# Hermite Functions and the Quantum Oscillator

| |
|---|
| **Background** |
| **Differentials Equations handout** |
| **The Laplace equation – solution and application** |
| **Concepts of primary interest:** |
| **Separation constants** |
| **Sets of orthogonal functions** |
| **Discrete and continuous eigenvalue spectra** |
| **Generating Functions** |
| **Rodrigues formula representation** |
| **Recurrence relations** |
| **Raising and lowering operators** |
| **Sturm-Liouville Problems** |
| **Sample calculations:** |
| **Tools of the trade:** |

**REVISE: Use the energy unit $\hbar\,({}^{k}/_{m})^{½}$ and include the roots of 2 from the beginning.**

**The Quantum Simple Harmonic Oscillator** is one of the problems that motivate the study of the Hermite polynomials, the $H_n(x)$. Q.M.S. (Quantum Mechanics says.):

$$-\frac{\hbar^2}{2m}\frac{d^2u_n}{dx^2}+(\tfrac{1}{2}k\,x^2-E_n)\,u_n(x)=0 \qquad \text{[Hn.1]}$$

This equation is to be attacked and solved by the numbers.

STEP ONE: Convert the problem from one in physics to one in mathematics. The equation as written has units of energy. The constant $\hbar$ has units of energy * time, $m$ has units of mass, and $k$ has units of energy per area. Combining, $\frac{\hbar^2}{mk}$ has units of

Contact: tank@alumni.rice.edu

$(\text{length})^4$ so a dimensioned scaling constant $\alpha = \left(\frac{m\,k}{\hbar^2}\right)^{1/4}$ is defined with units $(\text{length})^{-1}$ as a step toward defining a *dimensionless* variable $z = \alpha x$. . The equation itself is divided by the natural unit of energy ½ $\hbar$ $({}^{k}/_{m})^{½}$ leading to a dimensionless constant $\lambda_n = \frac{2\,E_n}{\hbar\,(k/m)^{1/2}}$ which is (proportional to) the eigenvalue, *the energy in natural units*.

The equation itself is now expressed in a dimensionless (*mathspeak*) form:

$$\frac{d^2u_n}{dz^2} + (\lambda_n - z^2)\,u_n(z) = 0\,. \quad \text{[Hn.2]} \qquad \text{(**\textit{See problem 2 for important details.})}$$

The advantage of this form is that one does not need to write down as many symbols.

**Exercise**: Divide equation [Hn.1] by the energy unit ½ $\hbar$ $({}^{k}/_{m})^{½}$. Note that the second derivative with respect to $x$ has dimensions $\text{length}^{-2}$ and that $x^2$ has units of $\text{length}^2$. Divide the coefficient of $x^2$ by the coefficient of the second derivative with respect to $x$, and you have a constant with dimensions $\text{length}^{-4}$. Compare the fourth root of this constant with the definition of $\alpha$.

STEP TWO: Identify and factor out the large $z$ behavior.[1] For large $z$, the $\lambda_n\, u_n$ term is negligible compared to $z^2\, u_n$. Study: $\frac{d^2u_n}{dz^2} = z^2\, u_n(x)$. It follows that, to leading order in $z$ the large $|z|$ limit is, $u(z) \approx A\; e^{-z^2/2} + B\; e^{+z^2/2}$. As the function $u(z)$ must be normalizable, the second behavior $e^{+z^2/2}$ *is discarded*.

**Exercise:** Show that $u_m(z) \approx A\, z^m\; e^{-z^2/2} + B\, z^m\; e^{+z^2/2}$ works as well (when terms lower order in $z$ are discarded). Conclude that we might try $g(z)\; e^{-z^2/2}$ where $g(z)$ is a polynomial in $z$.

[1] When the domain range runs to infinity, it is common to have an exponential regulating behavior that complicates the power series solution method so we begin by factoring out that large argument behavior. When the range ends at zero, we often factor out the small argument behavior as well although the method of Frobenius also handles the issue.

STEP THREE: Propose that the full solution is: $u_n(z) = g(z)\ e^{-z^2/2}$ where $g(z)$ is a slower-varying, well-behaved diverges more slowly than $e^{-z^2/2}$ vanishes to yield the full solution to the differential equation [Hn.2].

$$\frac{d}{dz}\left(g(z)\ e^{-z^2/2}\right) = \frac{dg}{dz}\ e^{-z^2/2} - z\, g(z)\ e^{-z^2/2}$$

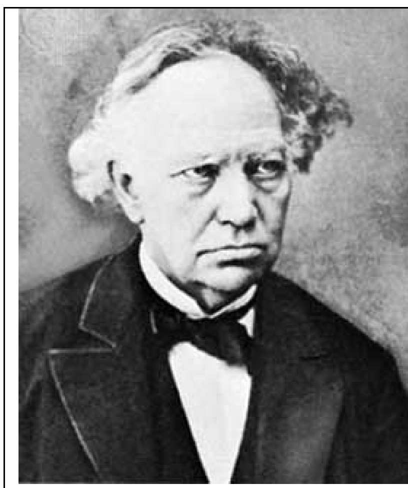
$$\frac{d^2}{dz^2}\left(g(z)\ e^{-z^2/2}\right) = \frac{d^2 g}{dz^2}\ e^{-z^2/2} - 2z\frac{dg}{dz}\ e^{-z^2/2} + z^2\, g(z)\ e^{-z^2/2}$$

After some substitutions and division by $e^{-z^2/2}$, it follows that $u_n(z)$ will satisfy equation [Hn.2] if $g(z)$ satisfies: $$\frac{d^2 g}{dz^2} - 2z\frac{dg}{dz} + (\lambda_n - 1)\, g = 0 \qquad \text{[Hn.3]}$$

This equation is the DE for the Hermite polynomials *if* $\lambda_n = 2n + 1$ (See problems 5 and 6.). The ratio and comparison tests indicate that the series solution to equation [Hn.3] diverges and that it diverges as fast as $e^{+z^2}$ or faster than $e^{-z^2/2}$ converges. The series must be terminated after a finite number of terms if the overall solution functions are to remain finite. Therefore the functions $g(z)$ are the Hermite polynomials, the $H_n(z)$ to within a multiplicative normalization constant. The conclusions flow forth as series termination requires that $\lambda_n = 2\,n + 1$ leading to energy eigenvalues $E_n = (n + ½)$ $\hbar(k/m)^{1/2} = (n + ½)\,\hbar\omega_o$ and spatial and temporal eigenfunctions: $u_n(z) = h_n(z) = [2^n\, n!\, \pi^{1/2}]^{-1/2}\, H_n(z)\ e^{-z^2/2}$ and $\psi(x, t) = [2^n\, n!\, \pi^{1/2}]^{-1/2}\, H_n(z)\ e^{-z^2/2}\ e^{-i(n+1/2)\omega t}$. $H_n(z)$ is the Hermite polynomial of order $n$, and the $h_n(z)$ are the spatial parts of the normalized wavefunctions for the quantum harmonic oscillator.

**Comment/Exercise**: Consider the original form of the equation $\frac{d^2u}{dz^2} + (\lambda - z^2)u(z) = 0$. Insert a template power series solution and isolate the coefficient of the $z^s$ terms. Show that the recurrence relation becomes $(s + 2)(s + 1)\, a_{s+2} + \lambda\, a_s - a_{s-2} = 0$. A *two-term* recurrence relation is a good thing. A *three-term* relation is an indication that you should factor out an asymptotic or other behavior out of the solution and try again. A recurrence relation relating only odd or only even index terms is *expected* for problems with symmetric domains.

**Exercise**: Consider $\frac{d^2g}{dz^2} - 2z\frac{dg}{dz} + (\lambda_n - 1)\,g = 0$. Attempt a solution using the power series methods. That is: insert a template power series solution $g(z) = \sum_{n=0}^{\infty} a_n z^n$ and isolate the coefficients of the $z^s$ terms. Show that the recurrence relation becomes $(s + 2)(s + 1)\,a_{s+2} - 2s\,a_s + (\lambda - 1)\,a_s = 0$. A *two-term* recurrence relation is a good thing. Find the requirement on $\lambda$ that will ensures that the power series terminates as a polynomial. Show that for $\lambda = 2n + 1$, the series terminates as an $n^{\text{th}}$ order polynomial.



**Charles Hermite** 1822-1901

Hermite made important contributions to number theory, algebra, orthogonal polynomials, and elliptic functions. He discovered his most significant mathematical results over the ten years following his appointment to the École Polytechnique. In 1848 he proved that doubly periodic functions can be represented as quotients of periodic entire functions. In 1849 Hermite submitted a memoir to the Académie des Sciences which applied Cauchy's residue techniques to doubly periodic functions. Sturm and Cauchy gave a good report on this memoir in 1851 but a priority dispute with Liouville seems to have prevented its publication.

MacTutor Archive on Mathematics History; University of St. Andrews Scotland

---

**Properties of the Hermite Polynomials**:

**The differential equation**: $\frac{d^2H_n}{dz^2} - 2z\frac{dH_n}{dz} + 2n\,H_n = 0$

**Normalization condition**: $H_n(z) = 2^n x^n$ + (*terms with powers of* $x^{n-2}$, $x^{n-4}$, …)

Hermite polynomials are alternately even and odd

**Orthogonality Relation:** $\int_{-\infty}^{\infty} e^{-x^2}\, H_n(x)\, H_m(x)\, dx = 2^n\, n!\sqrt{\pi}\,\delta_{mn}$

**Rodrigues Formula**: $H_n(z) = (-1)^n\, e^{z^2} \frac{d^n}{dz^n}\left(e^{-z^2}\right)$

**Generating Function**: $e^{(2zh-h^2)} = \sum_{n=0}^{\infty} \frac{h^n}{n!} H_n(z)$

**Recurrence Relations**: $\frac{d}{dz}\left(H_n(z)\right) = 2n\, H_{n-1}(z)$

$$\frac{d}{dz}\left(H_n(z)\right) = 2z\, H_n(z) - H_{n+1}(z)$$

$$2z\, H_n(z) = 2n\, H_{n-1}(z) + H_{n+1}(z)$$

**Sample Hermite Polynomials**: $H_0(z) = 1$ $\quad H_1(z) = 2z$ $\quad H_2(z) = 4z^2 - 2$

$H_3(z) = 8z^3 - 12z$ $\quad H_4(z) = 16z^4 - 48z^2 + 12$ $\quad H_5(z) = 32z^5 - 160z^3 + 120z$

**Mathematica syntax: HermiteH[n,z]** $\rightarrow$ $H_n(z)$

$$H_n(z) = (2z)^n - \frac{n(n-1)}{1!}(2z)^{n-2} + \frac{n(n-1)(n-2)(n-3)}{2!}(2z)^{n-4} - \ldots.$$

$$H_n(z) = \sum_{k=0}^{Int[n/2]} \frac{(-1)^k\; n!}{k!(n-2k)!}(2z)^{n-2k}$$

---

**Properties of the Harmonic Oscillator Wavefunctions**: $h_n(z) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}} H_n(z)\, e^{-z^2/2}$

**The differential equation**: $\frac{d^2 h_n}{dz^2} + (\lambda_n - z^2)\, h_n(x) = 0 \quad ; \qquad \lambda_n = 2n+1$

**Normalization condition**: $\int_{-\infty}^{\infty} \left[h_n(z)\right]^* h_m(z)\; dz = \delta_{mn}$ (The $h_n(z)$ are real-valued.)

**Rodrigues Formula**: $h_n(z) = [2^n\, n!\pi^{1/2}]^{1/2}\;\; (-1)^n\; e^{z^2/2} \frac{d^n}{dz^n}\left(e^{-z^2}\right)$

**Recurrence Relations**: $\frac{d}{dz}\left(h_n(z)\right) = \sqrt{n/2}\, h_{n-1}(z) - \sqrt{n+1/2}\, h_{n+1}(z)$

$$z\; h_n(z) = \sqrt{n/2}\, h_{n-1}(z) + \sqrt{n+1/2}\, h_{n+1}(z)$$

**Abstract Space Notation**: $\frac{d}{dz}|\, n\rangle = \sqrt{n/2}\;\; |\, n-1\rangle - \sqrt{n+1/2}\;\; |\, n+1\rangle$

$$z\,|\,n\rangle = \sqrt{n/2}\;\;|\,n-1\rangle + \sqrt{n+1/2}\;\;|\,n+1\rangle$$

**Sample Wavefunctions**: $h_o(z) = \dfrac{1}{\pi^{1/4}}\; e^{-z^2/2}$ $\quad h_1(z) = \dfrac{\sqrt{2}\,z}{\pi^{1/4}}\; e^{-z^2/2}$ $\quad h_2(z) = \dfrac{2\,z^2-1}{\sqrt{2}\;\;\pi^{1/4}}\; e^{-z^2/2}$

$$h_3(z) = \frac{2\,z^3-3\,z}{\sqrt{3}\;\;\pi^{1/4}}\; e^{-z^2/2} \qquad h_4(z) = \frac{4\,z^4-12\,z^2+3}{\sqrt{4!}\;\;\pi^{1/4}}\; e^{-z^2/2} \qquad h_5(z) = \frac{4\,z^5-20\,z^3+15\,z}{\sqrt{60}\;\;\pi^{1/4}}\; e^{-z^2/2}$$

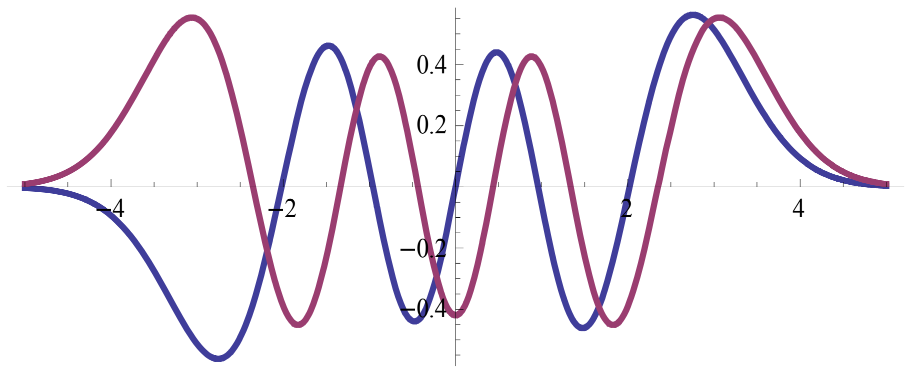
**Notation Alert:** The use of the zero vector notation $|\,0\rangle$ representing the additive identity is sometimes preempted by another convention. For example, in quantum mechanics, $|0\rangle$ represents the *ground state* (lowest energy state) for problems such as the quantum harmonic oscillator. In these cases the additive identity is to be represented as $|\text{ZERO}\rangle$ or $|\text{NULL}\rangle$. Stay alert; this conflict will arise when you study the quantum oscillator. That is $|\,0\rangle$ is the ground state, a state vector with ***non-zero*** magnitude, for the *QSHO* problem. Lowering $|\,1\rangle$ yields $|\,0\rangle$, the ground state; it does not annihilate the state. Lowering $|\,0\rangle$ results in annihilation.
**Ignore the last sentence if you have not heard of lowering.**

## Interlaced Zeros Property

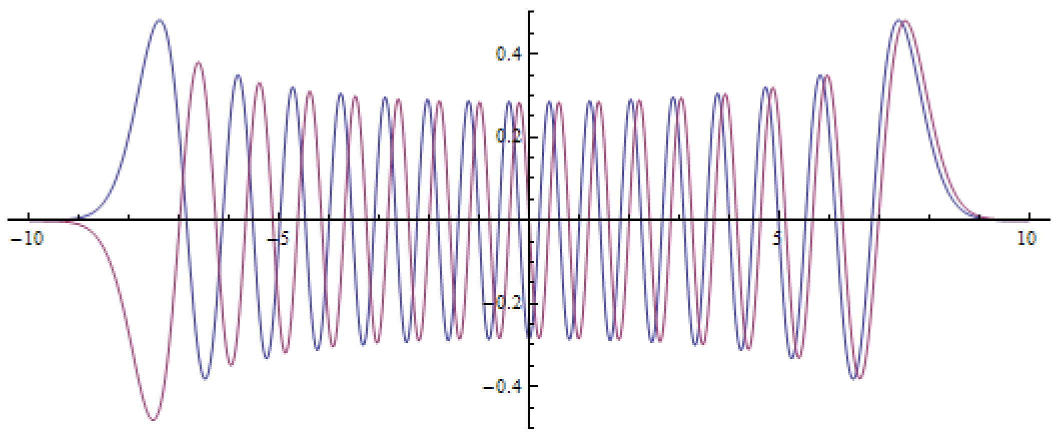
The eigenfunctions of a Sturm-Liouville operator (includes most Hamiltonians studied in the first year of quantum) have the properties that they can be chosen to be real valued and that the zeros of functions with *adjacent* eigenvalues are interlaced. This discussion assumes a discrete eigenvalue spectrum. Other than perhaps endpoint zeroes, a zero for the function with the higher eigenvalue will appear between any two zeros of the function with the next lower eigenvalue.

```
SHOwavefn[n_,z_]:= HermiteH[n,z] Exp[-(z^2)/2]*(1/Sqrt[2^n n! Sqrt[Pi]])
Plot[{SHOwavefn[5,z], SHOwavefn[6,z]},{z,-5,5}, AspectRatio→0.4]
```

This result does not mean that a function with a higher eigenvalue can never share an interior zero location with a lower eigenvalue function. It means that adjacent-eigenvalue functions will not share an interior zero location and that the wavefunctions gain a node for each step up in eigenvalue.




Plots of the $n$ = 5 and 6 QHO wavefunctions




Plots of the $n$ = 30 and 31 QHO wavefunctions

Given an eigenfunction, the next eigenfunction with a higher eigenvalue will have one zero between any two zeroes of that eigenfunction.

**Exercise**: Give an example in which a SHO wavefunction shares an interior zero location with a function with a lower eigenvalue.

The interlace behavior suggests that the higher eigenfunctions *wiggle* more rapidly and have smaller and smaller separations between their zero locations indicating that they might represent finer and finer spatial variations. The case that the eigenvalue spectrum is unbounded above might then suggest that the eigenfunctions can wiggle as fast as necessary to characterize any reasonable functions and hence that the set of eigenfunctions is a complete basis for all reasonable functions defined on the domain.

**Completeness**: The SHO wavefunctions $h_n(x)$ are orthonormal and so one can attempt to use them as an expansion set for a function $f(x)$.

$$f(x) = \sum_{n=0}^{\infty} a_n\, h_n(x) = \sum_{n=0}^{\infty} \frac{\langle h_n(x) | f(x) \rangle}{\langle h_n(x) | h_n(x) \rangle} h_n(x) = \sum_{n=0}^{\infty} \left\{ \int_{-\infty}^{\infty} h_n(x)\, f(x)\, e^{-x^2} dx \right\} h_n(x)$$

Recall that the $h_n(x)$ are normalized so that $\langle h_n(x) | h_n(x) \rangle = 1$.

The set is complete if expansions converge in the mean to all *reasonable* functions.

$$\underset{N\to\infty}{Limit} \left[ \int_{-\infty}^{\infty} \left| f(x) - \sum_{n=0}^{N} a_n\, h_n(x) \right|^2 e^{-x^2} dx \right] = 0 \;\; \forall \text{ reasonable } f(x)$$

Basically if the total integrated value of the square of the error in the series representation goes to zero, then no important parts of the behavior of $f(x)$ are absent. All our functions are faithfully represented so expansion set is adequate to provide a complete representation.

---

## Tools of the Trade

The following section will proceed in *discovery* mode. We will not just present the best solution by hindsight. Rather we will muddle through and adjust to more optimal definitions and approaches at the end.

**Ladder Operations and the Solution of Differential Equations**:

The form of the differential operator for the Hermite functions suggests an alternative approach to solving the equation for the Hermite functions.

$$-\frac{d^2 u_n}{dz^2} + z^2\, u_n(z) = \lambda_n u_n(z) \qquad \text{[Hn.4]}$$

that has the form of an eigenvalue problem for the dimensionless hamiltonian:

$$\hat{L}\,u_n(z) = \lambda_n u_n(z) \quad \text{where} \quad \hat{L} = -\frac{d^2}{dz^2} + z^2 \qquad \text{[Hn.5]}$$

The approach is motivated by the *great algebraic identity*: $x^2 - y^2 = (x - y)\,(x + y)$. One is tempted to express $\hat{L}$ as either $\hat{A}\hat{B}$ or $\hat{B}\hat{A}$ where $\hat{A} = z + \frac{d}{dz}$ and $\hat{B} = z - \frac{d}{dz}$.

Unfortunately, neither representation is correct due to the appearance of product rule terms in the derivative.

$$\hat{A}\hat{B}\;u_n(z) = \left(z + \tfrac{d}{dz}\right)\left(z - \tfrac{d}{dz}\right)u_n = \left[-\tfrac{d^2}{dz^2} + z^2\right]u_n + u_n = \left[\hat{L} + 1\right]u_n = \left(\lambda_n + 1\right)u_n \qquad \text{[Hn.6]}$$

$$\hat{B}\hat{A}\;u_n(z) = \left(z - \tfrac{d}{dz}\right)\left(z + \tfrac{d}{dz}\right)u_n = \left[-\tfrac{d^2}{dz^2} + z^2\right]u_n - u_n = \left[\hat{L} - 1\right]u_n = \left(\lambda_n - 1\right)u_n \qquad \text{[Hn.7]}$$

**Note**: The process seems to produce multipliers differing in value by 2. At this point, it is postulated that the spectrum for the eigenvalues $\lambda_n$ is discrete and consists of values separated by intervals of magnitude 2. **Thus $\lambda_{n+1}$ is assumed to be $\lambda_n$ + 2.** This problem arose in the study of the quantum harmonic oscillator and $\hat{L}$ is the dimensionless form of the Hamiltonian, the operator for the sum of the kinetic energy and the positive potential energy ½ $k\,x^2$. All the eigenvalues $\lambda_n$ should be positive. The spectrum of eigenvalues should start with a minimum positive value, and include values generated by incrementing that value by +2 multiple times.[1]

**Exercise**: What combination of the operators $\hat{A}$ and $\hat{B}$ would equal $\hat{L}$ ?

**Summary of the notation and results:**

$$\hat{L}\,u_n(z) = \lambda_n u_n(z) \quad \text{where} \quad \hat{L} = -\frac{d^2}{dz^2} + z^2$$

$$\hat{A} = z + \tfrac{d}{dz} \qquad\qquad \hat{B} = z - \tfrac{d}{dz} \qquad \text{[Hn.8]}$$

$$\hat{A}\hat{B}u_n(z) = \left[\hat{L} + 1\right]u_n = \left(\lambda_n + 1\right)u_n \qquad \hat{B}\hat{A}u_n(z) = \left[\hat{L} - 1\right]u_n = \left(\lambda_n - 1\right)u_n$$

---

[1] Rather than a minimum positive value, a more general requirement is that there should be a minimum or lowest eigenvalue such as – 13.6 *eV* for the hydrogen atom problem.

$$\text{Combining, } \left(\hat{A}\hat{B} - \hat{B}\hat{A}\right)u_n(z) = \left[\hat{A}, \hat{B}\right]u_n = 2u_n \qquad \text{[Hn.9]}$$

Clearly, the average of the two ordering reproduces the desired differential operator.

$$\hat{L}u_n = \left(\hat{A}\hat{B} + \hat{B}\hat{A}\right)u_n(z) = \lambda_n u_n \qquad \text{[Hn.10]}$$

Short calculations verify that the multiplication of the linear-differential operators $\hat{A}, \hat{B}$ and $\hat{L}$ is associative, but not commutative. $\hat{A}(\hat{B}\,\hat{A}) = (\hat{A}\,\hat{B})\,\hat{A}$, but $\hat{B}\,\hat{A} \neq \hat{A}\,\hat{B}$. In fact, $\hat{A}\,\hat{B} - \hat{B}\,\hat{A} = 2$.

**Exercise**: Verify that $\hat{A}(\hat{B}\,\hat{A}) = (\hat{A}\,\hat{B})\,\hat{A}$ and that the operator $\hat{A}\,\hat{B} - \hat{B}\,\hat{A}$ is equivalent to multiplication by 2.

**Raising and Lowering Operators**

Consider:

$$\hat{L}\hat{A}u_n = ½\left(\hat{A}\hat{B} + \hat{B}\hat{A}\right)\hat{A}u_n = ½(\hat{A}\hat{A}\hat{B} + \hat{A}\hat{B}\hat{A} - \hat{A}\hat{A}\hat{B} + \hat{B}\hat{A}\hat{A} - \hat{A}\hat{B}\hat{A} + \hat{A}\hat{B}\hat{A})u_n \qquad \text{[Hn.11]}$$

$$\hat{L}\hat{A}u_n = ½(\hat{A}\hat{A}\hat{B} + \hat{A}[\hat{B}, \hat{A}] + [\hat{B}, \hat{A}]\hat{A} + \hat{A}\hat{B}\hat{A})u_n = \hat{A}½(\hat{A}\hat{B} - 2 - 2 + \hat{A}\hat{B})u_n = \hat{A}\,(\hat{L} - 2)\,u_n$$

$$\hat{L}\left(\hat{A}u_n\right) = \hat{A}\,(\hat{L} - 2)\,u_n = (\lambda_n - 2)\hat{A}u_n \qquad \text{[Hn.12]}$$

Compare this result for $\hat{L}$ acting on an eigenfunction $u_k$ (See [Hn.10]). If $u_n$ is an eigenfunction of the scaled hamiltonian $\hat{L}$ with eigenvalue $\lambda_n$, then $\hat{A}u_n$ is an eigenfunction with eigenvalue $\lambda_n - 2$. We conclude that $\hat{A}$ acts as a lowering operator.

The same reasoning can be applied to $\hat{B}u_n$ to show that $\hat{L}\left(\hat{B}u_n\right) = (\lambda_n + 2)\hat{B}u_n$. We conclude that $\hat{B}$ acts as a raising operator.

$\hat{A}$ lowers the eigenfunction to (perhaps a multiple of) the eigenfunction with the next lowest eigenvalue and $\hat{B}$ raises the eigenfunction to (perhaps a multiple of) the one with the next highest eigenvalue. These operators seem to be joined together or associated. The operator $\hat{B}$ is to be relabeled $\hat{A}^{t}$ and dubbed the adjoint of $\hat{A}$ and read as '*A*-dagger'. Nothing has been said about the normalization and any multiple of an eigenfunction is a solution to the eigenvalue equation. The results are restated allowing for a loss of normalization when the operators raise (or lower) a function to the eigenfunction with the next higher (or lower) eigenvalue.

$$\hat{A}u_n(z) = c_n\, u_{n-1}(z) \qquad \hat{A}\left|n\right\rangle = c_n\left|n-1\right\rangle$$
$$\hat{A}^t u_n(z) = d_n\, u_{n+1}(z) \qquad \hat{A}^t\left|n\right\rangle = d_n\left|n+1\right\rangle \qquad \text{[Hn.13]}$$

Recalling previous result and converting them to abstract vector space notation,

$$\hat{A}\hat{A}^t u_n(z) = (\lambda_n + 1)u_n(z) \qquad \hat{A}\hat{A}^t\left|n\right\rangle = (\lambda_n + 1)\left|n\right\rangle \qquad \text{[Hn.14]}$$

$$\hat{A}^t\hat{A}u_n(z) = (\lambda_n - 1)u_n(z) \qquad \hat{A}^t\hat{A}\left|n\right\rangle = (\lambda_n - 1)\left|n\right\rangle \qquad \text{[Hn.15]}$$

As the $\lambda_n$ are positive and separated from one another by 2, there must be a least value of $\lambda$. Assume that the lowest value is $\lambda_o$ and that the corresponding eigenfunction is $u_o(z)$. It is impossible to lower the lowest eigenfunction as there is none lower. The action of $\hat{A}\ u_o(z)$ should be to *annihilate*[1] it (return zero as the result).

$$\hat{A}\ u_o(z) = 0 \ \text{ or } \ \left(z + \frac{d}{dz}\right)u_n(z) = 0 \quad \Rightarrow \quad \frac{du_{n(z)}}{dz} = -z\,u_n$$

This equation can be integrated to yield $u_o(z) = c\ e^{-z^2/2}$ where $c$ is a scalar constant. With the lowest eigenfunction in hand, its eigenvalue can by computed.

$$\hat{L}\,u_n(z) = \lambda_n u_n(z) \quad \text{where} \quad \hat{L} = -\frac{d^2}{dz^2} + z^2 \Rightarrow \hat{L}\,u_0(z) = \lambda_0 u_0(z)$$

$$\left[-\frac{d^2}{dz^2} + z^2\right]c\,e^{-\frac{1}{2}z^2} = c\,e^{-\frac{1}{2}z^2} = 1\left(c\,e^{-\frac{1}{2}z^2}\right)$$

The conclusion is that the lowest eigenvalue $\lambda_o$ is 1. The next task is to raise $u_o(z)$ to find $u_1(z)$.

[1] This behavior leads to the alternative name set of ***annihilation*** and ***creation*** for the lowering and raising operators.

$$\hat{A}^t u_0(z) = d_n\, u_n(z) \;\Rightarrow\; \left(z - \tfrac{d}{dz}\right) u_0(z) = d_n\, u_1(z) = (2z)\, e^{-\frac{1}{2}z^2}$$

The conclusion is that $u_1(z)$ is a multiple of $(2z)e^{-\frac{1}{2}z^2}$. The overall constant multiplier would be set by a normalization procedure. Even without normalization, we can find the eigenvalue for $u_1(z)$.

$$\left[-\frac{d^2}{dz^2} + z^2\right](2z)\, e^{-\frac{1}{2}z^2} = (6z)\, e^{-\frac{1}{2}z^2} = 3\left((2z)\, e^{-\frac{1}{2}z^2}\right)$$

The eigenvalue $\lambda_1 = 3$ which is $\lambda_0 + 2$ supporting the previous speculation about the spacing between eigenvalues and leading to the final result that $\lambda_n = 2\,n + 1$.

> The energy eigenvalues for the quantum harmonic oscillator follows from the values for the λ.
>
> $$\lambda_n = 2n + 1 = \frac{2E_n}{\hbar\sqrt{k/m}} \quad \Rightarrow E_n = (n + \tfrac{1}{2})\,\hbar\sqrt{k/m}$$

Combining the result $\lambda_n = 2\,n + 1$ with equations: [Hn.13], [Hn.14] and [Hn.15], the identifications $c_n = (2\,n)^{\frac{1}{2}}$ and $d_n = (2\,[n + 1])^{\frac{1}{2}}$ are possible. We need not look at the details until our operators have been renormalized. Our misstep was to choose the energy unit $\frac{1}{2}\,\hbar\,[k/m]^{\frac{1}{2}}$. If the energy unit $\hbar\,[k/m]^{\frac{1}{2}}$ had been chosen , we would have avoided several bothersome factors of 2. More later.

The choices of raising and lowering operators as defined to this point were based on an old algebraic identity. Now we add the normalization information. We can't get rid of the factors that depend on $n$, but we can dispense with the square roots of two. The new, improved raising and lowering operators are to be defined as:

$$\hat{a}^t = \tfrac{1}{\sqrt{2}}\,\hat{A}^t = \tfrac{1}{\sqrt{2}}\left[z - \frac{d}{dz}\right] \quad \text{and } \hat{a} = \tfrac{1}{\sqrt{2}}\,\hat{A} = \tfrac{1}{\sqrt{2}}\left[z + \frac{d}{dz}\right] \qquad \text{[Hn.16]}$$

We could have started with these operators if we had chosen the energy unit $\hbar\,[k/m]^{\frac{1}{2}}$.

**New Action Summary**:

$$\hat{a}\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle \qquad \hat{a}^t\left|n\right\rangle = \sqrt{n+1}\left|n+1\right\rangle \qquad \text{[Hn.17]}$$

$$(\hat{a}^t)^n\left|0\right\rangle = \sqrt{n!}\left|n\right\rangle \qquad u_n(z) = \tfrac{1}{\sqrt{2^n n!}}\left[z - \tfrac{d}{dz}\right]^n u_0(z) \qquad \text{[Hn.18]}$$

It follows that $\hat{a}^t\hat{a}\left|n\right\rangle = n\left|n\right\rangle$ and $\hat{a}\hat{a}^t\left|n\right\rangle = n+1\left|n\right\rangle$ leading to the identification of $\hat{a}^t\hat{a}$ as the number operator and of the relation $\hat{a}\hat{a}^t - \hat{a}^t\hat{a} = \left[\hat{a}, \hat{a}^t\right] = 1$. The action of this combination of $\hat{a}^t$ and $\hat{a}$ is to multiply the wavefunction by 1. Hence that operator combination, $\hat{a}\hat{a}^t - \hat{a}^t\hat{a} = \left[\hat{a}, \hat{a}^t\right]$, is completely equivalent to multiplication by 1. $\left[\hat{a}, \hat{a}^t\right] = \hat{a}\hat{a}^t - \hat{a}^t\hat{a}$ is called the commutator of $\hat{a}^t$ and $\hat{a}$.

If we adopt the need energy unit $\hbar\, [{}^k/_m]^{1/2}$, it follows that $\hat{h} = ½\left[\hat{a}\hat{a}^t + \hat{a}^t\hat{a}\right]$. Comparing with the eigenvalue equation,

$$\hat{h}\left|n\right\rangle = ½\left[\hat{a}\hat{a}^t + \hat{a}^t\hat{a}\right]\left|n\right\rangle = \gamma_n\left|n\right\rangle = (n+½)\left|n\right\rangle$$

| |
|---|
| The dimensioned Hamiltonian is $\hat{H} = ½\,\hbar\,({}^k/_m)^{1/2}\,\hat{L} = \hbar\,({}^k/_m)^{1/2}\,\hat{h}$ leading to $\hat{H}\left|n\right\rangle = (n+½)\,\hbar\,({}^k/_m)^{1/2}$. |

Using the relations [Hn.17], $\hat{h}\left|n\right\rangle = ½\left[\hat{a}\hat{a}^t + \hat{a}^t\hat{a}\right]\left|n\right\rangle = (n+½)\left|n\right\rangle$. The states $|n\rangle$ are eigenfunctions of $\hat{h}$ with eigenvalues $2n + 1$. The action of an operator on a state is to yield another state for the same problem. Let us consider $\hat{a}\left|n\right\rangle$.

$$\begin{aligned}\hat{h}\hat{a}\left|n\right\rangle &= ½\left(\hat{a}\hat{a}^t + \hat{a}^t\hat{a}\right)\hat{a}\left|n\right\rangle = ½\left(\hat{a}\hat{a}^t\hat{a} + \hat{a}^t\hat{a}\hat{a}\right)\left|n\right\rangle \\ &= ½\left(\hat{a}\hat{a}\hat{a}^t + \hat{a}\hat{a}^t\hat{a} - \hat{a}\hat{a}\hat{a}^t + \hat{a}\hat{a}^t\hat{a} - \hat{a}\hat{a}^t\hat{a} + \hat{a}^t\hat{a}\hat{a}\right)\left|n\right\rangle \\ &= ½\left(\hat{a}\hat{a}\hat{a}^t + \hat{a}[\hat{a}^t, \hat{a}] + \hat{a}\hat{a}^t\hat{a} + [\hat{a}^t, \hat{a}]\hat{a}\right)\left|n\right\rangle\end{aligned}$$

Use our commutator relation in reverse order: $\hat{a}\hat{a}^t - \hat{a}^t\hat{a} = \left[\hat{a}, \hat{a}^t\right] = 1$

$$\begin{aligned}\hat{h}\hat{a}\left|n\right\rangle &= ½\left(\hat{a}\hat{a}\hat{a}^t + \hat{a}(-1) + \hat{a}\hat{a}^t\hat{a} + (-1)\hat{a}\right)\left|n\right\rangle = \left\{½\,\hat{a}\left(\hat{a}\hat{a}^t + \hat{a}\hat{a}^t\hat{a}\right) - 1\,\hat{a}\right\}\left|n\right\rangle \\ &= ½\,\hat{a}\left(\hat{a}\hat{a}^t + \hat{a}\hat{a}^t\hat{a}\right)\left|n\right\rangle - 1\,\hat{a}\left|n\right\rangle = (n+½-1)\hat{a}\left|n\right\rangle\end{aligned}$$

We conclude that is $|n\rangle$ is an eigenfunction with eigenvalue $n + ½$, then $\hat{a}|n\rangle$ is an eigenfunction with eigenvalue $(n + ½ - 1)$, with an eigenvalue lowered by one.

Follow the same reasoning to show that $\hat{a}^\dagger|n\rangle$ is an eigenfunction with eigenvalue raised by one.

The dimensionless momentum operator is: $\hat{p}_z = -i\frac{d}{dz}$.

$$\hat{a}^t = \tfrac{1}{\sqrt{2}}\left[z - \tfrac{d}{dz}\right] \text{ and } \hat{a} = \tfrac{1}{\sqrt{2}}\left[z + \tfrac{d}{dz}\right] \text{ become } \hat{a}^t = \tfrac{1}{\sqrt{2}}\left[z - i\hat{p}_z\right] \text{ and } \hat{a} = \tfrac{1}{\sqrt{2}}\left[z + i\hat{p}_z\right]$$

Inverting the equations,

$$z = \tfrac{1}{\sqrt{2}}\left[\hat{a}^t + \hat{a}\right] \qquad \text{and} \qquad \hat{p}_z = \tfrac{i}{\sqrt{2}}\left[\hat{a}^t - \hat{a}\right]$$

[Hn.19]

The commutator of the position and momentum can now be computed in terms of the commutator: $\left[\hat{a}, \hat{a}^t\right] = \hat{a}\hat{a}^t - \hat{a}^t\hat{a}$ .

$$[z, \hat{p}_z] = \left[\tfrac{1}{\sqrt{2}}\left(\hat{a}^t + \hat{a}\right), \tfrac{i}{\sqrt{2}}\left(\hat{a}^t - \hat{a}\right)\right]$$

$$[z, \hat{p}_z] = \tfrac{i}{2}\left\{\left[\hat{a}^t, \hat{a}^t\right] - \left[\hat{a}^t, \hat{a}\right] + \left[\hat{a}, \hat{a}^t\right] - \left[\hat{a}, \hat{a}\right]\right\} = \tfrac{i}{2}\{0 - (-1) + (1) - (0)\} = i$$

This result is valid for our dimensionless operators. The fully dimensioned form is: $\left[x, \hat{p}_x\right] = i\hbar$. The value of the commutator is deduced by allowing the operator to act on an arbitrary function $f(x)$.

$$\begin{aligned}\left[x, \hat{p}_x\right] f(x) &= x(-i\hbar\tfrac{d}{dx}) f(x) - (-i\hbar\tfrac{d}{dx}) x\, f(x) \\ &= i\hbar\left[-x\frac{df}{dx} + x\frac{df}{dx} + f(x)\right] = i\hbar\ f(x)\end{aligned}$$

The action of the commutator on an arbitrary function is to multiply it by $i\hbar$ so the commutator is equivalent to multiplication by $i\hbar$.

**Developing the Rodrigues Formula**:

The machinery developed in the previous section provides a basis for developing the Rodrigues formula for the $u_n(z) \approx e^{z^2/2} \frac{d^n}{dz^n}\left(e^{-z^2}\right)$. Consider an arbitrary function $f(z)$.

$$e^{\frac{1}{2}z^2} \frac{d}{dz}\left[e^{-\frac{1}{2}z^2}\; f(z)\right] = e^{\frac{1}{2}z^2}\, e^{-\frac{1}{2}z^2} \left[\frac{d}{dz} - z\right] f(z) = \left[\frac{d}{dz} - z\right] f(z)$$

Next the induction step. It is assumed that:

$$\left[\frac{d}{dz} - z\right]^n g(z) = e^{\frac{1}{2}z^2} \frac{d^n}{dz^n}\left[e^{-\frac{1}{2}z^2}\; g(z)\right]$$

This assumption is used to establish the result for $n + 1$.

$$\left[\frac{d}{dz} - z\right]^{n+1} g(z) = \left[\frac{d}{dz} - z\right]\left\{\left[\frac{d}{dz} - z\right]^n g(z)\right\} = \left[\frac{d}{dz} - z\right]\left\{e^{\frac{1}{2}z^2} \frac{d^n}{dz^n}\left[e^{-\frac{1}{2}z^2}\; g(z)\right]\right\}$$

$$\left[\frac{d}{dz} - z\right]^{n+1} g(z) = \frac{d}{dz}\left\{e^{\frac{1}{2}z^2} \frac{d^n}{dz^n}\left[e^{-\frac{1}{2}z^2}\; g(z)\right]\right\} - z\left\{e^{\frac{1}{2}z^2} \frac{d^n}{dz^n}\left[e^{-\frac{1}{2}z^2}\; g(z)\right]\right\}$$

$$= \left\{z\, e^{\frac{1}{2}z^2} \frac{d^n}{dz^n}\left[e^{-\frac{1}{2}z^2}\; g(z)\right]\right\} + \left\{e^{\frac{1}{2}z^2} \frac{d^{n+1}}{dz^{n+1}}\left[e^{-\frac{1}{2}z^2}\; g(z)\right]\right\} - z\left\{e^{\frac{1}{2}z^2} \frac{d^n}{dz^n}\left[e^{-\frac{1}{2}z^2}\; g(z)\right]\right\}$$

$$\text{or } \left[\frac{d}{dz} - z\right]^{n+1} g(z) = \left\{e^{\frac{1}{2}z^2} \frac{d^{n+1}}{dz^{n+1}}\left[e^{-\frac{1}{2}z^2}\; g(z)\right]\right\}$$

With the $n = 1$ anchor step and the induction ($n \to n + 1$) step validated, the result is true for all $n$.

$$\left[\frac{d}{dz} - z\right]^n g(z) = \left\{e^{\frac{1}{2}z^2} \frac{d^n}{dz^n}\left[e^{-\frac{1}{2}z^2}\; g(z)\right]\right\} \;\; \forall\, n \text{ and well-behaved } g(z) \qquad \text{[Hn.20]}$$

To this point, $g(z)$ has been an arbitrary function; now $g(z)$ is identified with $u_0(z) = c\, e^{-\frac{1}{2}z^2}$. The operation begins with the lowest eigenfunction, the ground state and raises it $n$ times to generate a multiple of $u_n(z)$.

$$\left[\frac{d}{dz} - z\right]^n u_0(z) = \left[A^t\right]^n u_0(z) = d\; u_n(z) = \left\{e^{\frac{1}{2}z^2} \frac{d^n}{dz^n}\left[e^{-\frac{1}{2}z^2}\; c\, e^{-\frac{1}{2}z^2}\right]\right\}$$

$$\left(d/c\right) u_n(z) = \left\{e^{\frac{1}{2}z^2} \frac{d^n}{dz^n}\left[e^{-z^2}\right]\right\}$$

The factor $^d/_c$ provides for normalization if needed. It is claimed that the process has generated a multiple of the $n^{th}$ eigenfunction. Developments covered in the problem section establish that:

$$\left\{(-1)^n e^{\frac{1}{2}z^2} \frac{d^n}{dz^n}\left[e^{-z^2}\right]\right\} = e^{-\frac{1}{2}z^2}\left[(2z)^n + b_{n-2}z^{n-2} + b_{n-4}z^{n-4} + \dots\right] \Rightarrow = e^{-\frac{1}{2}z^2} H_n(z)$$

It follows that $e^{\frac{1}{2}z^2}\left\{(-1)^n e^{-\frac{1}{2}z^2} H_n(z)\right\} = H_n(z)$ or that $(-1)^n e^{z^2} \frac{d^n}{dz^n}\left[e^{-z^2}\right] = H_n(z)$.

Rodrigues got it right.

---

**Sturm – Liouville Problems** $\Rightarrow$ Almost all of our DEs

A homogeneous linear differential equation for $y(x)$ of the form:

$$\frac{d}{dx}\left[p(x)\frac{dy}{dx}\right] + \left[\lambda\, w(x) - q(x)\right] y(x) = 0 \qquad \text{[SL.21]}$$

Where $p(x)$, $q(x)$ and $w(x)$ are real-valued functions, $w(x) \ge 0$ and some rather general boundary conditions are met at $a$ and $b$, the ends of the interval over which the solutions are to be defined. The equation is found to possess physically meaningful solutions only if the parameter $\lambda$ is one of a certain set of characteristic values call *eigenvalues*. The permissible values of $\lambda$ are known as its *characteristic values* (or eigenvalues) $\lambda_k$, and the corresponding functions $y_k(x)$, which then satisfy the conditions of the problem when $\lambda = \lambda_k$, are known as the *characteristic functions* (or eigenfunctions)[1]. In most physics applications, the functions $p(x)$ and $w(x)$ are real and positive definite in the interval $[a,b]$, except possibly at one or both of the end points.

Consider the differential equation and its complex conjugate.

---

[1] ***Eigen*** is German for characteristic property. eigen, eigene, eigenes: own or its own; Eigenschaft (f): property

$$\frac{d}{dx}\left[p(x)\frac{dy_m}{dx}\right]+\left[\lambda_m\, w(x)-q(x)\right]y_m(x)=0$$
$$\frac{d}{dx}\left[p(x)\frac{dy_m^*}{dx}\right]+\left[\lambda_m^*\, w(x)-q(x)\right]y_m^*(x)=0 \qquad \text{[SL.22]}$$

Multiply the second equation by $y_n(x)$.

$$y_n(x)\frac{d}{dx}\left[p(x)\frac{dy_m^*}{dx}\right]+\left[\lambda_m^*\, w(x)-q(x)\right]y_n(x)\, y_m^*(x)=0$$

Prepare a copy with $m$ and $n$ interchanged and subtract it from the one above.

$$y_n(x)\frac{d}{dx}\left[p(x)\frac{dy_m^*}{dx}\right]-y_m^*(x)\frac{d}{dx}\left[p(x)\frac{dy_n}{dx}\right]=\left[\lambda_n-\lambda_m^*\right]w(x)\, y_n(x)\, y_m^*(x)=0$$

Integrate both sides over the range $a$ to $b$. Use integration by parts on the left-hand side:

$$p(x)\left[y_n(x)\frac{dy_m^*}{dx}-y_m^*(x)\frac{dy_n}{dx}\right]_a^b-\int_a^b\left(\frac{dy_m^*}{dx}\,p(x)\frac{dy_n}{dx}-\frac{dy_m^*}{dx}\,p(x)\frac{dy_n}{dx}\right)dx$$
$$=\left[\lambda_n-\lambda_m^*\right]\int_a^b y_m^*(x)y_n(x)\,w(x)\,dx \qquad \text{[SL.23]}$$

It is to be assumed that the following boundary condition is met:

$$p(x)\left[y_n(x)\frac{dy_m^*}{dx}-y_m^*(x)\frac{dy_n}{dx}\right]_a^b=0 \qquad \text{[SL.24]}$$

and it is clear that the second integral vanishes so the result is:

$$\left[\lambda_n-\lambda_m^*\right]\int_a^b y_m^*(x)y_n(x)\,w(x)\,dx=0 \qquad \text{[SL.25]}$$

Note that this procedure has generated a *natural inner product* for the functions associated with this differential equation. The function $w(x)$ is everywhere positive and is called the *weight* function.

$$\langle f(x)|g(x)\rangle=\int_a^b\left[f(x)\right]^* g(x)\,w(x)\,dx \qquad \text{[SL.26]}$$

In the case that $m = n$,

$$\left[\lambda_n - \lambda_n^*\right]\int_a^b y_n^*(x)\,y_n(x)\,w(x)\,dx = 0$$

and, as $\int_a^b y_n^*(x)\,y_n(x)\,w(x)\,dx > 0$ for non-trivial functions $y_n(x)$,

$$\lambda_n = \lambda_n^* \qquad \text{[SL.27]}$$

If a complex number is equal to its complex conjugate, it is a real number. The eigenvalues are real, and, as all the eigenvalues are real for Sturm-Liouville problems, the general case becomes:

$$\left[\lambda_n - \lambda_m\right]\int_a^b y_m^*(x)\,y_n(x)\,w(x)\,dx = 0$$

Solution functions $y_n(x)$ and $y_m(x)$ with distinct eigenvalues ($\lambda_n \neq \lambda_m$) are necessarily orthogonal.

$$\langle y_m | y_n \rangle = \int_a^b y_m^*(x)\,y_n(x)\,w(x)\,dx = 0 \quad \text{for} \quad \lambda_n \neq \lambda_m \qquad \text{[SL.28]}$$

**Eigenfunctions with distinct eigenvalues are orthogonal.**

In the cases that an eigenvalue is repeated, the several functions corresponding to the eigenvalue can be used to build a set of mutually orthogonal functions by applying the Gram-Schmidt procedure.

**COMPLETE BASIS**: The collection of the eigenfunctions that solve the differential equation is a ***complete set of basis functions*** for the problem. A well-behaved, general function defined over same interval can be expanded in a *generalized Fourier series* as:

$$f(x) = \sum_{m=1}^{\infty} a_m\, y_m(x) \quad \text{where} \quad a_m = \frac{\langle y_m | f \rangle}{\langle y_m | y_m \rangle} \qquad \text{[SL.29]}$$

**Exercise**: Show that the Hermite polynomial equation can be written as:

$$\frac{d}{dx}\left[e^{-x^2}\frac{dH_n}{dx}\right] + \left[2\,n\,e^{-x^2}\right]H_n(x) = 0$$

Compare this with the general Sturm-Liouville form to identify each function in the general form. What values are the allowed eigenvalues? What is the interval ($a$, $b$)?

$$\frac{d}{dx}\left[ p(x)\frac{dy}{dx}\right] + \left[\lambda\, w(x) - q(x)\right] y(x) = 0$$

Give the form of the *natural* inner product for the space spanned by the Hermite polynomials.

Is the condition $p(x)\left[ y_n(x)\frac{dy_m^*}{dx} - y_m^*(x)\frac{dy_n}{dx}\right]_a^b = 0$ met for the particulars of the Hermite problem?

**Tools of the Trade:**

**How does one get back to the dimensioned physics problem after solving the associated dimensionless math problem?**

The first step is to multiply the differential operator by ½ $\hbar\, \omega_o$ to recover the hamiltonian. $\hat{L}\left|n\right\rangle = ½\left[\hat{a}\hat{a}^t + \hat{a}^t\hat{a}\right]\left|n\right\rangle = \lambda_n\left|n\right\rangle = (2n+1)\left|n\right\rangle$

The dimensioned Hamiltonian is $\hat{H} = ½\,\hbar\,({}^k/_m)^{½}\,\hat{L}$ leading to $\hat{H}\left|n\right\rangle = (2n+1)\,½\,\hbar\,({}^k/_m)^{½}$. Hence the energy eigenvalues are: $E_n = (n + ½)\,\hbar\,\omega_o$. The problem also generates a characteristic length $\alpha^{-1} = \left(\frac{\hbar^2}{mk}\right)^{1/4} = \sqrt{\frac{\hbar}{m\omega_o}}$ leading to the assignment, $z = \alpha x$, and the inner product relation:

$$\int h_j^*(z)\,\left(h_k(z)\right)dz = \int h_j^*(\alpha x)\,\left(h_k(\alpha x)\right)\alpha\, dx = \int \alpha^{½} h_j^*(\alpha x)\,\left(\alpha^{½} h_k(\alpha x)\right)dx = \int \varphi_1^*(x)\,\left(\varphi_3(x)\right)dx$$

**Important**: We identify $\phi_n(x) = \alpha^{½}\, h_n(\alpha x)$. We have explicitly noted that $\phi_n$ and $h_n$ are *different* functions. Putting it all together,

$$h_n(z) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(z) e^{-z^2/2}; \qquad \phi_n(x) = \frac{\sqrt{a}}{\sqrt{2^n n! \sqrt{\pi}}} H_n(\alpha x) e^{-(\alpha x)^2/2}$$

Next we back-convert the operators. The coordinate is easy: $z \to \alpha x$ as is the derivative relation: $\partial/\partial z \to \alpha^{-1}\, \partial/\partial x$. Let's move on to the raising and lowering operators.

$$\hat{a} = \left(\tfrac{1}{\sqrt{2}}\right)\left[z + \tfrac{d}{dz}\right] = \left(\tfrac{1}{\sqrt{2}}\right)\left[\alpha x + \alpha^{-1}\tfrac{d}{dx}\right] = \left(\tfrac{1}{\sqrt{2\hbar m\omega_o}}\right)\left[m\omega_o x + i\left(-i\hbar \tfrac{d}{dx}\right)\right] = \left(\tfrac{1}{\sqrt{2\hbar m\omega_o}}\right)\left[m\omega_o x + i\hat{p}\right]$$

and $$\hat{a}^\dagger = \left(\tfrac{1}{\sqrt{2}}\right)\left[z - \tfrac{d}{dz}\right] = \left(\tfrac{1}{\sqrt{2}}\right)\left[\alpha x - \alpha^{-1}\tfrac{d}{dx}\right] = \left(\tfrac{1}{\sqrt{2\hbar m\omega_o}}\right)\left[m\omega_o x - i\hat{p}\right].$$

These relations can be inverted as well:

$$\hat{x} = \tfrac{\alpha^{-1}}{\sqrt{2}}\left(\hat{a}^\dagger + \hat{a}\right) \qquad \hat{x} = \tfrac{i\hbar\alpha}{\sqrt{2}}\left(\hat{a}^\dagger - \hat{a}\right)$$

**Application**:

$$\int_{-\infty}^{\infty} \varphi_m^*(x)\; x\; \varphi_n(x)\,dx = \int_{-\infty}^{\infty} \alpha^{½} h_m^*(z)\; \tfrac{\alpha^{-1}}{\sqrt{2}}\left(\hat{a}^\dagger + \hat{a}\right)\; \alpha^{½} h_n(z)\,dx = \int_{-\infty}^{\infty} h_m^*(z)\; \tfrac{\alpha^{-1}}{\sqrt{2}}\left(\hat{a}^\dagger + \hat{a}\right)\; h_n(z)\,dz$$

$$= \int_{-\infty}^{\infty} h_m^*(z)\; \tfrac{\alpha^{-1}}{\sqrt{2}}\left(\sqrt{n+1}\, h_{n+1}(z) + \sqrt{n}\; h_{n-1}(z)\right)\; dz = \tfrac{\alpha^{-1}}{\sqrt{2}}\left(\sqrt{n+1}\,\delta_{m,n+1} + \sqrt{n}\;\delta_{m,n-1}\right)$$

**Exercise**: Use the method of the application above to compute $\int_{-\infty}^{\infty} \varphi_m^*(x)\; \hat{p}\; \varphi_n(x)\,dx$.

---

**The Generating Function:** What is it good for?

Consider the generating function relation for the Hermite polynomials:

$$e^{(2zh - h^2)} = \sum_{n=0}^{\infty} \frac{h^n}{n!} H_n(z) \text{ and hence } \left[e^{(2zh-h^2)}\right]^2 = e^{(4zh - 2h^2)} = \left(\sum_{n=0}^{\infty} \frac{h^n}{n!} H_n(z)\right)\left(\sum_{m=0}^{\infty} \frac{h^m}{m!} H_m(z)\right).$$

Note that: Sums start at zero for the Hermite problem. Exercise (*what else*) the inner product.

$$\int_{-\infty}^{\infty} e^{(4zh-2h^2)}\, e^{-z^2}\, dz = \int_{-\infty}^{\infty} \left( \sum_{n=0}^{\infty} \frac{h^n}{n!} H_n(z) \right) \left( \sum_{m=0}^{\infty} \frac{h^m}{m!} H_m(z) \right) e^{-z^2}\, dz$$

$$e^{2h^2} \int_{-\infty}^{\infty} e^{-(z-2h)^2}\, dz = \sum_{m,n=0}^{\infty} \int_{-\infty}^{\infty} \frac{h^n}{n!} H_n(z) \frac{h^m}{m!} H_m(z) e^{-z^2}\, dz$$

We have shown that that the Hermite polynomials form a mutually orthogonal set.

$$\int_{-\infty}^{\infty} H_n(z) H_m(z)\, e^{-z^2}\, dz = \delta_{mn} \int_{-\infty}^{\infty} H_n(z) H_n(z)\, e^{-z^2}\, dz$$

$$e^{2h^2} \int_{-\infty}^{\infty} e^{-u^2}\, du = e^{2h^2} \sqrt{\pi} = \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \frac{h^{2n}}{(n!)^2} H_n(z) H_n(z) e^{-z^2}\, dz$$

Expanding the left-hand side:

$$e^{2h^2} \sqrt{\pi} = \sqrt{\pi} \sum_{n=0}^{\infty} \frac{2^n h^{2n}}{n!} = \sum_{n=0}^{\infty} \frac{h^{2n}}{(n!)^2} \int_{-\infty}^{\infty} H_n(z) H_n(z) e^{-z^2}\, dz$$

Each power of *h* is an independent function so the coefficient must match left to right.

$$2^n \frac{\sqrt{\pi}}{n!} = \frac{1}{(n!)^2} \int_{-\infty}^{\infty} H_n(z) H_n(z) e^{-z^2}\, dz \quad \text{or} \quad \int_{-\infty}^{\infty} H_n(z) H_n(z) e^{-z^2}\, dz = 2^n n \sqrt{\pi}$$

After incorporating the normalization and splitting the weight function between $u_m(x)^*$ and $u_n(x)$, the wavefunctions for the harmonic oscillator become:

$$u_n(z) = \frac{1}{\sqrt{2^n\, n!\sqrt{\pi}}} H_n(z)\, e^{-\frac{1}{2} z^2} \qquad \psi_n(z) = \frac{1}{\sqrt{2^n\, n!\sqrt{\pi}}} H_n(z)\, e^{-\frac{1}{2} z^2}\; e^{-i(n+\frac{1}{2})\omega_0 t}$$

CONCLUSION: The generating function may have application beyond being a difficult method to generate the eigenfunctions.

---

**Warm Up Problems**

WUP1. The constant $\alpha = \left( \frac{m k}{\hbar^2} \right)^{1/4}$ has dimensions of length inverse. It is used to define the dimensionless coordinate $z = \alpha x$.

a.) Provide an equation for *x* given *z*.

b.) The potential energy of a SHO is ½ $k\, x^2$. Give the expression for the potential energy as a function of *z*.

c.) Express $^{d}/_{dx}$ in terms of $^{d}/_{dz}$.

d.) Express $\hat{p} = -i\hbar \frac{\partial}{\partial x}$ in terms of a derivative with respect to $z$.

e.) Express the kinetic energy operator $\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ using derivatives with respect to $z$.

f.) What was identified as the natural energy unit for the SHO problem?

*Partial Answers*: $x = \alpha^{-1} z = \left(\frac{\hbar^2}{m k}\right)^{1/4} z$ kin. en. op. $= \frac{-\hbar^2}{2m}\alpha^2 \frac{\partial^2}{\partial z^2} = -\tfrac{1}{2}\hbar\sqrt{k/m}\,\frac{\partial^2}{\partial^2 z}$

WUP2. The Hermite polynomials are alternately even and odd and are normalized such that they have the form: $H_n(x) = (2x)^n + a_{n-2}\, x^{n-2} + a_{n-4}\, x^{n-4} + \dots$ .

Give the values of: $\frac{d^n H_n(x)}{dx^n}$; $\frac{d^{n+1} H_n(x)}{dx^{n+1}}$; $\frac{d^{n-1} H_n(x)}{dx^{n-1}}$

**WUP3**. Consider $\frac{d^2 g}{dz^2} - 2z\frac{dg}{dz} + (\lambda_n - 1)\, g = 0$. Attempt a solution using the power series methods. That is: insert a template power series solution $g(z) = \sum_{n=0}^{\infty} a_n z^n$ and isolate the coefficients of the $z^s$ terms. Show that the recurrence relation becomes $(s + 2)(s + 1)\, a_{s+2} - 2s\, a_s + (\lambda - 1)\, a_s = 0$. A *two-term* recurrence relation is a good thing. Find the requirement on $\lambda$ that will ensures that the power series terminates as a polynomial. Show that for $\lambda = 2n + 1$, the series terminates as an $n^{\text{th}}$ order polynomial

**WUP4**. We wish to prove that $\frac{d^n}{dz^n}(z^n) = n!$. Show that the formula works for $n = 1$. Assume that the formula works for $n$ and use this to prove that it works for $n + 1$ by starting with: $\frac{d^{n+1}}{dz^{n+1}}(z^{n+1}) = \frac{d^n}{dz^n}\frac{d}{dz}(z * z^n)$. Remember that the target result is $(n + 1)!$.

What is: $\frac{d^n}{dz^n}(2^n z^n)$ ?

## Problems

1.) Find the location of all the zeros of the seventh and eighth eigenfunctions for the harmonic oscillator in terms of their dimensionless argument. Locate the zeros to three significant figures.

$$h_n(z) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(z) e^{-z^2/2}$$

Do the zeros obey the interlaced-zeros hypothesis? Give a specific example in which a wavefunction has exactly the same location of an interior zero as does another wavefunction with a lower eigenvalue.

Use Mathematica: **n = 6; NSolve[HermiteH[n,x]==0,x,6]**

2.) Begin with the Shroedinger equation for the harmonic oscillator.

$$-\frac{\hbar^2}{2m}\frac{d^2 u_n}{dx^2} + (\tfrac{1}{2} k\, x^2 - E_n)\, u_n(x) = 0$$

As each term must have the same dimensions, argue that $\frac{\hbar^2}{mk}$ has units of (length)$^4$ and that $\hbar (k/m)^{1/2}$ has the dimensions of energy. Define $\alpha = \left(\frac{m\,k}{\hbar^2}\right)^{1/4}$ and use the change of variable $z = \alpha x$ and division by ½ $\hbar (k/m)^{1/2}$ to convert the Shroedinger equation a dimensionless form, a simple problem in mathematics. The DE becomes the dimensionless (*mathspeak*) form:

$$\frac{d^2 U_n}{dz^2} + (\lambda_n - z^2)\, U_n(z) = 0$$

Note that if one wants to be pure, $U_n(z) = U_n(\alpha\, x) = u_n(x)$. The variable $x$ has dimensions while $z$ is dimensionless. In the *mathform*, functions and their arguments are dimensionless. We are sloppy and often just write $\frac{d^2u_n}{dz^2}+(\lambda_n - z^2)u_n(z)=0$ even though we should be more careful. !This course is SP35*x*, not SM35*x*.

3.) Identify and factor out the large *z* behavior. For large *z,* the $\lambda_n\, u_n$ term is negligible compared to $z^2\, u_n$. Study: $\frac{d^2u_n}{dz^2}=z^2\, u_n(x)$. To leading order in z, $u(z) \approx A\; e^{-z^2/2}$ for $|z|$ very large. Show that:

$\frac{d^2}{dz^2}\left(e^{-z^2/2}\right)=z^2\, e^{-z^2/2}\left[1+\mathcal{O}(z^{-2})\right]$ where $\mathcal{O}(z^{-2})$ represents "*and terms of order that vanish as $z^{-2}$ or faster*". Why is the behavior $u(z) \approx A\; e^{+z^2/2}$, which works to the same order, banished for the list of possibilities? Propose that the full solution is: $u_n(z) = N_n\, H_n(z)\, e^{-z^2/2}$ where $N_n$ is a normalization constant, and show that $H_n(z)$ must satisfy $\frac{d^2H_n}{dz^2}-2\,z\frac{dH_n}{dz}+(\lambda_n-1)\,H_n=0$ if $u_n(z)$ is to satisfy the original equation . The equation $\frac{d^2H_n}{dz^2}-2\,z\frac{dH_n}{dz}+(\lambda_n-1)\,H_n=0$ is the DE for the Hermite polynomials (See problems 5 and 6.) The ratio and comparison tests indicate that the series diverges and that it diverges faster than $e^{-z^2/2}$ converges. The series must terminate to yield polynomials if the overall solution functions are to remain finite. The conclusions flow forth as series termination requires that $\lambda_n = 2\,n + 1$ leading to energy eigenvalues: $E_n = (n + {}^1/_2)\,\hbar\,(k/m)^{1/2} = (n + {}^1/_2)\;\hbar\,\omega_o$ and spatial and temporal eigenfunctions:

$u_n(z) = h_n(z) = [2^n\, n!\, \pi^{1/2}]^{-1/2}\, H_n(z)\; e^{-z^2/2}$ and $\psi(x,t) = [2^n\, n!\, \pi^{1/2}]^{-1/2}\, H_n(z)\; e^{-z^2/2}\, e^{-i(n+½)\omega_o t}$

4.) The normalized oscillator wave functions are: $u_m(x)=\left[\sqrt{2^m\, m!\,\sqrt{\pi}}\right]^{-1}\; H_m(x)\; e^{-x^2/2}$.

Verify this normalization for $u_o(x)$ and $u_2(x)$ and show that $u_o(x)$ and $u_2(x)$ are orthogonal. The quantum mechanics inner product: $\langle f\,|\,g\rangle = \int_{-\infty}^{\infty}[f(x)]^*\,g(x)\;dx$

5.) The **Hermite polynomials** are a family of polynomials central to the study of the harmonic oscillator in quantum mechanics and the transverse intensity pattern of laser beams. The governing differential equation is:

$$\frac{d^2H_n}{dx^2} - 2x\frac{dH_n}{dx} + (\lambda_n - 1)H_n = 0$$

Apply the power series method to find the indicial equation. If the series for $H_n$ is allowed to be infinite, it diverges by the ratio test. Identify the spectrum of values for $\lambda_n$ that terminate the series after a finite number of terms. Generate the form of the four lowest order polynomials using the recurrence relations for the coefficients in the power series trial solution and setting the lowest index coefficients $a_o$ and $a_1$ alternately to 1 and 0 or to 0 and 1. Renormalize the $m^{th}$ order polynomial by multiplying by whatever value makes the coefficient of the highest ($m^{th}$) power of $x$ equal to $2^m$. Compare with the forms given below and comment.

$$H_0(x) = 1 \;;\; H_1(x) = 2x \;;\; H_2(x) = 4x^2 - 2 \;;\; H_3(x) = 8x^3 - 12x$$

Quantum mechanics identifies $\lambda_n$ as $(2E_n)/[\hbar(k/m)^{1/2}]$ where the $E_n$ are the allowed energy levels for the harmonic oscillator. What are the allowed energy values?

6.) **Hermite Polynomials**: There are many ways to develop the Hermite polynomials. One method begins with the initial set of polynomials $\{\,1, x, x^2, x^3, \ldots\,, x^n, \,\ldots\,\}$ and uses the Gram-Schmidt procedure to generate an orthogonal set over the interval $(-\infty,\infty)$ using the inner product:

$$\int_{-\infty}^{\infty} H_\ell(x)\,H_m(x)\;e^{-x^2}\;dx = \langle H_\ell | H_m\rangle = 0 \quad \text{for } m \neq \ell$$

The weight function $e^{-x^2}$ is necessary to assure that the integrals over the infinite range converge. Assume that $H_0(x) = 1$ and that $H_1(x) = 2x$ is orthogonal to it. Start with $x^2$ and use the Gram-Schmidt procedure to get an $H_2(x)$ that is orthogonal to $H_0(x)$ and $H_1(x)$ and that has $2^n$ s the coefficient of the $x^n$. Continue to find $H_3(x)$. Starting at $x^0$ and proceeding up the list of powers, the Gram-Schmidt procedure guarantees that each new polynomial is orthogonal to all polynomials of lower order.

Use: $\int_{-\infty}^{\infty} e^{-x^2}\,dx = \sqrt{\pi}$ and $\int_{-\infty}^{\infty} x^{2n}\, e^{-x^2}\,dx = \sqrt{\pi}\,\left(n-\tfrac{1}{2}\right)\left(n-\tfrac{3}{2}\right)\ldots\left(\tfrac{1}{2}\right)$ for $n = 1,2, \ldots$

Partial Answer: $H_4(x) = 16\,x^4 - 48x^2 + 12.$

7.) Use the Rodrigues representation $H_n(x) = (-1)^n\, e^{x^2} \frac{d^n}{dx^n}\left(e^{-x^2}\right)$ for the Hermite polynomials to show that $\frac{d}{dx}\left(H_n(x)\right) = 2x\,H_n(x) - H_{n+1}(x)$. Use the first derivative of this result and the differential equation satisfied by the Hermite polynomials $\dfrac{d^2H_n}{dx^2} - 2x\dfrac{dH_n}{dx} + 2n\,H_n = 0$ to establish the recurrence relation $\frac{d}{dx}\left(H_n(x)\right) = 2n\,H_{n-1}(x)$. Continue to show that: $2x\,H_n(x) = 2n\,H_{n-1}(x) + H_{n+1}(x)$. Use recurrence properties of the Hermite polynomials to show that: $\frac{d^n}{dx^n}\left(H_n(x)\right) = 2^n\, n!\,H_0(x) = 2^n\, n!$.

8.) a.) Generate the first four Hermite polynomials be exercising the Rodrigues formula. Show that your results are consistent with

$$(-1)^n \frac{d^n}{dx^n}\left(e^{-x^2}\right) = \left[(2x)^n + a_{n-2}\,x^{n-2} + a_{n-4}\,x^{n-4} + \ldots\right] e^{-x^2} = H_n(x)e^{-x^2}$$

. That is the exponential times a polynomial with leading term $2^n x^n$ followed by terms that drop the power of $x$ by two as they step down to $x^1$ or $x^0$. Assume $p_n(x) = (2x)^n + a_{n-2}\,x^{n-2} + a_{n-4}\,x^{n-4} + \ldots$ and show that $-\frac{d}{dx}\left(p_n(x)e^{-x^2}\right) = \left[2x\,p_n(x) - \frac{d}{dx}(p_n(x))\right] e^{-x^2}$ leads to:

$$(-1)^{n+1} \frac{d^{n+1}}{dx^{n+1}}\left(e^{-x^2}\right) = \left[(2x)^{n+1} + a_{n-1}\,x^{n-1} + a_{n-3}\,x^{n-3} + \ldots\right] e^{-x^2} = H_{n+1}(x)e^{-x^2}.$$

Proving the result for $n = 0$ anchors the hypothesis. Assuming the result for the case $n$ and then proving it for the case $n + 1$ establishes the result for *all cases*. The $H_n(x)$ are alternately even and odd polynomials. Continue to argue that:

$\frac{d^n}{dx^n}\left(H_n(x)\right) = 2^n\, n!\, H_0(x) = 2^n\, n!$. Use this result in the problem below.

b.) Use the identity $\frac{d}{dx}\left(H_n(x)\right) = 2n\, H_{n-1}(x)$ to show that $\frac{d^n}{dx^n}\left(H_n(x)\right) = 2^n\, n!\, H_0(x) = 2^n\, n!$.

9.) Use the information in the previous two problems to evaluate: (Assume $m \geq n$)

$$\int_{-\infty}^{\infty} H_n(x)\, H_m(x)\, e^{-x^2}\, dx = \int_{-\infty}^{\infty} H_n(x)\left\{(-1)^m\; e^{x^2}\, \frac{d^m}{dx^m}\left(e^{-x^2}\right)\right\} e^{-x^2}\, dx = 2^n\, n!\sqrt{\pi}\;\; \delta_{mn}$$

Explain why one can assume $m \geq n$ without loss of generality. (The Hermite polynomial of higher order is represented by its Rodrigues formula.) Note that the results of this problem identify the orthonormal harmonic oscillator wavefunctions as $u_n(x) = \frac{1}{\sqrt{2^n\, n!\sqrt{\pi}}}\, H_n(x)\, e^{-x^2/2}$.

10.) The Hermite generating function relation is: $e^{(2xh - h^2)} = \sum_{n=0}^{\infty} \frac{h^n}{n!} H_n(x)$. Expand the left-hand side keeping all terms up to and including order $h^4$. Identify the Hermite polynomials $H_o$ to $H_4$.

11.) Give the value of $H_0(x)$. Prepare an argue that: $\frac{d^n}{dx^n}\left(H_n(x)\right) = 2^n\, n!\, H_0(x) = 2^n\, n!$ based on the recurrence relations. (short form of #8)

12.) Given the Hermite function definition: $\left|n\right\rangle = h_n(z) = \frac{1}{\sqrt{2^n\, n!\sqrt{\pi}}}\, H_n(z)\, e^{-z^2/2}$. Develop recurrence like expressions for $z\,|n\rangle$ and $({}^{d}/_{dz})\,|n\rangle$. Use the recurrence relations for the Hermite polynomials; do not assume those for the Hermite functions (SHO wavefunctions). What states are linked to $|n\rangle$ by $z$ and $\frac{d}{dz}$?

13.) Combine the Hermite function recurrence relations to find: $\left(\frac{1}{\sqrt{2}}\right)\left[z \pm \frac{d}{dz}\right]\left(h_n(z)\right)$.

Recast your results in the abstract vector space KET-style notation. What states are linked to $|n\rangle$ by $\hat{a} = \left(\frac{1}{\sqrt{2}}\right)\left[z + \frac{d}{dz}\right]$ and $\hat{a}^{\dagger} = \left(\frac{1}{\sqrt{2}}\right)\left[z - \frac{d}{dz}\right]$?

14.) Develop the recurrence relations based on $\frac{d^2}{dz^2}\left(h_n(z)\right)$ and $z^2 h_n(z)$. What states are linked to $|n\rangle$ by $z^2$ and the second derivative with respect to $z$?

15.) Given: $\phi_n(z) = h_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x)\, e^{-x^2/2}$, use the recurrence relations for the oscillator wave functions to evaluate: **All integrals are over the range -∞ το ∞.** Use the methods from the Tools of the Trade section.

$$\int \varphi_3^*(x)\; x^2 \varphi_1(x)\, dx \qquad \int \varphi_m^*(x)\; x^2 \varphi_n(x)\, dx \qquad \int \varphi_1^*(x)\, \frac{d}{dx}\left(\varphi_3(x)\right) dx \qquad \int \varphi_m^*(x)\, \frac{d}{dx}\left(\varphi_n(x)\right) dx$$

$$\int \varphi_m^*(x)\, \frac{d^2}{dx^2}\left(\varphi_n(x)\right) dx \quad \text{and} \quad \int \varphi_m^*(x) \left[-\frac{d^2}{dx^2} + x^2\right]\left(\varphi_n(x)\right) dx$$

16.) Use the methods from the Tools of the Trade section.

Given: $\phi_n(x) = \alpha^{1/2} h_n(\alpha x) = \frac{\alpha^{1/2}}{\sqrt{2^n n! \sqrt{\pi}}} H_n(\alpha x)\, e^{-(\alpha x)^2/2}$ Use the recurrence relations

$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$ $\qquad \hat{a}^t|n\rangle = \sqrt{n+1}\,|n+1\rangle$ to develop expressions for :

$x\varphi_n(x)$ and $\frac{d}{dx}\varphi_n(x)$. Continue to evaluate $\int \varphi_m^*(x)\, x \frac{d}{dx}\left(\varphi_n(x)\right) dx$, $\int \varphi_m^*(x)\, \frac{d}{dx}\left(x\varphi_n(x)\right) dx$

and $\int \varphi_m^*(x)\left[\frac{d}{dx}x - x\frac{d}{dx}\right]\left(\varphi_n(x)\right) dx$. **Both integrals are over the range -∞ το ∞.**

17. Starting with the linearly independent set of functions $\{1\, e^{-x^2/2}$, $x\, e^{-x^2/2}$, $x^2\, e^{-x^2/2}$, $x^3\, e^{-x^2/2}$, …. } over the domain (-∞,∞) construct the first three members of a set of orthonormal functions using the Gramm-Schmidt method with the inner product: $\langle f \,|\, g \rangle = \int_{-\infty}^{\infty} [\,f(x)]^*\, g(x)\; dx$ .

Hermite Functions: $h_o(x)$ = ________ ; $h_1(x)$ = ________ ; $h_2(x)$ = ____________

Companion problem for #6.

18. Identify and factor out the large $z$ behavior. For large $z$, the $\lambda_n\, u_n$ term is negligible compared to $z^2\, u_n$. Study: $\frac{d^2 u_n}{dz^2} = z^2\, u_n(x)$ . To leading order in $z$, $u(z) \approx A\; e^{-z^2/2}$ for $|z|$ very large. Show that:

$\frac{d^2}{dz^2}\left(e^{-z^2/2}\right) = z^2\, e^{-z^2/2}\, \left[1 + \mathcal{O}(z^{-2})\right]$ where $\mathcal{O}(z^{-2})$ represents "*and terms of order that vanish as $z^{-2}$ or faster*". Why is the behavior $u(z) \approx A\; e^{-z^2/2}$ which works to the same order banished for the list of possibilities? Propose that the full solution is: $u_n(z) = N_n\, H_n(z)\; e^{-z^2/2}$ where $N_n$ is a normalization constant, and find the equation satisfied by $H_n(z$ is

$\frac{d^2 H_n}{dz^2} - 2\,z\,\frac{dH_n}{dz} + (\lambda_n - 1)\, H_n = 0$ .

This equation is the DE for the Hermite polynomials (See problems 5 and 6.) The ratio and comparison tests indicate that the series diverges and that it diverges faster than $e^{-z^2/2}$ converges. The series must terminate to yield polynomials if the overall solution functions are to remain finite. The conclusions flow forth as series termination requires that $\lambda_n = 2\,n + 1$ leading to energy eigenvalues: $E_n = (n + {}^1/_2)\; \hbar\,(k/m)^{1/2} = (n + {}^1/_2)\; \hbar\,\omega_o$ and spatial and temporal eigenfunctions:

$$u_n(z) = h_n(z) = [2^n\, n!\, \pi^{1/2}]^{-1/2}\, H_n(z)\; e^{-z^2/2} \text{ and } \psi(x,t) = [2^n\, n!\, \pi^{1/2}]^{-1/2}\, H_n(z)\; e^{-z^2/2}$$

19.) The eigenvalue problem for the QSHO: $\left|n\right\rangle = h_n(z) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}} H_n(z)\, e^{-z^2/2}$

Find the recurrence relations for $\frac{d}{dz}\left(h_n(z)\right)$, $z\, h_n(z)$ and $\frac{d^2}{dz^2}\left(h_n(z)\right)$ and $z^2 h_n(z)$. Use then to evaluate $\left[-\frac{d^2}{dz^2} + z^2\right]\left(h_n(z)\right)$. Conclude that $h_n(z)$ is an eigenfunction of the operator $\left[-\frac{d^2}{dz^2} + z^2\right]$ with eigenvalue $2\,n + 1$. Recall that $\left[-\frac{d^2}{dz^2} + z^2\right]$ is the dimensionless form of the operator for the energy in terms of the energy unit $\frac{1}{2}\,\hbar\,(k/m)^{1/2}$.

20.) The eigenfunctions of the QSHO are known to be a complete set so any time independent solution can be represented as $u(z) = \sum_{m=0}^{\infty} a_m\, h_n(z)$ where the $h_m(z)$ are ortho-normal. The general form for a time dependent wave function is $\psi(z,t) = \sum_{m=0}^{\infty} a_m\, h_n(z)\, e^{-i(n+\frac{1}{2})\omega_0 t}$. Use this form to compute the normalization integral $\int_{-\infty}^{\infty} [\psi(z,t)]^*\, \psi(z,t)\, dz$. Be sure to use distinct dummy indices in the representations of the wavefunction and its complex conjugate. Use the orthogonality relation, $\int_{-\infty}^{\infty} h_m(z)\, h_n(z)\, dz = \delta_{mn}$. Express the probability that the particle is in the state $h_k(z)$ in terms of the expansion coefficients in the series representation of $\psi$.

21.) The eigenfunctions of the QSHO are known to be a complete set so any time independent solution can be represented as $u(z) = \sum_{m=0}^{\infty} a_m\, h_n(z)$ where the $h_m(z)$ are ortho-normal. The general form for a time dependent wave function is $\psi(z,t) = \sum_{m=0}^{\infty} a_m\, h_n(z)\, e^{-i(n+\frac{1}{2})\omega_0 t}$. Each state $h_n(z)\, e^{-i(n+\frac{1}{2})\omega_0 t}$ has an energy eigenvalue of $2\,n + 1$ (in units of $\frac{1}{2}\,\hbar\,(k/m)^{1/2}$) where $\left[-\frac{d^2}{dz^2} + z^2\right]$ is the operator for the energy. Compute the expectation value of the operator $\int_{-\infty}^{\infty}[\psi(z,t)]^*\left[-\frac{d^2}{dz^2}+z^2\right]\psi(z,t)\,dz$ using series representations for the wave function and its complex conjugate. Also use the orthogonality relation, $\int_{-\infty}^{\infty}h_m(z)\,h_n(z)\,dz=\delta_{mn}$. Discuss the result and the interpretation that $a_k{}^*a_k$ is the probability that the system is in the quantum state $k$ which has the (*dimensionless*) energy eigenvalue $2\,k+1$.

22. The eigenfunctions of the QSHO are known to be a complete set so any time independent solution can be represented as $u(z)=\sum_{m=0}^{\infty}a_m\,h_m(z)$ where the $h_m(z)$ are ortho-normal. The general form for a time dependent wave function is $\psi(z,t)=\sum_{m=0}^{\infty}a_m\,h_m(z)\,e^{-i(m+½)\omega_0 t}$. Find the expectation value of the coordinate $z$ in a general state of the QSHO. Compute that expectation value of position as: $\int_{-\infty}^{\infty}[\psi(z,t)]^*\,z\,\psi(z,t)\,dz$ using series representations for the wave function and its complex conjugate. Also use the orthogonality relation, $\int_{-\infty}^{\infty}h_m(z)\,h_n(z)\,dz=\delta_{mn}$. Make use of the recurrence relation: $z\,h_n(z) \;=\sqrt{n/2}\,h_{n-1}(z)\;+\sqrt{n+1/2}\,h_{n+1}(z)$. The result has two sums. Redefine the summation index in one sum as needed to make the summation ranges identical and show that the sums are the complex conjugates of one another. The result can be written as:

$$\langle z\rangle=\;\left[C^*\,e^{-i\omega_0 t}+C\,e^{+i\omega_0 t}\right]=\left[|C|e^{-i\delta}\,e^{-i\omega_0 t}+|C|e^{+i\delta}\,e^{+i\omega_0 t}\right]=A\cos[\omega_0 t+\delta]$$

where $C=|C|e^{i\delta}=(2)^{-½}\sum_{k=0}^{\infty}a_{k+1}^*\,a_k\,\sqrt{k+1}$ , $A = 2\,|C|$ (*Answer not verified*)

That is the expectation value of position has the same time dependence as does the position of a classical oscillator with the same $m$ and $k$. Note that the expectation value of the classical observable $z$ is real-valued.

This answer is for the dimensionless form of the problem. $\langle x\rangle = \alpha^{-1}\,\langle z\rangle$.

$$\langle x\rangle = 2\,|C|\left(\frac{\hbar^2}{mk}\right)^{1/4}\cos[\omega_0 t + \delta]$$

23. The eigenfunctions of the QSHO are known to be a complete set so any time independent solution can be represented as $u(z)=\sum_{m=0}^{\infty} a_m\,h_m(z)$ where the $h_m(z)$ are orthonormal. The general form for a time dependent wave function is $\psi(z,t)=\sum_{m=0}^{\infty} a_m\,h_m(z)\,e^{-i(m+½)\omega_0 t}$. Find the expectation value of the dimensionless momentum in a general state of the QSHO using its operator $-i\frac{\partial}{\partial z}$. Compute that expectation value of position as: $\int_{-\infty}^{\infty}[\psi(z,t)]^*\left(-i\frac{\partial}{\partial z}\right)\psi(z,t)\,dz$ using series representations for the wave function and its complex conjugate. Also use the orthogonality relation, $\int_{-\infty}^{\infty} h_m(z)h_n(z)\,dz=\delta_{mn}$. Make use of the recurrence relation:

$\frac{d}{dz}\,h_n(z)=\sqrt{n/2}\,h_{n-1}(z)-\sqrt{n+1/2}\,h_{n+1}(z)$. The result has two sums. Redefine the summation index in one sum as needed to make the summation ranges identical and show that the sums are the complex conjugates of one another. The result can be cast in the form:

$$\langle p\rangle = -\,B\sin[\omega_o\,t+\delta] = -\,2\,|C|\sin[\omega_o\,t+\delta]\quad\text{(see previous problem)}$$

That is the expectation value of position has the same time dependence as does the momentum of a classical oscillator with the same $m$ and $k$ and a position $\langle z\rangle$ = A $\cos[\omega_o\,t+\delta]$. Conclude that the expectation values of the quantum system obey the classical equations of motion. Note that the expectation value of the classical observable $p$ is real-valued. Compare with the previous problem.

With the dimensioned constants reasserted, $\hat{p}=-i\hbar\frac{\partial}{\partial x}=-i\hbar\left(\frac{mk}{\hbar^2}\right)^{1/4}\frac{\partial}{\partial z}$.

Show that in the dimensioned form $\langle p\rangle = m\, {}^{d}/_{dt}\, \langle x\rangle$. Expectation values obey the classical equations of motion.

24.) The most general form for a time dependent wave function for a quantum harmonic oscillator is $\psi(z,t) = \sum_{m=0}^{\infty} c_m\, h_m(z)\, e^{-i(m+\frac{1}{2})\omega_0 t} = \sum_{m=0}^{\infty} c_m \left|m\right\rangle e^{-i(m+\frac{1}{2})\omega_0 t}$. Compute: $\left\langle \psi \middle| \psi \right\rangle = \int_{-\infty}^{\infty} \psi(z,t)^* \,\psi(z,t)\, dz$. Use the orthogonality statement $\langle n|m\rangle = \delta_{nm}$.

Your answer should be: $\left\langle \psi \middle| \psi \right\rangle = \sum_{k=0}^{\infty} c_k^*\, c_k$. As it represents the normalization integral, $\langle\psi|\psi\rangle = 1$.What quantity is being normalized? Provide your best interpretation of $c_5^*\, c_5$ and $c_k^*\, c_k$.

25.) Consider our lowering and raising operators: $\hat{a} = \left(\frac{1}{\sqrt{2}}\right)\left[z + \frac{d}{dz}\right]$ and $\hat{a}^\dagger = \left(\frac{1}{\sqrt{2}}\right)\left[z - \frac{d}{dz}\right]$.

$$\hat{a}\left|n\right\rangle = \sqrt{n}\;\; \left|n-1\right\rangle \text{ and } \hat{a}^\dagger \left|n\right\rangle = \sqrt{n+1}\;\; \left|n+1\right\rangle$$

The ground state cannot be lowered. Rather, it is annihilated by the lowering operator. $\hat{a}\left|0\right\rangle = \sqrt{0}\;\; \left|n-1\right\rangle = 0$. Moving from abstract vector to function notation, this becomes $\left(\frac{1}{\sqrt{2}}\right)\left[z + \frac{d}{dz}\right] u_o(z) = 0$.

a.)Solve this equation to find the spatial form of the ground state wave function of a harmonic oscillator. Be sure to normalize your result.

b.) $\hat{a}^\dagger \left|n\right\rangle = \sqrt{n+1}\;\; \left|n+1\right\rangle$ translated into $\left(\frac{1}{\sqrt{2}}\right)\left[z - \frac{d}{dz}\right] u_n(z) = (n+1)^{\frac{1}{2}}\, u_{n+1}(z)$. Use the raising operator repetitively to generate $u_1(z)$ and $u_2(z)$ from your $u_o(z)$. Note that the process generates the properly normalized wave functions.

25.) The Hermite polynomials were developed by solving the DE using $g(z) = \sum_{n=0}^{\infty} a_n z^n$ and isolating the coefficients of the $z^s$ terms. The recurrence relation became $(s + 2)(s + 1)\, a_{s+2} - 2s\, a_s + (\lambda - 1)\, a_s = 0$. A *two-term* recurrence relation is a good thing. Find the requirement on λ that will ensures that the power series terminates as a polynomial. Show that for $\lambda = 2n + 1$, the series terminates as an $n^{\text{th}}$ order polynomial. Rewrite the recurrence relation using the value of λ. The $n^{\text{th}}$ order polynomial is normalized to have the leading tern $(2x)^n$. Use the recurrence relation to derive the evaluation scheme: $H_n(x) = (2x)^n - \frac{n(n-1)}{1!}(2x)^{n-2} + \frac{n(n-1)(n-2)(n-3)}{2!}(2x)^{n-2} - \ldots$ .

---

**References:**


1. Mary L. Boas, ***Mathematical Methods in the Physical Sciences***, 2nd Edition, chapter 3, John Wiley & Sons (1983).

2. K. F. Riley, M. P. Hobson and S. J. Bence, ***Mathematical Methods for Physics and Engineering***, 2nd Ed., Cambridge, Cambridge UK (2002).

3. The Wolfram web site: mathworld.wolfram.com/

4. M. Abramowitz and J. A. Stegun. ***Handbook of Mathematical Functions***, NIST (1964).


$$\frac{d}{dz}\left(H_n(z)\, e^{-z^2/2}\right) = \frac{dH_n}{dz}\, e^{-z^2/2} - z\, H_n(z)\, e^{-z^2/2}$$

$$\frac{d^2}{dz^2}\left(H_n(z)\, e^{-z^2/2}\right) = \frac{d^2 H_n}{dz^2}\, e^{-z^2/2} - 2z\frac{dH_n}{dz}\, e^{-z^2/2} + z^2\, H_n(z)\, e^{-z^2/2}$$

$$\frac{d^2 H_n}{dz^2} - 2\, z\frac{dH_n}{dz} + (\lambda_n - 1)\, H_n = 0$$