Spherical Harmonics and Matrix Elements

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Problem 1: Let's write a program to visualize the spherical harmonics $Y_l^m(\theta, \phi)$. From lecture, remember that the spherical harmonics are the solutions to the differential equation

$$\hat{\boldsymbol{L}}^2 Y_l^m(\theta, \phi) = \hbar^2 l(l+1) Y_l^m(\theta, \phi). \tag{1}$$

Python already has them included in the `scipy.special` module as the `sph_harmonic` function. Please note that θ and ϕ in this function are defined differently from how it is typically used in spherical coordinates, so take care when implementing it.

(a) You can use `matplotlib` and the 3D-plotting module `mpl_toolkits.mplot3d` to create 3-dimensional plots. First, note that since the spherical harmonics are complex functions, we can't plot them directly. However, it's possible to find a new and real-valued basis which is a superposition of the complex spherical harmonics. Conventionally, the following substitution is done:

$$Y_l^m \to \begin{cases} \sqrt{2}\mathrm{Re}(Y_l^m) & (m > 0) \\ \sqrt{2}\mathrm{Im}(Y_l^m) & (m < 0) \\ Y_l^m & (m = 0) \end{cases} \tag{2}$$

Typically, $|Y_l^m|$ is plotted using Y_l^m or $\mathrm{sign}(Y_l^m)$ as the color (to denote phase). Plot Y_4^4 and Y_4^{-4} in this way. How do they differ from each other? Can you say something general about how Y_l^m and Y_l^{-m} relate?

(b) Plot Y_0^0, Y_1^0, Y_2^0, and Y_3^0. Describe any patterns you see.

Problem 2: Similar to the radial dipole matrix elements, we will investigate the interaction between the angular parts of atomic states.

(a) What is an expression for:

$$\langle n', l', m' | \hat{f}(r) \hat{g}(\theta, \phi) | n, l, m \rangle\,, \tag{3}$$

where $\hat{f}$ and $\hat{f}$ are r- and (θ, ϕ)-dependent operators, resp. Highlight the angular part.

(b) Using the `romb` function from the `scipy.integrate` module, write a <u>function</u> that calculates the angular part of this expression for an arbitrary operator $\hat{g}$. Show that your function gets the correct results for the case where $\hat{g} = 1$. Why would we use the `romb` function over the obvious (simpler) alternative? Be quantitative in your comparison.

(c) Write the position vector operator $\hat{\boldsymbol{r}}$ as a function the spherical harmonics in the Cartesian coordinate system.

(d) Use the program from Problem 1(a) to visualize the angular parts of $\hat{x}$, $\hat{y}$, and $\hat{z}$. Since these operators are Hermitian (and their representation in coordinate space are therefore already real) you shouldn't have to make any substitutions. The results should make sense to you. Why?

(e) Write out the following operators as functions of spherical harmonics:

$$\begin{aligned} \hat{\sigma}_+ &= \tfrac{1}{\sqrt{2}}(\hat{x} + i\hat{y}) \\ \hat{\sigma}_- &= \tfrac{1}{\sqrt{2}}(\hat{x} - i\hat{y}) \\ \hat{\sigma}_0 &= \hat{z} \end{aligned} \tag{4}$$

What do these correspond to?

(f) Calculate the result of Eq. 3 using the operators from Eq. 4 and your program from Problem 2(b). You may choose whatever states you like to illustrate and describe all important behavior.

(g) The atom-light dipole interaction Hamiltonian is $\hat{H} = -e\,\hat{\boldsymbol{r}} \cdot \vec{E}$ where $\vec{E}$ is the electric field of the light. Describe how the work you have done in this problem set is relevant to this interaction.