Exploring the Harmonic Oscillator Wave Function Components

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Goal: To provide students with an opportunity to visualize the components of the harmonic oscillator wave functions, combine these components, and obtain a firm understanding of the harmonic oscillator wave functions.

Objectives: At the end of this set of exercises you should be able to:

1. Generate and plot the first few Hermite polynomials,
2. Identify the Hermite polynomials by function type,
3. Combine the Hermite polynomials with the exponential component and normalization factor to generate harmonic oscillator wave functions.
4. Explain the significance of each component of the wave function in terms of requiements for a well behaved wave function.
5. Relate the number of nodes of the harmonic oscillator wave functions to the energy of that quantum state.
6. Draw the conclusion that at high quantum numbers the quantum mechanical harmonic oscillator probability densities display classical behavior.

Prerequisites:

Users will need basic skills in creating and plotting functions within Mathcad. Users should also be familiar with the quantum mechanical harmonic oscillator up to and including obtaining the components of the differential equation that must be solved to obtain the solutions to the quantum mechanical harmonic oscillator problem. It is not necessary for students to be facile with solving differential equations by using series methods. If they know that a series of polynomials provides the solution then they can use this document to visualize the components of the solutions and the final solutions. Users should also know how components of the solutions satisfy the boundary conditions of the harmonic oscillator.

Step 1. Set up the constants and basic equations required for this exercise. Units are used throughout the document.

$h := 6.62608 \cdot 10^{-34} \cdot J \cdot s$ Plank 's constant

$$hbar := \frac{h}{2 \cdot \pi}$$

$k := 520 \cdot \frac{N}{m}$ for H2

The force constant for H_2

$xe := 74.16 \cdot 10^{-12} \cdot m$

Equilibrium bond length in H2

$m1 := \frac{.001}{6.023 \cdot 10^{23}} \cdot kg \qquad m2 := \frac{0.001}{6.023 \cdot 10^{23}} \cdot kg$

Defining the masses as m1 and m2 will permit you to adapt this template to other diatomics. Notice that you must use the mass of the atom.

$mu := \frac{m1 \cdot m2}{m1 + m2}$

Compute the reduced mass.

$Bsq := \frac{hbar}{\sqrt{mu \cdot k}} \qquad Bsq = 1.605 \times 10^{-22} m^2$

Be careful because Bsq is called $1/\alpha$ in some texts. It is important to note the units of Bsq

$B := \sqrt{Bsq} \qquad B = 1.267 \times 10^{-11} m$

The value of B gives you some idea of the range of the plot you will prepare later.

$x := \frac{-7.10 \cdot 10^{-11}}{B} \cdot m, \frac{-6.99 \cdot 10^{-11}}{B} \cdot m .. \frac{7.10 \cdot 10^{-11}}{B} \cdot m$

Here we define the range for the calculations and graphs. Notice the use of units here. The range was divide by B to permit integer values on the abscissa of the plots.

At this point you can check your text and examine the Quantum Mechanical Harmonic Oscillator Equation. You should be able to describe each part of the equation and understand how the equation was developed.

Step 2. Examining the harmonic oscillator wave function components.

The general solution to the harmonic oscillator consists of the product of a normalization constant, an exponential function, and a Hermite polynomial as shown here.

$$\Psi_v(x) = N_v H_v(x) e^{-\frac{x^2}{2}}$$

We will examine each component separately and then combine them in Step 3.

Thought Question: Why was it necessary to write the solution for the quantum mechanical harmonic oscillator equation as a product of three components? Explain the need for each component clearly in writing.

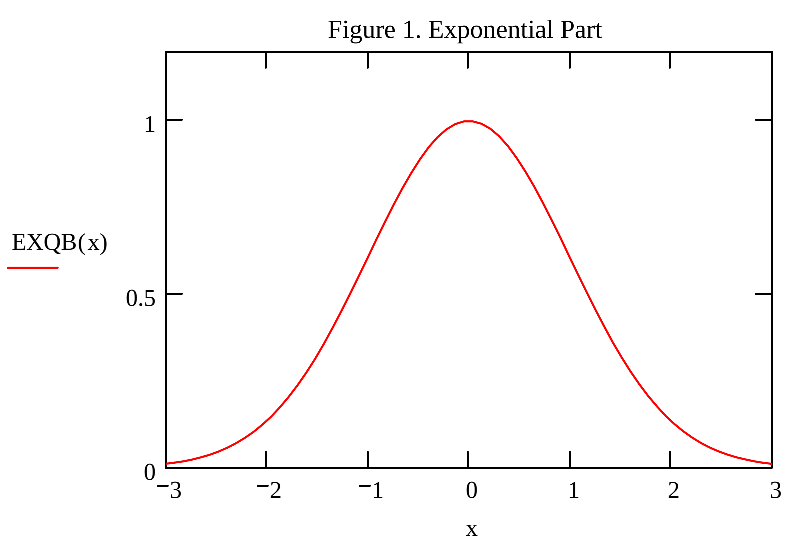
The Exponential Component (a Gaussian Function)

$$EXQB(x) := \exp\left(\frac{-x^2}{2}\right)$$

This expression defines the exponential factor of the harmonic oscillator wave function. The plot of this function is shown in Figure 1.

The exponential function is the same for all solutions to the Schrodinger equation for the harmonic oscillator. This function is shown in Figure 1.

Figure 1: The exponential part of the harmonic oscillator wave function.



The Normalization Factor

$$N_v(v) := \frac{1}{\left(2^v \cdot v!\right)^{\frac{1}{2}}} \cdot \left(\frac{1}{\pi}\right)^{\frac{1}{4}}$$

This expression computes the normalization factor for each harmonic oscillator wave function. a sample calculation for v=3 is shown.

$$N_v(3) = 0.108$$

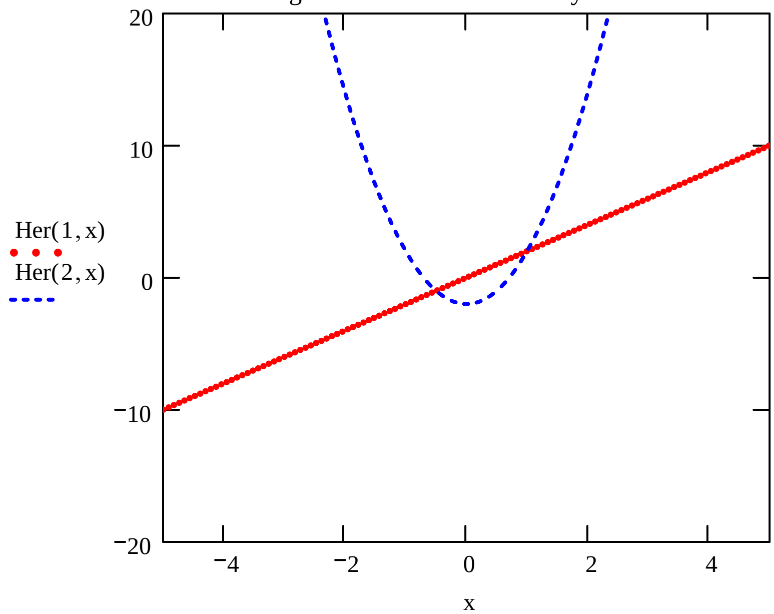
Exercise 1: Compute and tabulate the normalization factors for the first 10 harmonic oscillator wave functions. How do these factors vary with v?

The Hermite Polynomials

The third factor in the solutions to the harmonic oscillator Schrodinger equation is the Hermite polynomial. This is obtained easily by using the Her(n,x) Mathcad function.

Her(n,x) is the Mathcad function that returns the value of the Hermite polynomial of degree n at x where n is a non-negative integer and x is a real scalar. From the plots of various Her functions you can determine the type of polynomial for the specific v quantum state of the quantum mechanical harmonic oscillator. Figure 1 contains the plot of the first two Hermite polynomials.

Figure 2. Plot of Hermite Polynomials



Exercise 2 : Add two more Hermite polynomials to the plot above. Write a brief description of each curve in the plot after you have all four Hermite polynomials present. Be sure to identify the type of function you observe in each plot.

Generating Hermite Polynomials

At this point it is useful to generate the Hermite polynomials and examine their form. We will use a generating function to obtain various Hermite polynomials. You can find the explicit expression for the generating function in your text or some other reference.

Here we use n as the quantum number and q as the independent variable. This helps Mathcad function properly. The first example is for n=1.

$$n := 1$$

$$Hr(q) := (-1)^n \cdot \exp\left(q^2\right) \cdot \frac{d^n}{dq^n} \exp\left(-q^2\right)$$

Hermite Polynomial Generating Function

$$Hr(q) \rightarrow 2 \cdot \exp\left(q^2\right) \cdot q \cdot \exp\left(-q^2\right)$$

After I copied the right hand side and paste into this work sheet, I use Symbolics Simplify.

$$2 \cdot \exp\left(q^2\right) \cdot q \cdot \exp\left(-q^2\right)$$

$$2 \cdot q$$

Note the result. This is the Hermite polynomial arising when n=1 for the variable q. Your text may use v and x in the generating function.

Exercise 2. Note the mathematical function given here. Name this function and compare to the function you obtained using Her(x) above.

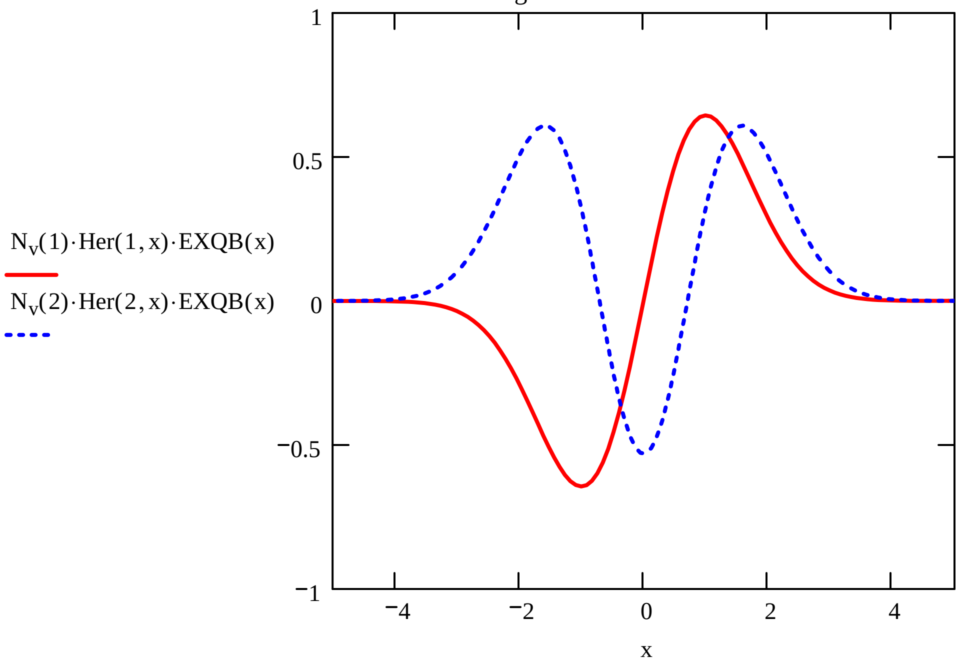
Exercise 3: Use the generating function for the Hermite polynomials provided and generate the first 10 Hermite polynomials. Compare the functions you obtain with the plots obtained using the Her(x,n) Mathcad function. Summarize your results in a separate Mathcad documnet to be sent to your instructor.

Step 3: Combining the parts and examining the Harmonic Oscillator wavefunctions.

Figure 3 shows the normalized harmonic oscillator wavefunctions as a product of the three components: normalization, Hermite polynomial, and exponential factor.

Exercise 4: What properties of well behaved wavefunctions required the use of each of the harmonic oscillator wave function components?

Figure 3. HO Wavefunctions



Exercise 5. Add two more wave functions to the figure above. Compare your results with those published in some text at your disposal.

Step 4. An alternative approach: Counting nodes.

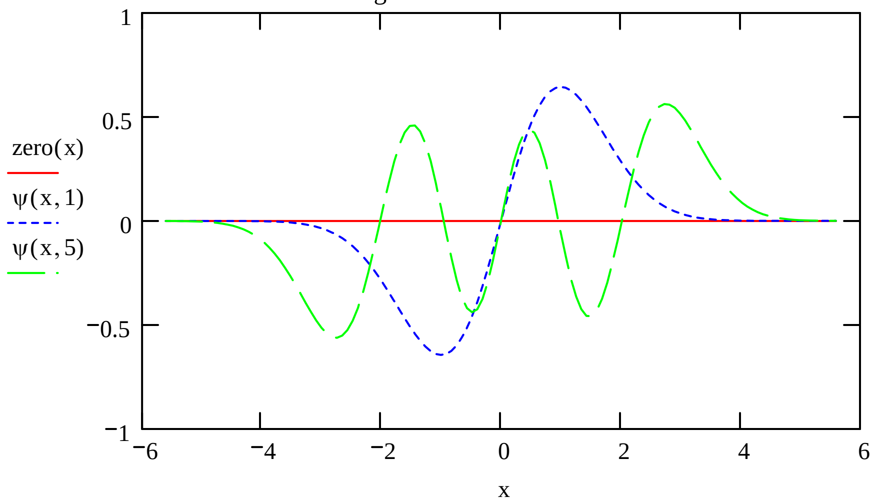
Let us write a general expression for the harmonic oscillator wavefunction.

$$\psi(x, v) := N_v(v) \cdot (Her(v, x)) \cdot EXQB(x)$$

$zero(x) := 0$ This is the zero base line.

Plotted here are the first and fifth harmonic oscillator wave functions.

Figure 4. HO wavefunctions

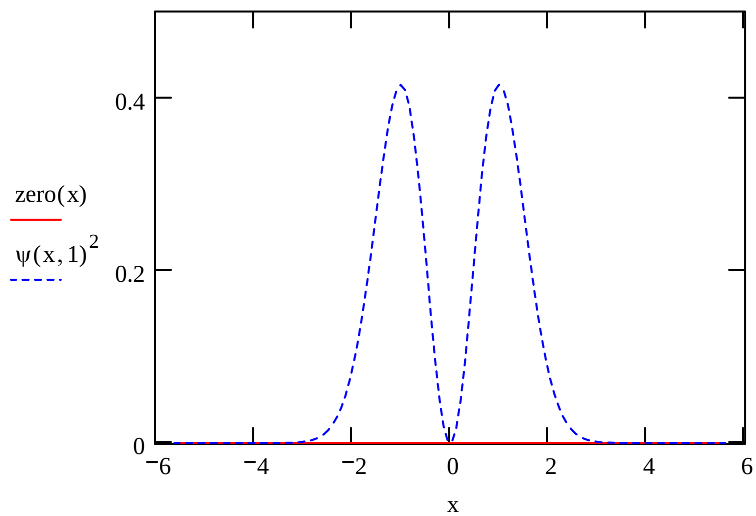


Exercise 6. Add additional wavefunctions to the plot above. Examine each curve and determine the number of nodes for each value of v. (Hint, do not count the approach to zero at the ends of the curves. If you do one quantum state at a time you will be better able to see the nodes. A crowded plot is no help at all.) Tabulate your results.

Exercise 7. Enter the expression for the energy for a harmonic oscillator quantum state. Compute the energy for each of the harmonic levels you studied above. How does the number of nodes vary with the energy of a quantum state?

Step 5. Probability Density Plots

Here we prepare the probability density function plots for the harmoinc oscillator wavefunctions. The curve for v=1 is shown here as a start.



Exercise 8. Prepare several more probability density plots for larger values of v. (for quantum numbers greater than 12 you must expand the absissa range that was set at the end of Step 1.) Reflect on the plots you obtain and state the most probable extensions for the oscillator at different energy levels. From observing the plots, as v increases, what can be said about the relationship between the quantum mechanical oscillator with large quantum number and the classical harmonic oscillator?

Exercise 9. Prepare a probability densit plot for a very large value of v. Discuss how the quantum mechanical result merges with the classical result as v increases.

Final Step: Collect all your work and submit to your instructor as directed in the course syllabus.

Selected References:

Atkins, P.,and de Paula, J., "Physical Chemistry," 7th edition (W.H. Freeman and Company, New York, NY, 2002), Chap. 12.

McQuarrie, D. A., and Simon, J. D., "Physical Chemistry: a Molecular Approach," (University Science Books, Sausalito, CA, 1997) Chap. 5.

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