Differential Operator Method on Simple Harmonics with the use of Mathematica

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1. Overview

The simple harmonics (or harmonic oscillator) is one of the most important topics in quantum mechanics. It can be solved in both classical and quantum mechanics. The annihilation operator $\hat{a}$ and creation operators $\hat{a}^+$ and are expressed in terms of the combination of the position operator $\hat{x}$ and the momentum operator $\hat{p}$, where the units of $\hat{a}$ and $\hat{a}^+$ are dimensionless. When undergraduate physics students start to learn such topics and encounters elegant form of $\hat{a}$ and $\hat{a}^+$ due to Dirac, they may have some struggles in understanding the physical meaning. The operator method for solving the quantum mechanics of simple harmonics appears to be magic.

In this article, we discuss how new operators $\hat{\xi}$ and $\hat{\kappa}$ (dimensionless) are related to $\hat{x}$ and $\hat{p}$,

$$\sqrt{\frac{m\omega}{\hbar}}\hat{x} = \beta\hat{x} = \hat{\xi} \qquad\qquad \frac{\hat{p}}{\sqrt{m\hbar\omega}} = \frac{\hat{p}}{\hbar\beta} = \frac{\hat{k}}{\beta} = \hat{\kappa},$$

with the commutation relation $[\hat{\xi},\hat{\kappa}] = i\hat{1}$. The annihilation operator and creation operator can be expressed by

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{\xi} + i\hat{\kappa}) , \qquad \hat{a}^+ = \frac{1}{\sqrt{2}}(\hat{\xi} - i\hat{\kappa}).$$

We also show that the eigenkets $|\xi\rangle$ and $|\kappa\rangle$ are related to $|x\rangle$ and $|p\rangle$ as

$$|\xi\rangle = \frac{1}{\sqrt{\beta}}|x\rangle, \qquad |\kappa\rangle = \sqrt{\hbar\beta}\,|p\rangle,$$

respectively. The eigenket $|\psi\rangle$ of the Hamiltonian in the $|\xi\rangle$ and $|\kappa\rangle$ representations are defined by $\langle\xi|\psi\rangle = \psi(\xi)$ and $\langle\kappa|\psi\rangle = \psi(\kappa)$. The function $\psi(\kappa)$ is the Fourier transform of the function $\psi(\xi)$

$$\langle\xi|\psi\rangle = \int d\kappa \langle\xi|\kappa\rangle\langle\kappa|\psi\rangle = \frac{1}{\sqrt{2\pi}}\int d\kappa e^{i\kappa\xi}\langle\kappa|\psi\rangle$$

using the closure relation with the transformation function.

Here we discuss the wave function of simple harmonics (quantum mechanics and classical limit) with the use of Mathematica. The differential operators of the creation operator and the annihilation operator is used for the derivation of the Hermite polynomials. We use the differential operators of $\hat{a}$ and $\hat{a}^+$,

$$\langle\xi|\hat{a}|\psi\rangle = \frac{1}{\sqrt{2}}(\xi + \frac{\partial}{\partial\xi})\psi(\xi), \qquad \langle\xi|\hat{a}^+|\psi\rangle = \frac{1}{\sqrt{2}}(\xi - \frac{\partial}{\partial\xi})\psi(\xi).$$

In Mathematica, we use the following expressions

$$\langle\xi|\hat{a}|\psi\rangle \to \frac{1}{\sqrt{2}}(\xi\#+D[\#,\xi])\&, \qquad \langle\xi|\hat{a}^+|\psi\rangle \to \frac{1}{\sqrt{2}}(\xi\#-D[\#,\xi])\&.$$

where the symbols (*D*, # and &) are used for the differential operators in the Mathematica program. The use of such notations may be useful to understanding the essential points in simple harmonics. Here we use "simple harmonics", instead of "harmonic oscillator. There are so many useful textbooks on the quantum mechanics on simple harmonics without the use of Mathematica.

2. Introduction of dimensionless operators $\hat{\kappa}$ and $\hat{\xi}$

The Hamiltonian of the simple harmonics is given by

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2,$$

where ω is the angular frequency, $\hat{p}$ and $\hat{x}$ are the momentum and position operators. Here we introduce the new operators ($\hat{\kappa}$ and $\hat{\xi}$) with the dimensionless units) instead of $\hat{p}$ and $\hat{x}$. To this end, we use the energy equipartition law in the classical limit, such that

$$\frac{1}{2m}p^2 = \frac{1}{2}\hbar\omega \qquad \frac{p}{\sqrt{m\hbar\omega}} = \frac{\hbar p}{\hbar\sqrt{m\hbar\omega}} = \frac{p}{\hbar\beta} = \frac{k}{\beta} = \kappa.$$

and

$$\frac{1}{2}m\omega^2 x^2 = \frac{1}{2}\hbar\omega \qquad \sqrt{\frac{m\omega}{\hbar}}x = \beta x = \xi$$

with

$$p = \hbar k = \hbar\beta\kappa$$

Here we note that the phase factor of the plane wave form wave function is given by

$$\frac{1}{\hbar}px = \frac{1}{\hbar}(\hbar\beta\kappa)\frac{\xi}{\beta} = \kappa\xi,$$

with

$$\xi = \beta x \qquad \kappa = \frac{k}{\beta}.$$

The parameter β is defined by

$$\beta = \sqrt{\frac{m\omega}{\hbar}} \qquad \text{(the units of } \beta\text{: 1/cm)}$$

The Hamiltonian can be rewritten as

$$\begin{aligned}\hat{H} &= \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 \\ &= \frac{1}{2m}\hbar^2\beta^2\hat{\kappa}^2 + \frac{1}{2}m\omega^2\frac{\hat{\xi}^2}{\beta^2} \\ &= \frac{1}{2}\hbar\omega(\hat{\kappa}^2 + \hat{\xi}^2)\end{aligned}$$

The commutation relation:

$$[\hat{\kappa}, \hat{\xi}] = [\frac{1}{\hbar\beta}\hat{p}, \beta\hat{x}] = \frac{1}{\hbar}[\hat{p}, \hat{x}] = \frac{1}{i}\hat{1}.$$

3. Creation operator and annihilation operators

Next, we introduce the annihilation and creation operators, The annihilation operator is defined by

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{\xi} + i\hat{\kappa}) \ , \qquad \hat{a}^{+} = \frac{1}{\sqrt{2}}(\hat{\xi} - i\hat{\kappa}).$$

The annihilation operator is

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{\xi} + i\hat{\kappa})$$
$$= \frac{1}{\sqrt{2}}(\beta\hat{x} + i\frac{\hat{k}}{\beta})$$
$$= \frac{1}{\sqrt{2}}(\beta\hat{x} + i\frac{\hat{p}}{\hbar\beta})$$
$$= \frac{1}{\sqrt{2}}\beta(\hat{x} + i\frac{\hat{p}}{\hbar\beta^2})$$

and the creation operator is

$$\hat{a}^+ = \frac{1}{\sqrt{2}}(\hat{\xi} - i\hat{\kappa})$$
$$= \frac{1}{\sqrt{2}}\beta(\hat{x} - i\frac{\hat{p}}{m\omega})$$

Note that the commutation relation is

$$[\hat{a}, \hat{a}^+] = \frac{1}{2}[\hat{\xi} + i\hat{\kappa}, \hat{\xi} - i\hat{\kappa}]$$
$$= \frac{1}{2}2i[\hat{\kappa}, \hat{\xi}]$$
$$= \hat{1}$$

or

$$[\hat{a}, \hat{a}^+] = \hat{1},$$

with $[\hat{\kappa}, \hat{\xi}] = \frac{1}{i}\hat{1}$.

4. Number operator

We note that the occupation number operator is definrd by

$$\begin{aligned}\hat{n} &= \hat{a}^{+}\hat{a} \\ &= \frac{1}{2}(\hat{\xi} - i\hat{\kappa})(\hat{\xi} + i\hat{\kappa}) \\ &= \frac{1}{2}(\hat{\xi}^2 + \hat{\kappa}^2 - i[\hat{\kappa}, \hat{\xi}]) \\ &= \frac{1}{2}(\hat{\xi}^2 + \hat{\kappa}^2 - \hat{1})\end{aligned}$$

or

$$\hat{\kappa}^2 + \hat{\xi}^2 = 2\hat{n} + \hat{1}.$$

So that, the Hamiltonian $\hat{H}$ can be rewritten as

$$\hat{H} = \frac{1}{2}\hbar\omega(\hat{\kappa}^2 + \hat{\xi}^2) = \hbar\omega(\hat{n} + \frac{1}{2}\hat{1}).$$

We note that

$$\hat{\xi} = \frac{1}{\sqrt{2}}(\hat{a} + \hat{a}^{+}),$$

$$\hat{\kappa} = \frac{1}{\sqrt{2}i}(\hat{a} - \hat{a}^{+}),$$

$$\begin{aligned}\hat{\xi}^2 &= \frac{1}{2}(\hat{a} + \hat{a}^{+})(\hat{a} + \hat{a}^{+}) \\ &= \frac{1}{2}[\hat{a}^2 + (\hat{a}^{+})^2 + \hat{a}\hat{a}^{+} + \hat{a}^{+}\hat{a}) \\ &= \frac{1}{2}[\hat{a}^2 + (\hat{a}^{+})^2 + 2\hat{a}^{+}\hat{a} + \hat{1}]\end{aligned}$$

$$\hat{\kappa}^2 = -\frac{1}{2}(\hat{a}-\hat{a}^+)(\hat{a}-\hat{a}^+)$$
$$= -\frac{1}{2}[\hat{a}^2 + (\hat{a}^+)^2 - \hat{a}\hat{a}^+ - \hat{a}^+\hat{a})$$
$$= -\frac{1}{2}[\hat{a}^2 + (\hat{a}^+)^2 - 2\hat{a}^+\hat{a} - \hat{1}]$$

The average:

$$\langle n|\hat{\xi}^2|n\rangle = \frac{1}{2}\langle n|[\hat{a}^2 + (\hat{a}^+)^2 + 2\hat{a}^+\hat{a} + \hat{1}]|n\rangle$$
$$= \frac{1}{2}\langle n|2\hat{n}^+ + \hat{1}|n\rangle$$
$$= n + \frac{1}{2}$$

$$\langle n|\hat{\kappa}^2|n\rangle = -\frac{1}{2}\langle n|[\hat{a}^2 + (\hat{a}^+)^2 - 2\hat{a}^+\hat{a} - \hat{1}]|n\rangle$$
$$= \frac{1}{2}\langle n|2\hat{n}^+ + \hat{1}|n\rangle$$
$$= n + \frac{1}{2}$$

The uncertainty:

$$(\Delta\xi)^2 = \langle n|\hat{\xi}^2|n\rangle - \langle n|\hat{\xi}|n\rangle^2$$
$$= n + \frac{1}{2}$$

$$(\Delta\kappa)^2 = \langle n|\hat{\kappa}^2|n\rangle - \langle n|\hat{\kappa}|n\rangle^2$$
$$= n + \frac{1}{2}$$

Heisenberg's principle of uncertainty:

$$(\Delta\xi)(\Delta\kappa) = n + \frac{1}{2} \geq \frac{1}{2}$$

We note that

$$\langle n|\hat{H}|n\rangle = \frac{1}{2}\langle n|\hat{\xi}^2 + \hat{\kappa}^2|n\rangle$$
$$= (n+\frac{1}{2})\hbar\omega$$

(equipartition law)

The matrix elements of $\hat{\xi}$ and $\hat{\kappa}$ is

$$\langle n'|\hat{\xi}|n\rangle = \frac{1}{\sqrt{2}}\langle n'|\hat{a} + \hat{a}^{+}|n\rangle$$
$$= \frac{1}{\sqrt{2}}[\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}]$$

$$\langle n'|\hat{\kappa}|n\rangle = \frac{1}{\sqrt{2}}\langle n'|\hat{a} - \hat{a}^{+}|n\rangle$$
$$= i\frac{1}{\sqrt{2}}(-\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1})$$

5. The eigenket of the Hamiltonian

$|n\rangle$ is the eigenket of the number operator;

$$\hat{n}|n\rangle = n|n\rangle .$$

So that, we have

$$\hat{H}|n\rangle = \hbar\omega(\hat{n} + \frac{1}{2}\hat{1})|n\rangle = \hbar\omega(n+\frac{1}{2}1)|n\rangle$$

We note that

$$\hat{a}^{+}\left|n\right\rangle = \sqrt{n+1}\left|n+1\right\rangle, \qquad \text{(creation operator)}$$

$$\hat{a}\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle, \qquad \text{(annihilation operator)}$$

where n = 0, 1, 2, 3, …. (integers). $\left|n\right\rangle$ can be expressed by

$$\left|n\right\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^{+})\left|0\right\rangle,$$

where $\hat{a}\left|0\right\rangle = 0$

6. Dirac notation

Here we introduce the kets $\left|\xi\right\rangle$ and $\left|\kappa\right\rangle$, which are defined by

$$\hat{\xi}\left|\xi\right\rangle = \xi\left|\xi\right\rangle \qquad \text{and} \qquad \hat{\kappa}\left|\kappa\right\rangle = \kappa\left|\kappa\right\rangle$$

From the definition of the Dirac delta function, we have

$$\begin{aligned}\left\langle \xi' | \xi'' \right\rangle &= \delta(\xi' - \xi'') \\ &= \delta(\beta x' - \beta x'') \\ &= \frac{1}{\beta}\delta(x' - x'') \\ &= \frac{1}{\beta}\left\langle x' | x'' \right\rangle\end{aligned}$$

and

$$\langle \kappa' | \kappa'' \rangle = \delta(\frac{k' - k''}{\beta})$$
$$= \beta\delta(k' - k'')$$
$$= \beta\langle k' | k'' \rangle$$

$$\langle p' | p'' \rangle = \delta[\hbar\beta(\kappa' - \kappa'')]$$
$$= \frac{1}{\hbar\beta}\langle \kappa' | \kappa'' \rangle$$

These results lead to the following relations for kets,

$$|\xi\rangle = \frac{1}{\sqrt{\beta}}|x\rangle, \qquad |\kappa\rangle = \sqrt{\beta}|k\rangle, \qquad |p\rangle = \frac{1}{\sqrt{\hbar\beta}}|\kappa\rangle$$

7. Transformation function

We have transformation function given by

$$\langle x | p \rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp(\frac{i}{\hbar}px)$$
$$= \frac{1}{\sqrt{2\pi\hbar}}\exp(\frac{i}{\hbar}\hbar\beta\kappa\frac{\xi}{\beta})$$
$$= \frac{1}{\sqrt{2\pi\hbar}}\exp(i\kappa\xi)$$

Since

$$\langle x | p \rangle = \frac{\sqrt{\beta}}{\sqrt{\hbar\beta}}\langle \xi | \kappa \rangle$$
$$= \frac{1}{\sqrt{\hbar}}\langle \xi | \kappa \rangle$$

we get a new transformation function

$$\langle \xi | \kappa \rangle = \frac{1}{\sqrt{2\pi}} \exp(i\kappa\xi), \qquad \langle \kappa | \xi \rangle = \langle \xi | \kappa \rangle^* = \frac{1}{\sqrt{2\pi}} \exp(-i\kappa\xi).$$

8. The $|\xi\rangle$ and $|\kappa\rangle$ and representation of $|\psi\rangle$

The $|\xi\rangle$ representation of $|\psi\rangle$ is related to the $|\kappa\rangle$ representation of $|\psi\rangle$ by the closure relation as

$$\begin{aligned}\langle \xi | \psi \rangle &= \int d\kappa \langle \xi | \kappa \rangle \langle \kappa | \psi \rangle \\ &= \frac{1}{\sqrt{2\pi}} \int d\kappa e^{i\kappa\xi} \langle \kappa | \psi \rangle\end{aligned}$$

and

$$\begin{aligned}\langle \kappa | \psi \rangle &= \int d\xi \langle \kappa | \xi \rangle \langle \xi | \psi \rangle \\ &= \frac{1}{\sqrt{2\pi}} \int d\xi e^{-i\kappa\xi} \langle \xi | \psi \rangle\end{aligned}$$

Note that

$$\begin{aligned}\langle \xi | \psi \rangle &= \int d\kappa \frac{1}{\sqrt{2\pi}} e^{i\kappa\xi} \langle \kappa | \psi \rangle \\ &= \frac{1}{2\pi} \int d\xi' \langle \xi' | \psi \rangle \int d\kappa e^{i\kappa(\xi - \xi')} \\ &= \frac{1}{2\pi} \int d\xi' \langle \xi' | \psi \rangle 2\pi\delta(\xi - \xi') \\ &= \int d\xi' \langle \xi' | \psi \rangle \delta(\xi - \xi') \\ &= \langle \xi | \psi \rangle\end{aligned}$$

with the use of the Dirac delta function

$$\int d\kappa e^{i\kappa(\xi-\xi')} = 2\pi\delta(\xi-\xi'),$$

and

$$\int d\xi e^{i\varsigma(\kappa-\kappa')} = 2\pi\delta(\kappa-\kappa').$$

9. Differential operators for the creation and annihilation operators

We start with the relation

$$\langle x|\hat{p}|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle$$

and

$$\langle p|\hat{x}|\psi\rangle = i\hbar\frac{\partial}{\partial p}\langle p|\psi\rangle$$

Using the relations

$$|\xi\rangle = \frac{1}{\sqrt{\beta}}|x\rangle, \qquad |\kappa\rangle = \sqrt{\beta}|k\rangle, \qquad |p\rangle = \frac{1}{\sqrt{\hbar\beta}}|\kappa\rangle$$

we get

$$\langle\xi|\hat{\kappa}|\psi\rangle = \frac{1}{i}\frac{\partial}{\partial\xi}\langle\xi|\psi\rangle$$

and

$$\langle\kappa|\hat{\xi}|\psi\rangle = i\frac{\partial}{\partial\kappa}\langle\kappa|\psi\rangle$$

Using the above relations, we find the expression of the differential operators for the annihilation and creating operators.

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{\xi} + i\hat{\kappa}), \qquad \hat{a}^{+} = \frac{1}{\sqrt{2}}(\hat{\xi} - i\hat{\kappa})$$

We get

$$\begin{aligned}\langle \xi | \hat{a} | \psi \rangle &= \frac{1}{\sqrt{2}} \langle \xi | \hat{\xi} + i\hat{\kappa} | \psi \rangle \\ &= \frac{1}{\sqrt{2}} (\xi + \frac{\partial}{\partial \xi}) \langle \xi | \psi \rangle\end{aligned}$$

and

$$\begin{aligned}\langle \xi | \hat{a}^{+} | \psi \rangle &= \frac{1}{\sqrt{2}} \langle \xi | \hat{\xi} - i\hat{\kappa} | \psi \rangle \\ &= \frac{1}{\sqrt{2}} (\xi - \frac{\partial}{\partial \xi}) \langle \xi | \psi \rangle\end{aligned}$$

Using the relations,

$$\hat{a}^{+} | n \rangle = \sqrt{n+1} | n+1 \rangle$$

and

$$\hat{a} | n \rangle = \sqrt{n} | n-1 \rangle$$

we get the general expression

$$|n\rangle = \frac{1}{\sqrt{n!}}\hat{a}^n |0\rangle$$

From this relation, we have

$$\langle \xi | n \rangle = \frac{1}{\sqrt{n!}} \langle \xi | \hat{a}^n | 0 \rangle$$
$$= \frac{1}{\sqrt{n!2^n}} (\xi - \frac{\partial}{\partial \xi})^n \langle \xi | 0 \rangle$$

10. Wave function of the ground state $\langle \xi | 0 \rangle$

The ground state $|0\rangle$ is defined by

$$\hat{a}|0\rangle = 0.$$

Using the relation,

$$\langle \xi | \hat{a} | 0 \rangle = \frac{1}{\sqrt{2}} \langle \xi | \hat{\xi} + i\hat{\kappa} | 0 \rangle$$
$$= \frac{1}{\sqrt{2}} (\xi + \frac{\partial}{\partial \xi}) \langle \xi | 0 \rangle$$

we get the first order differential equation

$$\frac{\partial}{\partial \xi} \langle \xi | 0 \rangle = -\xi \langle \xi | 0 \rangle$$

The solution of this first order differential equation is

$$\langle \xi | 0 \rangle = C \exp(-\frac{\xi^2}{2}),$$

where C can be determined from the normalization condition of the wave function

$$1 = \langle 0|0\rangle = \int_{-\infty}^{\infty} d\xi \langle 0|\xi\rangle\langle \xi|0\rangle = \int_{-\infty}^{\infty} d\xi \left|\langle \xi|0\rangle\right|^2$$

or

$$\int_{-\infty}^{\infty} d\xi \left|\langle \xi|0\rangle\right|^2 = |C|^2 \int_{-\infty}^{\infty} d\xi \exp(-\xi^2)$$
$$= |C|^2 \sqrt{\pi}$$

$$|C|^2 = \frac{1}{\pi^{1/2}}$$

$$C = \frac{1}{\pi^{1/4}}$$

Thus, we have

$$\langle \xi|0\rangle = \pi^{-1/4} \exp(-\frac{\xi^2}{2})$$

Then we get the expression of the wave function $\langle \xi|n\rangle$ as

$$\langle \xi|n\rangle = \frac{1}{\sqrt{n!}}\langle \xi|\hat{a}^{+}|0\rangle$$
$$= \frac{1}{\sqrt{n!}}\frac{1}{2^{n/2}}(\xi - \frac{\partial}{\partial \xi})^n \langle \xi|0\rangle$$
$$= \frac{1}{(2^n n!\sqrt{\pi})^{1/2}}(\xi - \frac{\partial}{\partial \xi})^n \exp(-\frac{\xi^2}{2})$$

As will be proofed using Mathematica, we get the formula

$$(\xi - \frac{\partial}{\partial \xi})^n \psi(\xi) = (-1)^n \exp(\frac{\xi^2}{2}) \frac{\partial^n}{\partial \xi^n} \exp(-\frac{\xi^2}{2}) \psi(\xi)$$

and

$$\begin{aligned}
(\xi - \frac{\partial}{\partial \xi})^n \exp(-\frac{\xi^2}{2}) &= [(-1)^n \exp(\frac{\xi^2}{2}) \frac{\partial^n}{\partial \xi^n} \exp(-\frac{\xi^2}{2})] \exp(-\frac{\xi^2}{2}) \\
&= (-1)^n \exp(\frac{\xi^2}{2}) \frac{\partial^n}{\partial \xi^n} \exp(-\xi^2) \\
&= (-1)^n \exp(-\frac{\xi^2}{2}) \exp(\xi^2) \frac{\partial^n}{\partial \xi^n} \exp(-\xi^2) \\
&= \exp(-\frac{\xi^2}{2}) H(n,\xi)
\end{aligned}$$

Here, the Hermite polynomial is defined by

$$H(n,\xi) = (-1)^n \exp(\xi^2) \frac{\partial^n}{\partial \xi^n} \exp(-\xi^2).$$

Using the above expression finally we get the form

$$\langle \xi | n \rangle = \frac{1}{(2^n n! \sqrt{\pi})^{1/2}} \exp(-\frac{\xi^2}{2}) H(n,\xi).$$

We also note that

$$\begin{aligned}\langle n|n'\rangle &= \int_{-\infty}^{\infty} d\xi \langle n|\xi\rangle\langle\xi|n'\rangle \\ &= \int_{-\infty}^{\infty} d\xi \langle\xi|n\rangle^{*}\langle\xi|n'\rangle \\ &= \frac{1}{(2^{n} n!\sqrt{\pi})^{1/2}}\frac{1}{(2^{n'} n'!\sqrt{\pi})^{1/2}}\int_{-\infty}^{\infty} d\xi \exp(-\xi^{2}) H(n,\xi) H(n',\xi) \\ &= \delta_{n,n'}\end{aligned}$$

or

$$\int_{-\infty}^{\infty} d\xi \exp(-\xi^{2}) H(n,\xi) H(n,\xi) = (2^{n} n!\sqrt{\pi})\delta_{n,n'}$$

((**Example**)) from Arfken

Show that

$$\int_{-\infty}^{\infty} \xi^{2} \exp(-\xi^{2}) H(n_{n},\xi) H(n_{n},\xi) = \sqrt{\pi}\, 2^{n} n!(n+\frac{1}{2})$$

((**Proof**)))

$$I = \int_{-\infty}^{\infty} \xi^{2} \exp(-\xi^{2}) H(n_{n},\xi) H(n_{n},\xi) = \sqrt{\pi}\, 2^{n} n!(n+\frac{1}{2})$$

Using the expression of $\langle\xi|n\rangle$,

$$\langle\xi|n\rangle = \frac{1}{\sqrt{\sqrt{\pi}\, 2^{n} n!}}\exp(-\frac{\xi^{2}}{2}) H_{n}(\xi)$$

$$
\begin{aligned}
I &= \sqrt{\pi}\, 2^n n! \int_{-\infty}^{\infty} \xi^2 \langle n|\xi\rangle\langle\xi|n\rangle H_n(\xi) \\
&= \sqrt{\pi}\, 2^n n! \langle n|\hat{\xi}^2|n\rangle \\
&= \sqrt{\pi}\, 2^n n! (n + \frac{1}{2})
\end{aligned}
$$

((**Mathematica Program-1**))

Creation operator and annihilation operator

$\hat{a}^{+}$ (CR; creation operator)

$\hat{a}$ (AN: annihilation operator)

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

$$\text{AN} := \frac{1}{\sqrt{2}} \left(\xi \# + \text{D}[\#, \xi]\right) \&;$$

$$\text{CR} := \frac{1}{\sqrt{2}} \left(\xi \# - \text{D}[\#, \xi]\right) \&;$$

Ground state wave function

```
f21 = AN[ψ1[ξ]] == 0 // Simplify
```

$\xi\, \psi 1[\xi] + \psi 1'[\xi] == 0$

```
f22 = DSolve[f21, ψ1[ξ], ξ]
```

$\left\{\left\{\psi 1[\xi] \to e^{-\frac{\xi^2}{2}}\, c_1\right\}\right\}$

$\psi 1[0, \xi\_] := \psi 1[\xi]\ /.\ \text{f22}[[1]]\ //.\ \left\{c_1 \to \pi^{-1/4}\right\}$

```
ψ1[0, ξ_] := ψ1[ξ] /. f22[[1]] //. {c₁ → π^(-1/4)}

ψ1[0, ξ]
```

$$\frac{e^{-\frac{\xi^2}{2}}}{\pi^{1/4}}$$

Wave function ψ2[n,ξ] in the real ξ space (in general case)

```
ψ1[n_, ξ_] := 1/Sqrt[n!] Nest[CR, ψ1[0, ξ], n] //
  FullSimplify

Table[{n, ψ1[n, ξ]}, {n, 0, 10}] //
 TableForm[#, TableHeadings →
    {None, {"n", "ψ[n,ξ]"}}] &
```

n	$\psi[n, \xi]$
0	$\frac{e^{-\frac{\xi^2}{2}}}{\pi^{1/4}}$
1	$\frac{\sqrt{2}\, e^{-\frac{\xi^2}{2}}\, \xi}{\pi^{1/4}}$
2	$\frac{e^{-\frac{\xi^2}{2}} \left(-1+2\,\xi^2\right)}{\sqrt{2}\,\pi^{1/4}}$
3	$\frac{e^{-\frac{\xi^2}{2}}\, \xi \left(-3+2\,\xi^2\right)}{\sqrt{3}\,\pi^{1/4}}$
4	$\frac{e^{-\frac{\xi^2}{2}} \left(3+4\,\xi^2 \left(-3+\xi^2\right)\right)}{2\sqrt{6}\,\pi^{1/4}}$
5	$\frac{e^{-\frac{\xi^2}{2}}\, \xi \left(15+4\,\xi^2 \left(-5+\xi^2\right)\right)}{2\sqrt{15}\,\pi^{1/4}}$
6	$\frac{e^{-\frac{\xi^2}{2}} \left(-15+90\,\xi^2-60\,\xi^4+8\,\xi^6\right)}{12\sqrt{5}\,\pi^{1/4}}$
7	$\frac{e^{-\frac{\xi^2}{2}}\, \xi \left(-105+210\,\xi^2-84\,\xi^4+8\,\xi^6\right)}{6\sqrt{70}\,\pi^{1/4}}$
8	$\frac{e^{-\frac{\xi^2}{2}} \left(105-840\,\xi^2+840\,\xi^4-224\,\xi^6+16\,\xi^8\right)}{24\sqrt{70}\,\pi^{1/4}}$
9	$\frac{e^{-\frac{\xi^2}{2}}\, \xi \left(945+8\,\xi^2 \left(-315+189\,\xi^2-36\,\xi^4+2\,\xi^6\right)\right)}{72\sqrt{35}\,\pi^{1/4}}$
10	$\frac{e^{-\frac{\xi^2}{2}} \left(-945+9450\,\xi^2+8\,\xi^4 \left(-1575+630\,\xi^2-90\,\xi^4+4\,\xi^6\right)\right)}{720\sqrt{7}\,\pi^{1/4}}$

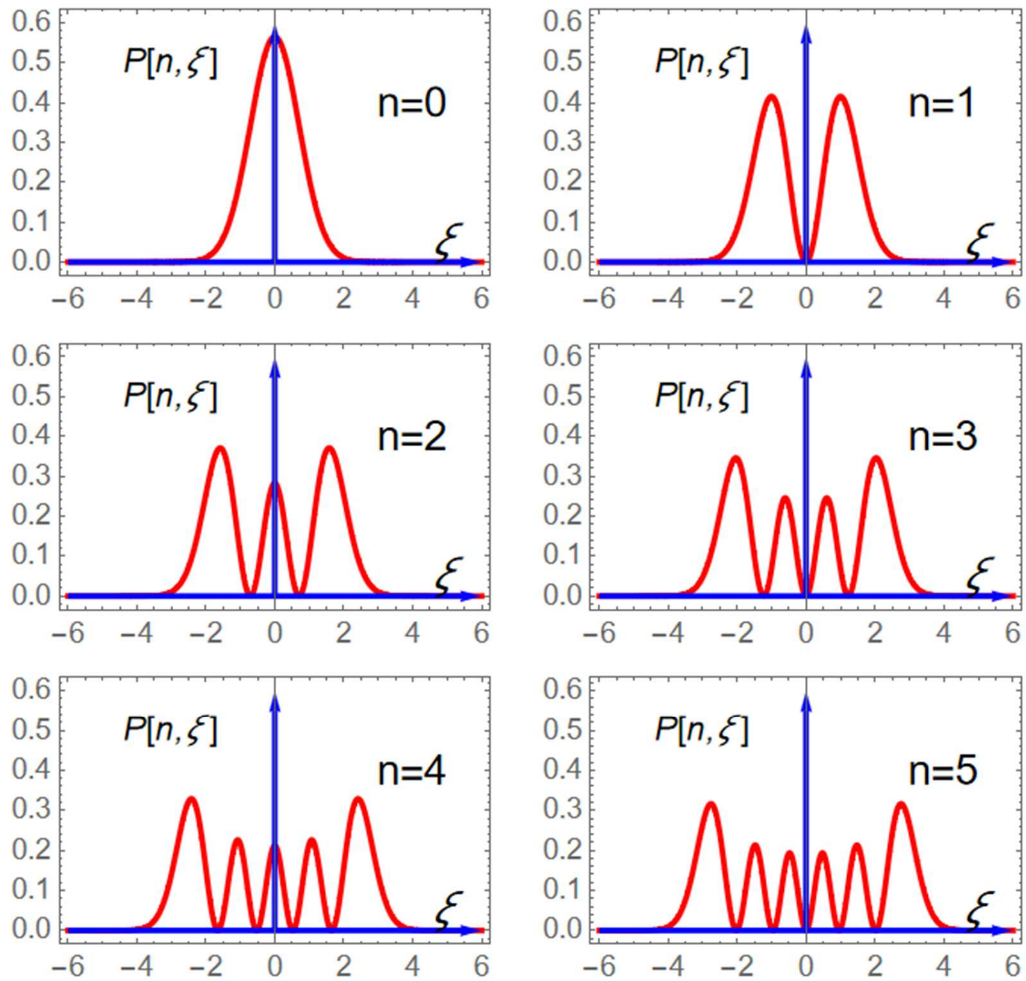
((**Mathematica Program-2**))

Simple Harmonics wave function

Plot of probability ; P[n,ξ]=ψ[n,ξ]^2

```
Clear["Global`*"];
ψ[n_, ξ_] := 2^(-n/2) π^(-1/4) (n !)^(-1/2) Exp[-ξ^2/2]
  HermiteH[n, ξ];
P[n_, ξ_] := ψ[n, ξ]^2;

pt1[n_] := Module[{f1, f2},
  f1 = Plot[Evaluate[P[n, ξ]], {ξ, -6, 6},
    PlotPoints → 100, PlotRange → All,
    PlotStyle → {Red, Thick},
    DisplayFunction → Identity, Frame → True];
  f2 =
   Graphics[
    {Text[Style["n=" <> ToString[n], Black, 15],
      {4, 0.4}], Arrowheads[0.05], Blue,
     Thick, Arrow[{{0, 0}, {0, 0.6}}],
     Arrow[{{-6, 0}, {6, 0}}],
     Text[Style["ξ", Black, Italic, 15],
      {5, 0.05}] ,
     Text[Style["P[n,ξ]", Black, Italic, 12],
      {-3, 0.5}]}];
  Show[f1, f2]];
```

```
pt2 = Evaluate[Table[pt1[n], {n, 0, 12}]];

Show[GraphicsGrid[Partition[pt2, 2]]]
```



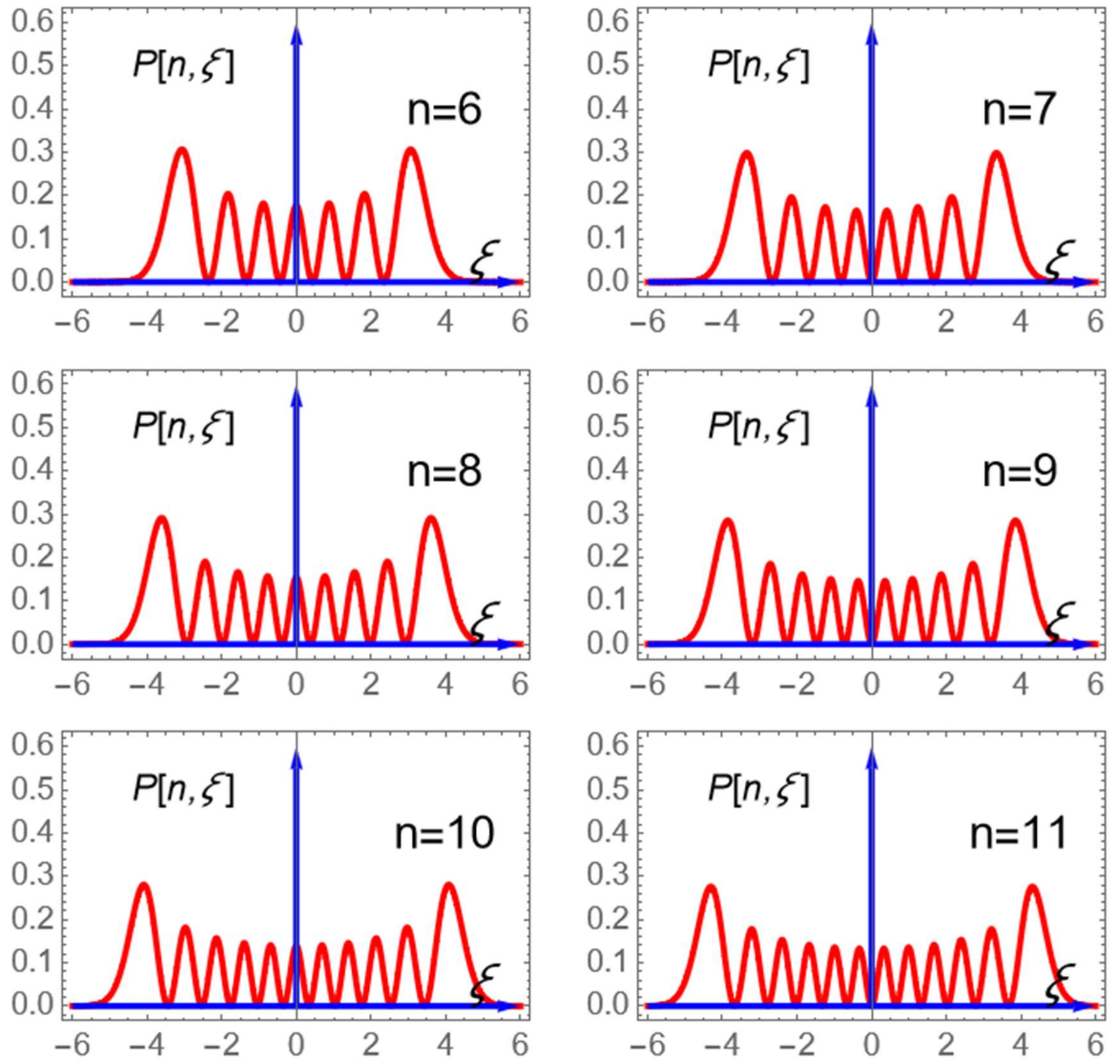


Fig. Plot of the probability density $P_n(\xi) = \left|\langle \xi | n \rangle\right|^2$ as a function of ξ for n = 1 - 11.

((Mathematica Program-3))

Formula

$(-1)^n \text{Exp}[\xi^2] \times D[\text{Exp}[-\xi^2], \{\xi, n\}]$==Hermite

H[n,ξ]

Proof

```
Clear["Global`*"];
H[n_, ξ_] :=
 (-1)^n Exp[ξ^2] × D[Exp[-ξ^2], {ξ, n}]

f1 = Table[{n, H[n, ξ]}, {n, 0, 5}] //
   Simplify //
  TableForm[#, TableHeadings →
     {None, {"n", "H[n,ξ]"}}] &
```

n	H[n,ξ]
0	1
1	2ξ
2	$-2+4\xi^2$
3	$4\xi(-3+2\xi^2)$
4	$4(3-12\xi^2+4\xi^4)$
5	$8\xi(15-20\xi^2+4\xi^4)$

```
f2 =
 Table[{n, HermiteH[n, ξ]}, {n, 0, 5}] //
  TableForm[#, TableHeadings →
     {None, {"n", "HermiteH[n,ξ]"}}] &
```

n	HermiteH[n,ξ]
0	1
1	$2\,\xi$
2	$-2+4\,\xi^2$
3	$-12\,\xi+8\,\xi^3$
4	$12-48\,\xi^2+16\,\xi^4$
5	$120\,\xi-160\,\xi^3+32\,\xi^5$

```
Table[{n, (H[n, ξ] - HermiteH[n, ξ])} //
   Simplify, {n, 0, 10}] // TableForm
```

0	0
1	0
2	0
3	0
4	0
5	0
6	0
7	0
8	0
9	0
10	0

((Mathematica Program-4))

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

$AN[\psi[\xi]] = \frac{1}{\sqrt{2}}(\xi\psi[\xi]+D[\psi[\xi],\xi])$

$CR[\psi[\xi]] = \frac{1}{\sqrt{2}}(\xi\psi[\xi]-D[\psi[\xi],\xi])$

$CR1[\psi[\xi]]=\xi\psi[\xi]-D[\psi[\xi],\xi]$

```
AN := 1/Sqrt[2] (ξ # + D[#, ξ]) &;
CR := 1/Sqrt[2] (ξ # - D[#, ξ]) &;
CR1 := (ξ # - D[#, ξ]) &;
```

Proof

J[n, ξ] = [n, (-1)^n Exp[ξ^2 / 2] D[Exp[-ξ^2 / 2] ψ[ξ] , {ξ, n}]

is equal to

$HE1[n,\xi] = (CR1)^n \psi[\xi] = Nest[CR1,\psi[\xi],n]$

```
J[n_, ξ_] := (-1)^n Exp[ξ^2 / 2] D[ Exp[-ξ^2 / 2] ψ[ξ] , {ξ, n}] //
   FullSimplify;
```

```
HE1[n_, ξ_] := Nest[CR1, ψ[ξ], n] // FullSimplify;
```

```
Table[{n, J[n, ξ]} // Simplify, {n, 0, 4}] //
 TableForm[#, TableHeadings → {None, {"n", "J[n,ξ]"}}] &
```

n	J[n,ξ]
0	$\psi[\xi]$
1	$\xi\,\psi[\xi] - \psi'[\xi]$
2	$\left(-1+\xi^2\right)\psi[\xi] - 2\,\xi\,\psi'[\xi] + \psi''[\xi]$
3	$\xi\left(-3+\xi^2\right)\psi[\xi] - 3\left(-1+\xi^2\right)\psi'[\xi] + 3\,\xi\,\psi''[\xi] - \psi^{(3)}[\xi]$
4	$\left(3-6\,\xi^2+\xi^4\right)\psi[\xi] - 4\,\xi\left(-3+\xi^2\right)\psi'[\xi] + 6\left(-1+\xi^2\right)\psi''[\xi] - 4\,\xi\,\psi^{(3)}[\xi] + \psi^{(4)}[\xi]$

```
Table[{n, HE1[n, ξ]} // FullSimplify, {n, 0, 4}] //
 TableForm[#, TableHeadings → {None, {"n", "HE1[n,ξ]"}}] &
```

n	HE1[n,ξ]
0	$\psi[\xi]$
1	$\xi\,\psi[\xi] - \psi'[\xi]$
2	$\left(-1+\xi^2\right)\psi[\xi] - 2\,\xi\,\psi'[\xi] + \psi''[\xi]$
3	$\xi\left(-3+\xi^2\right)\psi[\xi] - 3\left(-1+\xi^2\right)\psi'[\xi] + 3\,\xi\,\psi''[\xi] - \psi^{(3)}[\xi]$
4	$\left(3-6\,\xi^2+\xi^4\right)\psi[\xi] - 4\,\xi\left(-3+\xi^2\right)\psi'[\xi] + 6\left(-1+\xi^2\right)\psi''[\xi] - 4\,\xi\,\psi^{(3)}[\xi] + \psi^{(4)}[\xi]$

```
Table[{n, (J[n, ξ] - HE1[n, ξ])} // Simplify, {n, 0, 10}] //
 TableForm[#, TableHeadings → {None, {"n", "J[n,ξ]-HE1[n,ξ]"}}] &
```

n	J[n,ξ]-HE1[n,ξ]
0	0
1	0
2	0
3	0
4	0
5	0
6	0
7	0
8	0
9	0
10	0

11. Parity operator

We introduce the parity operator. The parity operator has the following properties.

$$\hat{\pi}\hat{\xi}\hat{\pi} = -\hat{\xi}, \qquad \hat{\pi}\hat{\kappa}\hat{\pi} = -\hat{\kappa}$$

$$\hat{\pi}^{+} = \hat{\pi}, \qquad \hat{\pi}^{2} = \hat{1}$$

$$\hat{\pi}|\xi\rangle = |-\xi\rangle, \qquad \langle\xi|\hat{\pi} = \langle-\xi|$$

$$\hat{\pi}|\kappa\rangle = |-\kappa\rangle, \qquad \langle\kappa|\hat{\pi} = \langle-\kappa|$$

Using these properties, ee show that

$$\hat{\pi}|0\rangle = |0\rangle \qquad \text{(even parity)}$$

$$\hat{\pi}|n\rangle = (-1)^{n}|n\rangle \qquad \text{(even parity for even n, odd parity for odd n)}$$

We start with the ground state wave function

$$\langle\xi|0\rangle = \frac{1}{\pi^{1/4}}\exp(-\frac{\xi^{2}}{2}) \qquad \text{(Gaussian)}$$

We note that

$$\langle\xi|\hat{\pi}|0\rangle = \langle-\xi|0\rangle = \frac{1}{\pi^{1/4}}\exp(-\frac{\xi^{2}}{2}) = \langle\xi|0\rangle$$

So that $\hat{\pi}|0\rangle = |0\rangle$.

12. Commutation relation between $\hat{H}$ and $\hat{\pi}$

The Hamiltonian $\hat{H}$ commutes with the parity operator

$$[\hat{\pi}, \hat{H}] = 0,$$

since

$$\begin{aligned}
\hat{\pi}\hat{H}\hat{\pi} &= \frac{1}{2}\hbar\omega\hat{\pi}(\hat{\kappa}^2 + \hat{\xi}^2)\hat{\pi} \\
&= \frac{1}{2}\hbar\omega(\hat{\pi}\hat{\kappa}\hat{\pi}\hat{\pi}\hat{\kappa}\hat{\pi} + \hat{\pi}\hat{\xi}\hat{\pi}\hat{\pi}\hat{\xi}\hat{\pi}) \\
&= \frac{1}{2}\hbar\omega[(-\hat{\kappa})^2 + (-\hat{\xi})^2] \\
&= \frac{1}{2}\hbar\omega(\hat{\kappa}^2 + \hat{\xi}^2) \\
&= \hat{H}
\end{aligned}$$

where $\hat{\pi}^2 = \hat{1}$, $\hat{\pi}\hat{\kappa}\hat{\pi} = -\hat{\kappa}$, $\hat{\pi}\hat{\xi}\hat{\pi} = -\hat{\xi}$.

So that, we have simultaneous eigenkets for $\hat{H}$ and $\hat{\pi}$

$$\hat{H}|n\rangle = \hbar\omega(n + \frac{1}{2})|n\rangle, \qquad \hat{\pi}|n\rangle = \lambda|n\rangle.$$

The eigenvalue λ is determined as follows.

$$\hat{\pi}^2|n\rangle = \lambda\hat{\pi}|n\rangle = \lambda^2|n\rangle = |n\rangle,$$

since $\hat{\pi}^2 = \hat{1}$. So that we have $\lambda = \pm 1$. We note that

$$\begin{aligned}
\hat{\pi}|n\rangle &= \frac{1}{\sqrt{n!}}\hat{\pi}(\hat{a}^+)^n\hat{\pi}\hat{\pi}|0\rangle \\
&= \frac{1}{\sqrt{n!}}(-\hat{a}^+)^n\hat{\pi}|0\rangle \\
&= (-1)^n\frac{1}{\sqrt{n!}}\hat{a}^{+n}|0\rangle \\
&= (-1)^n|n\rangle
\end{aligned}$$

or

$$\hat{\pi}\left|n\right\rangle = (-1)^n \left|n\right\rangle .$$

Here, we use the formula

$$\hat{\pi} f(\hat{a})\hat{\pi} = f(-\hat{a}) , \qquad \hat{\pi} g(\hat{a}^+)\hat{\pi} = g(-\hat{a}^+) ,$$

where *f* and *g* are any polynomial functions. Thus, we have

$$\left\langle \xi\right|\hat{\pi}\left|n\right\rangle = \left\langle -\xi\right|n\right\rangle = (-1)^n \left\langle \xi\right|n\right\rangle .$$

When n = 0, 2, 4, …, $\hat{\pi}\left|n\right\rangle = \left|n\right\rangle$ (even parity)

$\left\langle \xi\right|n\right\rangle$ is the even function of ξ.

When n = 1, 3, 4, …, $\hat{\pi}\left|n\right\rangle = -\left|n\right\rangle$ (odd parity parity)

$\left\langle \xi\right|n\right\rangle$ is the odd function of ξ.

13. The form of wave function $\left\langle \xi\right|n\right\rangle$

We now return to the form of wave function.

$$\left\langle \xi\right|n\right\rangle = \frac{1}{(2^n n!\sqrt{\pi})^{1/2}} \exp(-\frac{\xi^2}{2}) H(n,\xi)$$

$$\left\langle -\xi\right|n\right\rangle = \frac{1}{(2^n n!\sqrt{\pi})^{1/2}} \exp(-\frac{\xi^2}{2}) H(n,-\xi)$$

Since

$$\langle -\xi | n \rangle = (-1)^n \langle \xi | n \rangle$$

It is concluded that

$$H_n(-\xi) = (-1)^n H_n(\xi). \qquad \text{(the parity relation)}$$

14. Fourier Transform of $\langle \xi | 0 \rangle$

First, we calculate the Fourier transform of the ground state wave function $\langle \xi | 0 \rangle$. The Fourier transform of $\langle \xi | 0 \rangle$ is defined by

$$\begin{aligned}
\langle \kappa | 0 \rangle &= \int_{-\infty}^{\infty} d\xi \langle \kappa | \xi \rangle \langle \xi | 0 \rangle \\
&= \frac{1}{\sqrt{2\pi}} \frac{1}{\pi^{1/4}} \int_{-\infty}^{\infty} d\xi \exp(-i\kappa\xi) \exp(-\frac{\xi^2}{2}) \\
&= \frac{1}{\sqrt{2\pi}} \frac{1}{\pi^{1/4}} \exp(-\frac{\kappa^2}{2}) \int_{-\infty}^{\infty} d\xi \exp(-\frac{(\xi + i\kappa)^2}{2}) \\
&= \frac{1}{\pi^{1/4}} \exp(-\frac{\kappa^2}{2})
\end{aligned}$$

where

$$\int_{-\infty}^{\infty} d\xi \exp(-\frac{(\xi + i\kappa)^2}{2}) = \sqrt{2\pi} \; .$$

15. Fourier transform of $\langle \kappa | 0 \rangle$

We start with

$$\hat{a} | 0 \rangle = 0.$$

Thus, we have

$$\langle\kappa|\hat{a}|0\rangle = \frac{1}{\sqrt{2}}\langle\kappa|\hat{\xi}+i\hat{\kappa}|0\rangle$$
$$= \frac{1}{\sqrt{2}}i(\kappa+\frac{\partial}{\partial\kappa})\langle\kappa|0\rangle$$

in the $|\kappa\rangle$ representation,

or

$$(\kappa+\frac{\partial}{\partial\kappa})\langle\kappa|0\rangle = 0\,.$$

The solution of the first-order differential equation is

$$\langle\kappa|0\rangle = \pi^{-1/4}\exp(-\frac{\kappa^2}{2})\,.$$

16. Fourier transform of $\langle\kappa|n\rangle$

$$\langle\kappa|n\rangle = \frac{1}{\sqrt{n!}}\langle\kappa|(\hat{a}^{+})^{n}|0\rangle$$
$$= \frac{1}{\sqrt{n!}}\frac{1}{2^{n/2}}\langle\kappa|(\hat{\xi}-i\hat{\kappa})^{m}|0\rangle$$
$$= \frac{1}{\sqrt{n!}}\frac{1}{2^{n/2}}(-i)^{n}(\kappa-\frac{\partial}{\partial\kappa})^{n}\langle\kappa|0\rangle$$
$$= \frac{(-i)^{n}}{(2^{n}n!\sqrt{\pi})^{1/2}}(\kappa-\frac{\partial}{\partial\kappa})^{n}\exp(-\frac{\kappa^2}{2})$$
$$= \frac{(-i)^{n}}{(2^{n}n!\sqrt{\pi})^{1/2}}\exp(-\frac{\kappa^2}{2})H(n,\kappa)$$

with

$$(\kappa-\frac{\partial}{\partial\kappa})^n \exp(-\frac{\kappa^2}{2}) = (-1)^n \exp(-\frac{\kappa^2}{2})\exp(\kappa^2)\frac{\partial^n}{\partial\kappa^n}\exp(-\kappa^2)$$

$$= \exp(-\frac{\kappa^2}{2})H(n,\kappa)$$

$$\langle\kappa|n\rangle = \int_{-\infty}^{\infty} d\xi \langle\kappa|\xi\rangle\langle\xi|n\rangle$$

$$= \frac{1}{(2^n n!\sqrt{\pi})^{1/2}}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\xi \exp(-i\kappa\xi)\exp(-\frac{\xi^2}{2})H(n,\xi)$$

$$= \frac{(-i)^n}{(2^n n!\sqrt{\pi})^{1/2}}\exp(-\frac{\kappa^2}{2})H(n,\kappa)$$

$$(-i)^n \exp(\frac{-\kappa^2}{2})H(n,\kappa) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\xi \exp(-i\kappa\xi)\exp(\frac{-\xi^2}{2})H(n,\xi)$$

$$= \mathbf{F}[\exp(\frac{-\xi^2}{2})H(n,\xi)]$$

or

$$\mathbf{F}[\exp(\frac{-\xi^2}{2})H(n,\xi)] = (-i)^n \exp(\frac{-\kappa^2}{2})H(n,\kappa)$$

((**Mathematica Program-5**))

Simple Harmonics wave function

Fourier Transform of ψ[n,ξ]; ψ[n,κ]=Φ[n,κ]

```
Clear["Global`*"];
conjugateRule =
 {Complex[re_, im_] :→ Complex[re, -im]};
Unprotect[SuperStar];
SuperStar /: exp_* := exp /. conjugateRule;
Protect[SuperStar];
```

$$\psi[n\_,\ \xi\_] := 2^{-n/2}\ \pi^{-1/4}\ (n\,!)^{-1/2}\ \mathrm{Exp}\left[-\frac{\xi^2}{2}\right]$$

```
  HermiteH[n, ξ]
```

```
Φ[n_, κ_] := FourierTransform[ψ[n, ξ], ξ, κ,
  FourierParameters → {0, -1}]
```

```
Table[{n, Φ[n, κ]}, {n, 0, 5}] //
 TableForm[#,
   TableHeadings → {None, {"n", "Φ[n,κ]"}}] &
```

n	$\Phi[n,\kappa]$
0	$\frac{e^{-\frac{\kappa^2}{2}}}{\pi^{1/4}}$
1	$-\frac{i\sqrt{2}\,e^{-\frac{\kappa^2}{2}}\,\kappa}{\pi^{1/4}}$
2	$\frac{e^{-\frac{\kappa^2}{2}}\left(2-4\kappa^2\right)}{2\sqrt{2}\,\pi^{1/4}}$
3	$\frac{i\,e^{-\frac{\kappa^2}{2}}\,\kappa\left(-3+2\kappa^2\right)}{\sqrt{3}\,\pi^{1/4}}$
4	$\frac{e^{-\frac{\kappa^2}{2}}\left(3-12\kappa^2+4\kappa^4\right)}{2\sqrt{6}\,\pi^{1/4}}$
5	$-\frac{i\,e^{-\frac{\kappa^2}{2}}\,\kappa\left(15-20\kappa^2+4\kappa^4\right)}{2\sqrt{15}\,\pi^{1/4}}$

$$\chi[n\_,\kappa\_] := (-i)^{n}\, 2^{-n/2}\, \pi^{-1/4}\, (n!)^{-1/2}\, \mathrm{Exp}\left[-\frac{\kappa^2}{2}\right]$$

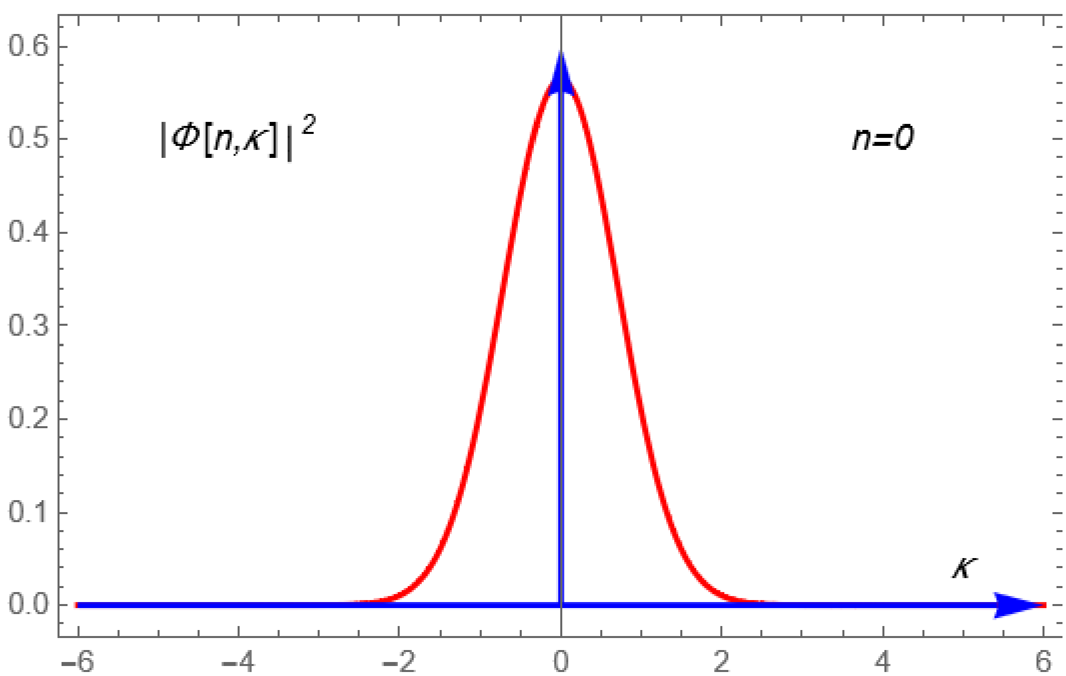
$$\mathrm{HermiteH}[n,\kappa]$$

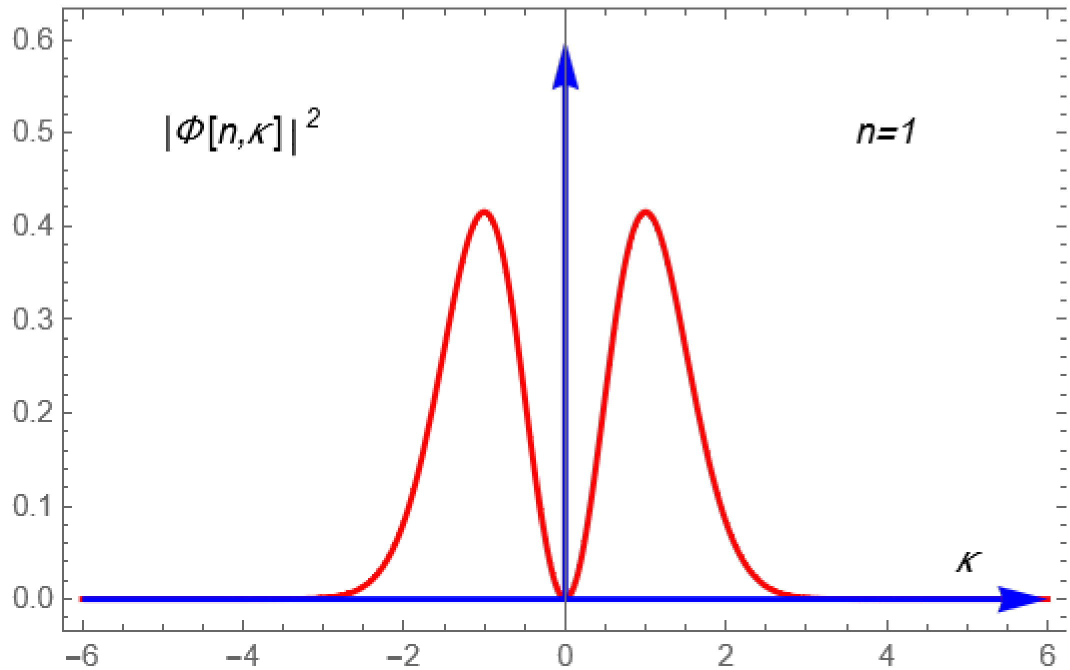
```
Table[{n, (Φ[n, κ] - χ[n, κ]) // Simplify},
  {n, 0, 10, 1}] //
 TableForm[#,
   TableHeadings → {None, {"n", "χ[n,κ]"}}] &
```

n	χ[n,κ]
0	0
1	0
2	0
3	0
4	0
5	0
6	0
7	0
8	0
9	0
10	0

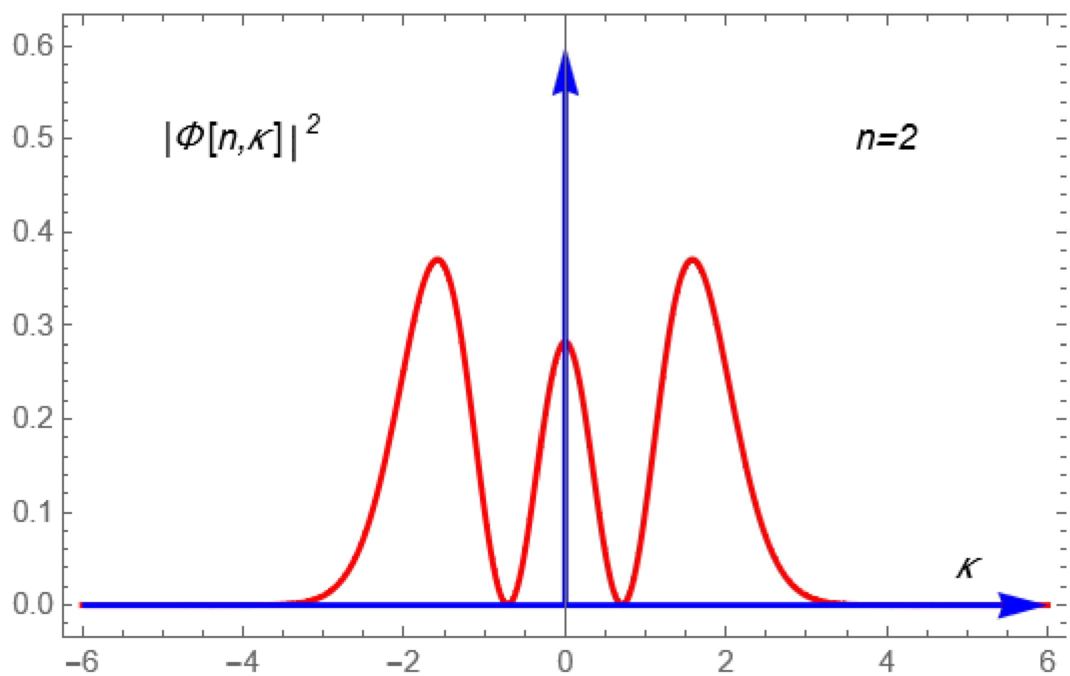
```
pt1[n_] := Module[{f1, f2},
   f1 = Plot[Evaluate[Φ[n, κ]* Φ[n, κ]],
     {κ, -6, 6}, PlotPoints → 100, PlotRange → All,
     PlotStyle → {Red, Thick}, Frame → True];
```

```
f2 = Graphics[
   {Text[Style["|Φ[n,κ]|²", Black, Italic,
      12], {-4, 0.5}],
    Text[Style["n=" <> ToString[n], Black,
      Italic, 12], {4, 0.5}],
    Text[Style["κ", Black, Italic, 12],
     {5, 0.04}], Blue, Thick, Arrowheads[0.05],
    Arrow[{{0, 0}, {0, 0.6}}],
    Arrow[{{-6, 0}, {6, 0}}]}];
  Show[f1, f2]];

pt2 = Evaluate[Table[pt1[n], {n, 0, 8}]];
Show[GraphicsGrid[Partition[pt2, 1]]]
```

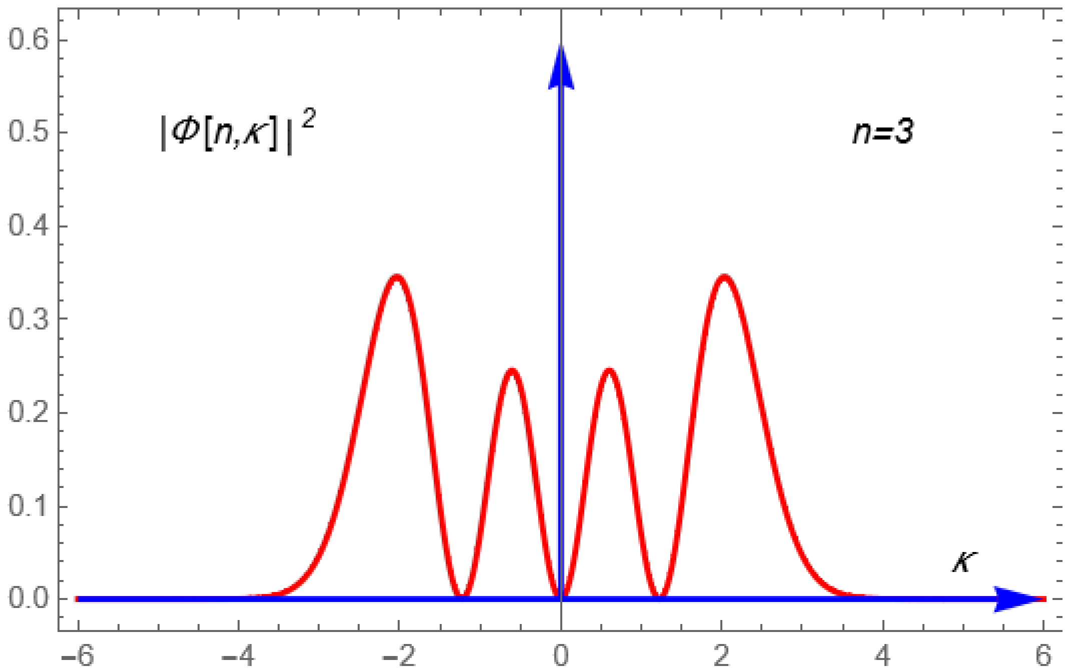


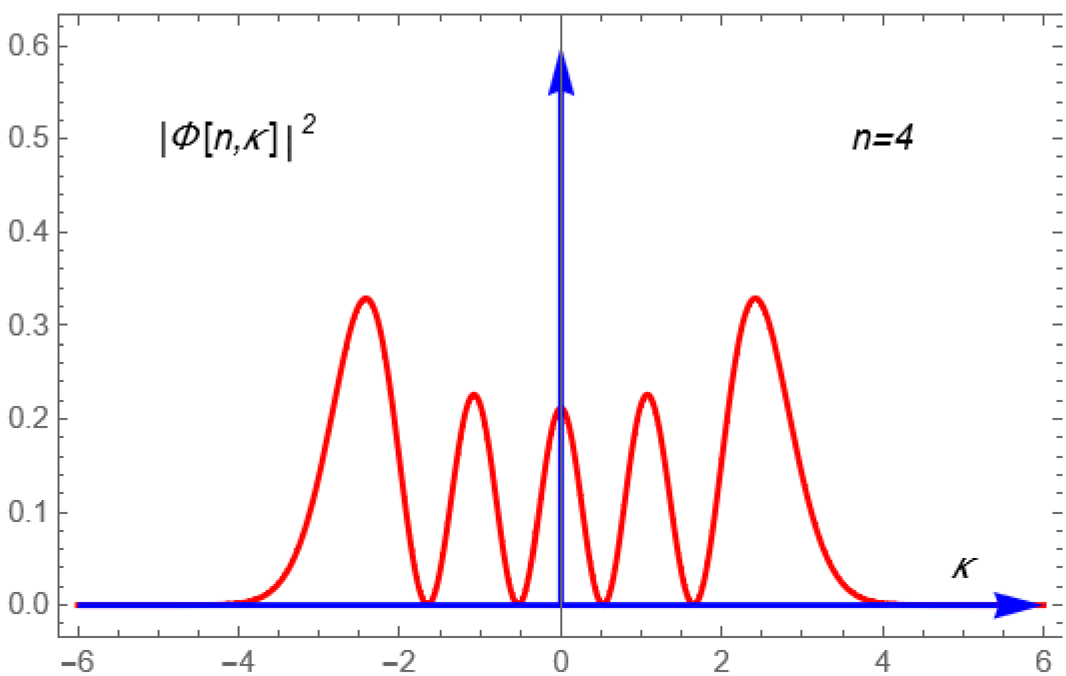


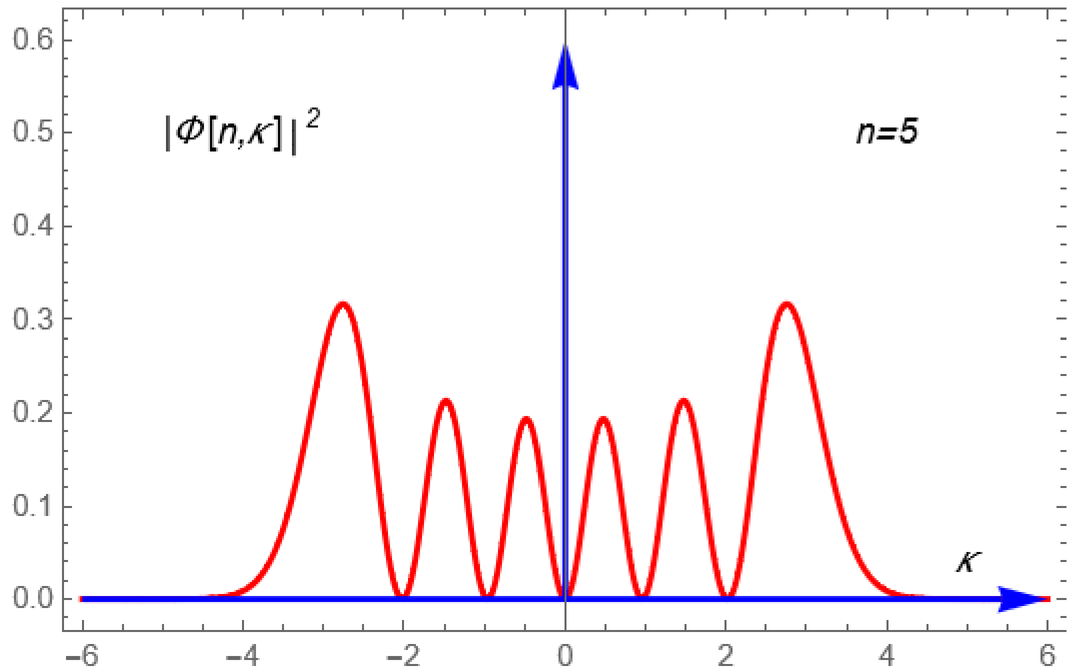
|Φ[n,κ]|^2
n=1
κ



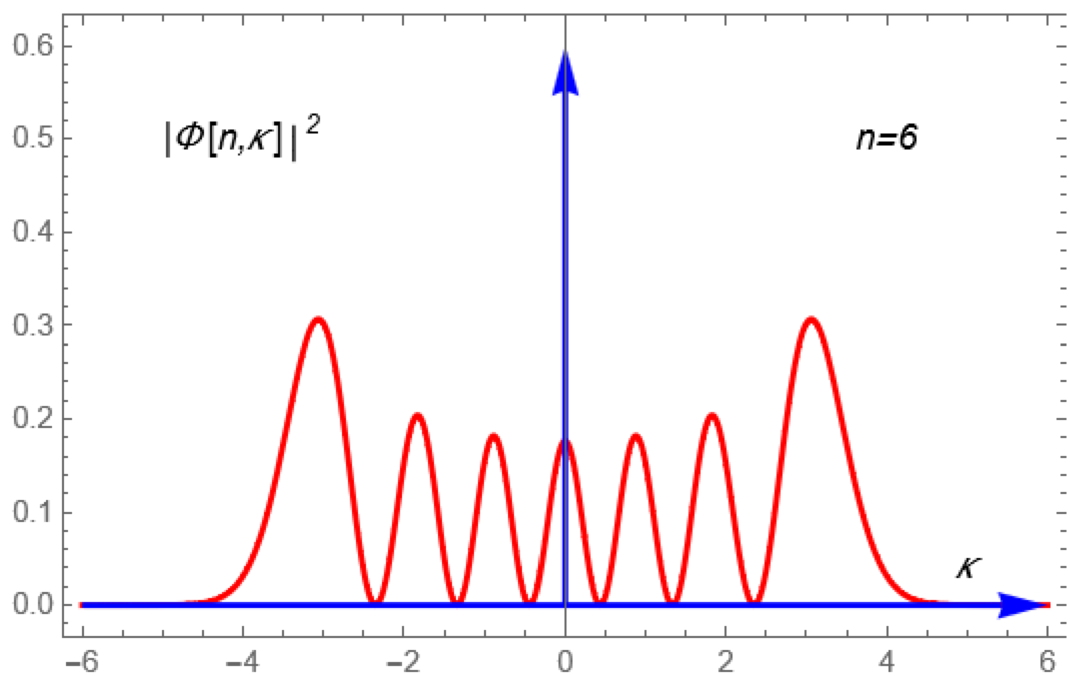
|Φ[n,κ]|^2
n=2
κ


|Φ[n,κ]|²
n=3
κ

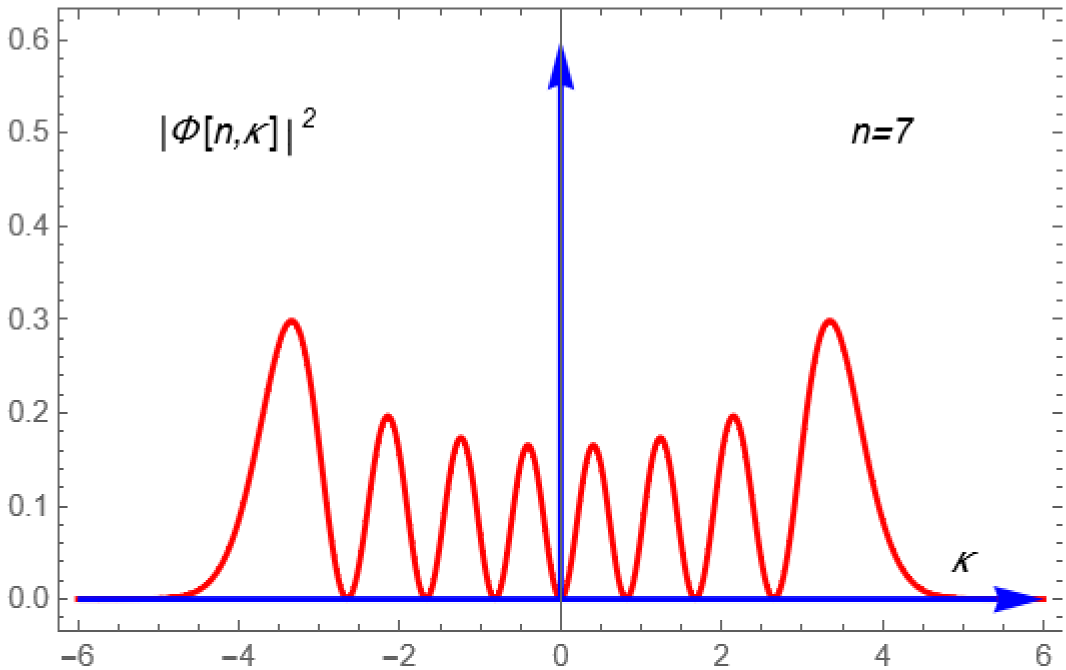

|Φ[n,κ]|²
n=4
κ

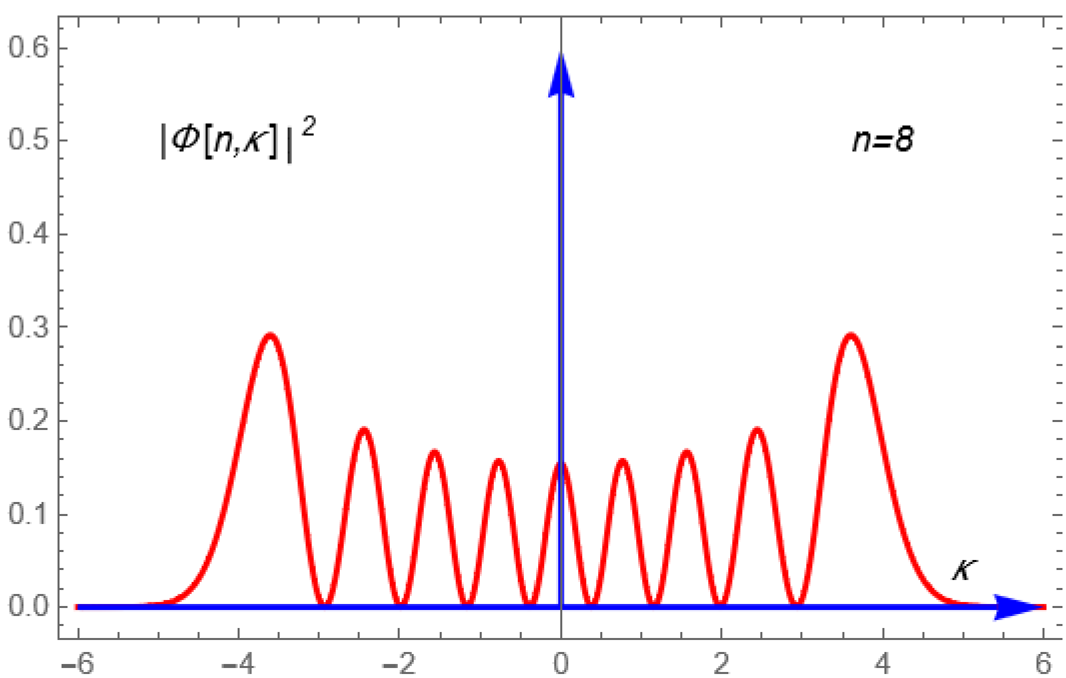


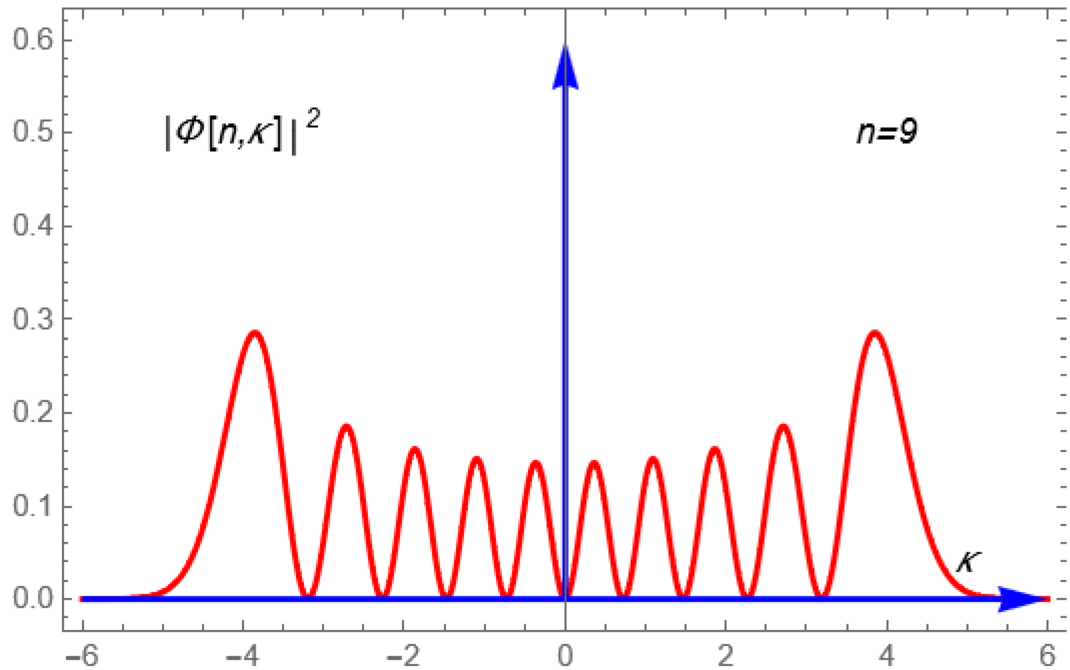
|Φ[n,κ]|²
n=5
κ



|Φ[n,κ]|²
n=6
κ


|Φ[n,κ]|²
n=7
κ
0.6
0.5
0.4
0.3
0.2
0.1
0.0
−6
−4
−2
0
2
4
6


|Φ[n,κ]|²
n=8
κ
0.6
0.5
0.4
0.3
0.2
0.1
0.0
−6
−4
−2
0
2
4
6



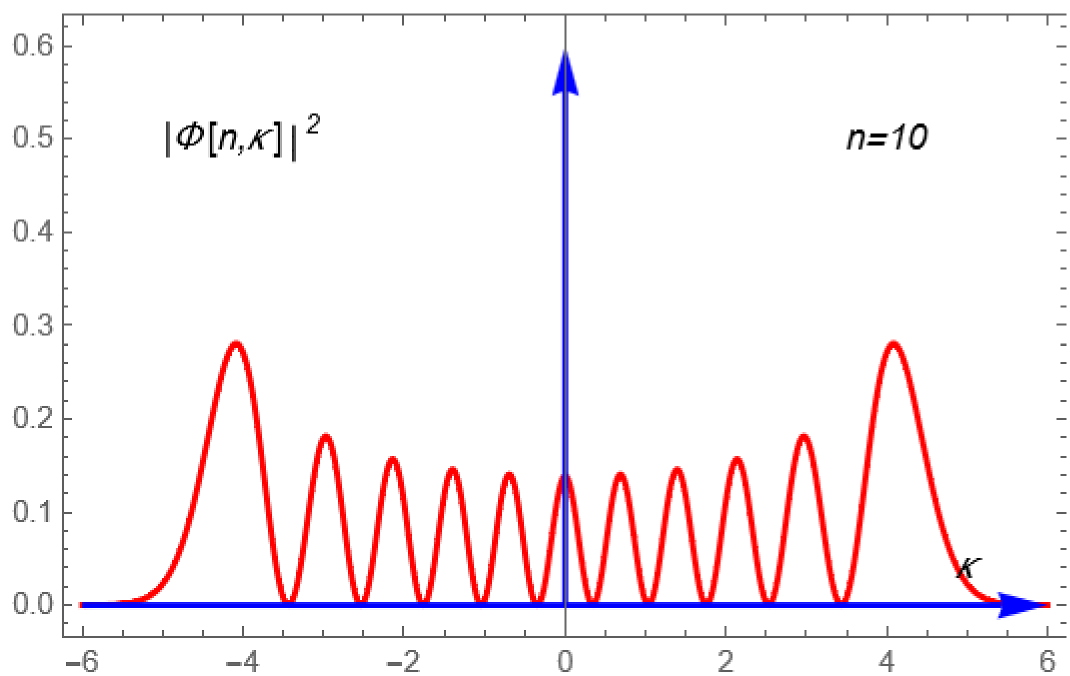


Fig. Plot of $|\langle \kappa | n \rangle|^2$ for n = 0 - 70, as a function of κ for n = 1 - 10.

17. Classical mechanics

$$
\begin{aligned}
H &= \frac{1}{2m} p^2 + \frac{1}{2} m\omega^2 x^2 \\
&= \frac{1}{2m} (\hbar \beta \kappa)^2 + \frac{1}{2} m\omega^2 (\frac{\xi}{\beta})^2 \\
&= \frac{1}{2} \hbar\omega (\kappa^2 + \xi^2) \\
&= \hbar\omega (n + \frac{1}{2})
\end{aligned}
$$

$$
\kappa^2 + \xi^2 = 2n + 1
$$

Equation of motion:

$$
\frac{dx}{dt} = \frac{p}{m} \qquad \frac{d\xi}{dt} = \omega\kappa
$$

The probability density P is obtained from

$$
\begin{aligned}
P_{cl}(\xi) d\xi &= \frac{2dt}{T} \\
&= \frac{2}{\frac{2\pi}{\omega}} \frac{1}{\omega\kappa} d\xi \\
&= \frac{1}{\pi} \frac{d\xi}{\kappa} \\
&= \frac{1}{\pi} \frac{d\xi}{\sqrt{2n + 1 - \xi^2}}
\end{aligned}
$$

where $T = \frac{2\pi}{\omega}$ is the period. The factor $2dt$ comes from the passing of the particle in the region $d\xi$ during the round trip of the movement.

$$
P_{cl}(\xi) = \frac{1}{\pi} \frac{1}{\sqrt{2n + 1 - \xi^2}}
$$

We mote that

$$\int_{-\sqrt{2n+1}}^{\sqrt{2n+1}} P_{cl}(\xi) = \frac{1}{\pi}\int_{-\sqrt{2n+1}}^{\sqrt{2n+1}} \frac{d\xi}{\sqrt{2n+1-\xi^2}}$$
$$= \frac{2}{\pi}\int_{0}^{\sqrt{2n+1}} \frac{d\xi}{\sqrt{2n+1-\xi^2}}$$
$$= 1$$

Classical probability

$$P_{cl}(\xi) = \frac{1}{\pi}\frac{1}{\sqrt{2n+1-\xi^2}}$$

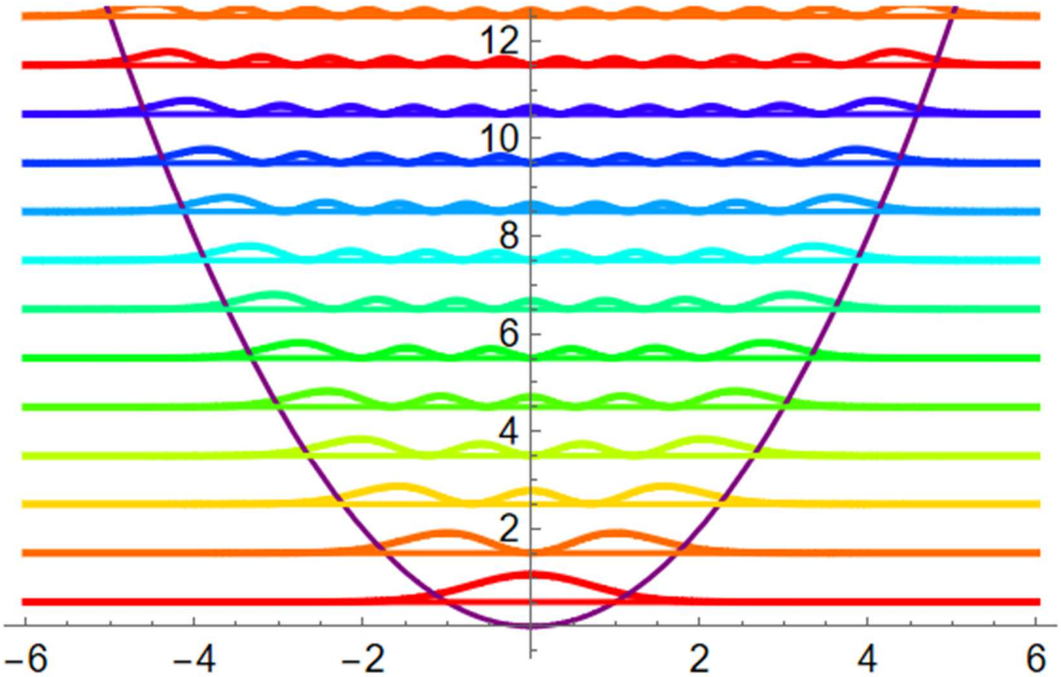
The classical turning point is

$$\xi_{cl} = \pm\sqrt{2n+1}\,.$$

((**Mathematica Program-6**))

Classical limit of the simple harmonics

```
Clear["Global`*"];
ψ[n_, ξ_] := 2^(-n/2) π^(-1/4) (n!)^(-1/2) Exp[-ξ^2/2]
  HermiteH[n, ξ];
plot1 =
 Plot[
  Table[ψ[n, ξ]^2 + n + 0.5, {n, 0, 12}] //
   Evaluate, {ξ, -6, 6},
  PlotStyle → Table[{Hue[0.07 i], Thick},
    {i, 0, 10}]];
plot2 = Plot[ξ^2/2, {ξ, -6, 6},
  PlotStyle → {Purple, Thickness[0.005]}];
plot3 =
 Plot[Table[n + 0.5, {n, 0, 12}] // Evaluate,
  {ξ, -6, 6},
  PlotStyle → Table[Hue[0.07 i], {i, 0, 10}],
  Prolog → AbsoluteThickness[2]];
f1 = Show[plot1, plot2, plot3,
  PlotRange → {{-6, 6}, {0, 12}}]
```




```
f2 = Show[plot1, plot2, plot3,
  PlotRange → {{-4, 4}, {0, 4}}]
```

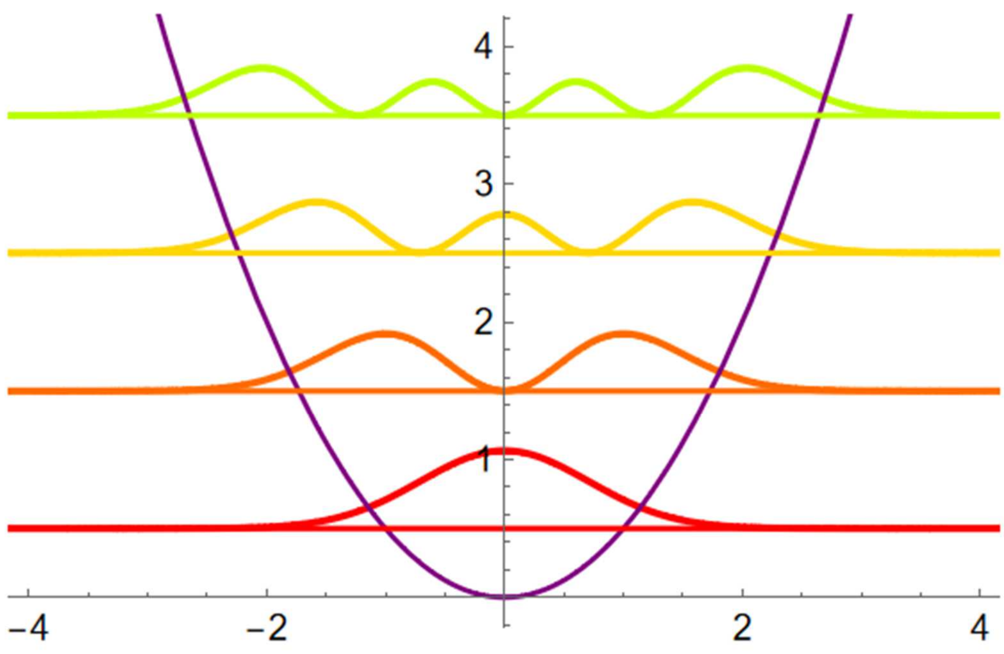


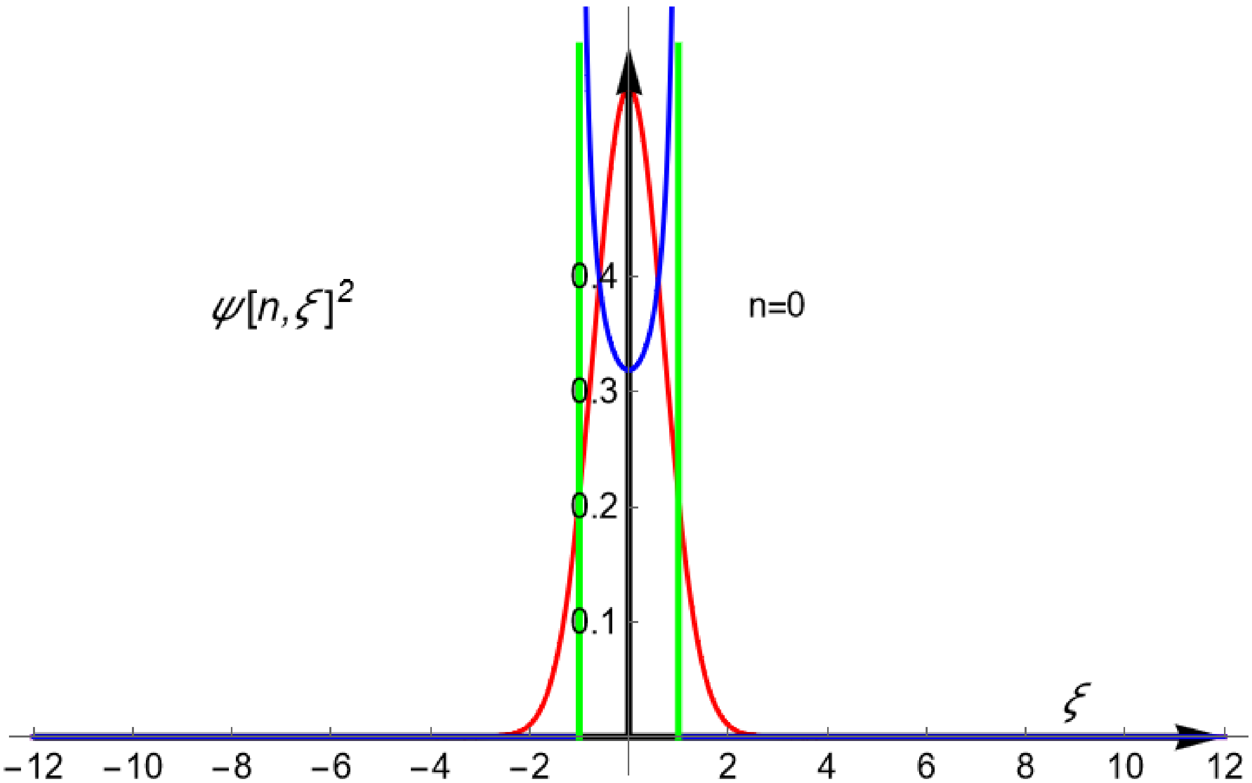
Fig. The classical turning point (or classical limit) is the point where the potential energy $\frac{1}{2}\xi^2$ is equal to $n+\frac{1}{2}$ for each quantum number *n*. *n* = 0, 1, 2, 3, ...

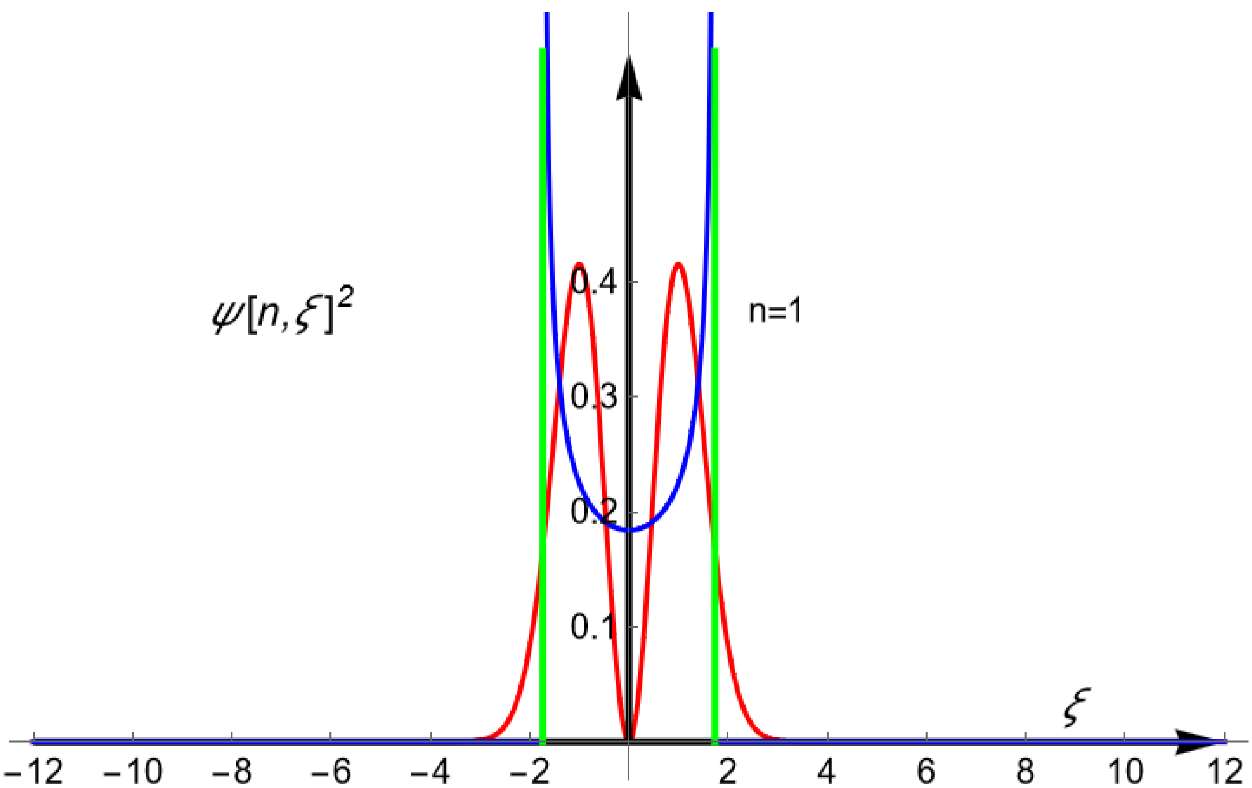
((**Mathematica Program-7**))

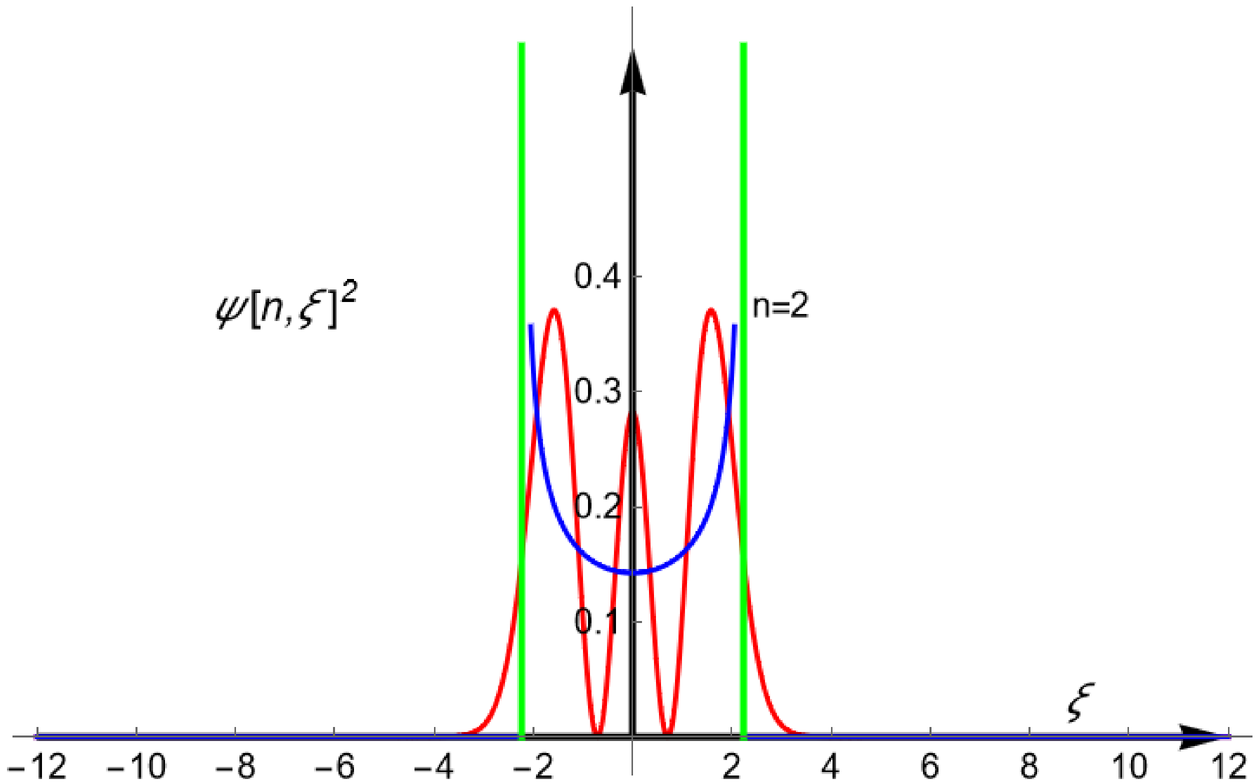
Classical limit→

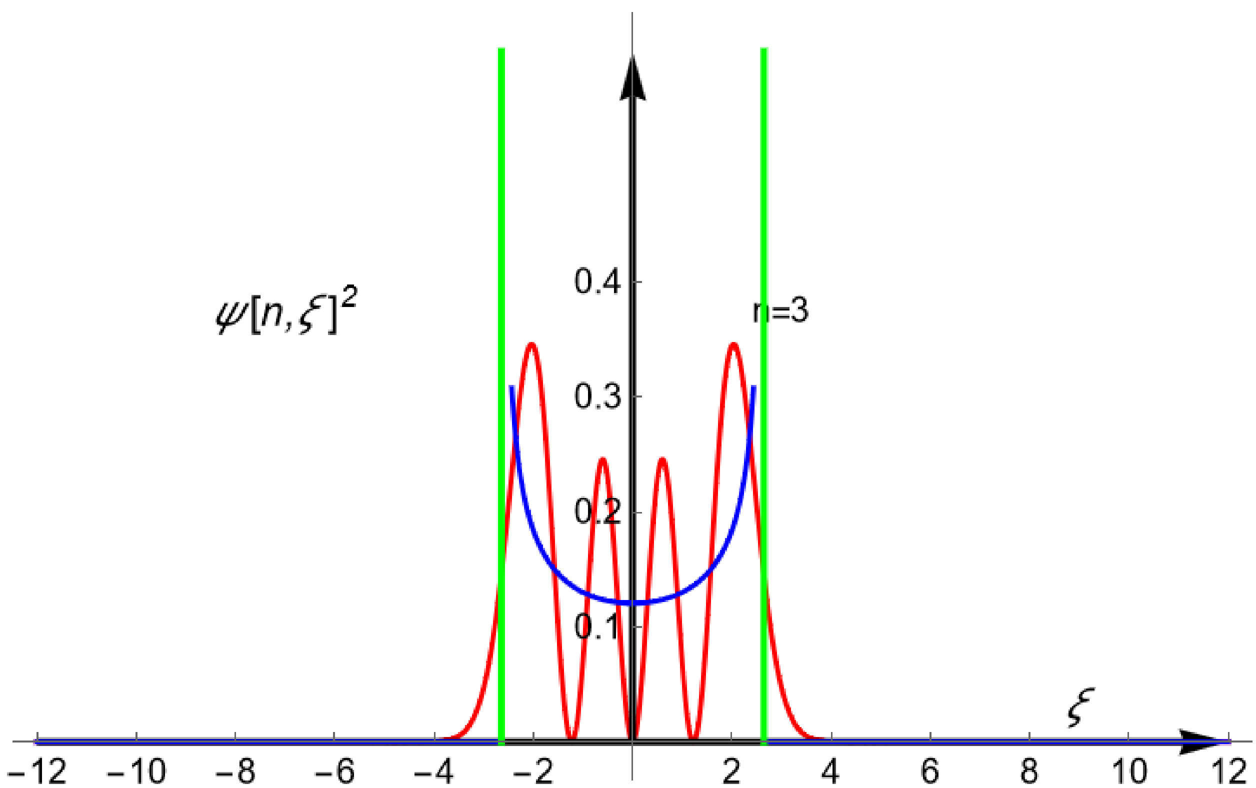
```
Clear["Global`*"];
wc[n_, ξ_] := Which[-√(2 n + 1) ≤ ξ ≤ √(2 n + 1),
   (1/π) 1/√(2 n + 1 - ξ^2), ξ ≥ √(2 n + 1), 0,
   ξ ≤ -√(2 n + 1) , 0];

ψ[n_, ξ_] := 2^(-n/2) π^(-1/4) (n !)^(-1/2) Exp[-ξ^2/2]
   HermiteH[n, ξ];

Class[n1_] :=
 Module[{f1, f2},
  f1 = Plot[Evaluate[wc[n1, ξ]], {ξ, -12, 12},
    PlotStyle → {Blue, Thickness[0.004]},
    PlotPoints → 200];
```

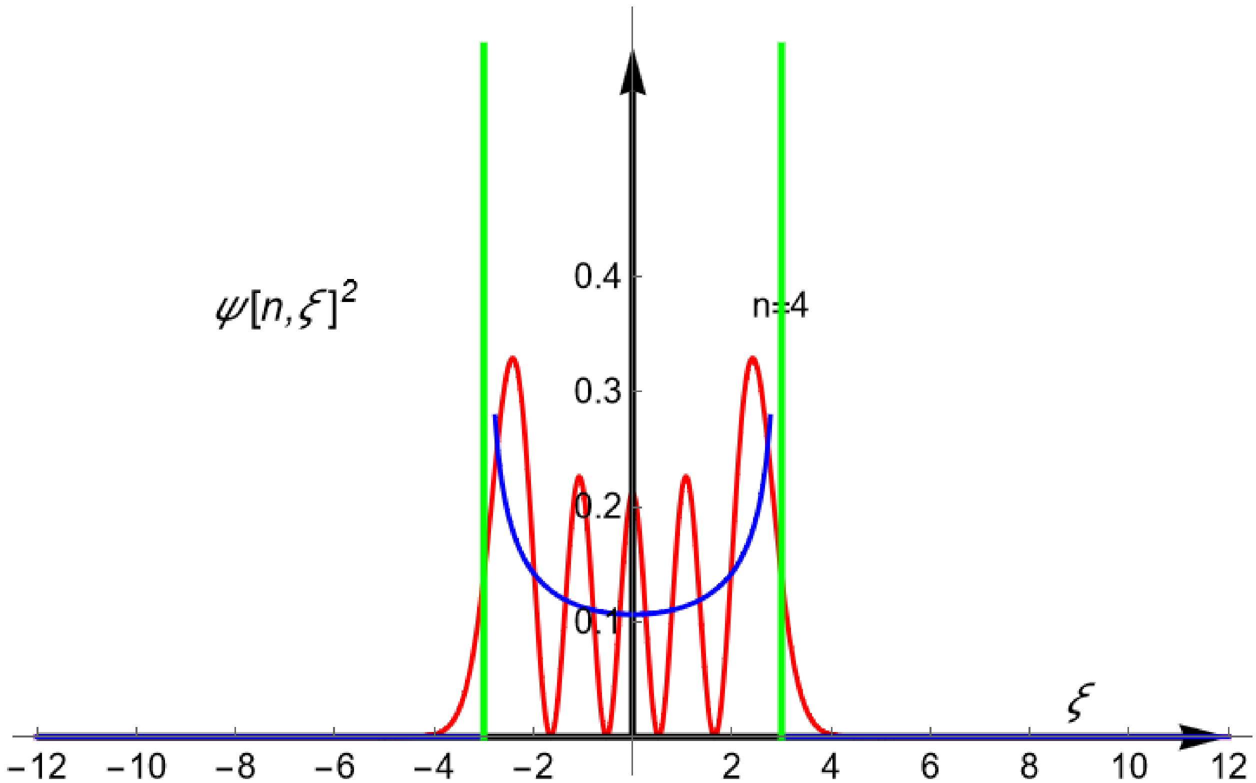
```
f2 = Graphics[{Green, Thick,
    Line[{{-√(2 n1 + 1), 0},
      {-√(2 n1 + 1), 0.6}}],
    Line[{{√(2 n1 + 1), 0},
      {√(2 n1 + 1), 0.6}}]}]; Show[f1, f2]];
Prob[n1_] := Module[{g1, g2, g3},
  g1 = Plot[ψ[n1, ξ]^2, {ξ, -12, 12},
    PlotStyle → {Red, Thickness[0.004]},
    PlotPoints → 200,
    Ticks → {Range[-12, 12, 2],
      Range[0, 0.40, 0.1]}, PlotRange → All];
  g2 = Graphics[
    {Text[Style["ξ", Black, 12, Italic],
      {9, 0.03}],
     Text[Style["ψ[n,ξ]^2", Black, 12, Italic],
      {-7, 0.375}],
     Text[Style["n=" <> ToString[n1]],
      {3, 0.375}], Black, Thick,
     Arrowheads[0.04],
     Arrow[{{0, 0}, {0, 0.6}}],
     Arrow[{{-12, 0}, {12, 0}}]}];
  g3 = Show[g1, g2]];
PC[n1_] := Show[Prob[n1], Class[n1],
  PlotRange → {{-12, 12}, {0, 0.6}}];
```


ψ[n,ξ]^2
n=0
0.1
0.2
0.3
0.4
ξ
−12 −10 −8 −6 −4 −2 2 4 6 8 10 12

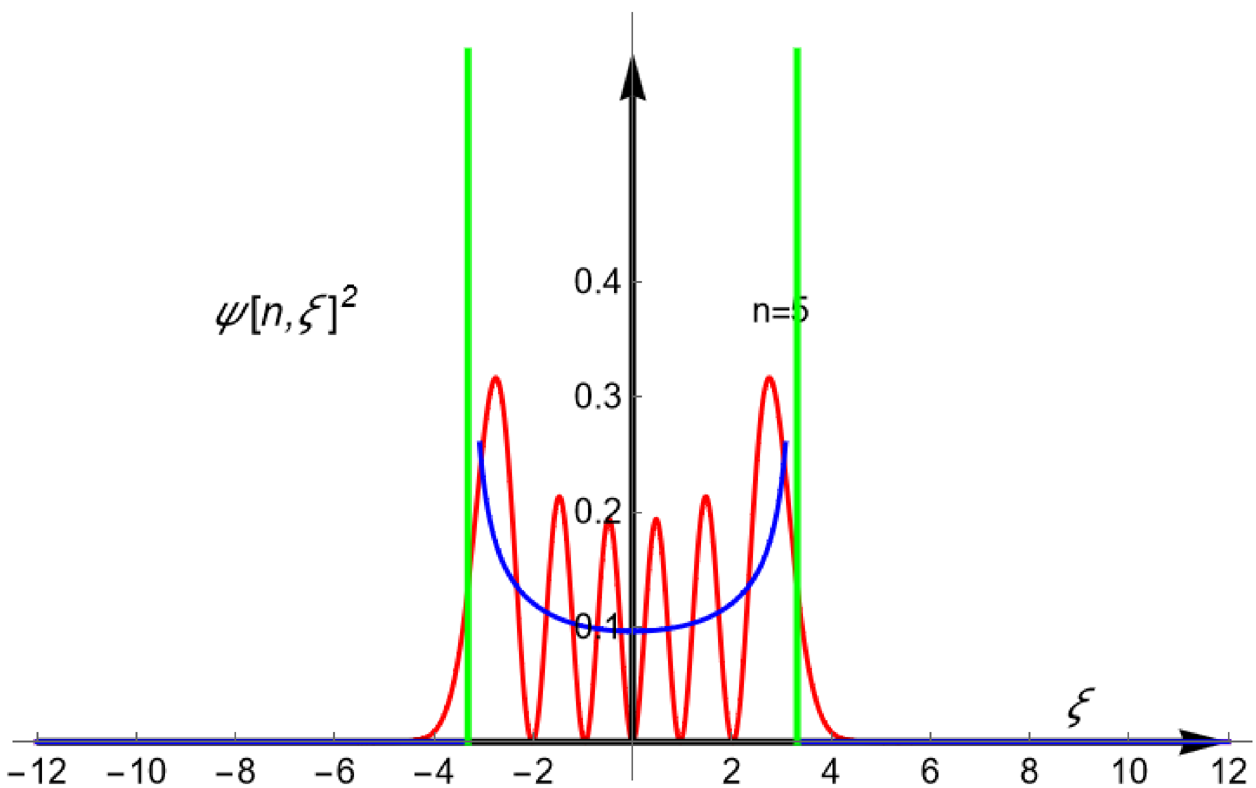

ψ[n,ξ]^2
n=1
0.1
0.2
0.3
0.4
ξ
−12 −10 −8 −6 −4 −2 2 4 6 8 10 12


0.4
0.3
0.2
0.1
ψ[n,ξ]^2
n=2
ξ
−12 −10 −8 −6 −4 −2 2 4 6 8 10 12

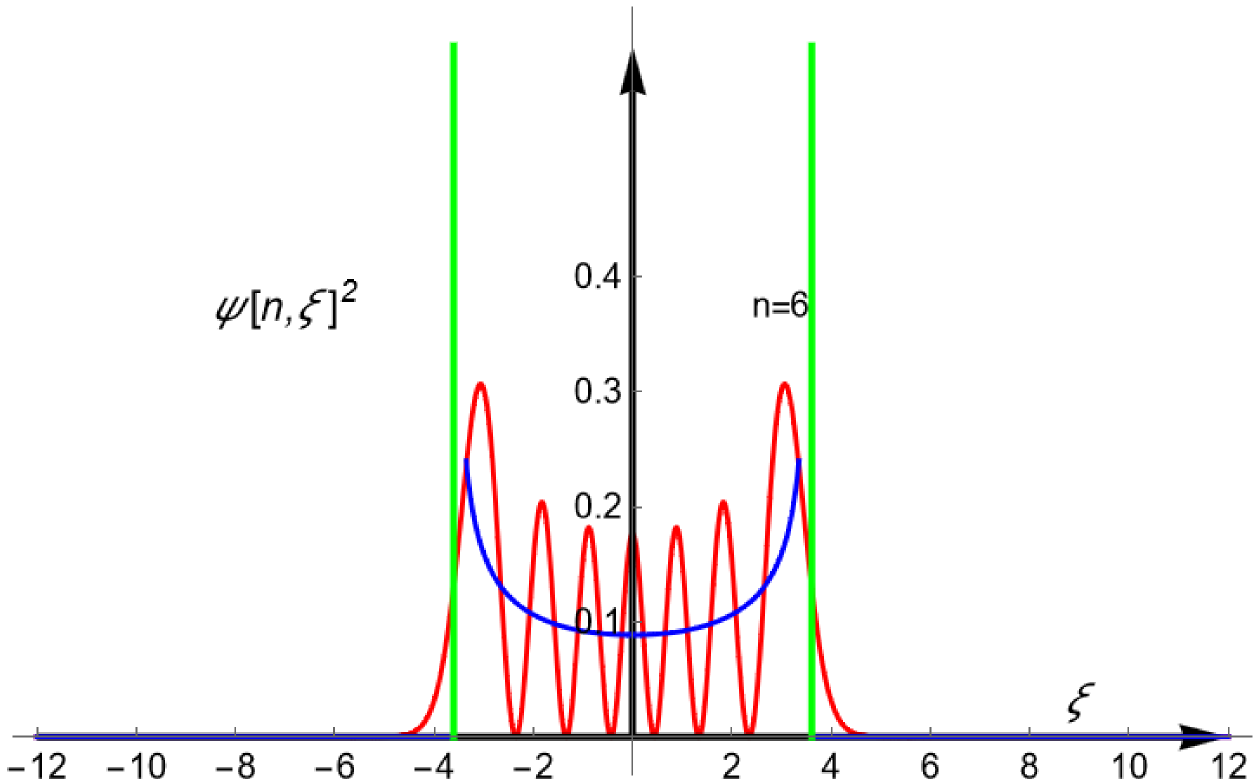

0.4
0.3
0.2
0.1
ψ[n,ξ]^2
n=3
ξ
−12 −10 −8 −6 −4 −2 2 4 6 8 10 12

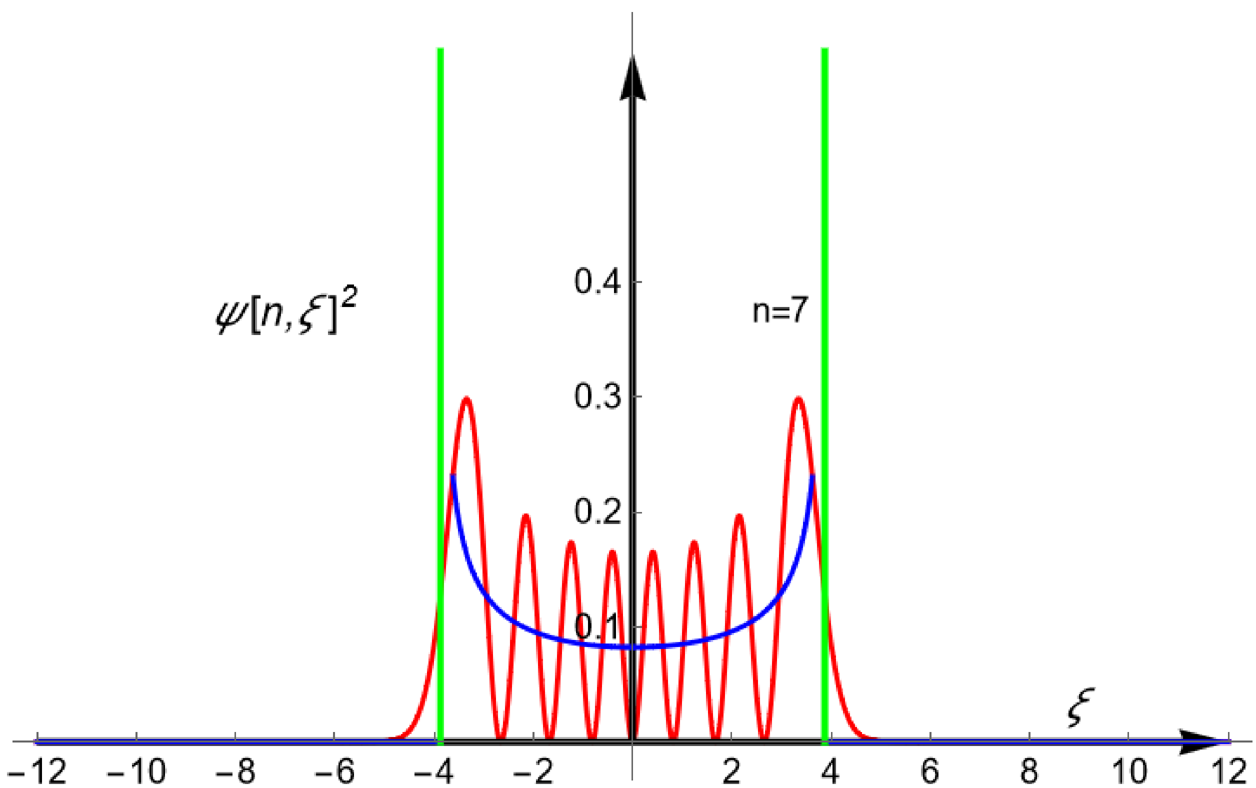


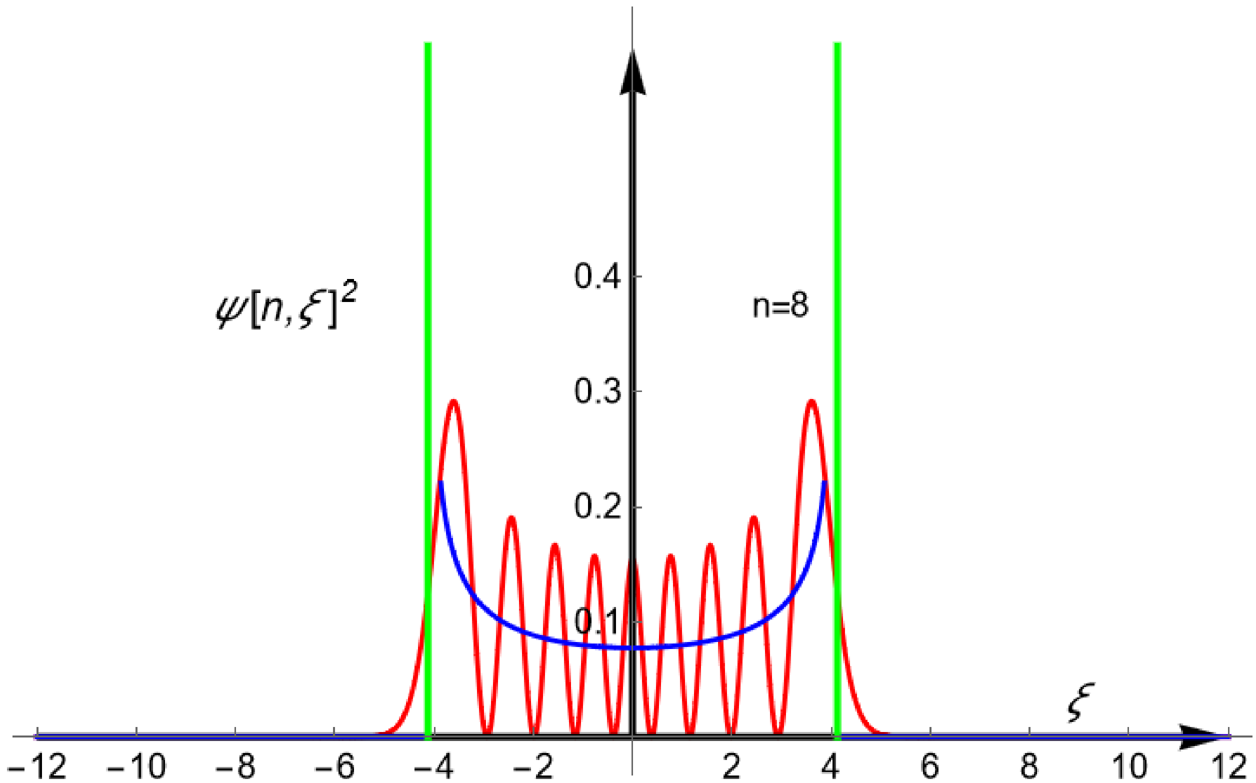
$\psi[n,\xi]^2$
n=4
0.4
0.3
0.2
0.1
ξ
−12 −10 −8 −6 −4 −2 2 4 6 8 10 12

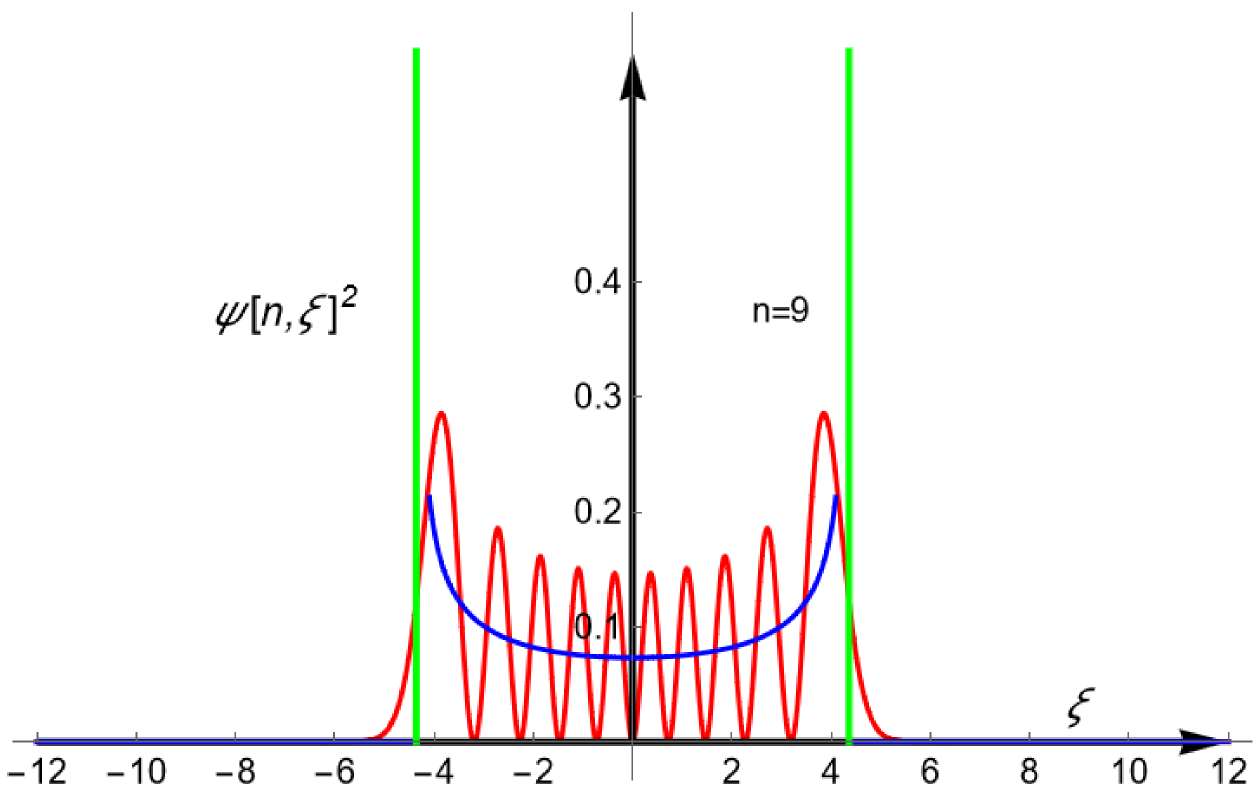


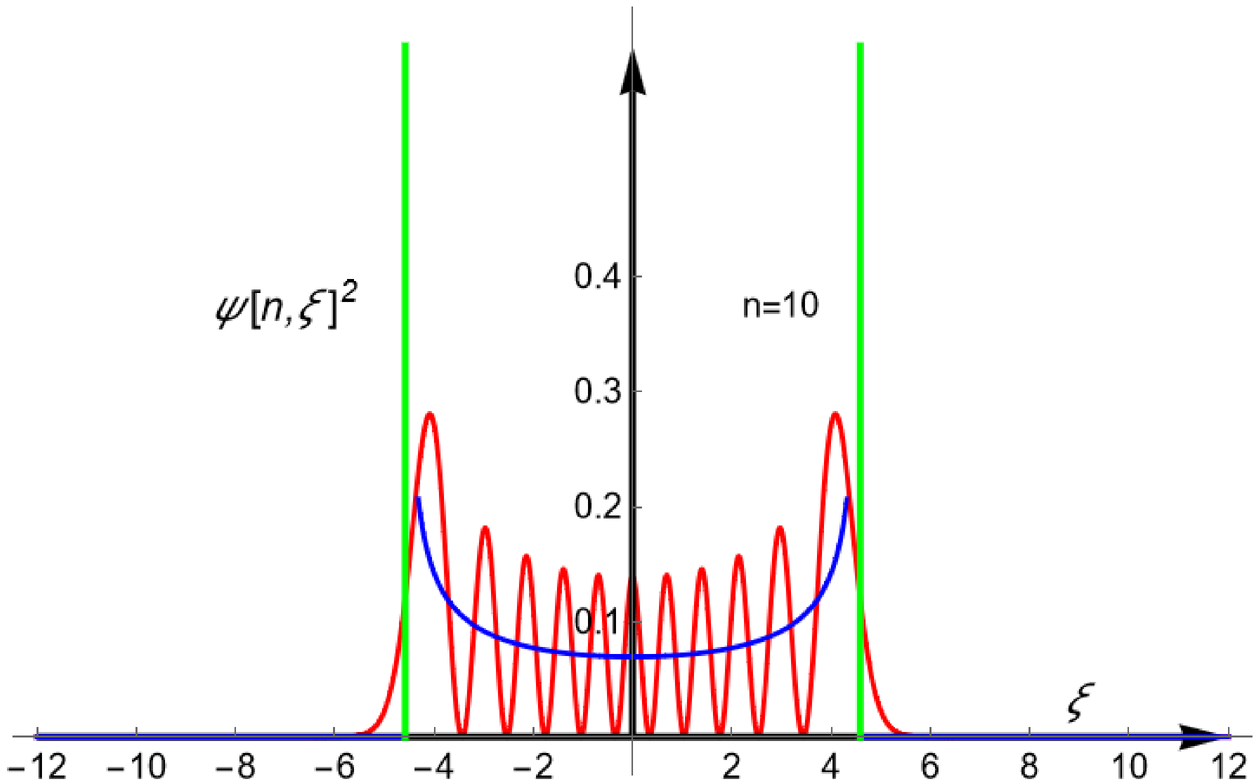
$\psi[n,\xi]^2$
n=5
0.4
0.3
0.2
0.1
ξ
−12 −10 −8 −6 −4 −2 2 4 6 8 10 12


ψ[n,ξ]^2
n=6
ξ
0.4
0.3
0.2
0.1
−12 −10 −8 −6 −4 −2 2 4 6 8 10 12

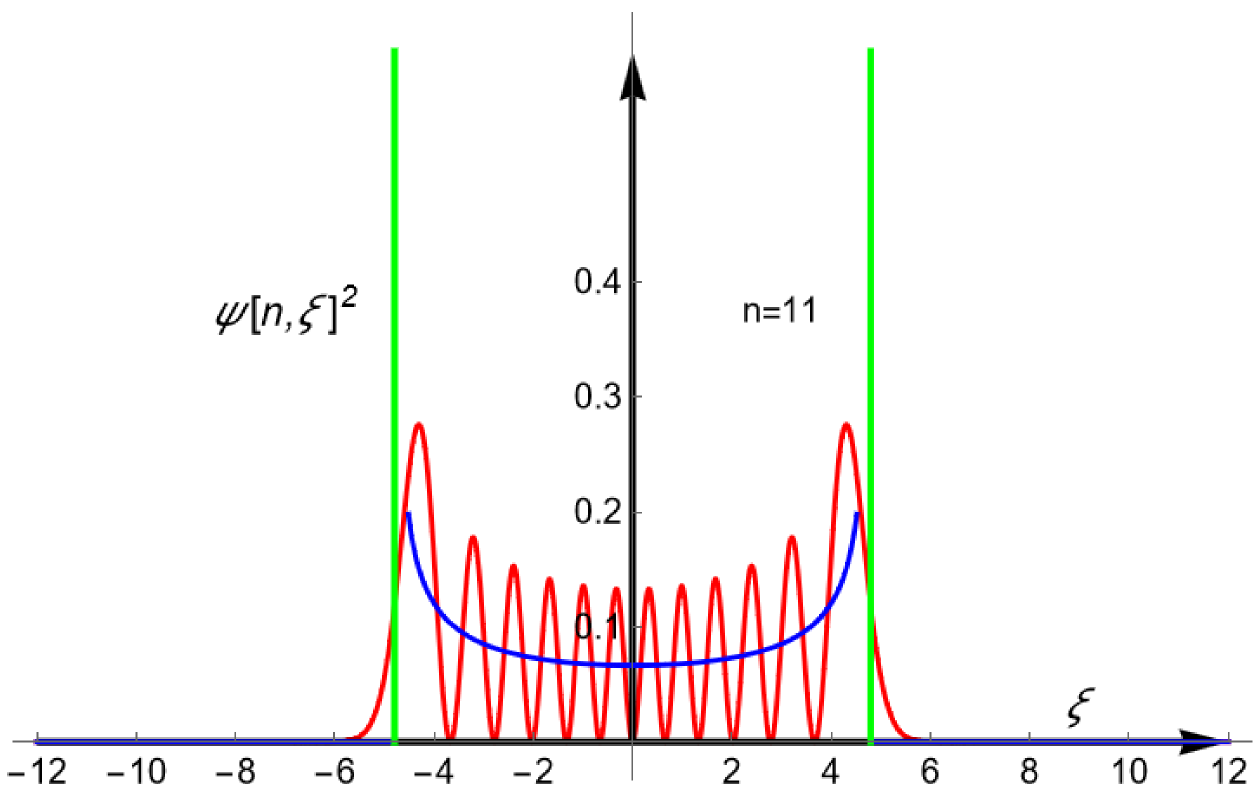

ψ[n,ξ]^2
n=7
ξ
0.4
0.3
0.2
0.1
−12 −10 −8 −6 −4 −2 2 4 6 8 10 12


ψ[n,ξ]^2
n=8
0.4
0.3
0.2
0.1
ξ
−12 −10 −8 −6 −4 −2 2 4 6 8 10 12

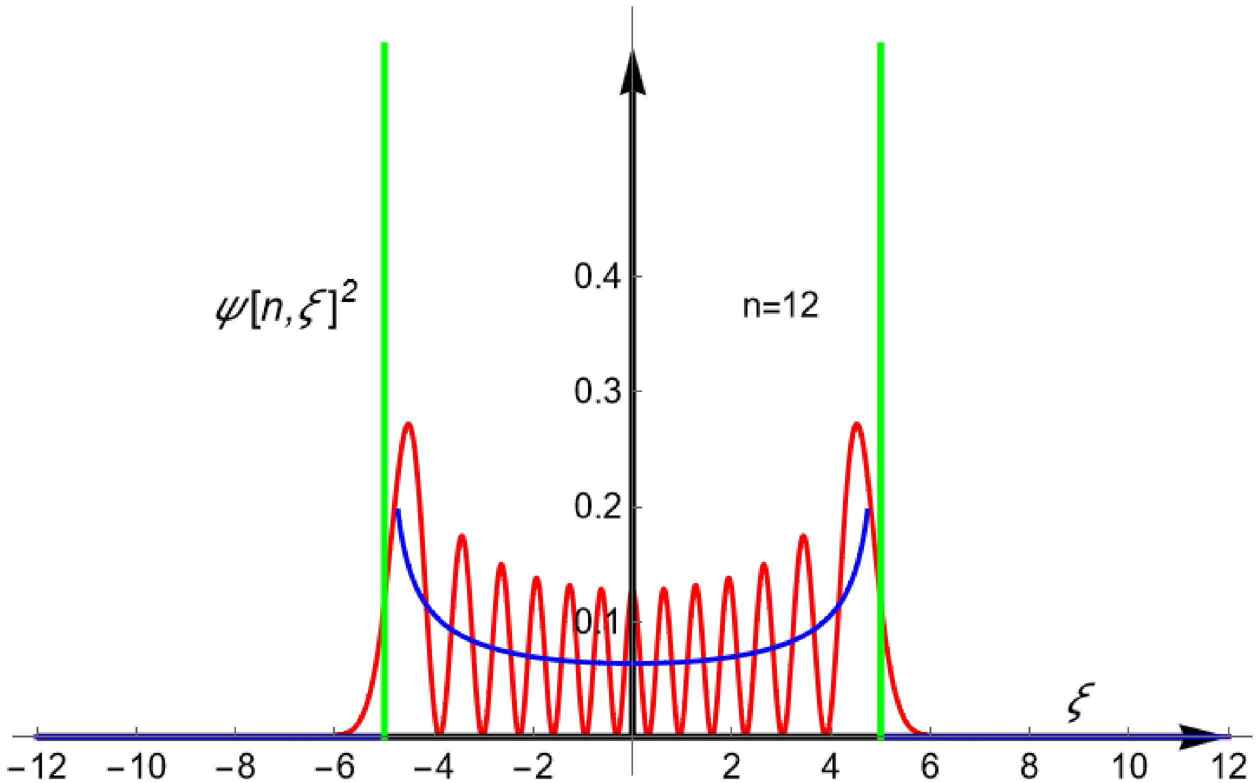

ψ[n,ξ]^2
n=9
0.4
0.3
0.2
0.1
ξ
−12 −10 −8 −6 −4 −2 2 4 6 8 10 12

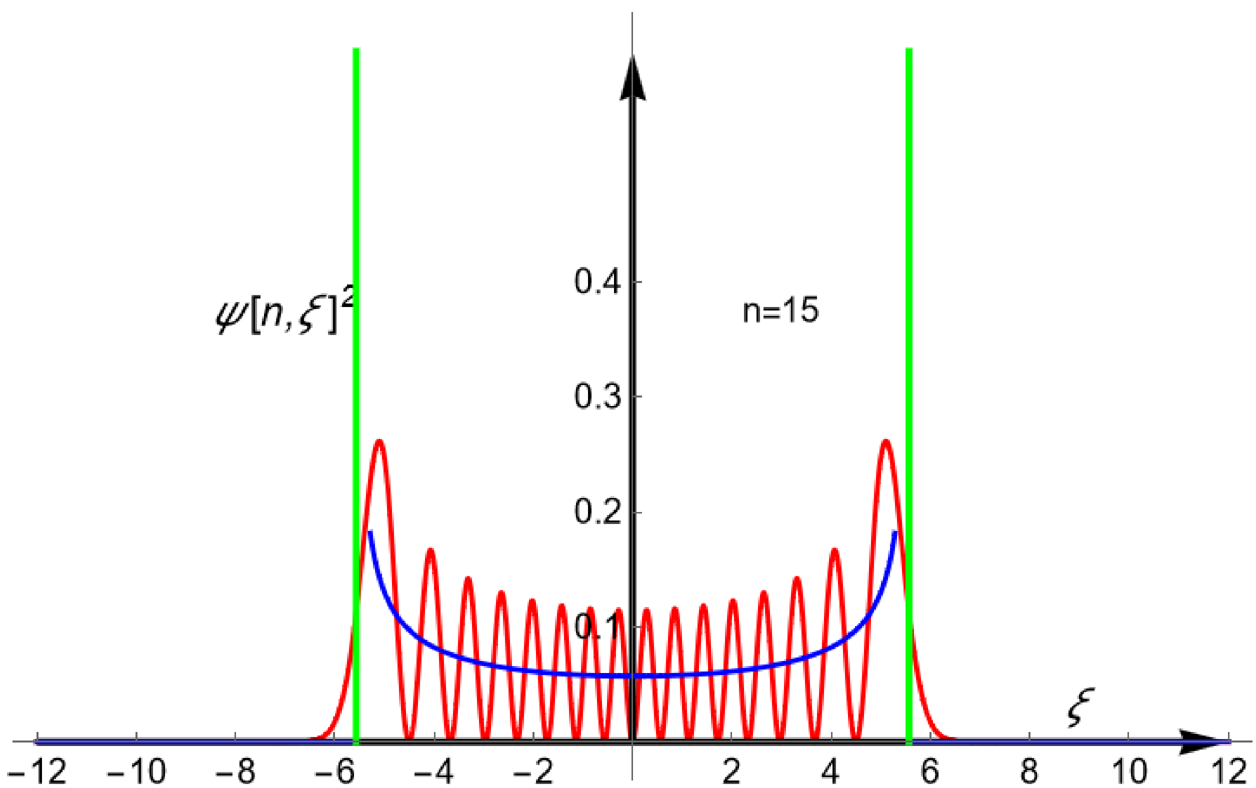


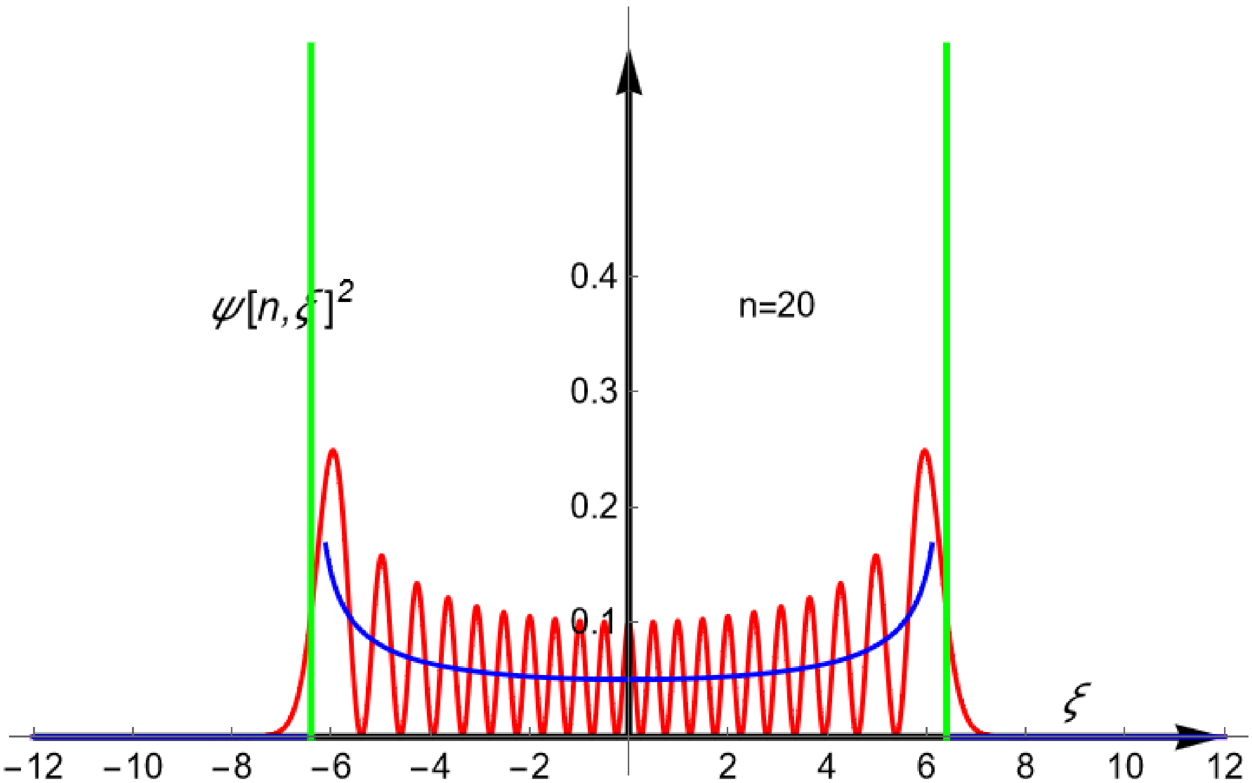
ψ[n,ξ]^2
n=10
0.4
0.3
0.2
0.1
ξ
−12 −10 −8 −6 −4 −2 2 4 6 8 10 12

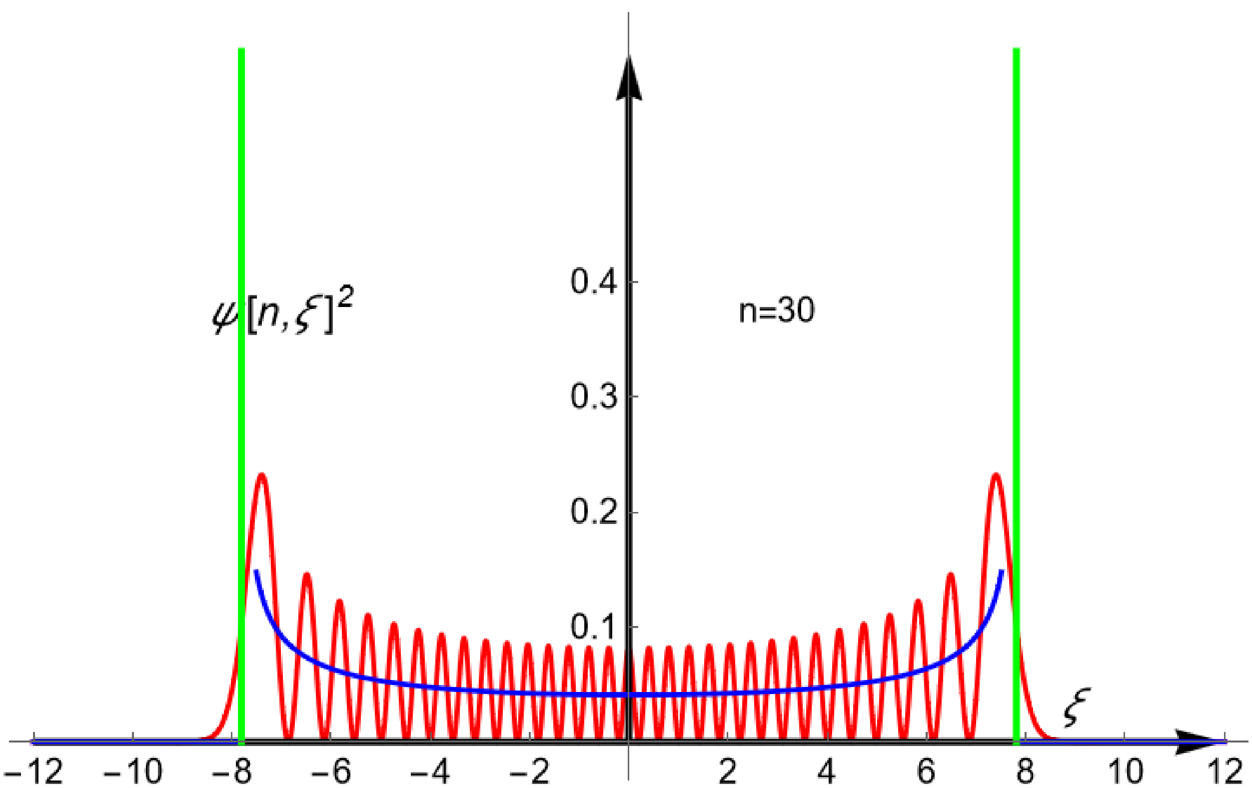


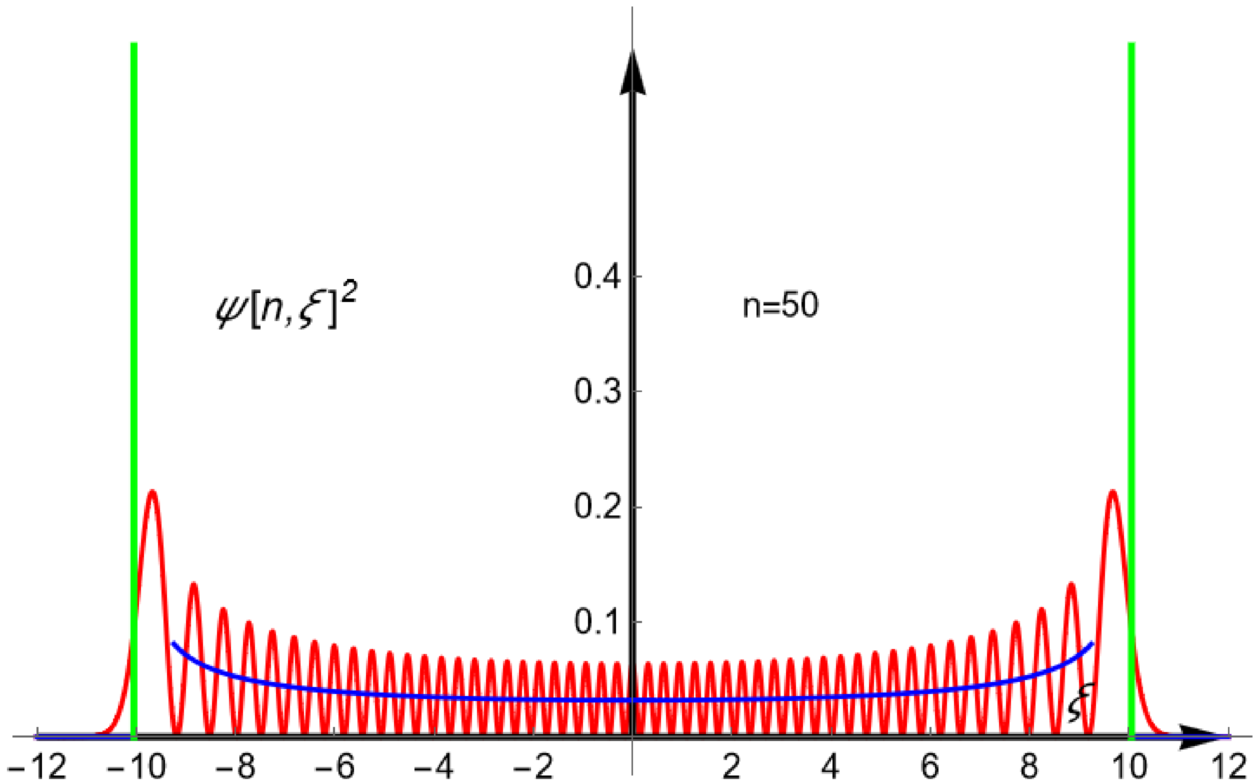
ψ[n,ξ]^2
n=11
0.4
0.3
0.2
0.1
ξ
−12 −10 −8 −6 −4 −2 2 4 6 8 10 12

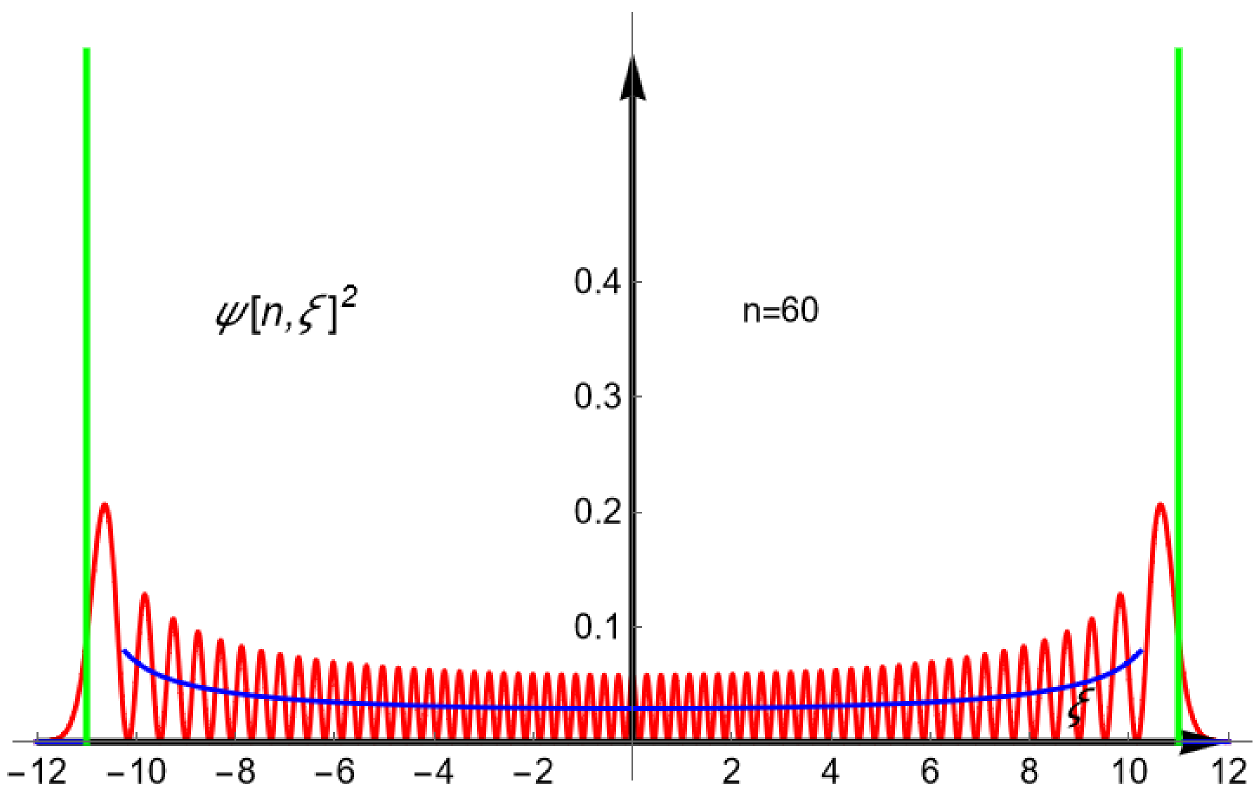

$\psi[n,\xi]^2$
n=12
0.4
0.3
0.2
0.1
ξ
−12
−10
−8
−6
−4
−2
2
4
6
8
10
12


$\psi[n,\xi]^2$
n=15
0.4
0.3
0.2
0.1
ξ
−12
−10
−8
−6
−4
−2
2
4
6
8
10
12


ψ[n,ξ]²
n=20
0.4
0.3
0.2
0.1
ξ
−12 −10 −8 −6 −4 −2 2 4 6 8 10 12


ψ[n,ξ]²
n=30
0.4
0.3
0.2
0.1
ξ
−12 −10 −8 −6 −4 −2 2 4 6 8 10 12


ψ[n,ξ]^2
n=50
0.4
0.3
0.2
0.1
ξ
−12
−10
−8
−6
−4
−2
2
4
6
8
10
12


ψ[n,ξ]^2
n=60
0.4
0.3
0.2
0.1
ξ
−12
−10
−8
−6
−4
−2
2
4
6
8
10
12

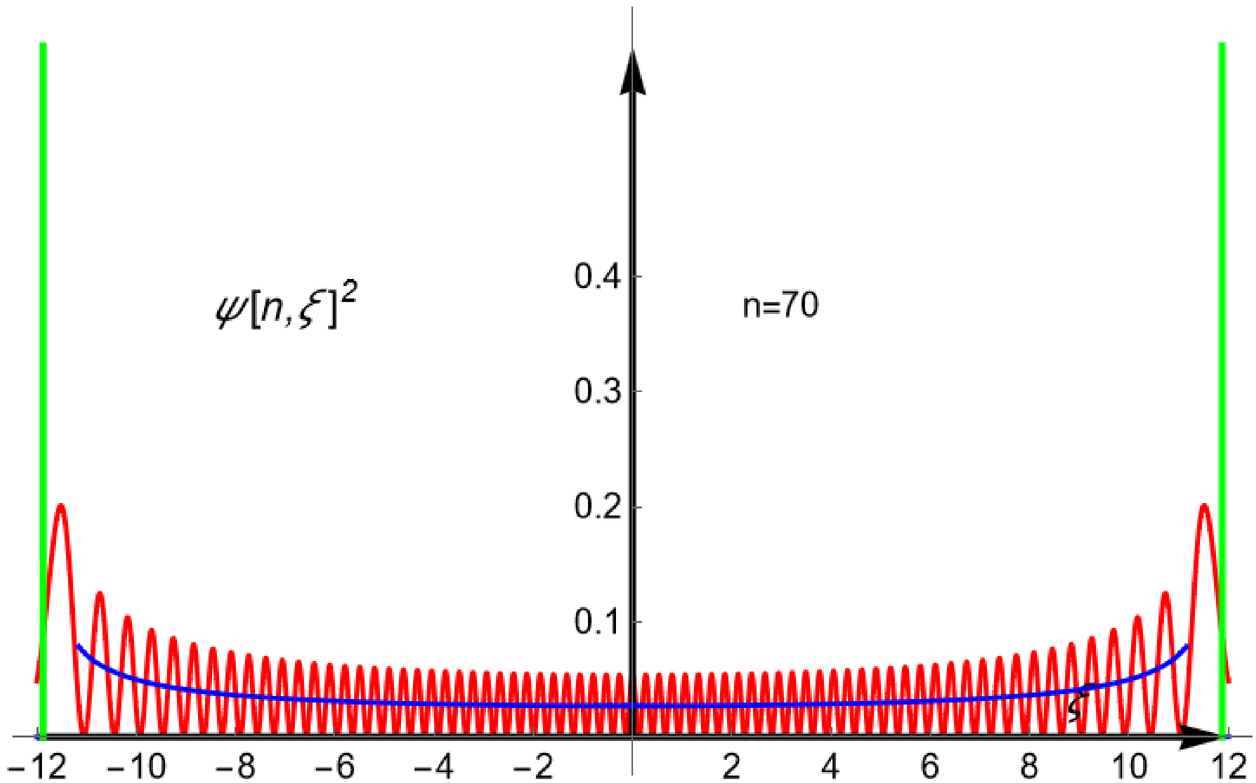


Fig. The quantum probability density $\left|\langle \xi | n \rangle\right|^2$ and classical probability P_{cl} (the blue line) for n = 0 - 70 with the same energy, as a function of ξ. The vertical green line denotes the classical limits.

18. Coherent state

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$$

$$|\alpha\rangle = \exp(-\frac{|\alpha|^2}{2})\sum_n \frac{(\alpha\hat{a}^+)^n}{n!}|0\rangle$$

$$
\begin{aligned}
\langle \xi | \alpha \rangle &= \exp(-\frac{|\alpha|^2}{2})\sum_n \frac{\alpha^n}{n!}\langle \xi | (\hat{a}^+)^n | 0 \rangle \\
&= \exp(-\frac{|\alpha|^2}{2})\sum_n \frac{\alpha^n}{2^{n/2} n!}(\xi - \frac{\partial}{\partial \xi})^n \langle \xi | 0 \rangle \\
&= \frac{1}{\pi^{1/4}}\exp(-\frac{|\alpha|^2}{2})\sum_n \frac{\alpha^n}{2^{n/2} n!}[(\xi - \frac{\partial}{\partial \xi})^n \exp(-\frac{\xi^2}{2})] \\
&= \frac{1}{\pi^{1/4}}\exp(-\frac{|\alpha|^2}{2})\sum_n \frac{\alpha^n}{2^{n/2} n!}\exp(-\frac{\xi^2}{2})H(n,\xi) \\
&= \exp(-\frac{|\alpha|^2}{2})\sum_n \frac{\alpha^n}{\sqrt{n!}}\frac{1}{(\pi^{1/2} 2^n n!)^{1/2}}\exp(-\frac{\xi^2}{2})H(n,\xi)
\end{aligned}
$$

19. Fourier transform of the coherent state

$$
\begin{aligned}
\langle \kappa | \alpha \rangle &= \exp(-\frac{|\alpha|^2}{2})\sum_n \frac{\alpha^n}{n!}\langle \kappa | (\hat{a}^+)^n | 0 \rangle \\
&= \exp(-\frac{|\alpha|^2}{2})\sum_n \frac{\alpha^n}{2^{n/2} n!}(-i)^n(\kappa - \frac{\partial}{\partial \kappa})^n \langle \kappa | 0 \rangle \\
&= \frac{1}{\pi^{1/4}}\exp(-\frac{|\alpha|^2}{2})\sum_n \frac{\alpha^n}{2^{n/2} n!}(-i)^n[(\kappa - \frac{\partial}{\partial \kappa})^n \exp(-\frac{\kappa^2}{2})] \\
&= \frac{1}{\pi^{1/4}}\exp(-\frac{|\alpha|^2}{2})\sum_n \frac{\alpha^n}{2^{n/2} n!}(-i)^n \exp(-\frac{\kappa^2}{2})H(n,\kappa) \\
&= \exp(-\frac{|\alpha|^2}{2})\sum_n \frac{\alpha^n}{\sqrt{n!}}\frac{(-i)^n}{(\pi^{1/2} 2^n n!)^{1/2}}\exp(-\frac{\kappa^2}{2})H(n,\kappa)
\end{aligned}
$$

where

$$
(\xi - \frac{\partial}{\partial \xi})^n \exp(-\frac{\xi^2}{2}) = \exp(-\frac{\xi^2}{2})H(n,\xi)
$$

$$
(\kappa - \frac{\partial}{\partial \kappa})^n \exp(-\frac{\kappa^2}{2}) = \exp(-\frac{\kappa^2}{2})H(n,\kappa)
$$

20. Differential operator for creation and annihilation operator

(**Mathematica**)

$$AN := \frac{1}{\sqrt{2}}(\# + D[\#, \xi])\,\&$$

$$CR := \frac{1}{\sqrt{2}}(\# - D[\#, \xi])\,\&$$

$$CR[\psi[\xi]] = \frac{1}{\sqrt{2}}(\psi[\xi] - \frac{\partial}{\partial \xi}\psi[\xi])$$

$$AN[\psi[\xi]] = \frac{1}{\sqrt{2}}(\psi[\xi] + \frac{\partial}{\partial \xi}\psi[\xi])$$

$$[\hat{a}, \hat{a}^{+}] = \hat{1}$$

$$\begin{aligned} AN[CR[\psi(\xi)] - CR[AN[\psi(\xi)] &= \frac{1}{2}[(\xi + \frac{d}{d\xi})(\xi\psi(\xi) - \psi'(\xi) - \frac{1}{2}(\xi - \frac{d}{d\xi})(\xi\psi(\xi) + \psi'(\xi)] \\ &= \frac{1}{2}[\xi^2\psi(\xi) - \xi\psi'(\xi) + \psi(\xi) + \xi\psi'(\xi) - \psi''(\xi)] \\ &\quad -\frac{1}{2}[\xi^2\psi(\xi) + \xi\psi'(\xi) - \psi(\xi) - \xi\psi'(\xi) - \psi''(\xi)] \\ &= \psi(\xi) \end{aligned}$$

((**Mathematica Program-8**))

Commutation relations for the creation and annihilation operators

```
Clear["Global`"];
CR := 1/Sqrt[2] (ξ # - D[#, ξ]) &;
AN := 1/Sqrt[2] (ξ # + D[#, ξ]) &;
N1 := CR[AN[#]] &;
N11 := (CR[AN[#]] + AN[CR[#]]) &;
```

$[a, (a^{+})^2] = 2a+$

```
f11 = AN[CR[CR[ψ[ξ]]]] - CR[CR[AN[ψ[ξ]]]] //
  Simplify
```

$\sqrt{2}\ (\xi\,\psi[\xi] - \psi'[\xi])$

```
f12 = 2 CR[ψ[ξ]] // Simplify
```

$\sqrt{2}\ (\xi\,\psi[\xi] - \psi'[\xi])$

```
f11 - f12 // Simplify
```

0

$[a^{+}, a^2] = -\,2a$

```
f21 = CR[AN[AN[ψ[ξ]]]] - AN[AN[CR[ψ[ξ]]]] //
  Simplify
```

$-\sqrt{2}\ (\xi\,\psi[\xi] + \psi'[\xi])$

```
f22 = -2 AN[ψ[ξ]] // Simplify
```

$-\sqrt{2}\ (\xi\,\psi[\xi] + \psi'[\xi])$

```
f21 - f22 // Simplify
```

0

$$\left[a^2,\ (a^+)^2\right] = 2\ (a^+ a + a\ a^+]$$

```
f31 =
 AN[AN[CR[CR[ψ[ξ]]]]] - CR[CR[AN[AN[ψ[ξ]]]]] //
  Simplify
```

$2\,\xi^2\,\psi[\xi] - 2\,\psi''[\xi]$

```
f32 = 2 N11[ψ[ξ]] // Simplify
```

$2\,\xi^2\,\psi[\xi] - 2\,\psi''[\xi]$

```
f31 - f32 // Simplify
```

0

$[a,(a^{+})^{3}] = 3\,(a+)^{2}$

```
f41 =
 AN[CR[CR[CR[ψ[ξ]]]]] - CR[CR[CR[AN[ψ[ξ]]]]] //
  Simplify
```

$$\frac{3}{2}\left(\left(-1+\xi^{2}\right)\psi[\xi]-2\,\xi\,\psi'[\xi]+\psi''[\xi]\right)$$

```
f42 = 3 CR[CR[ψ[ξ]]] // Simplify
```

$$\frac{3}{2}\left(\left(-1+\xi^{2}\right)\psi[\xi]-2\,\xi\,\psi'[\xi]+\psi''[\xi]\right)$$

```
f41 - f42 // Simplify
```

0

$[a^2, (a^+)^3] = 2\ (a^+)^2 a + 2 a (a^+)^2 + 2 a^+ a\ a^+$

```
f51 = 2 CR[CR[AN[ψ[ξ]]]] + 2 AN[CR[CR[ψ[ξ]]]] +
   2 CR[AN[CR[ψ[ξ]]]] // Simplify
```

$$\frac{1}{\sqrt{2}} 3 \left(\xi \left(-1+\xi^2\right) \psi[\xi] - \left(1+\xi^2\right) \psi'[\xi] - \xi \psi''[\xi] + \psi^{(3)}[\xi]\right)$$

```
f52 =
 AN[AN[CR[CR[CR[ψ[ξ]]]]]] -
   CR[CR[CR[AN[AN[ψ[ξ]]]]]] // Simplify
```

$$\frac{1}{\sqrt{2}} 3 \left(\xi \left(-1+\xi^2\right) \psi[\xi] - \left(1+\xi^2\right) \psi'[\xi] - \xi \psi''[\xi] + \psi^{(3)}[\xi]\right)$$

```
f52 - f51 // FullSimplify
```

0

21. Sturm-Liouville differential equation

Eigenvalue problem

$$\langle \xi | \hat{H} | \psi \rangle = \hbar\omega \langle \xi | \hat{a}^+ \hat{a} + \frac{1}{2}\hat{1} | \psi \rangle = \hbar\omega (n + \frac{1}{2}) \langle \xi | \psi \rangle$$

or

$$\langle \xi | \hat{a}^+ \hat{a} | \psi \rangle = n \langle \xi | \psi \rangle$$

or

$$\frac{1}{2}\langle\xi|(\hat{\xi}-i\hat{\kappa})(\hat{\xi}+i\hat{\kappa}|\psi\rangle = n\langle\xi|\psi\rangle$$

or

$$(\xi-\frac{\partial}{\partial\xi})(\xi+\frac{\partial}{\partial\xi})\psi(\xi) = 2n\psi(\xi)$$

$$\psi''(\xi)-(2n+1-\xi^2)\psi(\xi) = 0$$

We assume that

$$\psi(\xi) = \exp(-\frac{\xi^2}{2})H(n,\xi)$$

where $H(n,\xi)$ satisfies the Hermite differential equation

$$H''(n,\xi)-2\xi H'(n,\xi)+2nH(n,\xi) = 0$$

This can be rewritten in the form of Sturm-Liouville type differential equation as

$$\begin{aligned}\frac{d}{d\xi}[\exp(-\xi^2)H'(n,\xi)] &= \exp(-\xi^2)H''(n,\xi)-2\xi\exp(-\xi^2)H'(n,\xi)\\ &= \exp(-\xi^2)[H''(n,\xi)-2\xi H'(n,\xi)]\\ &= -2n\exp(-\xi^2)H(n,\xi)\end{aligned}$$

((**Mathematica Program-9**))

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

Derivative operator of Hamiltonian of SH

$$AN := \frac{1}{\sqrt{2}} (\xi \# + D[\#, \xi]) \&;$$

$$CR := \frac{1}{\sqrt{2}} (\xi \# - D[\#, \xi]) \&;$$

$$H1 := \hbar\, \omega \left(CR[AN[\#]] + \frac{1}{2} \#\right) \&;$$

Schrodinger equation of

SH;
$$\left(1 + 2\,n - \xi^2\right) \psi[\xi] + \psi''[\xi]\Big) = 0$$

$$g1 = H1[\psi[\xi]] - \hbar\, \omega \left(n + \frac{1}{2}\right) \psi[\xi] \;//$$

FullSimplify

$$-\frac{1}{2}\, \omega\, \hbar \left(\left(1 + 2\,n - \xi^2\right) \psi[\xi] + \psi''[\xi]\right)$$

We assume that $\psi(\xi) = \text{Exp}\left[-\frac{\xi^2}{2}\right] \text{H0}(\xi)$

```
rule1 = {ψ → (Exp[-#^2/2] H0[#] &)};
```

```
g11 = g1 /. rule1 // Simplify
```

$$-\frac{1}{2} e^{-\frac{\xi^2}{2}} \omega \hbar \left(2 n \text{H0}[\xi] - 2 \xi \text{H0}'[\xi] + \text{H0}''[\xi]\right)$$

H0(ξ) satisfies the Hermite differential equation.

H0(ξ)=HermiteH[n,ξ]

```
g2 = 2 n H0[ξ] - 2 ξ H0'[ξ] + H0''[ξ];
```

```
DSolve[g2 == 0, H0[ξ], ξ]
```

$$\left\{\left\{\text{H0}[\xi] \to c_1 \text{HermiteH}[n, \xi] + c_2 \text{Hypergeometric1F1}\left[-\frac{n}{2}, \frac{1}{2}, \xi^2\right]\right\}\right\}$$

```
Table[{n, HermiteH[n, ξ]}, {n, 0, 10}] //
 TableForm[#, TableHeadings → {None, {"n", "HermiteH[n,ξ]"}}] &
```

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

22. Differential operator for Hermite polynomial

We prove that

$$(2\xi-\frac{d}{d\xi})^n 1=H(n_n,\xi),$$

which can be also used for the discussion of recursion relation.

((**Mathematica Program-10**))

Prove that

$\left(2\xi - \frac{d}{d\xi}\right)^n 1$=Hermite[n,ξ]

```
Clear["Global`*"];
G1 := (2 ξ # - D[#, ξ]) &;
G[n_, ξ_] := Nest[G1, 1, n] // Expand;
Table[{n, G[n, ξ]}, {n, 0, 6}] //
 TableForm[#,
   TableHeadings →
    {None, {"n", "Hn(ξ)"}}] &
```

n	$H_n(\xi)$
0	1
1	2ξ
2	$-2+4\xi^2$
3	$-12\xi+8\xi^3$
4	$12-48\xi^2+16\xi^4$
5	$120\xi-160\xi^3+32\xi^5$
6	$-120+720\xi^2-480\xi^4+64\xi^6$

23. Derivation of $H(n,\xi)$ from Generating function

From the generating function

$$S(\xi,t)=\exp(-t^2+2t\xi),$$

we show that the Hermite polynomials $H(n,\xi)$ can be obtained as

$$\frac{d^n}{dt^n} S(\xi, t)|_{t=0} = H(n, \xi).$$

The proof of this equation can be done with the use of Mathematica.

((**Mathematica Program-11**))

S[ξ,t]=Exp[-t^2+2t ξ]

$\frac{d^n}{dt^n}$S[ξ,t] | $_{t=0}$=Hermite[n,ξ]

```
Clear["Global`*"];
D1 := D[#, t] &;
S[ξ_, t_] := Exp[-t^2 + 2 t ξ];
G1[n_, ξ_] := Nest[D1, S[ξ, t], n] /. t → 0;
Table[{n, G1[n, ξ]}, {n, 0, 6}] //
 TableForm[#,
   TableHeadings → {None, {"n", "Hn(ξ)"}}] &
```

n	$H_n(\xi)$
0	1
1	2ξ
2	$-2+4\xi^2$
3	$-12\xi+8\xi^3$
4	$12-48\xi^2+16\xi^4$
5	$120\xi-160\xi^3+32\xi^5$
6	$-120+720\xi^2-480\xi^4+64\xi^6$

24. Recursion relation for Hermite polynomial

The Hermite polynomials satisfy the recurrence relations,

$$H(n+1,\xi) = 2\xi H(n,\xi) - 2nH(n,\xi)$$

This relation can be proved with the use of Mathematica as follows, using the formula

$$(2\xi - \frac{d}{d\xi})^n 1 = H(n,\xi)$$

25. Properties of the Hermite polynomials.

(1) Property-1

The Hermite polynomials satisfy the recurrence relations,

$$H(n+1,\xi) = 2\xi H(n,\xi) - \frac{d}{d\xi}H(n,\xi)$$

((**Proof**))

$$\begin{aligned} H(n+1,\xi) &= (2\xi - \frac{d}{d\xi})^{n+1} 1 \\ &= (2\xi - \frac{d}{d\xi})[(2\xi - \frac{d}{d\xi})^n 1] \\ &= (2\xi - \frac{d}{d\xi})H(n,\xi) \\ &= 2\xi\, H(n,\xi) - \frac{d}{d\xi}H(n,\xi) \end{aligned}$$

(2) The property-II

$$\frac{d}{d\xi}H(n,\xi) = 2nH(n-1,\xi)$$

((**Proof**))

$$\begin{aligned}\frac{d}{d\xi}H(n,\xi) &= \frac{d}{d\xi}[(2\xi-\frac{d}{d\xi})^n 1] \\ &= \frac{d}{d\xi}(2\xi-\frac{d}{d\xi})(2\xi-\frac{d}{d\xi})^{n-1}1 \\ &= \frac{d}{d\xi}(2\xi-\frac{d}{d\xi})H(n-1,\xi) \\ &= \frac{d}{d\xi}[2\xi H(n-1,\xi)-\frac{d}{d\xi}H(n-1,\xi)] \\ &= 2H(n-1,\xi)-H''(n-1,\xi)+2\xi H'(n-1,\xi) \\ &= 2nH(n-1,\xi)\end{aligned}$$

since

$$H''(n-1,\xi)-2\xi H'(n-1,\xi)=-2(n-1)H(n-1,\xi).$$

26. Conclusion

Here we have discussed the wave function of simple harmonics with the use of Mathematica. We have shown the application of differential operator techniques. Such method has a number of properties and a variety of uses. The objective of this method is to derive all the quantum mechanics while keeping the properties of the state vectors as simple as possible.

The annihilation operator and creation operator can be expressed in terms of the differential operators, where the symbols of D, #, & are used. We note that in a textbook written by David Bohm, similar discussions on the wave functions of simple harmonics were extensively done, using differential operators of annihilation and creation operators without Mathematica. It seems that the mathematics used in the book of David Bohm is complicated to beginners who just starts to study the quantum mechanics.

((**Goswami**))

We have three important operators for the simple harmonics; creation operator, annihilation operator, and the number operator. " the late Dr. Sakurai (J.J.)used to joke, using his knowledge of Hindu mythology, that $\hat{a}^+$ is like Brahma, the creator, $\hat{a}$ is like Shiva, the destroyer, and $\hat{n}$ the benign Vishnu, the preserver."

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APPENDIX` Formula

The derivation of the following formula is discussed in the above sections.

$$\sqrt{\frac{m\omega}{\hbar}}\hat{x} = \beta\hat{x} = \hat{\xi} \qquad \frac{\hat{p}}{\sqrt{m\hbar\omega}} = \frac{\hat{p}}{\hbar\beta} = \frac{\hat{k}}{\beta} = \hat{\kappa}$$

$$\hat{a} = \frac{1}{\sqrt{2}}(\hat{\xi} + i\hat{\kappa}) \ , \qquad \hat{a}^+ = \frac{1}{\sqrt{2}}(\hat{\xi} - i\hat{\kappa})$$

$$[\hat{\xi}, \hat{\kappa}] = i\hat{1} \ .$$

$$|\xi\rangle = \frac{1}{\sqrt{\beta}}|x\rangle , \qquad |\kappa\rangle = \sqrt{\hbar\beta}\,|p\rangle$$

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 = \frac{1}{2}\hbar\omega(\hat{\kappa}^2 + \hat{\xi}^2)$$

$$\langle\xi|\hat{a}|\psi\rangle=\frac{1}{\sqrt{2}}(\xi+\frac{\partial}{\partial\xi})\psi(\xi), \qquad \langle\xi|\hat{a}^{+}|\psi\rangle=\frac{1}{\sqrt{2}}(\xi-\frac{\partial}{\partial\xi})\psi(\xi)$$

$$\hat{a}|n\rangle=\sqrt{n}|n-1\rangle, \qquad \hat{a}^{+}|n\rangle=\sqrt{n+1}|n+1\rangle$$

$$\hat{a}|0\rangle=0$$

$$|n\rangle=\frac{1}{\sqrt{n!}}(\hat{a}^{+})|0\rangle$$

$$\langle\xi|n\rangle=\frac{1}{\sqrt{n!2^{n}}}(\xi-\frac{\partial}{\partial\xi})^{n}\langle\xi|0\rangle$$

$$\langle\xi|n\rangle=\frac{1}{(2^{n}n!\sqrt{\pi})^{1/2}}\exp(-\frac{\xi^{2}}{2})H(n,\xi)$$

$$\hat{\pi}|n\rangle=(-1)^{n}|n\rangle$$

$$\langle\xi|0\rangle=\pi^{-1/4}\exp(-\frac{\xi^{2}}{2})$$

$$\langle\kappa|0\rangle=\pi^{-1/4}\exp(-\frac{\kappa^{2}}{2})$$

$$\langle\xi|\kappa\rangle=\frac{1}{\sqrt{2\pi}}\exp(i\kappa\xi)$$

$$(\xi-\frac{\partial}{\partial\xi})^{n}\psi(\xi)=(-1)^{n}\exp(\frac{\xi^{2}}{2})\frac{\partial^{n}}{\partial\xi^{n}}\exp(-\frac{\xi^{2}}{2})\psi(\xi)$$

$$\langle\kappa|n\rangle=\frac{1}{\sqrt{n!}}\langle\kappa|(\hat{a}^{+})^{n}|0\rangle=\frac{(-i)^{n}}{(2^{n}n!\sqrt{\pi})^{1/2}}\exp(-\frac{\kappa^{2}}{2})H(n,\kappa)$$

$$\mathbf{F}[\exp(\frac{-\xi^{2}}{2})H(n,\xi)]=(-i)^{n}\exp(\frac{-\kappa^{2}}{2})H(n,\kappa)$$

$$P_{cl}(\xi)=\frac{1}{\pi}\frac{1}{\sqrt{2n+1-\xi^{2}}}$$

$$H(n,\xi)=(-1)^{n}\exp(\xi^{2})\frac{\partial^{n}}{\partial\xi^{n}}\exp(-\xi^{2})$$

$$H_{n}(-\xi)=(-1)^{n}H_{n}(\xi)$$

$$(2\xi-\frac{d}{d\xi})^{n}1=H(n,\xi)$$

$$S(\xi,t) = \exp(-t^2 + 2t\xi) \qquad \text{(generating function)}$$

$$\frac{d^n}{dt^n} S(\xi,t)|_{t=0} = H(n,\xi)$$

$$H(n+1,\xi) = 2\xi\, H(n,\xi) - \frac{d}{d\xi} H(n,\xi)$$

$$\frac{d}{d\xi} H(n,\xi) = 2nH(n-1,\xi)$$

$$H''(n,\xi) - 2\xi H'(n,\xi) + 2nH(n,\xi) = 0$$

$$\psi''(n,\xi) - (2n+1-\xi^2)\psi(n,\xi) = 0$$

$$\hat{a}\left|\alpha\right\rangle = \alpha\left|\alpha\right\rangle$$

$$\left|\alpha\right\rangle = \exp(-\frac{|\alpha|^2}{2})\sum_n \frac{(\alpha\hat{a}^+)^n}{n!}\left|0\right\rangle$$

$$\left\langle\xi\middle|\alpha\right\rangle = \exp(-\frac{|\alpha|^2}{2})\sum_n \frac{\alpha^n}{\sqrt{n!}} \frac{1}{(\pi^{1/2}2^n n!)^{1/2}} \exp(-\frac{\xi^2}{2}) H(n,\xi)$$

$$\left\langle\kappa\middle|\alpha\right\rangle = \exp(-\frac{|\alpha|^2}{2})\sum_n \frac{\alpha^n}{\sqrt{n!}} \frac{(-i)^n}{(\pi^{1/2}2^n n!)^{1/2}} \exp(-\frac{\kappa^2}{2}) H(n,\kappa)$$