

Special Functions - The Harmonic Oscillator Hermite Polynomials

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Abstract

A one dimensional harmonic oscillator (HO) can be used to represent a variety of fundamental concepts within physics. The HO is "an idealization of the potential experienced by an object trapped near a minimum" [1]. While the previously examined potential square well illustrated the concept of quantization, it is uncommon to have such an unrealistic scenario where the particle does not interact with the environment beyond the well and is entirely discrete. Contrast this to the HO, which is commonly observed in day to day life. Classical examples include a mass on a spring, a swinging pendulum, and the rocking of a cradle. In quantum mechanics, it is typically used as a limiting case of the way particles within an atom or crystal lattice structure interact with one another. For this very reason, the potential of the HO describes a particle confined to a smooth potential well. In this project, we generate Hermite polynomials to the energy eigenvalues of the time-independent Schrödinger's Equation idealized as a HO and examine the limit of excitation for the HO.

1 Introduction

1.1 Hermite Polynomials and Harmonic Oscillator

As established with the finite and infinite potential well, a particle confined to a potential well exhibits wave like properties. The potential of a HO is as follows:

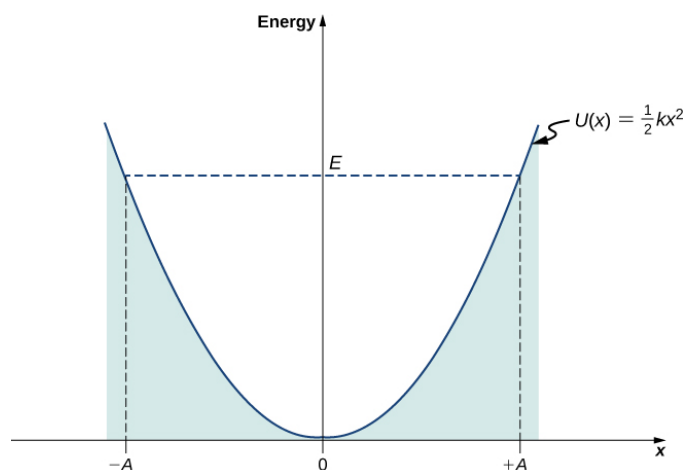


Figure 1: Harmonic Oscillator Potential Well

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$$V_{HO} = \frac{1}{2}m\omega^2 x^2 \quad (1)$$

Where m is mass and ω is angular frequency of the oscillator. From this potential we are able to take the Hamiltonian of the system. The Hamiltonian H is a system operator that describes the total energy of the system as the kinetic and potential energy. In terms of the HO Shrödinger Equation, the eigenvalues of these energies are the possible quantized energy states that the particle is able to fall into. The Hamiltonian of a mass moving in a HO potential is as follows [1]:

$$H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2 \quad (2)$$

Note that the first term of the Hamiltonian represents kinetic energy where as the latter represents potential. Ordinarily, the momentum and position would be represented as vectors, however, because we are dealing only with one dimension, the Hamiltonian has been simplified. Quantum mechanically, the Hamiltonian is written as an operator [1]:

$$\hat{H} = \frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \quad (3)$$

Utilizing the Hamiltonian to first construct the time-independent Shrödinger Equation, we can mathematically simplify this system as a second-order ordinary differential equation. The eigenvalue and eigenfunctions that describe the system of the HO Shrödinger Equation yield the discrete energies and wave functions respectively.

$$\hat{H}\psi(x) = E\psi(x) \quad (4)$$

$$\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + (\frac{1}{2}m\omega^2 x^2 - E)\psi(x) = 0 \quad (5)$$

$$E \longrightarrow \gamma = \frac{E}{\frac{1}{2}\hbar\omega} \quad (6)$$

If we do a change of variables where ρ is some dimensionless quantity:

$$\rho = \sqrt{\frac{m\omega}{\hbar}} x \quad (7)$$

$$\frac{\hbar^2}{2m} \frac{d^2\psi}{d\rho^2} + (\gamma - \rho^2)\psi(\rho) = 0 \quad (8)$$

The solution to this differential equation only exists for discrete values:

$$\left\{ E_n = (2n + 1)\frac{1}{2}\hbar\omega \quad n = 0, 1, 2, \dots \right. \quad (9)$$

With eigenfunction:

$$\psi_n(\rho) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{-\frac{\rho^2}{2}} H_n(\rho) \quad (10)$$

Where H_n are Hermite polynomials of degree n . By substituting (10) into (9), we can see that the Hermite polynomials are a solution that can be expressed as a power series for both odd and even powers of ρ [1]. We are able to generate the Hermite utilized the following recursion relation:

$$H_{n+1}(\rho) = 2\rho H_n(\rho) - 2n H_{n-1}(\rho) \quad (11)$$

The first few Hermite polynomials for the first 6 orders are as follows:

$$\begin{aligned}
H_0(\rho) &= 1 \\
H_1(\rho) &= 2\rho \\
H_2(\rho) &= 4\rho^2 - 2 \\
H_3(\rho) &= 8\rho^3 - 12\rho \\
H_4(\rho) &= 16\rho^4 - 48\rho^2 + 12 \\
H_5(\rho) &= 32\rho^5 - 160\rho^3 + 120\rho
\end{aligned}$$

The coefficients can be expressed as:

$$H_{n+1,k}(\rho) = 2a_{n,k-1} - 2na_{n-1,k} \quad (12)$$

We will use the fact that $H_0(\rho) = 1$ and $H_1(\rho) = 2\rho$ to determine the starting values:

$$a_{0,0} = 1 \qquad a_{1,0} = 0 \qquad a_{0,1} = 2$$

Beginning with these initial coefficients, we are able to propagate an array of dimension n and k to determine the corresponding polynomial coefficients. These coefficients can then be utilized to determine a value's corresponding Hermite polynomial function. From this function, we can plot the Hermite polynomials as well and finally, the HO wave function $\psi(\rho)$ which satisfies the Shrödinger Equation.

2 Procedure

The goal is to solve for the allowed energies and wave function of the Shrödinger Equation idealized as a Harmonic Oscillator using the Hermite polynomials. The following are the steps to complete this process.

Argument List:

- NARY: Two-dimensional array for all the coefficients up to order NDMN
- NDMN: Dimension of array NARY
- n & k : Order of the Hermite Polynomial

1. Initialize
 2. Create an array called *NARY* of dimensions $NDMN + 1$ by $NDMN + 1$
 3. Fill the array *NARY* with zeros
 4. Initialize the array using the coefficients $a_{0,0} = 1$ for $H_0(\rho)$ and $a_{1,0} = 0, a_{0,1} = 2$ for $H_1(\rho)$
5. Determine Hermite coefficients
 6. Find the non-vanishing coefficients using (12)
 7. Print the results in the array NARY
8. Determine Hermite polynomials

9. Utilize (11) to determine the Hermite polynomial values, and append these into arrays of H_n
10. Plot polynomial values $\frac{H_n}{n^3}$ by ρ so that the curve is within the same range
11. Plot $\psi(\rho)$
 12. Append the values of $\psi(\rho)$ from (10) into arrays of $\psi_n(\rho)$, whether the Hermite polynomials are divided by 3^n will not change the overall shape of the curves
 13. Plot wave function $\psi_n(\rho)$ by ρ to examine excitation of the system
 14. Examine excitation of the system for values of large n

3 Discussion

The array $NARY$ corresponds to the Hermite coefficients, thus its values should agree with the first few lines of the Hermite polynomials following (11). The following table describes the array generated from the Hermite coefficients relationship (12) with dimensions 7 by 7:

Table 1: Resulting Generated Array of Hermite Coefficients with Corresponding Energy Levels and Polynomials

	ρ^0	ρ^1	ρ^2	ρ^3	ρ^4	ρ^5	ρ^6
n=0	1	0	0	0	0	0	0
n=1	0	2	0	0	0	0	0
n=2	-2	0	4	0	0	0	0
n=3	0	-12	0	8	0	0	0
n=4	12	0	-48	0	16	0	0
n=5	0	120	0	-160	0	32	0
n=6	-120	0	720	0	-480	0	64

This is in agreement with the polynomial coefficient values previously mentioned following (11).

A particle confined to a smooth potential well near a minimum can be described by the Shrödinger Equation idealized as a Harmonic Oscillator. Examining the following figure, we are able to see that the greater the energy levels n represent more excited states of the harmonic oscillator. Note that the eigenvalues of the eigenfunction correspond to the Hermite polynomials as solutions to the Hermite function.

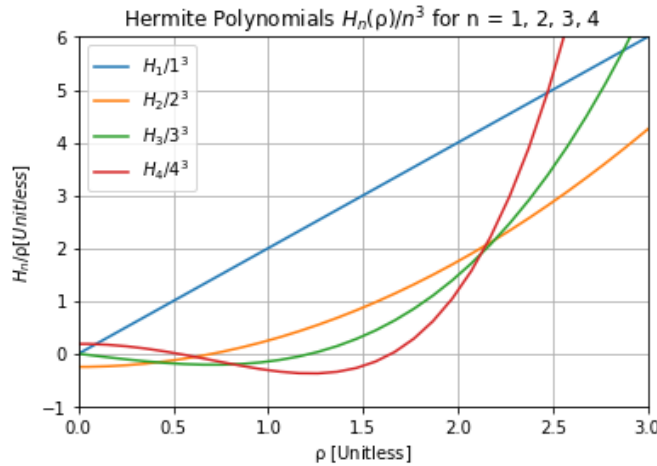


Figure 2: Hermite Polynomials H_n for $n = 1, 2, 3, 4$, showcasing the eigenvalue solutions of the Hermite eigenfunction

We used these coefficients to plot the wave function $\psi(\rho)$ which satisfies the Shroedinger Equation. This allows us to examine the way the system reacts at large excitation levels of n . The following figure showcases the energy of the particle and its wave like properties once confined to a smooth potential well.

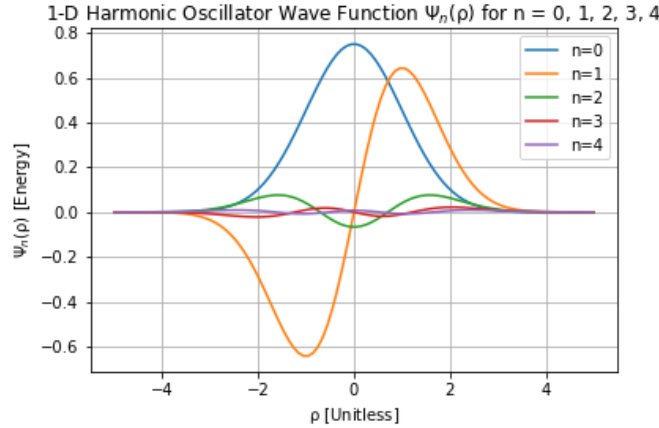


Figure 3: Wave Functions $\psi(\rho)$ that satisfy the Harmonic Oscillator Shrödinger Equation

Examining the way in which the system reacts at large energy levels in the following figure, we see that at larger energies there is greater excitation of the particle. This phenomenon is described by the Correspondence Principle of the Quantum Oscillator. At high excitation energies, the particle has enough energy to possibly escape its potential confinement, thus may be found outside of the well. The large scale oscillations of the probability of a particle being within the well prevents us from being able to determine the particles position without affecting the state of the particle and/or oscillator itself [2]. This is exactly what we expect with the uncertainty principle. The oscillator begins to take the shape of the classical oscillator at large excitation energies with the ends crossing into the initially forbidden region outside of the well [2].

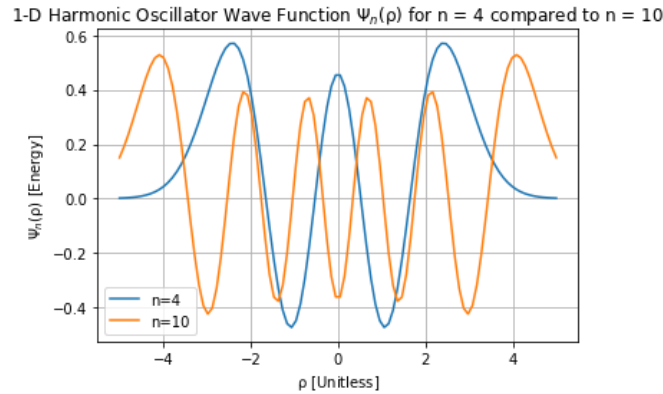


Figure 4: Wave Functions $\psi(\rho)$ at levels $n = 4$ and $n = 10$ showcasing increasingly variable excitation.

4 Conclusion

In this project, we determine the Hermite coefficients, their corresponding polynomials, and the wave function for a particle confined to a smooth potential well. This smooth potential well corresponds to the Schroedinger Equation in the form of a Harmonic Oscillator. We see that at large excitation levels, we are unable to determine the position and/or energy of a particle and that the particle is more likely to be

found outside the well as its energy increases to a point where it is able to leave the confinement of the well. This is in agreement with the Uncertainty Principle, and is described by the correspondence Principle.

References

- [1] S.S.M Wong. *Computational Methods in Physics and Engineering*.
- [2] <http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hosc6.htmlc1>.