Lecture 4: 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 $x = a$,

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

which will converge more or less quickly depending of f and a. Popular Taylor series include the trig functions:

$$\begin{cases} \sin(x) & = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \cdots \\ \cos(x) & = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \cdots \end{cases}$$

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

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

And there are many, many other ways to express a function in some basis. You've probably been learning about some general approaches in quantum right now (involving bras and kets).

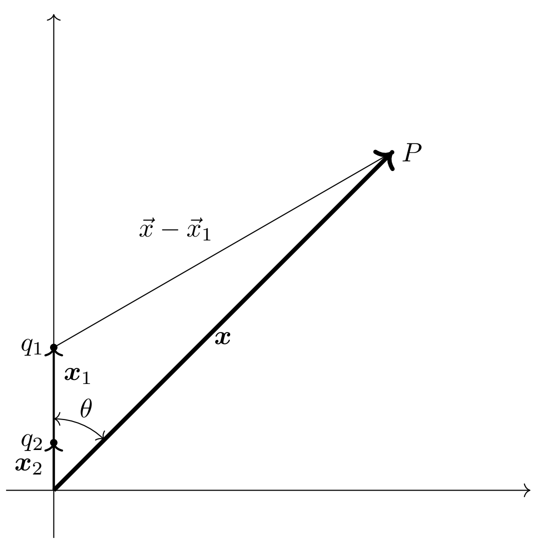
In electrostatics, the basic potential function for a point at the origin goes like $1/r$:

$$V_{\text{point}} = \frac{k\ q}{r}$$

More complicated systems (including points charges not situated at the origin) make more complicated potentials, but if we're decently far away we'll be able to expand $V(\boldsymbol{x})$ as a reciprocal power series:

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

We call this the *multipole expansion*, for reasons that will become apparent. By convention, we set this up so that r is actually the spherical radial coordiate r, not $|\boldsymbol{x} - \boldsymbol{x'}|$.
Let's start with a simple example: two point charges of different sizes q_1 and q_2 at locations $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$. 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

$$V(\boldsymbol{x}) = \frac{k\ q_1}{|\boldsymbol{x} - \boldsymbol{x}_1|} + \frac{k\ q_2}{|\boldsymbol{x} - \boldsymbol{x}_2|}$$

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

$$\frac{1}{|\boldsymbol{x}-\boldsymbol{x}_1|} = \frac{1}{\sqrt{r^2 - 2rr_1\cos\theta + r_1^2}} \qquad \text{where } |\boldsymbol{x}| = r \quad \text{and} \quad |\boldsymbol{x}_1| = r_1.$$

We're assuming we're pretty far away so $r \gg r_1 + r_2$, and the angles θ for the sources are about the same. Pulling out an r,

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

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

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

Keeping those first three terms, we get

$$\begin{aligned}\frac{1}{|\boldsymbol{x}-\boldsymbol{x}_1|} = \frac{1}{r}\left(1 - \frac{r_1^2 - 2rr_1\cos\theta}{r^2}\right)^{-1/2} &= \frac{1}{r}\left[1 + \frac{1}{2}\frac{2rr_1\cos\theta - r_1^2}{r^2} + \frac{3}{8}\left(\frac{4r^2r_1^2\cos^2\theta - 4rr_1^3\cos\theta + r_1^4}{r^4}\right)\right] \\ &= \frac{1}{r} + \frac{r_1\cos\theta}{r^2} - \frac{r_1^2}{2r^3} + \frac{3}{2}\frac{r_1^2}{r^3}\cos^2\theta - \frac{3}{2}\frac{r_1^3}{r^4}\cos\theta + \frac{3}{8}\frac{r_1^4}{r^5}\end{aligned}$$

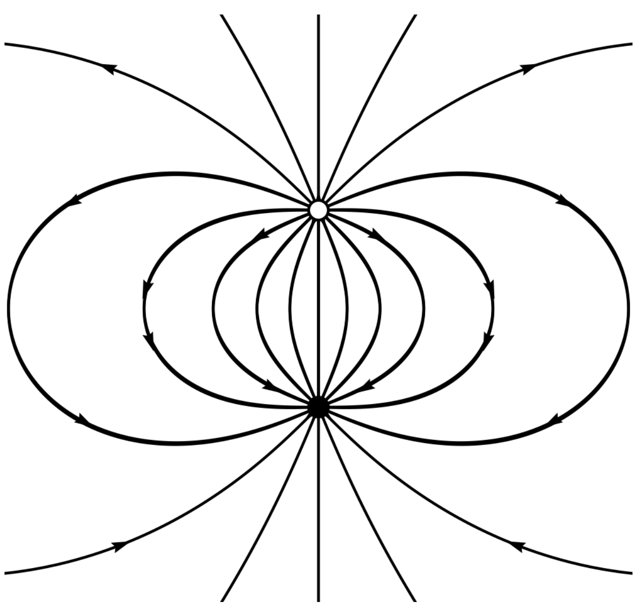
Let's drop all terms higher order than $1/r^3$, and also include q_2. Then our three-term multipole expansion of this potential becomes

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

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 that goes like $1/r^2$). A system of charges has a term in its voltage that goes like $\dfrac{k\ q_{\text{total}}}{r}$, where q_{total} is the total charge of the system.

A standard dipole 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 and opposite charges screen away some, but not all of V.

The dipole moment of this pair is defined as

$$\boldsymbol{p} \equiv q\boldsymbol{d},$$

And its potential far away looks like

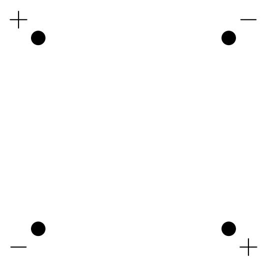
$$V(\boldsymbol{x}) = \frac{\boldsymbol{p}\cdot\hat{\boldsymbol{r}}}{4\pi\epsilon_o}$$

And a general definition for the dipole moment of any charge system is

$$\boldsymbol{p} \equiv q\boldsymbol{x'},$$

where $\boldsymbol{x'}$ is the location of the charge. So something that looks like $\dfrac{q_1 r_1 \cos\theta}{r^2}$ is exactly a dipole potential. Note that most molecules are polar to some degree. You can also find tables of dipole moments easily enough.

A quadrupole is two dipole 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.



$V \propto \frac{1}{r^3}, \qquad E \propto \frac{1}{r^4}$

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,

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

where Q_{net} is the monopole moment of the whole system: $Q_{\text{net}} = \displaystyle\int \rho(\boldsymbol{x})d^3x$, $\boldsymbol{p}$ is the dipole moment of the system, $\boldsymbol{p} = \displaystyle\int \boldsymbol{x'}\rho(\boldsymbol{x'})d^3x'$.
And $\overleftrightarrow{Q}$ is the quadrupole moment: $\overleftrightarrow{Q} = \dfrac{1}{2}\displaystyle\int \left(3\boldsymbol{x}\boldsymbol{x} - r^2\overleftrightarrow{I}\right)\rho(\boldsymbol{x})\ d^3x$.

You may be wondering what the hell I just wrote.
The monopole moment needs no orientation. It's a scalar. A dipole moment has orientation. It's a vector. 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 indentity tensor, which in two-dimensions 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 $\hat{\boldsymbol{r}}\cdot\boldsymbol{p}$, where the dot product "picks out" the component of $\boldsymbol{p}$ that lies along our observation axis. Similarly, we pick out elemnts of $\overleftrightarrow{Q}$.

An example: I'll calculate $\hat{\boldsymbol{r}}\cdot\overleftrightarrow{I}\cdot\hat{\boldsymbol{r}}$. It's nothing more than matrix operations. Let's do it in 2D to make it easier.
We can write $\hat{\boldsymbol{r}} = \begin{pmatrix} r_x/r \\ r_y/r \end{pmatrix}$, with $r_x^2 + r_y^2 = r^2$. Then

$$\overleftrightarrow{I} \cdot \hat{\boldsymbol{r}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} r_x/r \\ r_y/r \end{pmatrix} = \begin{pmatrix} r_x/r \\ r_y/r \end{pmatrix}.$$

And

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

So that means that $\hat{\boldsymbol{r}} \cdot \overleftrightarrow{I} \cdot \hat{\boldsymbol{r}} = 1$, which makes an odd kind of sense, if you stop and think about it.
One last fun fact: $V(\boldsymbol{x})$ *does not* change when you change your origin. But that's okay as long as $-\nabla V$ doesn't.

Storytime with Pat

Electrostatics, industrial London, and coal.