6 Multipole expansion and spherical harmonics

Charge and current distributions in a small region of space may be very complicated, and the potentials will generally not be simple. For example, a water molecule is electrically neutral as a whole, but one side of the molecule is slightly positive ($+q$), while the other side is slightly negative ($-q$). If the two charges are separated by a distance $\mathbf{d}$, the potential of each is

$$\Phi_+(\mathbf{r}) = -\frac{q}{4\pi\epsilon_0|\mathbf{r}|} \quad \text{and} \quad \Phi_-(\mathbf{r}) = \frac{q}{4\pi\epsilon_0|\mathbf{r}-\mathbf{d}|}\,. \tag{6.1}$$

Using the superposition principle to find the scalar potential of the combined charges Φ, we find ($r \gg d$)

$$\Phi(\mathbf{r}) = -\frac{q|\mathbf{r}-\mathbf{d}|}{4\pi\epsilon_0|\mathbf{r}||\mathbf{r}-\mathbf{d}|} + \frac{q|\mathbf{r}|}{4\pi\epsilon_0|\mathbf{r}||\mathbf{r}-\mathbf{d}|} \simeq \frac{qd\cos\theta}{4\pi\epsilon_0 r^2}\,, \tag{6.2}$$

where θ measures the angle between $\mathbf{d}$ and $\mathbf{r}$. This is the so-called *dipole* potential. Note that it is no longer a $1/r$ potential but falls off faster, with $1/r^2$. If, for some reason the potentials in Eq. (6.1) had different charges q_1 and $q_2 = -q_1 - \delta$, then the scalar potential would be

$$\Phi(\mathbf{r}) = -\frac{q_1}{4\pi\epsilon_0|\mathbf{r}|} + \frac{q_1+\delta}{4\pi\epsilon_0|\mathbf{r}-\mathbf{d}|} \simeq \frac{\delta}{4\pi\epsilon_0 r} + \frac{q_1 d\cos\theta}{4\pi\epsilon_0 r^2}\,. \tag{6.3}$$

Now the scalar potential is a superposition of a monopole and a dipole contribution. In general, the scalar potential of a charge distribution will have a *multipole expansion*, and the same will apply to the vector potential. Let's look at this in a bit more detail.

6.1 Multipole expansion of a charge density

Suppose that we have a localized (meaning enclosed in a volume V) static charge density $\rho(\mathbf{r})$, which gives rise to a scalar potential

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\int \frac{\rho(\mathbf{r}')\,d\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}\,. \tag{6.4}$$

Far away from the charge density, the potential looks mainly like that of a point charge, but with some higher-order corrections. These corrections are the multipoles, and we can find them by looking at the Taylor expansion of Eq. (6.4). Let

$$f(\mathbf{r}-\mathbf{r}') = \frac{1}{|\mathbf{r}-\mathbf{r}'|} = \frac{1}{\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}}\,. \tag{6.5}$$

Now we make a Taylor expansion of $f(\mathbf{r}-\mathbf{r}')$ around $\mathbf{r}'=0$:

$$f(\mathbf{r}-\mathbf{r}') = f(\mathbf{r}) - \sum_{i=1}^{3} r'_i \left.\frac{\partial f}{\partial r_i}\right|_{\mathbf{r}'=0} + \frac{1}{2}\sum_{i,j=1}^{3} r'_i r'_j \left.\frac{\partial^2 f}{\partial r_i \partial r_j}\right|_{\mathbf{r}'=0} + \ldots \tag{6.6}$$

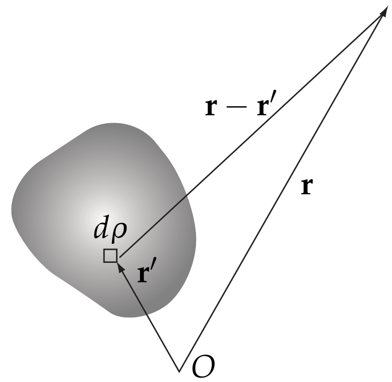

Figure 10: The field at position $\mathbf{r}$ far away from a charge distribution $\rho(\mathbf{r})$ can be expressed conveniently in terms of a multipole expansion. O denotes the origin of the coordinate system.

This can be rewritten in compact form as

$$\begin{aligned} \frac{1}{|\mathbf{r}-\mathbf{r}'|} &= \frac{1}{r} - \mathbf{r}'\cdot\nabla\frac{1}{r} + \frac{1}{2}(\mathbf{r}'\cdot\nabla)^2\frac{1}{r} + \ldots \\ &= \frac{1}{r} + \sum_{i=1}^{3}\frac{r_i r_i'}{r^3} + \frac{1}{2}\sum_{i,j=1}^{3}\frac{r_i(3r_i'r_j' - r'^2\delta_{ij})r_j}{r^5} + \ldots \end{aligned} \tag{6.7}$$

where $r = \sqrt{r_1^2 + r_2^2 + r_3^2} = |\mathbf{r}|$ is the magnitude of the vector with components r_i. After substituting this into the generic form of the scalar potential in Eq. (6.4), we find

$$\begin{aligned} \Phi(\mathbf{r}) &= \frac{1}{4\pi\epsilon_0}\int\frac{\rho(\mathbf{r}')\,d\mathbf{r}'}{r} + \frac{1}{4\pi\epsilon_0}\sum_{i=1}^{3}\int\frac{r_i' r_i}{r^3}\rho(\mathbf{r}')\,d\mathbf{r}' \\ &\quad + \frac{1}{8\pi\epsilon_0}\sum_{i,j=1}^{3}\int\frac{3r_i'r_j' - r'^2\delta_{ij}}{r^5}r_i r_j\rho(\mathbf{r}')\,d\mathbf{r}' + \ldots \end{aligned} \tag{6.8}$$

$$= \frac{1}{4\pi\epsilon_0}\left[\frac{Q}{r} + \sum_{i=1}^{3}\frac{Q_i r_i}{r^3} + \frac{1}{2}\sum_{i,j=1}^{3}\frac{r_i Q_{ij} r_j}{r^5} + \ldots\right]. \tag{6.9}$$

The multipole moments of the charge distribution are the *total charge* Q, the *dipole* moment Q_i, the *quadrupole* moment Q_{ij}, etc. They are defined as follows:

$$Q = \int \rho(\mathbf{r}')\,d\mathbf{r}' \tag{6.10}$$

$$Q_i = \int r_i'\,\rho(\mathbf{r}')\,d\mathbf{r}' \tag{6.11}$$

$$Q_{ij} = \int (3r_i'r_j' - r'^2\delta_{ij})\,\rho(\mathbf{r}')\,d\mathbf{r}' \tag{6.12}$$

$$\vdots \tag{6.13}$$

The quadrupole moment has nine components, but it is easy to see that $Q_{ij} = Q_{ji}$, and

$$\sum_{i=1}^{3} Q_{ii} = \sum_{i=1}^{3} \int (3r_i r_i - r^2)\rho(\mathbf{r})\, d\mathbf{r} = \int \left[\left(3 \sum_{i=1}^{3} r_i r_i \right) - 3r^2 \right] \rho(\mathbf{r})\, d\mathbf{r} = 0\,. \tag{6.14}$$

The quadrupole moment is therefore characterised by five independent variables.

6.2 Spherical harmonics and Legendre polynomials

It is clear from the previous section that we can continue the multipole expansion to octupoles and higher, but it is also pretty obvious that the polynomials in the definitions of $Q_{ijk\ldots}$ get quite unwieldy very quickly. Luckily, there is a more systematic approach based on *spherical harmonics*. These are functions of the spherical coordinates θ and ϕ of a vector $\mathbf{r}$, and the function f can then be written as

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{r'^l}{r^{l+1}} \sqrt{\frac{4\pi}{2l+1}}\, Y_{lm}(\theta, \phi) \sqrt{\frac{4\pi}{2l+1}}\, Y^*_{lm}(\theta', \phi') \tag{6.15}$$

with

$$Y_{lm}(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l+m)!}{(l-m)!}}\, \frac{e^{im\phi}}{\sin^m \theta} \left[\frac{d}{d\cos\theta} \right]^{l-m} \frac{(\cos^2\theta - 1)^l}{2^l l!}\,. \tag{6.16}$$

This is still rather complicated, but the advantage is that this is valid for all l. Note also that the spherical harmonics are complex, but Eq. (6.15) is still real due to the sum over m. You should think of the Y_{lm} as basis functions that can be used to write arbitrary functions (of θ and ϕ) as a series, just like any polynomial can be written as a series $\sum_n a_n x^n$, or a periodic function as a Fourier series. Like any proper set of basis functions, the Y_{lm} obey an orthogonality relation:

$$\int d\Omega\; Y^*_{lm}(\theta, \phi) Y_{l'm'}(\theta, \phi) \equiv \int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\phi\; Y^*_{lm}(\theta, \phi) Y_{l'm'}(\theta, \phi) = \delta_{ll'}\delta_{mm'}\,, \tag{6.17}$$

where we introduced the integration over the sold angle $d\Omega$.

We can now define the *Legendre polynomials* as

$$P_l(w) = \left[\frac{d}{dw} \right]^l \frac{(w^2 - 1)^l}{2^l l!}\,, \tag{6.18}$$

with normalisation $P_l(1) = 1$. In the spherical harmonics, we have set $w = \cos\theta$. The Legendre polynomials also obey an orthogonality relation

$$\int_{-1}^{1} dw\; P_l(w) P_{l'}(w) = \frac{2}{2l+1}\, \delta_{ll'}\,. \tag{6.19}$$

D Tensors and tensor fields

D.1 Cartesian tensor fields in 3-dimensional space

We start with the following list of tools:

– The 3-dimensional[1] space with an orthonormal axis system XYZ.
– A number n which we call *rank* or *order*.
– A set of 3^n functions $f_i : \mathbb{R}^3 \mapsto \mathbb{C} : (x, y, z) \mapsto f_i(x, y, z) = a_i$ which make every point (x, y, z) in the 3-dimensional space correspond with a number a_i (real or complex).

With these tools we now define *tensor fields of rank* n, and will see how they behave when XYZ is rotated into X'Y'Z':

– Scalar field: a tensor field of rank 0
  Because $n = 0$ we need only 1 $(= 3^0)$ function $f_1 : \mathbb{R}^3 \mapsto \mathbb{C} : (x, y, z) \mapsto f_1(x, y, z) = a_1$. With every point in space $(x, y, z,)$ corresponds a number a_1, which we call a *(cartesian) scalar*. The collection of all these scalars is called a *(cartesian) scalar field* defined by f_1. But not every f_1 defines a scalar field. The good f_1's are those for which the a_1's are invariant under a rotation of XYZ into X'Y'Z'. This is the defining property for a scalar field[2]:

$$[f_1(x', y', z')] = [1][f_1(x, y, z)] \qquad \textit{or} \qquad [a'_1] = [1][a_1] \tag{D.1}$$

  (x', y', z') are the coordinates of the point (x, y, z) in the rotated system X'Y'Z'. For later use we note that the matrix [1] is a 1-dimensional representation[3] of the group R_3 of all possible rotations of XYZ.

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[1] Because of this choice for 3-dimensional space, we define here 3-tensors. One can start also from m-dimensional space to define m-tensors. A physical example are the space-time 4-vectors from general relativity.

[2] The matrixnotation is redundant here, but is used for similarity with tensors of higher rank.

[3] Representing a group by matrices means associating a matrix with every element of the group, such that the product between the two representatives of two group elements equals the representative of the product of these two group elements. In the present case, the matrix [1] is associated with every element of the rotation group.

An trivial example of a cartesian scalar field is the one defined by the identical function $f_1(x,y,z) = \alpha$. Another example is the distance field $f_1(x,\,y,\,z) = \sqrt{x^2+y^2+z^2}$.

– Vector field : a tensor field of rank 1
  To define a tensor field of rank 1, 3 $(= 3^1)$ functions f_i are needed. Every point in space (x,y,z) is now associated with a triplet (called a *(cartesian) vector*) in the following way:

$$(x,y,z) \mapsto \begin{bmatrix} f_1(x,\,y,\,z) \\ f_2(x,\,y,\,z) \\ f_3(x,\,y,\,z) \end{bmatrix} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} \tag{D.2}$$

  The collection of all these vectors is a *(cartesian) vector field* defined by f_i. Not every set of f_i defines a vector field however. The required property is that the triplets behave in the following way under a rotation of XYZ:

$$\begin{bmatrix} f_1(x',\,y',\,z') \\ f_2(x',\,y',\,z') \\ f_3(x',\,y',\,z') \end{bmatrix} = \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{bmatrix} \begin{bmatrix} f_1(x,\,y,\,z) \\ f_2(x,\,y,\,z) \\ f_3(x,\,y,\,z) \end{bmatrix} \tag{D.3}$$

  or

$$\begin{bmatrix} a'_1 \\ a'_2 \\ a'_3 \end{bmatrix} = \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} \tag{D.4}$$

  or

$$a'_i = \sum_{j=1}^{3} b_{ij}\, a_j \tag{D.5}$$

  Here b_{ij} is the cosine of the angle between the old i-axis and the new j-axis (direction cosine). The matrices $[b_{ij}]$ form a 3-dimensional representation of the rotation group R_3.
  An example of a cartesian vector field is:

$$\begin{cases} f_1(x,\,y,\,z) = \alpha x \\ f_2(x,\,y,\,z) = \alpha y \\ f_3(x,\,y,\,z) = \alpha z \end{cases} \tag{D.6}$$

  α must be a scalar. If $\alpha = 1$, equation D.6 defines the field of position vectors in space. If $\alpha = \frac{q}{4\pi\epsilon_0\,(x^2+y^2+z^2)}$, equation D.6 defines the electric field of a point charge q put at the origin of XYZ.

– Tensor field of rank 2
  To define a tensor field of rank 2 we need 9 $(= 3^2)$ functions f_i. Every point in space (x,y,z) is now associated with a 9-fold object (called a *(cartesian) tensor of rank 2*) in the following way:

$$(x,y,z) \mapsto \begin{bmatrix} f_1(x,\,y,\,z) \\ f_2(x,\,y,\,z) \\ \cdots \\ f_9(x,\,y,\,z) \end{bmatrix} = \begin{bmatrix} a_1 \\ a_2 \\ \cdots \\ a_9 \end{bmatrix} \tag{D.7}$$

The collection of all these tensors constitutes a *(cartesian) tensor field of rank 2 defined by* f_i. Not every set f_i defines a tensor field however. The required property is that the tensors (which we can arrange either as a 9×1-matrix or as a 3×3-matrix) behave in the following way under a rotation of XYZ:

$$f_{ij}(x',\, y',\, z') = \sum_{k=1}^{3}\sum_{l=1}^{3} b_{ik}b_{jl}\, f_{kl}(x,\, y,\, z) \qquad \text{(D.8)}$$

or

$$a'_{ij} = \sum_{k=1}^{3}\sum_{l=1}^{3} b_{ik}b_{jl}\, a_{kl} \qquad \text{(D.9)}$$

The subscripts i, j, k, and l all run from 1 to 3, which is a convenient notation if the tensor is arranged as a 3×3-matrix. If the tensor is arranged as a 9×1-matrix, the 81 objects $b_{ik}b_{jl}$ can be arranged in a 9×9-matrix. The b_{ik} and b_{jl} are the same direction cosines as used in equation D.3. The 9×9-matrices form a 9-dimensional representation of the rotation group R_3.
An example of a cartesian tensor field of rank 2 is given by the following functions f_{ij} (the arguments $(x,\, y,\, z)$ are omitted):

$$\begin{array}{lll} f_1 = f_{11} = x^2 & f_2 = f_{12} = xy & f_3 = f_{13} = xz \\ f_4 = f_{21} = yx & f_5 = f_{22} = y^2 & f_6 = f_{23} = yz \\ f_7 = f_{31} = zx & f_8 = f_{32} = zy & f_9 = f_{33} = z^2 \end{array} \qquad \text{(D.10)}$$

If the product between x and y is commutative, then $f_{12} = f_{21}$ etc.
A physical example of a cartesian tensor field of rank 2 is the susceptibility tensor field $\boldsymbol{\chi}$. For every point in space (the space is thought to be filled with a given material), χ_{ij} gives the polarization in the i-direction induced by an electric field in the j-direction. A susceptibility tensor is used in the following equation (which can be written for every point in space), where also the electric field and the polarization vector appear (both are vectors of two different tensor fields of rank 1, evaluated at the same point in space):

$$\begin{bmatrix} P_x \\ P_y \\ P_z \end{bmatrix} = \epsilon_0 \begin{bmatrix} \chi_{xx} & \chi_{xy} & \chi_{xz} \\ \chi_{yx} & \chi_{yy} & \chi_{yz} \\ \chi_{zx} & \chi_{zy} & \chi_{zz} \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} \qquad \text{(D.11)}$$

Note from this example that multiplication between tensors of different rank is possible. We knew this already for the familiar case of the multiplication of a vector by a scalar.

– Tensor field of rank n
The above definitions can be generalized to define (cartesian) tensor fields of rank n. There will be needed 3^n functions f_i. Tensors of rank n can be arranged in a $3^n \times 1$-matrix, and in the required transformation property

a $3^n \times 3^n$-matrix containing products between n direction cosines will appear. The latter matrices form a n-dimensional representation of the rotation group R_3.

D.2 Reducing cartesian tensors

Without going too deep into the mathematical meaning of the word, a tensor field of rank n defined by a set of functions f_i can be *equivalent*[4] to another tensor field of the same rank defined by a set of functions g_i. Two equivalent tensor fields have the same basic mathematical properties and only apparently look different. Also the $n^2 \times n^2$-matrices in the equation describing the transformation properties will look different between two equivalent tensor fields. In fact, it can be proven that for any tensor field $\boldsymbol{F}$ it is always possible to find an equivalent tensor field $\boldsymbol{G}$ such that their transformation matrices relate in the following way:

$$\begin{bmatrix} \bowtie & \bowtie & \cdots & \bowtie \\ \bowtie & \bowtie & \cdots & \bowtie \\ \vdots & \vdots & \ddots & \vdots \\ \bowtie & \bowtie & \cdots & \bowtie \end{bmatrix} \Longleftrightarrow \begin{bmatrix} \bowtie & \cdots & \bowtie & & & \\ \vdots & \ddots & \vdots & & 0 & \\ \bowtie & \cdots & \bowtie & & & \\ & & & \bowtie & \cdots & \bowtie \\ & 0 & & \vdots & \ddots & \vdots \\ & & & \bowtie & \cdots & \bowtie \end{bmatrix} \tag{D.12}$$

The matrix on the right hand side in the above equation is said to be in *block form*. The tensor field $\boldsymbol{F}$ is said to have been *reduced* into the tensor field $\boldsymbol{G}$. Equation D.12 tells nothing about the size of the different subblocks. It can happen that the size of the smallest block equals the size of the complete matrix. Then the tensor field is *irreducible* and their transformation matrices form an *irreducible representation* of the rotation group R_3.

Cartesian tensor fields of rank 2 are reducible. Their 9×9 transformation matrices can be proven to have a block form consisting out of a 5×5-block, a 3×3-block and a 1×1-block. If a tensor field of rank 2 is described by the functions g_i yielding the block form, then under a rotation of XYZ the first 5 components of a new tensor are linear combinations of the first 5 components of an old tensor. The same happens for components number 6 to 8, while component number 9 remains unchanged. To put it in other words: the transformation leaves a 5-dimensional, 3-dimensional and 1-dimensional subspace invariant.

[4] In mathematical language this means the tensor field defined by f_i can be transformed by a unitary transformation into the tensor field defined by g_i.

D.3 Spherical tensors in 3-dimensional space

We now leave the cartesian tensor fields for a while and define spherical tensor fields. For a spherical tensor field of rank n we need only $2n+1$ defining functions f_i. Every point in space – now preferably described by spherical coordinates $(r,\,\theta,\,\phi)$ – is associated to an object with $2n+1$ components:

$$(r,\,\theta,\,\phi) \mapsto \begin{cases} f_1(r,\,\theta,\,\phi) \\ f_2(r,\,\theta,\,\phi) \\ \dots \\ f_{2n+1}(r,\,\theta,\,\phi) \end{cases} \Longleftrightarrow \begin{cases} f_n^n(r,\,\theta,\,\phi) \\ f_{n-1}^n(r,\,\theta,\,\phi) \\ \dots \\ f_q^n(r,\,\theta,\,\phi) \\ \dots \\ f_{-n}^n(r,\,\theta,\,\phi) \end{cases} \Longleftrightarrow \begin{cases} a_n^n \\ a_{n-1}^n \\ \dots \\ a_q^n \\ \dots \\ a_{-n}^n \end{cases} \tag{D.13}$$

Not every such an object is a spherical tensor. The defining property is that it should behave in the following way under a rotation of XYZ:

$$\begin{aligned} \left[\, f_n^n(r',\,\theta',\,\phi')\; f_{n-1}^n(r',\,\theta',\,\phi') \cdots f_{-n+1}^n(r',\,\theta',\,\phi')\; f_{-n}^n(r',\,\theta',\,\phi') \right] &= \\ \left[\, f_n^n(r,\,\theta,\,\phi)\; f_{n-1}^n(r,\,\theta,\,\phi) \cdots f_{-n+1}^n(r,\,\theta,\,\phi)\; f_{-n}^n(r,\,\theta,\,\phi) \right] &\cdot \\ \begin{bmatrix} \dots & \dots & \dots \\ \dots & \dots & \dots \\ \dots & D_{q'q}^n(\alpha,\,\beta,\,\gamma) & \dots \\ \dots & \dots & \dots \\ \dots & \dots & \dots \end{bmatrix} & \end{aligned} \tag{D.14}$$

or

$$f_q^n(r',\,\theta',\,\phi') = \sum_{q'=-n}^{n} \mathcal{D}_{q'q}^n(\alpha,\beta,\gamma)\, f_{q'}^n(r,\,\theta,\,\phi) \tag{D.15}$$

Here we follow the usual convention that the components of spherical tensors are given as $1 \times (2n+1)$ row-matrices (and not as column matrices). The angles α, β and γ are the Euler angles which specify the orientation of the new axis system with respect to the old one (see Appendix F for the exact definition used in this book). The $\mathcal{D}_{q'q}^n(\alpha,\,\beta,\,\gamma)$ are matrix elements of the Wigner rotation matrix $\mathcal{D}^n$ of order $2n+1$, which is a $(2n+1)$-dimensional *irreducible* representation of the rotation group R^3. Symmetry properties and explicit expressions for these matrix elements are given in Appendix H.

As for cartesian tensor fields, one has here scalar fields (rank 0), vector fields (rank 1) and tensor fields (rank ≥ 2). Note that from rank 2 on, a spherical tensor field has less components than a cartesian tensor field of the same rank. Moreover, spherical tensor fields can also be defined for n being an integer multiple of 1/2. An example of a spherical tensor field of rank n (integer) is the following one:

$$a_q^n = f_q^n(r,\,\theta,\phi) = \sqrt{\frac{4\pi}{2n+1}}\, r^n\, Y_n^q(\theta,\,\phi) \tag{D.16}$$

The Y_q^n are the spherical harmonics defined in appendix G. We will use this for physics important tensor field as an example on the following pages[5]. The special property which makes spherical tensors interesting, is their irreducibility.

D.4 Cartesian form of spherical tensor fields

Because of their irreducibility, the 5, 3 and 1 components of a cartesian tensor field are equivalent to a spherical tensor field of rank 2 (5 components), rank 1 (3 components) and rank 0 (1 component), which make 9 components in total. It is easier to describe a physical property by these 3 spherical tensor fields than by the single cartesian one, because of the lower dimensionalities involved and because of the easy transformation properties by Wigner matrices.

In this course we work a lot with spherical tensor fields, especially of rank 2. Sometimes we will express them by means of spherical harmonics (equation D.16) and sometimes by their 'cartesian form'. The latter is an explicit expression for a *spherical* tensor field in a *cartesian* axis system, and must not be confused with a cartesian tensor field. The relation between the $2n+1$ spherical components a_q^n and the $2n+1$ components a_i of the cartesian form are:

– Scalar field (rank 0):

$$a_1 = a_0^0 \tag{D.17}$$

For the example of equation D.16 (n=0), $a_0^0 = 1$, and hence $a_1 = 1$.

– Vector field (rank 1):
Being given a spherical tensor field of rank 1, the corresponding 3 components of its cartesian form are found by:

$$\begin{aligned} a_1 &= \frac{\sqrt{2}}{2}\left(a_{-1}^1 - a_{+1}^1\right) \\ a_2 &= \frac{\sqrt{2}}{2} i\left(a_{-1}^1 + a_{+1}^1\right) \\ a_3 &= a_0^1 \end{aligned} \tag{D.18}$$

Check that for the example given in equation D.16, the cartesian components $(a_1,\, a_2,\, a_3)$ are $(x,\, y,\, z)$: for rank 1, this example is the position field we defined earlier. The inverse relations are given by:

$$a_{-1}^1 = \frac{1}{\sqrt{2}}\left(a_1 - i a_2\right)$$

[5] See also Sec. 2.1, equation 2.6 for the use of this tensor field in physics.

$$a^1_{+1} = -\frac{1}{\sqrt{2}}(a_1 + ia_2) \qquad \text{(D.19)}$$
$$a^1_0 = a_3$$

- Tensor field of rank 2:
  For spherical scalar and vector fields, the cartesian form has as many components as the spherical form. For the cartesian form of a spherical tensor field of rank 2 the cartesian form will have 9 components in stead of the expected 5, but relations between these components will reduce the number of free choices again to 5. Indeed, the cartesian form of a tensor field of rank 2 is given by *traceless*[6] *symmetric matrices*. The cartesian form then looks like:

$$\boldsymbol{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{bmatrix} \qquad \textit{with } Tr(\boldsymbol{A}) = a_{11} + a_{22} + a_{33} = 0 \qquad \text{(D.20)}$$

Being given a spherical tensor field of rank 2, the corresponding 6 components of its cartesian form (only 5 of them are independent) are found by:

$$\begin{aligned} a_{11} &= \frac{\sqrt{6}}{2}\left(a^2_2 + a^2_{-2}\right) - a^2_0 \\ a_{22} &= -\frac{\sqrt{6}}{2}\left(a^2_2 + a^2_{-2}\right) - a^2_0 \\ a_{33} &= 2a^2_0 \end{aligned} \qquad \text{(D.21)}$$

$$\begin{aligned} a_{12} &= -\frac{\sqrt{6}}{2} i\left(a^2_2 - a^2_{-2}\right) \\ a_{13} &= -\frac{\sqrt{6}}{2}\left(a^2_1 - a^2_{-1}\right) \\ a_{23} &= \frac{\sqrt{6}}{2} i\left(a^2_1 + a^2_{-1}\right) \end{aligned} \qquad \text{(D.22)}$$

Verify that with the example of equation D.16 you find in this way the *quadrupole tensor* Q, with $Q_{ij} = 3x_i x_j - r^2\delta_{ij}$:

$$Q = \begin{bmatrix} 3x^2 - r^2 & 3xy & 3xz \\ 3xy & 3y^2 - r^2 & 3yz \\ 3xz & 3yz & 3z^2 - r^2 \end{bmatrix} \qquad \text{(D.23)}$$

The inverse relations are:

$$a^2_0 = \frac{1}{2} a_{33}$$

[6] The trace of a rectangular matrix is the sum of its diagonal elements. A traceless matrix has zero trace.

$$a^2_{\pm 1} = \mp \frac{1}{\sqrt{6}} (a_{13} \pm i a_{23}) \qquad \text{(D.24)}$$
$$a^2_{\pm 2} = \frac{1}{2\sqrt{6}} (a_{11} - a_{22} \pm 2 i a_{12})$$

There is a close relationship between the reduction of a cartesian tensor (3×3-matrix) and matrix algebra. It can be proven that any 3 × 3-matrix can be written as the sum of i) a traceless symmetric matrix, ii) an antisymmetric matrix (which is automatically traceless) and iii) a multiple of the unity matrix with the trace of the original matrix. These 3 matrices have 5, 3 and 1 degrees of freedom respectively and can be considered to be cartesian forms of spherical tensors of rank 2, 1 and 0 (for rank 2 this is indeed the cartesian form we introduced above, for rank 1 and rank 0 we used simpler cartesian forms).

D.5 The dot product

The dot product between two cartesian tensors of rank n $\boldsymbol{A}$ and $\boldsymbol{B}$ is defined as:

$$\boldsymbol{A} \cdot \boldsymbol{B} = a_1 b_1 + a_2 b_2 + \ldots + a_{3^n} b_{3^n} \qquad \text{(D.25)}$$

For rank 1 this is the familiar dot product between vectors. The dot product is a scalar quantity: it does not change upon a rotation of XYZ. The dot product between two spherical tensors of rank n $\boldsymbol{A}^n$ and $\boldsymbol{B}^n$ is defined as:

$$\boldsymbol{A}^n \cdot \boldsymbol{B}^n = \sum_{q=-n}^{n} A^{n^*}_q B^n_q \qquad \text{(D.26)}$$

For the tensors we will encounter in this course, this is equivalent to:

$$\boldsymbol{A}^n \cdot \boldsymbol{B}^n = \sum_{q=-n}^{n} (-1)^q A^n_{-q} B^n_q \qquad \text{(D.27)}$$

Verify by equation D.19 that both definitions make sense.

If a spherical tensor of rank 2 is given by its cartesian form, then it can be proven that the dot product between two such tensors equals:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{bmatrix} \cdot \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{12} & b_{22} & b_{23} \\ b_{13} & b_{23} & b_{33} \end{bmatrix} = a_{11} b_{11} + a_{12} b_{12} + \ldots + a_{33} b_{33} \qquad \text{(D.28)}$$

Do not confuse this notation with a matrix product!

D.6 Principal axis system

When considering a spherical tensor of any rank, corresponding to a particular point in the three-dimensional space[7], one can ask whether an axis system X'Y'Z' exists in which this tensor is expressed easier – this means: with as many components as possible being zero – then in any other system. Such an axis system is called a *principal axis system (PAS)* for that tensor.
For a scalar this question is irrelevant. For a vector, many principal axis systems exist. This can easily be visualized for a position field: as long as one of the axes is parallel to a particular position vector, only the component along that axis is non-zero in the cartesian form. As a practical convention, the Z-axis is chosen parallel to the vector (X- and Y-axes do not matter). A vector $\boldsymbol{A}$ with length A has in its PAS the following cartesian and spherical components:

$$\begin{array}{ll} a_x = 0 & a_0^1 = A \\ a_y = 0 & a_1^1 = 0 \\ a_z = A & a_{-1}^1 = 0 \end{array} \tag{D.29}$$

A principal axis system for a spherical tensor of rank 2 is an axis system in which the 3×3-matrix of the cartesian form of this tensor is diagonal (for symmetric matrices this is always possible). Once XYZ is rotated such that the matrix is diagonal, the axes are renamed by convention such that $|a_{zz}| \geq |a_{yy}| \geq |a_{xx}|$. The cartesian form in the PAS is now:

$$\begin{bmatrix} a_{xx} & 0 & 0 \\ 0 & a_{yy} & 0 \\ 0 & 0 & a_{zz} \end{bmatrix} \tag{D.30}$$

The trace of matrix is invariant upon rotation of the axis system and therefore remains zero. It means we have only 2 degrees of freedom in D.30. Because there are also 3 degrees of freedom needed to specify the PAS with respect to the original XYZ (e.g. 3 Euler angles), we retain the 5 degrees of freedom expected for a spherical tensor of rank 2. From D.24 we see that the spherical components in the PAS are:

$$\begin{aligned} a_0^2 &= \frac{1}{2}\, a_{zz} \\ a_{\pm 1}^2 &= 0 \\ a_{\pm 2}^2 &= \frac{1}{2\sqrt{6}}\, (a_{xx} - a_{yy}) \end{aligned} \tag{D.31}$$

Because $a_{+2}^2 = a_{-2}^2$ also in the spherical components only 2 apparent degrees of freedom are left. Again because of the 3 degrees of freedom needed to specify the PAS, we find back the 5 degrees of freedom which are needed.

[7] A PAS will be a property of a particular *tensor*, not of the entire tensor *field*.

D.7 Summarizing exercise

To check your ability to work with coordinate transformations, spherical tensors and Wigner rotation matrices, you might verify – by using spherical tensors – the statement which is proven in Appendix F by Cartesian arguments:

Take the (cartesian) vector (1, 0, 0) in an 'old' axis system. Now consider a 'new' axis system, which is defined by the Euler angles (90°, 90°, 90°) with respect to the old one. From Appendix F, you know that the coordinates of this vector in the new axis system are (−1, 0, 0). Show that this is true by the following chain of arguments:

- Transform the original vector into a spherical tensor of rank 1 (equation D.19).
- Write the explicit Wigner rotation matrix for this case (Appendix H).
- Transform the spherical tensor into the new axis system (equation D.14).
- Transform the resulting spherical tensor back into a cartesian vector (equation D.18).

If all the formulae in this book are consistent with each other[8] and if you didn't make mistakes, you should find (−1, 0, 0) in the end.

[8] Which is a never-ending source of sleepless nights for the authors of this text…