

## Multipole expansions

We should be getting used to the idea that we can expand complex functions in terms of simpler functions. In calculus, we learn about Taylor expansions:

For  $f(x)$  near  $x=a$ ,

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)(x-a)^2}{2!} + \frac{f'''(a)(x-a)^3}{3!} + \dots$$

which will converge more or less quickly depending on  $f(x)$  and  $a$ .

Popular Taylor series include the trig functions:

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \dots$$

$$\cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \dots$$

You've also seen Fourier series expansions - re-expressions of complicated functions in terms of sines & cosines:

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos(nx) + \sum_{n=1}^{\infty} b_n \sin(nx)$$

And there are many, many other ways to express a function in some basis. You're probably learning some general approaches in quantum right now, involving bras & kets.

In electrostatics, the basic potential function for a point at the origin goes like  $1/r$ :

$$V_{\text{point}}(r) = Kq/r$$

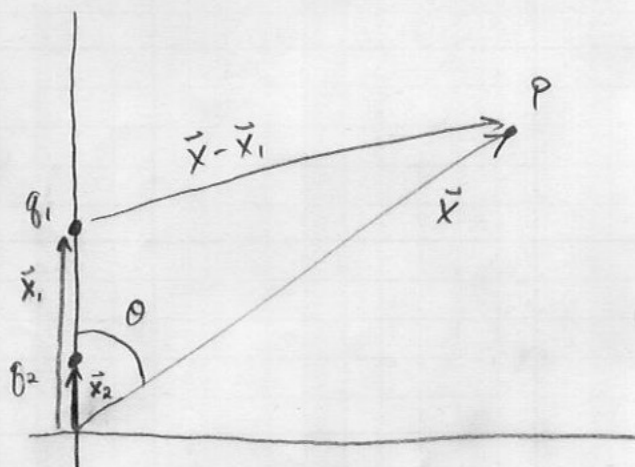
More complicated systems (including points off the origin) make more complicated potentials, but if we're decently far away we'll be able to expand  $V(\vec{x})$  as a reciprocal power series:

$$V(\vec{x}) = \frac{\text{thing}_1}{r} + \frac{\text{thing}_2}{r^2} + \frac{\text{thing}_3}{r^3} + \dots$$

We call this the multipole expansion, for reasons that will become apparent. Note that conventionally, we set this up so that  $r$  is actually the radial coordinate  $r$ , not  $|\vec{x}-\vec{x}'|$ .

Let's start with a simple example: Two point charges of different sizes  $q_1$  and  $q_2$  at locations  $\vec{x}_1$  and  $\vec{x}_2$ .

I'll let the  $\theta=0$  axis lay along the line that includes the charges:



We want to find the voltage at point  $P$ , which is at some arbitrary angle  $\theta$ .

The exact expression is:

$$V(\vec{x}) = \frac{Kq_1}{|\vec{x}-\vec{x}_1|} + \frac{Kq_2}{|\vec{x}-\vec{x}_2|}$$

Let's use the law of cosines to expand the denominators:

$$\frac{1}{|\vec{x}-\vec{x}_1|} = \frac{1}{\sqrt{r^2 - 2r r_1 \cos\theta + r_1^2}}$$

where  $|\vec{x}| = r$ ,  $|\vec{x}_1| = r_1$ , and

we're assuming we're pretty far away, so  $r \gg r_1, r_2$ , and the  $\theta$ s for the different sources are about the same.

Pulling out a  $1/r$ ,

$$\frac{1}{|\vec{x}-\vec{x}_1|} = \frac{1}{r} \frac{1}{\sqrt{1 + \frac{r_1^2 - 2r r_1 \cos\theta}{r^2}}} = \frac{1}{r} \left( 1 - \frac{r_1^2 - 2r r_1 \cos\theta}{r^2} \right)^{-1/2}$$

The thing in the parentheses is of the form  $(1 + \text{small})^n$ , which is ripe for a binomial expansion. We know

$$(1+x)^{-1/2} \approx 1 - \frac{1}{2}x + \frac{3}{8}x^2 - \text{higher order terms}$$

Keeping those first three terms, we get

$$\frac{1}{r} \left[ 1 + \frac{1}{2} \frac{2r r_1 \cos\theta - r_1^2}{r^2} + \frac{3}{8} \left( \frac{4r^2 r_1^2 \cos^2\theta - 4r r_1^3 \cos\theta + r_1^4}{r^4} \right) \right] \quad (1)$$

$$= \frac{1}{r} + \frac{r_1 \cos\theta}{r^2} - \frac{r_1^2}{2r^3} + \frac{3}{2} \frac{r_1^2 \cos^2\theta}{r^3} - \frac{3}{2} \frac{r_1^3 \cos\theta}{r^4} + \frac{3r_1^4}{8r^5}$$

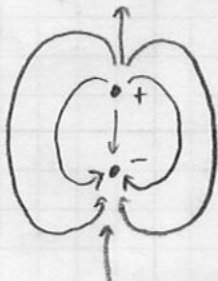
Let's drop all terms higher order than  $1/r^3$ , and also include  $q_2$ . Then our three-term multipole expansion of this potential becomes:

$$V(r, \theta) = k \left[ \frac{q_1 + q_2}{r} + \frac{(q_1 r_1 + q_2 r_2) \cos\theta}{r^2} + \frac{q_1 r_1^2 + q_2 r_2^2}{2r^3} (3\cos^2\theta - 1) \right]$$

These terms are referred to as the monopole, dipole, and quadrupole terms, respectively. Physically, we interpret them as follows:

A point charge (a monopole) makes a voltage that goes like  $1/r$  (and a field like  $1/r^2$ ). A system of charges has a term in its voltage that goes like  $kq_{\text{tot}}/r$ , where  $q_{\text{tot}}$  is the total charge of the system.

A standard dipole is two charges of the same magnitude <sup>(q)</sup> and opposite sign, separated by some distance  $d$ :



The net charge of a true dipole is zero, so far away it has no  $1/r$  potential. It does, however, have some leftover  $1/r^2$  potential. The equal & opposite charges screen away some, but not all, of  $V$ .

The dipole moment of this pair is defined as

$$\vec{p} \equiv q\vec{d}$$

And its potential far away looks like

$$V(\vec{x}) = \frac{\vec{p} \cdot \vec{r}}{4\pi\epsilon_0 r^2}$$

$$V \propto 1/r$$

$$E \propto 1/r^3$$

And a general definition for the dipole moment of any charge is  $\vec{p} = q\vec{x}'$ , where  $\vec{x}'$  is the location of the charge.

So something that looks like  $\frac{q_1 r_1 \cos\theta}{r^2}$  is exactly a

dipole potential. Note that most molecules are polar to some degree. You can find tables of dipole moments for them easily enough.

A quadrupole is two dipoles back to back in such a way that their dipole moments cancel, as do their voltages that go like  $1/r^2$ , leaving a  $1/r^3$  remainder

+o     o-      $V \propto 1/r^3, \quad E \propto 1/r^4$

-o     o+     We've used quads in field session, in particular the mass spectrometry unit.

Deriving an expression for  $V$  for a quadrupole takes a bit more work but is essentially what we did before. For now, take my word for it that the third term in (1) is a quadrupole-like term.

So now we can see what a multipole expansion is, physically. We're expanding a potential function in a basis, where the elements of the basis include the kinds of field made by a monopole, a dipole, a quadrupole and so on.

What we did with the two charge system above is generalizable. For any localized charge distribution, if we're far from the source,

$$V(\vec{x}) \approx k \left[ \frac{Q_{\text{net}}}{r} + \frac{\hat{r} \cdot \vec{p}}{r^2} + \frac{\hat{r} \cdot \overleftrightarrow{Q} \cdot \hat{r}}{r^3} \right]$$

where  $Q_{\text{net}}$  is the monopole moment of the whole system,  $Q_{\text{net}} = \int \rho(\vec{x}') d^3x'$   
 $\vec{p}$  is the dipole moment of the system,  $\vec{p} = \int \vec{x}' \rho(\vec{x}') d^3x'$

And  $\vec{Q}$  is the quadrupole moment,  $\vec{Q} = \frac{1}{2} \int (3\vec{x}\vec{x} - r^2\vec{I}) \rho(\vec{x}) d^3x$

You may well be wondering what the hell I just wrote.

The monopole moment needs no orientation. It's a scalar. ( $Q$ )

A dipole moment has orientation. It's a vector. ( $\vec{p}$ )

And a quadrupole has a higher degree of ordering, and is a second-rank tensor. I'm indicating those with a double headed arrow.

A rank-2 tensor is basically a matrix that obeys certain additional rules, which we won't worry about here.

$\vec{I}$  is the identity tensor, which in 2D is  $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Now,  $V$  is always a scalar, never a tensor or a vector. You'll notice the expansion of  $V$  includes an  $\hat{r} \cdot \vec{p}$ , where the dot product picks out the component of  $\vec{p}$  that lies along our observation axis. Similarly, we pick out elements of  $\vec{Q}$ .

An example: I'll calculate  $\hat{r} \cdot \vec{I} \cdot \hat{r}$ . It's just representing matrix operations. Let's do it in 2D to make it easier.

We can write  $\hat{r} = \begin{pmatrix} r_x/r \\ r_y/r \end{pmatrix}$  (with  $r_x^2 + r_y^2 = r^2$ )

Then  $\vec{I} \cdot \hat{r} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} r_x/r \\ r_y/r \end{pmatrix} = \begin{pmatrix} r_x/r \\ r_y/r \end{pmatrix}$

And  $\hat{r} \cdot (\vec{I} \cdot \hat{r}) = \begin{pmatrix} r_x/r & r_y/r \end{pmatrix} \begin{pmatrix} r_x/r \\ r_y/r \end{pmatrix} = \frac{r_x^2}{r^2} + \frac{r_y^2}{r^2} = 1$

$\Rightarrow \hat{r} \cdot \vec{I} \cdot \hat{r} = 1$  Which makes an odd kind of sense, if you stop and think about it.

One last fun fact:  $V(\vec{x})$  does change when you change your origin. But that's okay as long as  $-\nabla V$  doesn't.

Storytime with Pat: Electrostatics, industrial London, & coal.