Simple harmonics
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1. Classical mechanics

We consider a particle moving under the harmonic potential given by

$$V(x) = \frac{1}{2} m\omega_0^2 x^2 .$$

Equation of motion is given by

$$F = -\frac{\partial V}{\partial x} = -m\omega_0^2 x ,$$

$$m\frac{d^2 x}{dt^2} = F = -\frac{\partial V}{\partial x} = -m\omega_0^2 x ,$$

which leads to a simple harmonics oscillation,

$$\frac{d^2 x}{dt^2} = -\omega_0^2 x .$$

The solution of this differential equation is

$$x = x_M \cos(\omega_0 t - \varphi)$$

where x_M is the amplitude of the oscillation. The momentum p is given by

$$p = m\frac{dx}{dt} = -m\omega_0 x_M \sin(\omega t - \varphi) .$$

The total energy of the system is a sum of the kinetic energy and potential energy

$$E = \frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 x^2 = \frac{1}{2} m\omega_0^2 x_M^2$$

(Conservative system)

2. Quantum Mechanics

The Hamiltonian of the simple harmonics is given by

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{m\omega_0^2}{2}\hat{x}^2 .$$

The eigenvalue problem of the simple harmonics is defined by

$$\hat{H}\varphi_n(x) = \varepsilon_n\varphi_n(x) ,$$

with the energy eigenvalue,

$$\varepsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega_0$$

where n = 0, 1, 2, 3,.... The wave function of the simple harmonics can be described as

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega_0^2}{2}x^2\right)\varphi_n(x) = \varepsilon_n\varphi_n(x) .$$

We now introduce ξ as

$$\xi = \beta x$$

with

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}} \text{ [unit of cm}^{-1}]$$

The wave function of the ground state satisfies

$$(\xi + \frac{\partial}{\partial\xi})\varphi_0 = 0 .$$

The solution of this differential equation is obtained as

$$\varphi_0(\xi) = A_0 e^{-\frac{\xi^2}{2}}$$

Normalization:

$$1 = \int_{-\infty}^{\infty}|\varphi_0(\xi)|^2 d\xi = |A_0|^2\int_{-\infty}^{\infty}e^{-\xi^2}d\xi = |A_0|^2\pi$$

leading to $A_0 = \pi^{-\frac{1}{4}}$. Here we assume that A_0 is real.
Note that

$$\varphi_n(\xi) = \frac{1}{\sqrt{\beta}}\varphi_n(x).$$

and $\varphi_n(\xi)$ is given by

$$\varphi_n(\xi) = (\sqrt{\pi}2^n n!)^{-\frac{1}{2}}(\xi - \frac{\partial}{\partial\xi})^n e^{-\frac{\xi^2}{2}}.$$

or

$$\varphi_n(\xi) = (\sqrt{\pi}2^n n!)^{-\frac{1}{2}}(-1)^n e^{\frac{\xi^2}{2}}\frac{\partial^n}{\partial\xi^n}e^{-\xi^2}.$$

Since the Hermite polynomial is defined by

$$H_n(\xi) = (-1)^n e^{\xi^2}\frac{\partial^n}{\partial\xi^n}e^{-\xi^2}$$

we have the final form of the wavefunctions

$$\varphi_n(\xi) = (\sqrt{\pi}2^n n!)^{-\frac{1}{2}}e^{-\frac{\xi^2}{2}}H_n(\xi).$$

((Note))

$$(\xi - \frac{\partial}{\partial\xi})^n e^{-\xi^2/2} = (-1)^n e^{\xi^2/2}\frac{\partial^n}{\partial\xi^n}e^{-\xi^2}.$$

$$H_n(\xi) = (-1)^n e^{\xi^2}\frac{\partial^n}{\partial\xi^n}e^{-\xi^2} = e^{\xi^2/2}(\xi - \frac{\partial}{\partial\xi})^n e^{-\xi^2/2}.$$

The Hermite polynomial satisifies the differential equation

$$(\frac{d^2}{d\xi^2} - 2\xi\frac{d}{d\xi} + 2n)H_n(\xi) = 0.$$

3. Mathematica-1

Hermite polynomials

```
H[x_, n_] := (-1)^n Exp[x^2] D[Exp[-x^2], {x, n}];

Prepend[Table[{n, HermiteH[n, x]}, {n, 0, 10}], {"n", " H[x,n]"}] //
 TableForm
```

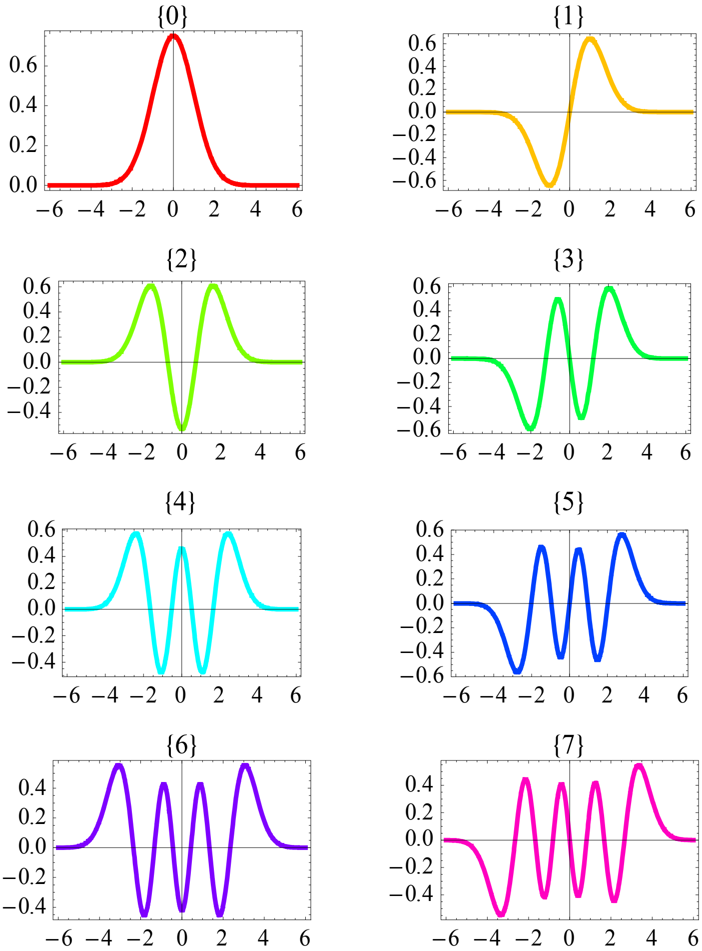
n	H[x,n]
0	1
1	$2x$
2	$-2+4x^2$
3	$-12x+8x^3$
4	$12-48x^2+16x^4$
5	$120x-160x^3+32x^5$
6	$-120+720x^2-480x^4+64x^6$
7	$-1680x+3360x^3-1344x^5+128x^7$
8	$1680-13440x^2+13440x^4-3584x^6+256x^8$
9	$30240x-80640x^3+48384x^5-9216x^7+512x^9$
10	$-30240+302400x^2-403200x^4+161280x^6-23040x^8+1024x^{10}$

4. Mathematica-2

Plot of the wave function

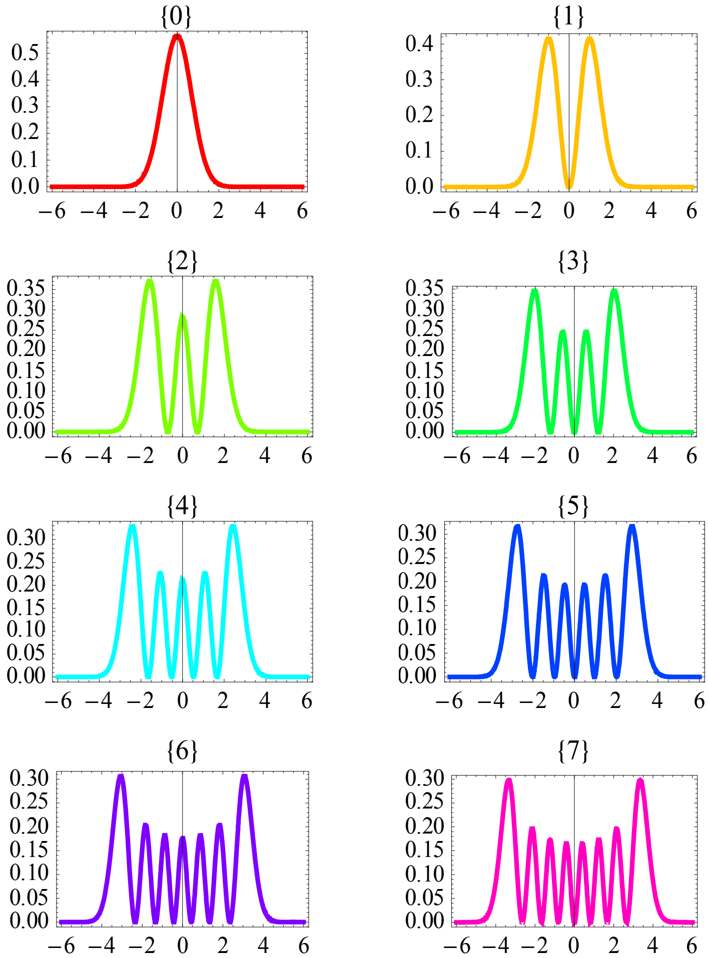
$$\varphi_n(\xi) = (\sqrt{\pi}\,2^n n!)^{-1/2} e^{-\xi^2/2} H_n(\xi)$$

where $n = 0, 1, 2,...$



5. Mathematica-3

Plot of $|\varphi_n(\xi)|^2$ where n = 0, 1, 2, ...,



6. Mathematica-4

Proof of

$$(\xi - \frac{\partial}{\partial \xi})^n \chi(\xi) = (-1)^n e^{\frac{\xi^2}{2}} \frac{\partial^n}{\partial \xi^n} e^{-\frac{\xi^2}{2}} \chi(\xi)$$

for any function $\chi(\xi)$.

```
Clear["Global`*"]; CR1 := (ξ # - D[#, ξ]) &; φ0[ξ_] := π^(-1/4) Exp[-ξ^2/2];

f[n_] := Nest[CR1, χ[ξ], n] // Simplify;
g[n_] := (-1)^n Exp[ξ^2/2] D[Exp[-ξ^2/2] χ[ξ], {ξ, n}] // Simplify;
Prepend[Table[{n, f[n]}, {n, 1, 4}], {"n", "f(n)= g(n)"}] // TableForm
```

n	f(n)= g(n)
1	$\xi\,\chi[\xi]-\chi'[\xi]$
2	$(-1+\xi^2)\,\chi[\xi]-2\,\xi\,\chi'[\xi]+\chi''[\xi]$
3	$\xi\,(-3+\xi^2)\,\chi[\xi]-3\,(-1+\xi^2)\,\chi'[\xi]+3\,\xi\,\chi''[\xi]-\chi^{(3)}[\xi]$
4	$(3-6\,\xi^2+\xi^4)\,\chi[\xi]-4\,\xi\,(-3+\xi^2)\,\chi'[\xi]-6\,\chi''[\xi]+6\,\xi^2\,\chi''[\xi]-4\,\xi\,\chi^{(3)}[\xi]+\chi^{(4)}[\xi]$

13. Mathematica-5:

```
ψ[ξ_, n_] := 1/Sqrt[n!] Nest[CR, φ0[ξ], n] // Simplify;
Prepend[Table[{n, ψ[ξ, n]}, {n, 0, 6}], {"n", "ψ[ξ,n]"}] // TableForm
```

n	ψ[ξ,n]
0	$\frac{e^{-\frac{\xi^2}{2}}}{\pi^{1/4}}$
1	$\frac{\sqrt{2}\,e^{-\frac{\xi^2}{2}}\,\xi}{\pi^{1/4}}$
2	$\frac{e^{-\frac{\xi^2}{2}}\,(-1+2\,\xi^2)}{\sqrt{2}\,\pi^{1/4}}$
3	$\frac{e^{-\frac{\xi^2}{2}}\,\xi\,(-3+2\,\xi^2)}{\sqrt{3}\,\pi^{1/4}}$
4	$\frac{e^{-\frac{\xi^2}{2}}\,(3-12\,\xi^2+4\,\xi^4)}{2\,\sqrt{6}\,\pi^{1/4}}$
5	$\frac{e^{-\frac{\xi^2}{2}}\,\xi\,(15-20\,\xi^2+4\,\xi^4)}{2\,\sqrt{15}\,\pi^{1/4}}$
6	$\frac{e^{-\frac{\xi^2}{2}}\,(-15+90\,\xi^2-60\,\xi^4+8\,\xi^6)}{12\,\sqrt{5}\,\pi^{1/4}}$

14. Comparison with Classical Mechanics

Classical mechanics

$$x = x_M \cos(\omega t - \varphi)$$

$$p = m\frac{dx}{dt} = -m\omega_0 x_M \sin(\omega t - \varphi)$$

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 x^2 = \frac{1}{2}m\omega_0^2 x_M{}^2$$

Comparison (classical mechanics and quantum mechanics)

We choose $\varphi = \pi/2$.

$$x = x_M \sin(\omega t)$$

$$p = m\frac{dx}{dt} = m\omega_0 x_M \cos(\omega t)$$

We define a classical "positional probability" as

$$W_{class}(x)dx = \frac{dt}{T}$$

where dt is the amount of time within dx and $T = 2\pi/\omega$.

$$dx = \omega x_M \cos(\omega t)dt = \omega x_M dt\sqrt{1-\sin^2(\omega t)} = \omega x_M dt\sqrt{1-(\frac{x}{x_M})^2}$$

since

$$\cos(\omega t) = \pm\sqrt{1-\sin^2(\omega t)} = \pm\sqrt{1-\left(\frac{x}{x_M}\right)^2}$$

we get

$$W_{class}(x)\omega x_M dt\sqrt{1-(\frac{x}{x_M})^2} = \frac{dt}{T} = \frac{\omega dt}{2\pi}$$

or

$$W_{class}(x) = \frac{1}{2\pi}\frac{1}{x_M\sqrt{1-(\frac{x}{x_M})^2}}$$

But this expression is not correct. Requiring that the total probability of finding the particle between $-x_M$ and x_M is unity determine the following correct expression

$$W_{class}(x) = \frac{1}{\pi} \frac{1}{x_M \sqrt{1-(\frac{x}{x_M})^2}}$$

In fact

$$\int_{-x_M}^{x_M} W_{class}(x)dx = \int_{-x_M}^{x_M} \frac{1}{\pi} \frac{1}{x_M \sqrt{1-(\frac{x}{x_M})^2}} dx = 1$$

The reason for the factor 2 is as follows. The particle passes between x and x +dx twice during a period

Here we have

$$x_M = \sqrt{\frac{2E}{m\omega_0{}^2}} = \sqrt{\frac{2\hbar\omega_0(n+\frac{1}{2})}{m\omega_0{}^2}} = \sqrt{2n+1}\sqrt{\frac{\hbar}{m\omega_0}} = \frac{\sqrt{2n+1}}{\beta}$$

Since

$$W_{class}(\xi)d\xi = W_{class}(x)dx$$

or

$$W_{class}(\xi)d\xi = W_{class}(x)dx = W_{class}(x)\frac{1}{\beta}d\xi$$

or

$$W_{class}(\xi) = W_{class}(x)\frac{1}{\beta}$$

and

$$\xi = \beta x$$

$$W_{class}(\xi)d\xi = W_{class}(x)dx = \frac{\beta}{\pi\sqrt{2n+1}} \frac{1}{\sqrt{1-(\frac{\xi}{\sqrt{2n+1}})^2}} \frac{d\xi}{\beta}$$

$$W_{class}(\xi) = \frac{1}{\pi\sqrt{2n+1}} \frac{1}{\sqrt{1-(\frac{\xi}{\sqrt{2n+1}})^2}} .$$

The classical limit is given by

$$\frac{\xi^2}{2} = n + \frac{1}{2}$$

The intercepts of the parabora ($\xi^2/2$) with horizontal lines (n+1/2) are the positions of the classical turning points. $W_{class}(\xi)$ is compared with $|\varphi_n(\xi)|^2$ (quantum mechanics).

$$W_{class}(\xi) = \underset{n\to\infty}{Lim} \frac{1}{2\varepsilon} \int_{\xi-\varepsilon}^{\xi+\varepsilon} \left|\varphi_n(\xi)^2\right| d\xi$$

Finally we calculate the probability of the particle in the forbidden region of the classical mechanics.

$$P(n) = 2 \int_{\sqrt{2n+1}}^{\infty} |\varphi_n(\xi)|^2 d\xi$$

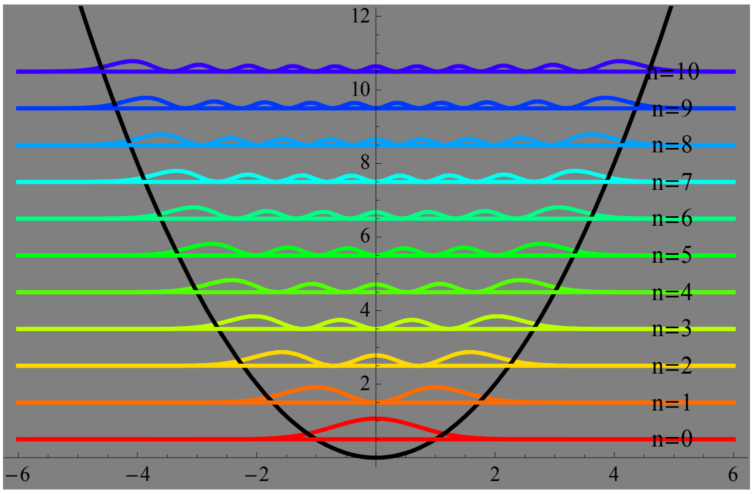
15. Mathematica-6

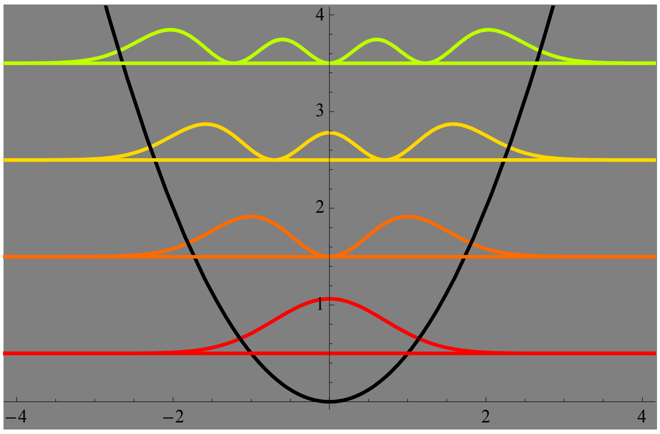
Probability beyond the classical limit

```
Clear["Global`*"];
φ[n_, ξ_] := 2^(-n/2) π^(-1/4) (n!)^(-1/2) Exp[-ξ^2/2] HermiteH[n, ξ];
Prob[n_] := 2 ∫_{√(2 n+1)}^∞ φ[n, ξ]^2 dξ // N;
Prepend[Table[{n, Prob[n], 1 - Prob[n]}, {n, 0, 10}],
  {"n", "Prob(n)", "1-Prob{n)"}] // TableForm
```

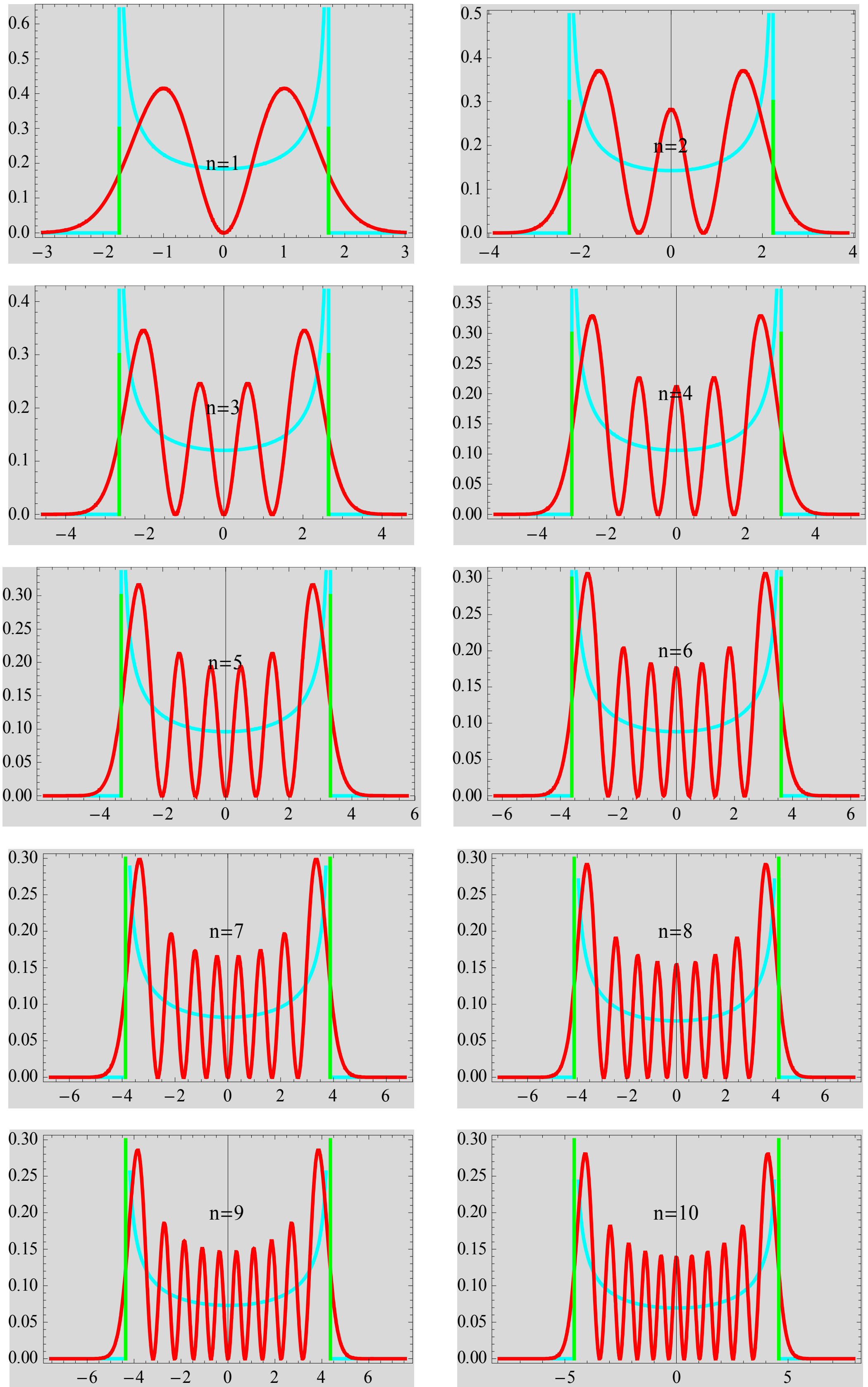
n	Prob(n)	1-Prob{n)
0	0.157299	0.842701
1	0.11161	0.88839
2	0.0950694	0.904931
3	0.0854829	0.914517
4	0.0789264	0.921074
5	0.0740342	0.925966
6	0.0701809	0.929819
7	0.0670313	0.932969
8	0.0643863	0.935614
9	0.0621191	0.937881
10	0.0601438	0.939856

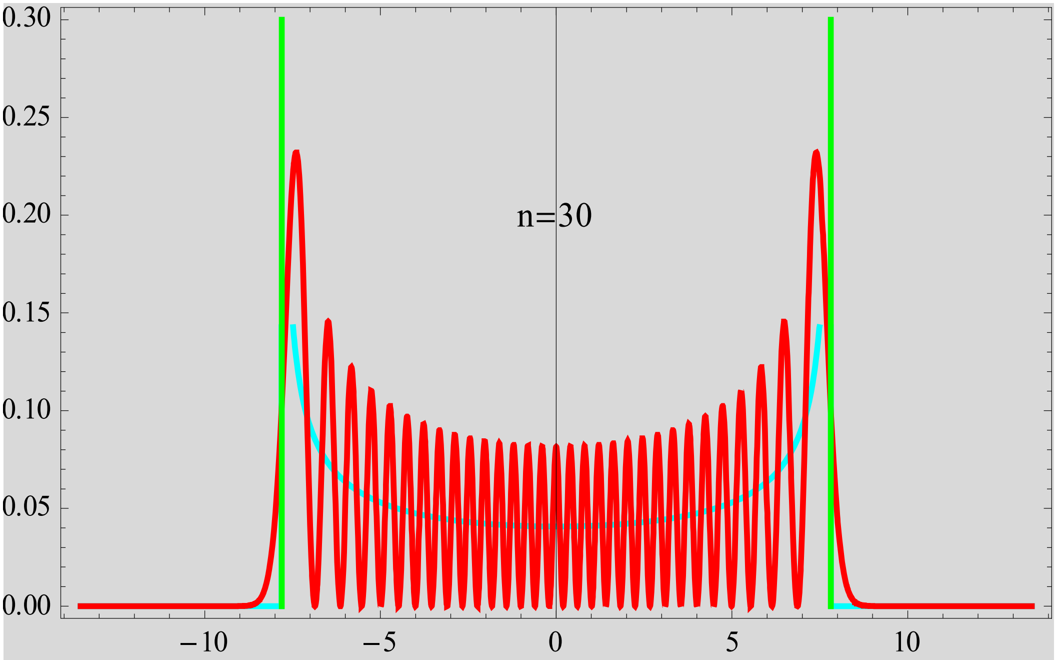
16. Mathematica-7





17. Mathematica-8


n=1
n=2
n=3
n=4
n=5
n=6
n=7
n=8
n=9
n=10



18. Differential equation (Series expansion method)

$$[\frac{d^2}{d\xi^2} - (\xi^2 - 2\varepsilon)]\varphi(\xi) = 0$$

where

$$\varepsilon = \frac{E}{\hbar\omega_0}$$

Let us try to predict intuitively the behavior of $\varphi(\xi)$ for very large ξ.

$$(\frac{d^2}{d\xi^2} - \xi^2)\varphi(\xi) = 0$$

To do this, consider

$$G_{\pm}(\xi) = e^{\pm\frac{\xi^2}{2}}$$

satisfies

$$[\frac{d^2}{d\xi^2} - (\xi^2 \pm 1)]G_\pm(\xi) = 0$$

When ξ approaches infinity, $\xi^2 \pm 1 \approx \xi^2 \approx \xi^2$-2ε.

We choose

$$G_\pm(\xi) = e^{-\frac{\xi^2}{2}}$$

from a physical point of view.

$$\lim_{\xi \to \infty} G_\pm(\xi) = 0$$

Now we set

$$\varphi(\xi) = e^{-\frac{\xi^2}{2}} h(\xi)$$

Here $h(\xi)$ satisfies the differential equation.

$$[\frac{d^2}{d\xi^2} - 2\xi \frac{d}{d\xi} + (2\varepsilon - 1)]h(\xi) = 0$$

$h(\xi)$ should be either even or odd functions.

$$h(\xi) = \xi^p (a_0 + a_2 \xi^2 + a_4 \xi^4 + ...) = \sum_{m=0}^{\infty} a_{2m} \xi^{2m+p}$$

with $a_0 \neq 0$.

$$h'(\xi) = \sum_{m=0}^{\infty} a_{2m} (2m + p) \xi^{2m+p-1}$$

$$h''(\xi) = \sum_{m=0}^{\infty} a_{2m} (2m + p)(2m + p - 1) \xi^{2m+p-2}$$

$$\sum_{m=0}^{\infty} a_{2m}(2m+p)(2m+p-1)\xi^{2m+p-2} - 2\sum_{m=0}^{\infty} a_{2m}(2m+p)\xi^{2m+p} h_n(\xi)$$

$$++\sum_{m=0}^{\infty}(2\varepsilon-1)a_{2m}\xi^{2m+p} = 0$$

$$a_0 p(p-1)\xi^{p-2} + a_2(p+2)(p+1)\xi^p + [-2a_0 p\xi^p + (2\varepsilon-1)a_0\xi^p] + ... = 0$$

The coefficient of ξ^{p-2}

$$a_0 p(p-1) = 0$$

Then $p = 0$ or 1.

....

In general, for the co-efficient of ξ^{2m+p}

$$a_{2m}(2\varepsilon - 1 - 4m - 2p) + a_{2m+2}(2m+p+2)(2m+p+1) = 0$$

or

$$a_{2m+2} = -\frac{2\varepsilon - (4m+2p+1)}{(2m+p+1)(2m+p+2)} a_{2m} \qquad (1)$$

with $p = 0$ or 1.

We consider what happens when ε is not expressed by

$$2\varepsilon = 4m_0 + 2p + 1$$

where m_0 is some positive integer.

$$\lim_{m\to\infty} \frac{a_{2m+2}}{a_{2m}} = \lim_{m\to\infty}\left[\frac{-2\varepsilon + (4m+2p+1)}{(2m+p+1)(2m+p+2)}\right] = \frac{1}{m}$$

Now we consider the power series of e^{ξ^2}

$$e^{\xi^2} = \sum_{m=0}^{\infty} b_{2m}\xi^{2m}$$

with

$$b_{2m} = \frac{1}{m!}$$

Thus

$$\lim_{m\to\infty} \frac{b_{2m+2}}{b_{2m}} \approx \frac{1}{m}$$

This means that

$$h(\xi) \approx e^{\xi^2}$$

or

$$\varphi(\xi) = e^{-\frac{\xi^2}{2}} h(\xi) \approx e^{-\frac{\xi^2}{2}} e^{\xi^2} \approx e^{\frac{\xi^2}{2}}$$

which become infinity when ξ tends to infinity. We must reject this solution. This solution makes no sense physically.

The numerator of Eq.(1) goes to zero for a value m_0 of m.

$$a_{2m} \neq 0 \text{ for } m \le m_0$$

and

$$a_{2m} = 0 \text{ for } m > m_0$$

or

$$4m_0 + 2p - 2\varepsilon + 1 = 0$$

or

$$\varepsilon = 2m_0 + p + \frac{1}{2} = \frac{E}{\hbar\omega}$$

If we set $n = 2m_0 + p$

(n = even for p = 0 and n = odd for p = 1.)

$$E_n = \hbar\omega(n + \frac{1}{2})$$

and

$$h_n(\xi) = \xi^p (a_0 + a_2\xi^2 + a_4\xi^4 + ... + a_{2m_0}\xi^{2m_0})$$

Then $p = 0$ or 1.

We consider the two cases.

(a) $p = 0$.

The coefficients of ξ^0, ξ^2, ξ^4, ξ^6, ξ^8,......

ξ^0 $(2\varepsilon - 1)a_0 + 2a_2 = 0$

ξ^2 $(2\varepsilon - 5)a_2 + 12a_4 = 0$

ξ^4 $(2\varepsilon - 9)a_4 + 30a_6 = 0$

ξ^6 $(2\varepsilon - 13)a_6 + 56a_8 = 0$

ξ^8 $(2\varepsilon - 17)a_8 + 90a_{10} = 0$

ξ^{10} $(2\varepsilon - 21)a_{10} + 132a_{12} = 0$

ξ^{12} $(2\varepsilon - 25)a_{12} + 182a_{14} = 0$

ξ^{14} $(2\varepsilon - 29)a_{14} + 240a_{16} = 0$

ξ^{16} $(2\varepsilon - 33)a_{16} + 306a_{18} = 0$

ξ^{18} $(2\varepsilon - 37)a_{18} + 380a_{20} = 0$

....

(b) $p = 1$

The coefficients of ξ^1, ξ^3, ξ^5, ξ^7,......

ξ^1 $(2\varepsilon - 3)a_0 + 6a_2 = 0$

ξ^3 $(2\varepsilon - 7)a_2 + 20a_4 = 0$

ξ^5 $(2\varepsilon - 11)a_4 + 42a_6 = 0$

ξ^7 $(2\varepsilon - 15)a_6 + 72a_8 = 0$

ξ^9 $(2\varepsilon - 19)a_8 + 110a_{10} = 0$

ξ^{11} $\quad (2\varepsilon-23)a_{10}+156a_{12}=0$

ξ^{13} $\quad (2\varepsilon-27)a_{12}+210a_{14}=0$

ξ^{15} $\quad (2\varepsilon-31)a_{14}+272a_{16}=0$

ξ^{17} $\quad (2\varepsilon-35)a_{16}+342a_{18}=0$

ξ^{19} $\quad (2\varepsilon-39)a_{18}+420a_{20}=0$

19. Mathematica-9

Hermite differential equation (series expansion)

```
Clear["Global`*"];

Eq1=D[φ[ξ],{ξ,2}]-(ξ^2-2 ε) φ[ξ];

rule1={φ→(Exp[-#^2/2] h[#]&)};

Eq2=Eq1/.rule1//Simplify;

Eq3=Eq2 e^(ξ^2/2) //Simplify
(-1 + 2 ε) h[ξ] - 2 ξ h′[ξ] + h″[ξ]

Eq4=(-1+2 ε) h[ξ]-2 ξ h′[ξ]+h″[ξ]
(-1 + 2 ε) h[ξ] + h″[ξ] - 2 ξ h′[ξ]

f[x_] := x^p Sum[a[2 m + 2 k] x^(2 m+2 k), {k, -2, 2}]

f[ξ] // Expand
ξ^(2 m+p) a[2 m] + ξ^(-4+2 m+p) a[-4 + 2 m] + ξ^(-2+2 m+p) a[-2 + 2 m] + ξ^(2+2 m+p) a[2 + 2 m] + ξ^(4+2 m+p) a[4 + 2 m]

rule2 = {h → (f[#] &)};

Eq5 = Eq4 /. rule2 // Simplify
```

$$-\frac{1}{\xi^4}\Big((1+4m+2p-2\varepsilon)\,\xi^{4+2m+p}\,a[2m]+$$
$$(-7+4m+2p-2\varepsilon)\,\xi^{2m+p}\,a[-4+2m]+\xi^2\Big((-3+4m+2p-2\varepsilon)\,\xi^{2m+p}\,a[-2+2m]+$$
$$(5+4m+2p-2\varepsilon)\,\xi^{4+2m+p}\,a[2+2m]+9\,\xi^{6+2m+p}\,a[4+2m]+4m\,\xi^{6+2m+p}\,a[4+2m]+$$
$$2p\,\xi^{6+2m+p}\,a[4+2m]-2\varepsilon\,\xi^{6+2m+p}\,a[4+2m]-\xi^2\,(f[\#1]\,\&)''[\xi]\Big)\Big)$$

```
Eq6 = Eq5 ξ^(6-2 m-p) // FullSimplify
```

$$\xi^{2-2m-p}\Big(-\xi^{2m+p}\Big((1+4m+2p-2\varepsilon)\,\xi^4\,a[2m]+(-7+4m+2p-2\varepsilon)\,a[-4+2m]+$$
$$\xi^2\Big((-3+4m+2p-2\varepsilon)\,a[-2+2m]+(5+4m+2p-2\varepsilon)\,\xi^4\,a[2+2m]+$$
$$(9+4m+2p-2\varepsilon)\,\xi^6\,a[4+2m]\Big)\Big)+\xi^4\,(f[\#1]\,\&)''[\xi]\Big)$$

```
list1=Table[{2 n,Coefficient[Eq6,ξ,2 n]},{n,0,6}]//Simplify//TableForm
```

0	0
2	$(7-4m-2p+2\varepsilon)\,a[-4+2m]$
4	$(3-4m-2p+2\varepsilon)\,a[-2+2m]$
6	$-(1+4m+2p-2\varepsilon)\,a[2m]$
8	$-(5+4m+2p-2\varepsilon)\,a[2+2m]$
10	$-(9+4m+2p-2\varepsilon)\,a[4+2m]$
12	0

We pick up the recursion formula :

$$-(1+4m+2p-2\varepsilon)\,a[2m]+\big(2+4m^2+3p+p^2+m\,(6+4p)\big)\,a[2+2m]$$

```
seq1 = -(1 + 4 m + 2 p - 2 ε) a[2 m] + (2 + 4 m^2 + 3 p + p^2 + m (6 + 4 p)) a[2 + 2 m] == 0
```

$$(-1-4m-2p+2\varepsilon)\,a[2m]+\big(2+4m^2+3p+p^2+m\,(6+4p)\big)\,a[2+2m]==0$$

```
Solve[seq1, a[2 + 2 m]] // Simplify
```

$$\Big\{\Big\{a[2+2m]\to\frac{(1+4m+2p-2\varepsilon)\,a[2m]}{2+4m^2+3p+p^2+m\,(6+4p)}\Big\}\Big\}$$

```
Factor[2 + 4 m^2 + 3 p + p^2 + m (6 + 4 p)]
```

$$(1+2m+p)\,(2+2m+p)$$

20. Stationary wave function))

Ground state ($n = 0$)

$\varepsilon = 1/2$

$m_0 = 0$, $p = 0$, $\qquad a_2 = 0$, $a_0 \neq 0$.

$$h(\xi) = a_0$$

$$\varphi_0(\xi) = a_0 e^{-\frac{\xi^2}{2}} \quad \text{(even function)}$$

Normalization:

$$\int_{-\infty}^{\infty} |\varphi_0(\xi)|^2 d\xi = \int_{-\infty}^{\infty} |a_0|^2 \exp(-\xi^2) d\xi = |a_0|^2 \sqrt{\pi} = 1$$

or

$$\varphi_0(\xi) = \pi^{-1/4}\frac{1}{\sqrt{2^0 0!}}e^{-\frac{\xi^2}{2}}$$

<u>$n = 1$ state</u>
$\varepsilon = 3/2$
$m_0 = 0, p = 1.$ $a_2 = 0, a_0 \neq 0.$

$$h(\xi) = a_0\xi$$

$$\varphi_1(\xi) = e^{-\frac{\xi^2}{2}}a_0\xi$$

$$\int_{-\infty}^{\infty}|\varphi_1(\xi)|^2 d\xi = \int_{-\infty}^{\infty}|a_0|^2\xi^2\exp(-\xi^2)d\xi = |a_0|^2\frac{\sqrt{\pi}}{2} = 1$$

$$\varphi_1(\xi) = \pi^{-1/4}\frac{1}{\sqrt{2^1 1!}}(2\xi)e^{-\frac{\xi^2}{2}}$$

<u>$n = 2$ state</u>
$\varepsilon = 5/2$, or $E = \hbar\omega_0(2 + \frac{1}{2})$
$m_0 = 1, p = 0.$ $2a_2 + 4a_0 = 0$
$a_2 = -2a_0$

$$\varphi_2(\xi) = e^{-\frac{\xi^2}{2}}a_0(1 - 2\xi^2)$$

$$\int_{-\infty}^{\infty}|\varphi_2(\xi)|^2 d\xi = \int_{-\infty}^{\infty}|a_0|^2(1-2\xi^2)^2\exp(-\xi^2)d\xi = |a_0|^2 2\sqrt{\pi} = 1$$

$$\varphi_2(\xi) = \pi^{-1/4}\frac{1}{\sqrt{2^2 2!}}(-2 + 4\xi^2)e^{-\frac{\xi^2}{2}}$$

<u>$n = 3$ state</u>
$\varepsilon = 7/2$, or $E = \hbar\omega_0(3 + \frac{1}{2})$
$m_0 = 1, p = 1.$ $6a_2 + 4a_0 = 0$

$$\varphi_3(\xi) = e^{-\frac{\xi^2}{2}} a_0 \xi (1 - \frac{2}{3}\xi^2)$$

$$\int_{-\infty}^{\infty} |\varphi_3(\xi)|^2 d\xi = \int_{-\infty}^{\infty} |a_0|^2 \xi^2 (1 - \frac{2}{3}\xi^2)^2 \exp(-\xi^2) d\xi = |a_0|^2 \frac{\sqrt{\pi}}{3} = 1$$

$$\varphi_3(\xi) = e^{-\frac{\xi^2}{2}} \pi^{-1/4} \frac{1}{\sqrt{2^3 3!}} (-12\xi + 8\xi^3)$$

$n = 4$ state

$\varepsilon = \frac{9}{2}$ or $E = \hbar\omega_0 (4 + \frac{1}{2})$

$p = 0$, $m_0 = 2$, $\quad a_4 = -\frac{1}{12}(2\varepsilon - 5)a_2 = -\frac{1}{3}a_2 = -\frac{1}{3}(-4a_0) = \frac{4}{3}a_0$

$$a_2 = -\frac{1}{2}(2\varepsilon - 1)a_0 = -4a_0$$

$$h_4(\xi) = a_0 (1 - 4\xi^2 + \frac{4}{3}\xi^4) = a_0'(12 - 48\xi^2 + 16\xi^4)$$

$$\varphi_4(\xi) = \exp[-\frac{\xi^2}{2}] h_4(\xi)$$

Normalization

$$\int_{-\infty}^{\infty} \exp[-\xi^2] |a_0'|^2 (12 - 48\xi^2 + 16\xi^4)^2 d\xi = |a_0'|^2 \sqrt{\pi} 2^4 4! = 1$$

or

$$a_0' = \pi^{-1/4} \frac{1}{\sqrt{2^4 4!}}$$

Thus we have

$$\varphi_4(\xi) = \pi^{-1/4} \frac{1}{\sqrt{2^4 4!}} \exp[-\frac{\xi^2}{2}] H_4(\xi)$$

((Note))

$H_n(\xi)$ is the Hermite polynomial.

$H_0(\xi) = 1$

$H_1(\xi) = 2\xi$

$H_2(\xi) = 4\xi^2 - 2$

$H_3(\xi) = 8\xi^3 - 12\xi$

$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12$

$H_5(\xi) = 32\xi^5 - 160\xi^3 + 120\xi$

$H_n(\xi)$ satisfies the differential equation given by

$$\left(\frac{d^2}{d\xi^2} - 2\xi\frac{d}{d\xi} + 2n\right)H_n(\xi) = 0$$

28. Normalization of the wave function of the simple harmonics

The wave function is given by

$$\varphi_n(\xi) = (\sqrt{\pi}2^n n!)^{-1/2} e^{-\xi^2/2} H_n(\xi)$$

where

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{\partial^n}{\partial \xi^n} e^{-\xi^2}$$

We show that

$$\int_{-\infty}^{\infty} \varphi_n^*(\xi)\varphi_n(\xi) d\xi = 1$$

or

$$\int_{-\infty}^{\infty} e^{-\xi^2} H_n(\xi) H_n(\xi) d\xi = 2^n n!\sqrt{\pi}$$

((Proof))

$$\int_{-\infty}^{\infty} e^{-\xi^2} H_n(\xi) H_n(\xi) d\xi = (-1)^n \int_{-\infty}^{\infty} e^{-\xi^2} H_n(\xi)[e^{\xi^2} \frac{\partial^n}{\partial \xi^n} e^{-\xi^2}] d\xi$$

$$= (-1)^n \int_{-\infty}^{\infty} H_n(\xi) \frac{\partial^n}{\partial \xi^n} e^{-\xi^2} d\xi = (-1)^n (-1)^n \int_{-\infty}^{\infty} e^{-\xi^2} \frac{\partial^n}{\partial \xi^n} H_n(\xi) d\xi$$

$H_n(\xi)$ is the Hermite polynomial and is a function of ξ. The highest power is ξ^n and the coefficient for the power ξ^n is 2^n.

$$\frac{\partial^n}{\partial \xi^n} H_n(\xi) = 2^n n!$$

Thus we have

$$\int_{-\infty}^{\infty} e^{-\xi^2} H_n(\xi) H_n(\xi) d\xi = 2^n n! \int_{-\infty}^{\infty} e^{-\xi^2} d\xi = 2^n n! \sqrt{\pi}$$

or

$$\int_{-\infty}^{\infty} \varphi_n^*(\xi)\varphi_n(\xi) d\xi = 1 .$$