Tutorial for Mathematica-Sims
"Single Spherical Harmonic" and "Superposition of Two Spherical Harmonics"[*]

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With these simulations (sims), we will explore the properties of spherical harmonics and their superposition. The tutorial is meant for undergraduate and graduate level introductory quantum mechanics courses. It can be used, e.g., for homework, or in-class simulations. We assume that the quantum mechanical treatment of the rigid rotator has been introduced already.

Some Technical Notes:

Before you begin using the sims make sure that you either have Mathematica installed on your computer, or that you have downloaded and installed the free Computable Document Format (CDF) player from the Wolfram website. Once you have installed the software, open a browser that supports 32-bit plugins (Mozilla, Internet Explorer, Safari) and you're ready to begin! Go to

<div align="center">http://jila.colorado.edu/weberlabs/single_ylm.html</div>

or to   http://jila.colorado.edu/weberlabs/sup_ylm.html.

Note that the sims may run a bit slow on older computers or on machines that are not meant for number crunching and fast graphics. We are working on an implementation in HTML5 format that will be better for slower machines.

If you are color vision impaired, you can pick a color scheme that suits your needs. The center of the color bar represents the numerical value zero. Since you will think a lot about the nodal lines in this tutorial, you should pick a color scheme that gives you a sharply defined "zero" color and different colors for negative ("left") and positive ("right") values.

Ready? OK, let's start!

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1. **Single Spherical Harmonic – Static Simulations**

The sim shows the values of a spherical harmonic $Y_\ell^m(\theta,\varphi)$ projected onto the surface of a sphere. The variable B is the rotational constant of a rigid rotator. You can display the real or imaginary part of $Y_\ell^m(\theta,\varphi)$ or its absolute value, $|Y_\ell^m(\theta,\varphi)|^2$.

a. Describe the positions of the nodal lines for all m-values of ℓ=1. Do you think that the positions depend on the value of B? Test your prediction.

b. For ℓ>0, the nodal lines look like circles of latitude and longitude. Formulate a rule for the number of nodal lines forming circles of "latitude" and "longitude" as a function of ℓ and m. You can rotate the sphere in space by clicking/dragging the mouse inside the box showing the coordinate system.

c. Interpret the position of the nodal line for ℓ=1, m=0. Can you relate the nodal line with the motion of a classical particle on a sphere? How is this different for ℓ=1, m=1?

d. Interpret the nodal line structure for ℓ=3, m=0 in the picture of a classical particle moving on the sphere. What changes in your interpretation as you go to ℓ=3, m=1,2 and 3. Draw a schematic vector diagram representing the angular momentum vectors for each of these 4 situations.

e. Display the absolute value of the spherical harmonics. What is the difference in the nodal line structure between the absolute value and the real and imaginary parts? Why is there a difference? Can you rationalize the difference between real and imaginary part using Euler's formula?

f. Recall that atomic p-orbitals have ℓ=1. Do the shapes of the ℓ=1 spherical harmonics represent p orbitals? Are there some that do while others don't?

2. Simulations with Time Dependence

The time dependent part of the sim attributes a phase factor to each spherical harmonic, corresponding to the energy levels of a rigid rotator. It therefore visualizes the wave functions and probability densities belonging to a rigid rotator.

Click on the + sign at the end of the "Relative Time" sliding bar. Note that this part only works well if your computer has the computational power to calculate and display the graphics quickly enough. If the sim seems to run very unsteadily, lower B as much as possible. Explain why this should help, thinking about the difference between H_2 (B = 60.809 cm^{-1}) and N_2 (B = 2.010 cm^{-1}). In addition, click the down arrows until the simulation slows down enough. If all else fails, don't use the "Play" button at all, rather manipulate the slider manually.

a. Run the sim for ℓ=m=0. What do you observe, and why?

b. Run the sim for ℓ=1, m=0, displaying the real part. Can you tell from your observation why the wave function cannot be described with only the real part? Display the absolute value. What do you observe, and why?

c. **Before** you run the sim accordingly, do you expect the plane of the nodal line in the real and imaginary part for ℓ=1, m= ±1 to change with time? Check your prediction by running the sim, and explain the result.

d. **Before** you run the sim accordingly, do you expect the absolute value to change with time? Check your prediction by running the sim, and explain the result.

e. Run the sim with increasing ℓ, but the same m. You have already explored how the spatial distribution of Y_ℓ^m changes in that case (activity 1.d). What else changes, now looking at the time dependence of the function? Explain your observations.

f. Run the sim with constant ℓ and m of your choice (play around with this!), and vary B. Describe your observations and interpret. Think of diatomic molecules like H_2 and N_2 and their moments of inertia.

3. **Superpositions of Spherical Harmonics – Static Simulations**

This time we look at the superpositions of two spherical harmonics. You can choose ℓ and m for the two just like you did earlier for the single $Y_\ell{}^m$ functions. You can add or subtract the two with the "-1/1" selector.

a. Recall activity 1.f. about atomic orbitals. Use superpositions of two ℓ=1 spherical harmonics to create p_x and p_y orbitals. Which linear combinations do you use?

b. Now build the various d orbitals. Which linear combinations do you use to get d(xy), d(xz), d(x^2-y^2) and d(yz)? What do you do to get d(z^2)?

c. Can you construct any hybrid orbitals with this sim? If yes, which ones, and why? Check your prediction.

4. **Superpositions of Spherical Harmonics –Simulations with Time Dependence**

a. Make a superposition of ℓ=0, m=0 and ℓ=1, m=1. Run the time dependence and describe your observation. In particular, look at the absolute of the function. How do you interpret what you see there? How can you explain the difference to what you observed in activity 2.d.?

b. **Before** you run the sim accordingly, predict what changes if you superimpose the two functions in phase vs. out of phase, i.e. you add or subtract the two? Check your prediction by running the sim .

c. How can you change the direction of rotation keeping the same combination of ℓ? What part of the equation displayed at the top of the sim determines the direction of rotation?

d. Repeat the experiment for ℓ=1, m=0 and ℓ=1, m=1. Explain the difference between what you observe here and in activity 4.a. Argue with the expression at the top of the sim.

e. **Before** you run the sim accordingly, predict what happens if you increase ℓ on the second function, keeping the first function as $Y_0{}^0$. Check your prediction by running the sim.