

Details on Problem 7-31

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The formula for $1/r_{12}$ given by McQuarrie and Simon in problem 7-31 is exact, but its derivation is not at all obvious. At least, the way Shervin and I found to derive it¹ is not at all obvious; maybe someone else has a smoother way! However, it is instructive, and we'd like to show you that we don't just pull these things out of our thin air.

The main procedure we're going to follow is the following:

$$\begin{aligned} \frac{1}{r_{12}} &\rightarrow \frac{1}{\sqrt{r_>^2 + r_<^2 - 2r_>r_<\cos(\gamma)}} \rightarrow \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} P_l(\cos(\gamma)) \\ &\rightarrow \sum_{l=0}^{\infty} \sum_{m=-l}^l \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_l^m(\theta_1, \phi_1) Y_l^{m*}(\theta_2, \phi_2) \end{aligned}$$

Using the Law of Cosines

Hopefully, you remember the Law of Cosines from a previous geometry or trigonometry class. It says, quite simply, that given the picture in figure 1, we have the relation

$$r_{12} = \sqrt{r_1^2 + r_2^2 - r_1 r_2 \cos(\gamma)}$$

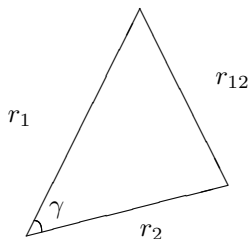


Figure 1: The Law of Cosines

Note that in the expression for r_{12} , it doesn't matter whether r_1 or r_2 is larger; either way we get:

$$r_{12} = \sqrt{r_<^2 + r_>^2 - 2r_<r_>\cos(\gamma)}$$

¹I'm overstating by calling this a "derivation" — the second step is lacking in rigor. If I figure out a way to make it more rigorous, I'll update this.

So that directly gives us:

$$\frac{1}{r_{12}} = \frac{1}{\sqrt{r_{<}^2 + r_{>}^2 - 2r_{<}r_{>} \cos(\gamma)}} \quad (1)$$

Obtaining a Taylor Expansion

We'll continue from equation (1) by making the two-variable system into a one-variable system, which we'll be able to Taylor-expand.

$$\frac{1}{\sqrt{r_{>}^2 + r_{<}^2 - 2r_{>}r_{<} \cos(\gamma)}} = \frac{1}{r_{>} \sqrt{1 + \frac{r_{<}^2}{r_{>}^2} - 2\frac{r_{<}}{r_{>}} \cos(\gamma)}}$$

Now, we make the variable substitution $x = \frac{r_{<}}{r_{>}}$:

$$\frac{1}{r_{12}} = \frac{1}{r_{>}} \frac{1}{\sqrt{1 + x^2 - 2x \cos(\gamma)}}$$

Now we'll begin to Taylor-expand the second term in that product. Since we'll be taking the Taylor expansion to infinity, this is not actually an approximation; it is exact.² As a reminder, the Taylor series around zero (also known as the MacLaurin series) is the expansion:

$$f(x) = \sum_{l=0}^{\infty} x^l f^{(l)}(0)$$

As you can probably already see, the goal of this step will therefore be to show that

$$\left. \frac{d^l}{dx^l} \frac{1}{\sqrt{1 + x^2 - 2x \cos(\gamma)}} \right|_{x=0} = P_l(\cos(\gamma))$$

Here's where we cheat: instead of actually showing this, we're just going to show it for the first few, and then say, "uh, it works for $l = 0$, $l = 1$, and $l = 2$, so obviously it works for everything else!" and hope that no one notices. This is *bad math*, but until I figure out something prettier, it's all I can give you.

So this will give us

$$\begin{aligned} \frac{1}{r_{12}} &= \frac{1}{r_{<}} \sum_{l=0}^{\infty} x^l P_l(\cos(\gamma)) \\ &= \sum_{l=0}^{\infty} \frac{r_{<}^l}{r_{>}^{l+1}} P_l(\cos(\gamma)) \end{aligned}$$

which is the second result in the sketch given at the beginning.

²Strictly speaking, we need to show that this function converges over a given radius of convergence. We'll leave that to a complex analysis class, shall we?

The Addition Relation for Spherical Harmonics

The last step of the derivation is given directly what is known as the “addition theorem for spherical harmonics:”

$$P_n(\cos(\gamma)) = \frac{4\pi}{2n+1} \sum_{m=-n}^n Y_l^m(\theta_1, \phi_1) Y_l^{m*}(\theta_2, \phi_2)$$

where the directions (θ_1, ϕ_1) and (θ_2, ϕ_2) are separated by the angle γ .

I won't go through the details of the derivation, which can be found in Arfken and Weber's "Mathematical Methods for Physicists."

Plugging that in, we get the result given by McQuarrie and Simon in exercise 7-31:

$$\frac{1}{r_{12}} = \sum_{l=0}^{\infty} \sum_{m=-l}^l \frac{4\pi}{2l+1} \frac{r_{<}^l}{r_{>}^{l+1}} Y_l^m(\theta_1, \phi_1) Y_l^{m*}(\theta_2, \phi_2)$$