}_i = \lambda_i \vec{v}_i,$$

where the eigenvectors can again span eigenspaces, and degeneracies may arise. However, in general it is not entirely simple to determine now possible eigenspectra and eigenvalues. Especially, they may be continuous. However, this question will be central in many areas of physics, and in particular quantum physics.

Consider as an example the differential operator. Then the eigenvalue equation

$$\frac{d}{dx}f(x) = \lambda f(x)$$

becomes a differential equation. It is solved by $f(x) = a\exp(\lambda x)$, and therefore there is a continuous and infinite set of eigenvalues, λ, with eigenvectors $a\exp(\lambda x)$. The prefactor a plays in this case the role of the arbitrary normalization.

Formally, it is possible to define the determinant and trace of a linear operator by the sum and product of the eigenvalues.

Interestingly, it is also possible to define properties like hermiticity or unitarity for linear operators. In particular, the equivalent of the spectral theorem can be proven also for hermitian operators. Thus, the eigenspace of a hermitian operator will form a basis of the vector space at hand. Especially, also its eigenvalues will be real. Also this will play a central role in quantum physics and many other areas of physics.

10.5 Morphisms

Since the restriction of the linear operators to those which map a vector space in itself appeared repeatedly, it is useful to classify this property. It is also these class of linear operators which are the most important ones, and the most frequently appearing ones, in physics.

The basic concept is the morphism. A morphism is a map which preserves the structure of the space it acts on. For a vector space, this structure is vector addition and multiplication by an element of the field. Since a linear operator on a vector space by definition maintains this structure, any linear operator is a morphism. This is also called a homomorphism, and for the present case of linear operators on vector spaces both denote the same. This may be different in other areas of mathematics.

If a linear operator maps a vector space into the same vector space, it is called an endomorphism. If it has an inverse, i. e. the matrix representing the linear operator

can be inverted, it is called an isomorphism. Finally, if a linear operator is both, an endomorphism and an isomorphism, it is called an automorphism. It should be noted that linear operators with a non-trivial kernel can never be an isomorphism. On the other hand, a unitary matrix or an orthogonal matrix is automatically an automorphism. Thus basis transformations are also automorphisms.

In this context, also the other designations from section 7.4.5 are again relevant. A linear operator is called injective, if it maps two different vectors to two different vectors. This is also called one-to-one. A surjective linear operator reaches every vector in the target space, i. e. for every vector in the target space, there is one or more vectors from the original space which are mapped on this vector. If a linear operator is both injective and surjective, and therefore has a unique result for any vector, it is called bijective. Note that bijective operators are automatically invertible: Since there is a unique map, just inverting the map defines the inverse operator. Note that a bijective operator is not necessarily an isomorphism, as it is not required to be an endomorphism.

These designations are important, as it is often possible to make general statements about the category itself. Then, as soon as it is clear that a map or operator belongs to any of these categories it is certain that it fulfills all these statements.

Chapter 11

Non-Euclidean geometry

So far, everything discussed was about the topic of spaces with an Euclidean metric, i. e. spaces with a positive semi-definite scalar product. However, especially in physics non-Euclidean geometries play an important role, i. e. spaces with an indefinite scalar product. This is particularly true for special relativity and general relativity, but also applies to particle physics. It is therefore useful to collect a few results on such spaces.

11.1   Non-Euclidean metrics

The simplest examples occur when the metric g defining the scalar product does not lead to a positive-definite scalar product. The simplest example has been on a real[1] vector space the metric

$$g = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$ (11.1)

for which the scalar product takes the form

$$\vec{x}^T g \vec{y} = x_1 y_1 - x_2 y_2$$

and which can now also be recognized as a particular matrix-vector product.

The first consequence is that orthogonal transformations O no longer leave the scalar product invariant

$$\vec{x}^T O^T g O \vec{y} \neq \vec{x}^T g \vec{y}$$

since

$$\begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} = \begin{pmatrix} \cos(2\alpha) & -2\cos\alpha\sin\alpha \\ -2\cos\alpha\sin\alpha & -\cos(2\alpha) \end{pmatrix} \neq g,$$

and likewise in other cases.

However, it is possible to define transformations which leave the metric invariant, as

$$\Lambda^T g \Lambda = g$$ (11.2)

---

[1]All of the following can also be done for complex vector spaces, but for simplicity here only real vector spaces will be considered. Also, this is the case relevant to special relativity.

which in two dimensions for this particular metric have the form

$$\Lambda = \begin{pmatrix} \cosh\alpha & \sinh\alpha \\ \sinh\alpha & \cosh\alpha \end{pmatrix}, \tag{11.3}$$

and are therefore not orthogonal matrices. Note that $\Lambda^T = \Lambda$. That this is indeed the case can be seen by an explicit calculation,

$$\begin{pmatrix} \cosh\alpha & \sinh\alpha \\ \sinh\alpha & \cosh\alpha \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \cosh\alpha & \sinh\alpha \\ \sinh\alpha & \cosh\alpha \end{pmatrix}$$

$$= \begin{pmatrix} \cosh\alpha & \sinh\alpha \\ \sinh\alpha & \cosh\alpha \end{pmatrix} \begin{pmatrix} \cosh\alpha & \sinh\alpha \\ -\sinh\alpha & -\cosh\alpha \end{pmatrix}$$

$$= \begin{pmatrix} \cosh^2\alpha - \sinh^2\alpha & \cosh\alpha\sinh\alpha - \cosh\alpha\sinh\alpha \\ \cosh\alpha\sinh\alpha - \cosh\alpha\sinh\alpha & \sinh^2\alpha - \cosh^2\alpha \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

where it has been used that $\cosh^2\alpha - \sinh^2\alpha = 1$.

Thus, a scalar product is invariant under these new transformations. Matrices of this type are called SO(1,1), similar to the SO(2) matrices discussed in section 8.8, since the rotation plane includes 1 axis with negative metric element and 1 with positive metric element, and the determinant is 1.

11.2 Covariant and contravariant vectors

As in chapter 9, this situation is now used to define covariant and contravariant tensors. Especially, a vector $\vec{v}$ which transforms as

$$\vec{v}' = \Lambda\vec{v}$$

is defined to be a covariant vector. A contravariant vector $\vec{w}$ is a vector which transforms in the opposite way, i. e. like

$$\vec{w}' = \Lambda^{-1}\vec{v}.$$

As already noted in section 9, the components of a covariant vector will be denoted as v_i and of a contravariant vector as w^i. However, the relation (11.2) implies

$$\Lambda^{-1}(g\vec{v}) = \Lambda^{-1}\Lambda^T g\Lambda\vec{v} = \Lambda^{-1}\Lambda g\Lambda\vec{v} = g\vec{v}' = (g\vec{v})'.$$

Thus $(g\vec{v})$ transforms like a contravariant vector. As a consequence, the metric is given two contravariant indices, and it is defined that

$$g^{ij}v_j = v^i$$

to signify this fact: The metric can be used to raise and lower the indices of a tensor. Since $gg^{-1} = 1$, the inverse metric is denoted to have lower indices. Note that this needs

to be read as $g_{ij}g^{jk} = 1_i^k$ in components. Thus, the metric with lower indices is defined to lower the indices, turning a contravariant vector into a covariant one.

$$g_{ij}w^j = w_i$$

This also implies that the scalar product can be considered to be a combination of a contravariant and a covariant vector,

$$w_i g^{ij} v_j = w^i v_i.$$

The consequence of the metric being, in a sense, its own inverse is then that

$$g_{ij}g^{jk} = \delta_i^k,$$

and thus a δ with one index up and one index down is the corresponding unit matrix.

The consequence of such a metric is that scalar products are no longer positive semi-definite. Especially

$$\vec{v}^T g \vec{w} = a$$

can now be greater, smaller or equal zero, even if $\vec{v} = \vec{w}$. Thus, vectors can be classified by the fact whether they have positive, negative, or zero length. Examples for all possibilities in two dimensions for the metric (11.1) are

$$\vec{v}_1 = \begin{pmatrix} a \\ 0 \end{pmatrix}$$
$$\vec{v}_2 = \begin{pmatrix} b \\ b \end{pmatrix}$$
$$\vec{v}_3 = \begin{pmatrix} 0 \\ c \end{pmatrix},$$

where these vectors have positive, zero, and negative norm. This also implies that the 'angle'

$$\frac{v^i w_i}{|\vec{v}||\vec{w}|}$$

between two vectors needs no longer to be a real angle, and in fact this expression needs no longer to vary between -1 and 1, as it does in Euclidean metric. Rather, as with rotations before, this should be considered to be a generalized angle η, and this expression is equal to $\cosh\eta$.

11.3   Four-dimensional Minkowski case

These results can be generalized to higher dimensions, especially to the physically relevant case of the so-called Minkowski metric[2]

$$g = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{11.4}$$

in four dimensions dimensions.

However, the situation is now quite different from the two-dimensional case discussed previously. Three of the four directions form a conventional Euclidean vector space, with a positive semi-definite scalar product, instead of a semi-scalar product. Thus, it is necessary to carefully distinguish the fourth direction and the other three directions.

Especially, rotations only along the three normal axes are generated by again a normal three-dimensional orthogonal matrix. But whenever the direction of rotation has a component in the fourth direction, the rotation occurs in a non-Euclidean subspace, and therefore requires a generalization of the matrix (11.3).

In total, there are then six different rotations, corresponding to the six planes which can be formed using four axes. Three are ordinary rotations, where the rotation plane contains two directions which have ordinary metric coefficients. But there are also three rotation planes, where one of the directions is the direction which is different. In analogy to the Euclidean case of SO(4), this is called SO(1,3), since there is one different axis, and three 'normal' axes. A general rotation is therefore composed out of the three conventional rotation matrices

$$J_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\alpha & \sin\alpha & 0 \\ 0 & -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}; \quad J_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\beta & 0 & \sin\beta \\ 0 & 0 & 1 & 0 \\ 0 & -\sin\beta & 0 & \cos\beta \end{pmatrix}; \quad J_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos\gamma & \sin\gamma \\ 0 & 0 & -\sin\gamma & \cos\gamma \end{pmatrix}$$

as well as the three 'special' rotations

$$J_4 = \begin{pmatrix} \cosh\eta & \sinh\eta & 0 & 0 \\ \sinh\eta & \cosh\eta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}; \quad J_5 = \begin{pmatrix} \cosh\xi & 0 & \sinh\xi & 0 \\ 0 & 1 & 0 & 0 \\ \sinh\xi & 0 & \cosh\xi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}; \quad J_6 = \begin{pmatrix} \cosh\zeta & 0 & 0 & \sin\zeta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \cosh\zeta & 0 & 0 & \sinh\zeta \end{pmatrix}.$$

In the context of relativity, these are called boosts. Restricting only to these six special, so called Lorentz, transformations, is not necessary. It is possible to also permit determinants of ±1, which then require the matrices $\text{diag}(-1,1,1,1)$ and $\text{diag}(1,-1,-1,-1)$, which correspond to the different possible mirroring, which cannot be created using just rotations.

---

[2]Everything works in the same way by replacing g with $\text{diag}(-1,1,1,1)$. It is thus a matter of convention which to use.

Together, these forms the so-called Lorentz group O(1,3), while SO(1,3) is sometimes also called proper Lorentz group.

It should be noted that now not always $J_i = J_i^T$, and thus to show the changes from covariant to contravariant vectors by the metric requires to make separate calculations for J_{1-3} and J_{4-6}, but in the end the result is always the same.

11.4 Symplectic geometry

Another non-trivial example is so-called symplectic geometry, which plays an important role in the mathematical foundations of mechanics, and thus physics in general. It will again be sufficient to consider two real dimensions. Consider the metric

$$g = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{11.5}$$

It has the peculiar property that it yields zero length for any vector

$$\vec{v}^T g \vec{v} = (x, y) g \begin{pmatrix} x \\ y \end{pmatrix} = (x, y) \begin{pmatrix} y \\ -x \end{pmatrix} = xy - xy = 0.$$

Thus, this metric is certainly not creating an ordinary inner product. It satisfies also $g^{-1} = g^T = -g$ and $g^2 = -1$

This can now be generalized to arbitrary even dimensions, by just using blocks of g instead of ones[3].

Again, there are transformations J which leave such a metric invariant. These are the so-called symplectic matrices, $\mathrm{Sp}(d)$. These are matrices J which again need to satisfy

$$J^T g J = g \tag{11.6}$$

$$\tag{11.7}$$

It can be shown that for the 2×2 submatrices of the matrix J

$$J = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

holds that

$$\begin{aligned}
(A^T C)^T &= A^T C \\
(B^T D)^T &= B^T D \\
A^T D - C^T B &= 1.
\end{aligned}$$

This can be seen by explicit calculation. Using an explicit 2×2 block form,

$$\begin{aligned}
J^T g J &= \begin{pmatrix} A^T & C^T \\ B^T & D^T \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} A^T & C^T \\ B^T & D^T \end{pmatrix} \begin{pmatrix} C & D \\ -A & -B \end{pmatrix} \\
&= \begin{pmatrix} A^T C - C^T A & A^T D - C^T B \\ B^T C - D^T A & B^T D - B D^T \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.
\end{aligned}$$

---

[3]The fact that this is only possible in even dimensions hints already at the very important fact that even and odd dimensions are fundamentally different.

Thus, such transformation leave the metric invariant.

As before, it is possible to distinguish covariant and contravariant tensors, transforming differently.

Using (11.6) and the properties of the metric it is possible to show that

$$J^{-1} = g^{-1} J^T g = -g J^T g.$$

Note that in this case raising and lowering of indices with the metric is more involved.

11.5   Other symmetries

Finally, it should be illustrated that relevant transformations in vector spaces are not necessarily linear. The following works, no matter whether the metric is positive or not.

First, consider the so-called sphere inversion transformation

$$x_\mu \to \frac{a x_\mu}{\vec{x}^2}.$$

It is not a linear transformation, as it does not respect the conditions (10.1-10.3). Consequently, it also impossible to describe it by a constant, i. e. x-independent, matrix.

This transformation rescales a vector by a position-dependent factor, and thus is non-linear. It has the property to leave the angles between the vectors invariant,

$$(|\vec{x}||\vec{y}|\cos\theta)' = \vec{x}^{T'}\vec{y}' = \frac{a^2}{x^2 y^2}\vec{x}^T \vec{y} = |\vec{x}'||\vec{y}'|\cos\theta.$$

Geometrically, as the name suggests, it describes how points in the interior of a sphere of radius $\sqrt{|a|}$ are moved to the outside, and the points outside into the inside. The center of the sphere is distributed to a sphere at infinity, by definition. Such transformations are useful, as they invert the concepts of near and far.

As a second example consider the two transformations

$$
\begin{aligned}
x^\mu &\to \lambda x^\mu \\
x^\mu &\to \frac{x^\mu + a^\mu \vec{x}^2}{1 + 2x^\nu a_\nu + \vec{a}^2 \vec{x}^2},
\end{aligned}
$$

The first is a scale transformation, also known as dilatation. It is a linear operation. The second is not, and a is just a fixed vector. It is called a special conformal transformation However, consider the length of a transformed vector

$$x'^2 = \frac{x^2 + 2(ax)\vec{x}^2 + \vec{a}^2(\vec{x}^2)^2}{(1 + 2ax + \vec{a}^2\vec{x}^2)^2} = \frac{\vec{x}^2}{1 + 2ax + \vec{a}^2\vec{x}^2}$$

Thus, this transformation is not length-preserving. In fact, it can be rewritten as

$$x'_\mu = \frac{x^2}{1 + 2ax + \vec{a}^2\vec{x}^2}\left(\frac{x_\mu}{\vec{x}^2} + a_\mu\right).$$

Thus, it is equivalent to a position-dependent rescaling, followed by a translation, and finally another rescaling.

A physical system in d dimensions, which is invariant under rotations, being that those mediated by the conventional $\mathrm{SO}(d)$ matrices or by the Lorentz group $\mathrm{SO}(1,d-1)$, and both dilatation and special conformal transformations are said to have conformal symmetry. Systems exhibiting such symmetries play an important role in many physical applications. E. g., substances undergoing a second-order phase transition behave exactly at the phase transition as if they would have conformal symmetry, which has very far-reaching implications.

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