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 $1/r$:

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

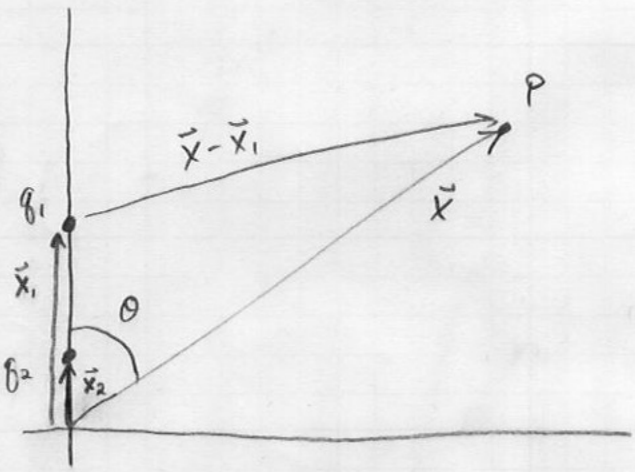
More complicated systems (including points off the origin) make more complicated potentials, but if we're decently far away we'll be able to expand $V(\vec{x})$ as a reciprocal power series:

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

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

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 θ

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:

$$\frac{1}{|\vec{x}-\vec{x}_1|} = \frac{1}{\sqrt{r^2 - 2rr_1\cos\theta + r_1^2}}$$

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 θs for the different sources are about the same.

Pulling out a $1/r$,

$$\frac{1}{|\vec{x}-\vec{x}_1|} = \frac{1}{r}\frac{1}{\sqrt{1 - \frac{2rr_1\cos\theta + r_1^2}{r^2}}} = \frac{1}{r}\left(1 - \frac{2rr\cos\theta + r_1^2}{r^2}\right)^{-1/2}$$

The thing in the parentheses is of the form $(1 + \text{small})^{\wedge}$, 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

$$\frac{1}{r}\left[1 + \frac{1}{2}\,\frac{2rr_1\cos\theta - r_1^2}{r^2} + \left(\frac{4r^2r_1^2\cos^2\theta - 4rr_1^3\cos\theta + r_1^4}{r^4}\right)\right] \qquad (1)$$

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

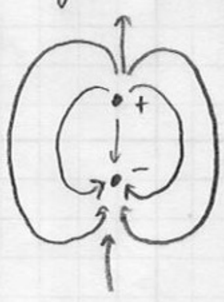
Let's drop all terms higher order than $1/r^3$, and also include q_2. Then our three-term multipole expansion of this potential becomes:

$$V(r,\theta) = k\left[\frac{q_1+q_2}{r} + \frac{(q_1r_1 + q_2r_2)\cos\theta}{r^2} + \frac{q_1r_1^2 + q_2r_2^2}{2r^3}\left(3\cos^2\theta - 1\right)\right]$$

These terms are referred to as the <u>monopole</u>, <u>dipole</u>, and <u>quadrupole</u> 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_{tot}/r, where q_{tot} is the total charge of the system.

A standard <u>dipole</u> is two charges of the same magnitude (q) 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

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

$V \propto 1/r^2$

$E \propto 1/r^3$

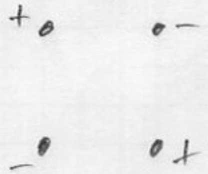
And its potential far away looks like

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

And a general definition for the dipole moment of any charge is $\vec{p} \equiv q\vec{x}'$, 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 <u>quadrupole</u> 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



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

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,

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

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

$\vec{p}$ is the dipole moment of the system, $\vec{p} = \int \vec{x}'\,\rho(\vec{x}')\,d^3x'$

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

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.

$\overleftrightarrow{I}$ 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 $\overleftrightarrow{Q}$.

An example: I'll calculate $\hat{r}\cdot\overleftrightarrow{I}\cdot\hat{r}$. 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 $\overleftrightarrow{I}\cdot\hat{r} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} r_x/r \\ r_y/r \end{pmatrix} = \begin{pmatrix} r_x/r \\ r_y/r \end{pmatrix}$

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

$\Rightarrow \boxed{\hat{r}\cdot\overleftrightarrow{I}\cdot\hat{r} = 1}$ 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 $-\vec{\nabla}V$ doesn't.

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