Simple harmonics

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The model of the simple harmonics plays an important role in quantum mechanics as it does in classical mechanics. In our discussion of the simple harmonics we stress operator techniques using the creation operator and annihilation operator, rather than the coordinate representation (Schrödinger equation) because of the generality of the former approach. Such quantum mechanics treatment of the simple harmonics is very useful for our understanding various kinds of quantum phenomena such as the lattice vibration (as phonon) in solids and the quantization of the electromagnetic field (as photons).

The quantum mechanics of simple harmonics can be discussed in terms of (i) the wave function of the Schrodinger equation (ii) the operator method with the commutationrelations. The latter method is the more powerful tool in discussing the physics of simple harmonics.

((**L. Susskind and A. Friedman))**
Quantum Mechanics, the theoretical minimum, Basic Book 2014)) **The operator methods have tremendous power.**

"The operation method reduces the entire study of wave functions and wave equations to a very small number of algebraic tricks, which almost always involve the commutation relations. In fact, whenever you see a pair of operators, my advice is to figure out their commutator. If the commutator is a new operator that you have not seen before, find its commutator with the original pair. That is when the fun happens. Obviously, this advice can lead to an unending chain of boring computations. But once in a while you may get lucky and find a set of operators that close under commutation. Whenever that happens, you are in business; as we will see, operator methods have tremendous power."

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,

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

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)

Then we have

$$x_M = \sqrt{\frac{2E}{m\omega_0^{\,2}}}\,.$$

((**Note-1**)) Equi-partition of energy for simple harmonics

Suppose that the kinetic energy and the potential enegy are the same.

$$\frac{p^2}{2m} = \frac{1}{2}\hbar\omega_0\,, \qquad p = \sqrt{m\hbar\omega_0}$$

$$\frac{1}{2}m\omega_0^2 x^2 = \frac{1}{2}\hbar\omega_0 \qquad x = \sqrt{\frac{\hbar}{m\omega_0}}$$

Thus $\frac{p}{\sqrt{m\hbar\omega_0}}$,and $x\sqrt{\frac{m\omega_0}{\hbar}}$ are dimensionless variables.

We use a parameter

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}. \qquad [\mathrm{cm}^{-1}]$$

Then we get

$$x\sqrt{\frac{m\omega_0}{\hbar}} = \beta x\,,$$

$$\frac{p}{\sqrt{m\hbar\omega_0}} = \frac{p}{\sqrt{m\hbar\omega_0}}\beta\sqrt{\frac{\hbar}{m\omega_0}} = \beta\frac{p}{m\omega_0}\,.$$

((**Note-2**))
We consider the Hamiltonian of the simple harmonics divided by $\hbar\omega_0$. Using the notation β, we have

$$\begin{aligned}
\frac{\hat{H}}{\hbar\omega_0} &= \frac{1}{2m\hbar\omega_0}\hat{p}^2 + \frac{m\omega_0^2}{2\hbar\omega_0}\hat{x}^2 \\
&= \frac{1}{2m\hbar\omega_0}\hat{p}^2 + \frac{m\omega_0}{2\hbar}\hat{x}^2 \\
&= \frac{1}{2m\hbar\omega_0}(\frac{\hbar}{m\omega_0}\beta^2)\hat{p}^2 + \frac{1}{2}\beta^2\hat{x}^2 \\
&= \frac{1}{2}\frac{1}{m^2\omega_0{}^2}\beta^2\hat{p}^2 + \frac{1}{2}\beta^2\hat{x}^2 \\
&= \frac{1}{2}\beta^2(\hat{x}^2 + \frac{1}{m^2\omega_0{}^2}\hat{p}^2)
\end{aligned}$$

This notation leads to the form of creation operator and annihilation operator,

$$\hat{a} = \frac{\beta}{\sqrt{2}}(\hat{x} + \frac{i\hat{p}}{m\omega_0})\,,$$

$$\hat{a}^+ = \frac{\beta}{\sqrt{2}}(\hat{x} - \frac{i\hat{p}}{m\omega_0})\,.$$

We note that

$$\frac{i\hat{p}}{m\omega_0} \to \frac{i}{m\omega_0}\frac{\hbar}{i}\frac{\partial}{\partial x} = \frac{\hbar}{m\omega_0}\frac{\partial}{\partial x} = \frac{1}{\beta^2}\frac{\partial}{\partial x}\,.$$

2. Creation and annihilation operators

The commutation relation is given by

$$[\hat{x}, \hat{p}] = i\hbar\hat{1}.$$

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

$$\hat{H}|n\rangle = \varepsilon_n|n\rangle,$$

with the energy eigenvalue,

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

where n = 0, 1, 2, 3,....

In the $\{|x\rangle\}$ representation, the wave function of the simple harmonics can be described as

$$(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega_0^2}{2}x^2)\langle x|n\rangle = \varepsilon_n\langle x|n\rangle.$$

Here we introduce the creation operator and annihilation operator given by

$$\hat{a} = \frac{\beta}{\sqrt{2}}(\hat{x} + \frac{i\hat{p}}{m\omega_0}) = \frac{1}{\sqrt{2}}(\sqrt{\frac{m\omega_0}{\hbar}}\hat{x} + \frac{i\hat{p}}{\sqrt{m\hbar\omega_0}}),$$

$$\hat{a}^+ = \frac{\beta}{\sqrt{2}}(\hat{x} - \frac{i\hat{p}}{m\omega_0}) = \frac{1}{\sqrt{2}}(\sqrt{\frac{m\omega_0}{\hbar}}\hat{x} - \frac{i\hat{p}}{\sqrt{m\hbar\omega_0}}),$$

with

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}.$$

The operators $\hat{x}$ and $\hat{p}$ are given by

$$\hat{x} = \frac{1}{\sqrt{2}\beta}\left(\hat{a} + \hat{a}^+\right) = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\hat{a} + \hat{a}^+\right)$$

$$\hat{p} = \frac{1}{\sqrt{2}\beta}\frac{m\omega_0}{i}\left(\hat{a} - \hat{a}^+\right) = \frac{1}{i}\sqrt{\frac{m\hbar\omega_0}{2}}\left(\hat{a} - \hat{a}^+\right)$$

where

$$[\hat{x}, \hat{p}] = \frac{1}{\left(\sqrt{2}\beta\right)^2}\frac{m\omega_0}{i}[\hat{a} + \hat{a}^+, \hat{a} - \hat{a}^+] = -\frac{\hbar}{i}[\hat{a}, \hat{a}^+].$$

Since $[\hat{x}, \hat{p}] = i\hbar\hat{1}$, the commutation relation $[\hat{a}, \hat{a}^+]$ is obtained as

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

Noting that

$$\begin{aligned}
\hat{a}^+\hat{a} &= \frac{\beta^2}{2}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right)\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right) \\
&= \frac{\beta^2}{2}\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega_0^2} - i\frac{1}{m\omega_0}[\hat{p}, \hat{x}]\right) \\
&= \frac{m\omega_0}{2\hbar}\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega_0^2} - \frac{\hbar}{m\omega_0}\hat{1}\right)
\end{aligned}$$

or

$$\begin{aligned}
\hbar\omega_0\hat{a}^+\hat{a} &= \frac{m\omega_0{}^2}{2}\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega_0^2} - \frac{\hbar}{m\omega_0}\hat{1}\right) \\
&= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0{}^2\hat{x}^2 - \frac{1}{2}\hbar\omega_0
\end{aligned}$$

the Hamiltonian of the simple harmonics can be expressed by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0{}^2\hat{x}^2 = \hbar\omega_0\left(\hat{a}^+\hat{a} + \frac{1}{2}\hat{1}\right) = \hbar\omega_0\left(\hat{n} + \frac{1}{2}\hat{1}\right),$$

where

$$\hat{n} = \hat{a}^+\hat{a}.$$

The number operator $\hat{n}$ is Hermitian since

$$\hat{n}^+ = \left(\hat{a}^+\hat{a}\right)^+ = \hat{a}^+\hat{a} = \hat{n}.$$

The eigenvectors of $\hat{H}$ are those of $\hat{n}$, and vice versa since $[\hat{H},\hat{n}]=0$.

$$\hat{H}|n\rangle = \hbar\omega_0\left(\hat{n}+\frac{1}{2}\right)|n\rangle = \hbar\omega_0\left(n+\frac{1}{2}\right)|n\rangle = E_n|n\rangle$$

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

((**Note**)) The eigenvalue ε_n should be positive.

$$\begin{aligned}\varepsilon_n &= \frac{1}{\langle n|n\rangle}\langle n|\hat{H}|n\rangle \\ &= \frac{1}{\langle n|n\rangle}[\langle n|\frac{\hat{p}^2}{2m}|n\rangle + \langle n|\frac{m\omega^2}{2}\hat{x}^2|n\rangle \\ &= \frac{1}{\langle n|n\rangle}[\langle n|\frac{\hat{p}^+\hat{p}}{2m}|n\rangle + \langle n|\frac{m\omega^2}{2}\hat{x}^+\hat{x}|n\rangle \geq 0\end{aligned}$$

((**Note**))

$$\langle n|\hat{a}^+\hat{a}|n\rangle = \langle n|\hat{n}|n\rangle = n\langle n|n\rangle \geq 0$$

$n = 0$ is the minimum value.

where

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

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

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

Thus we have the relations

$$[\hat{n},\hat{a}] = -\hat{a},$$

and

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

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

From the relation

$$[\hat{n}, \hat{a}]|n\rangle = -\hat{a}|n\rangle ,$$

or

$$(\hat{n}\hat{a} - \hat{a}\hat{n})|n\rangle = -\hat{a}|n\rangle ,$$

we get

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

which implies that $\hat{a}|n\rangle$ is the eigenket of $\hat{n}$ with the eigenvalue (n-1).

$$\hat{a}|n\rangle \approx |n-1\rangle$$

Similarly, from the relation

$$[\hat{n}, \hat{a}^+]|n\rangle = \hat{a}^+|n\rangle ,$$

or

$$(\hat{n}\hat{a}^+ - \hat{a}^+\hat{n})|n\rangle = \hat{a}^+|n\rangle ,$$

we get

$$\hat{n}\hat{a}^+|n\rangle = (n+1)\hat{a}^+|n\rangle ,$$

which implies that $\hat{a}^+|n\rangle$ is the eigenket of $\hat{n}$ with the eigenvalue (n+1).

$$\hat{a}^+|n\rangle \approx |n+1\rangle .$$

Now we need to show that n should be either zero or positive integers: n = 0, 1, 2, 3,…..
We note that

$$\langle n|\hat{a}^+\hat{a}|n\rangle = \langle n|\hat{n}|n\rangle = n\langle n|n\rangle \geq 0 ,$$

and

$$\langle n|\hat{a}\hat{a}^+|n\rangle = \langle n|\hat{a}^+\hat{a}+1|n\rangle = (n+1)\langle n|n\rangle \geq 0\,.$$

The norm of a ket vector is non-negative and the vanishing of the norm is a necessary and sufficient condition for the vanishing of the ket vector. In other words, $n \geq 0$.

If $n = 0$, $\hat{a}|n\rangle = 0$.

If $n \neq 0$, $\hat{a}|n\rangle$ is a nonzero ket vector of norm $n\langle n|n\rangle$.

If n>0, one successively forms the set of eigenkets,

$$\hat{a}|n\rangle, \hat{a}^2|n\rangle, \hat{a}^3|n\rangle, \ldots., \hat{a}^p|n\rangle,$$

belonging to the eigenvalues, n-1, n-2, n-3,….., n-p.

This set is certainly limited since the eigenvalues of $\hat{N}$ have a lower limit of zero. In other words, the eigenket $\hat{a}^p|n\rangle \approx |n-p\rangle$, or n - p = 0. Thus n should be a positive integer.

Similarly, one successively forms the set of eigenkets,

$$\hat{a}^+|n\rangle, \hat{a}^{+2}|n\rangle, \hat{a}^{+3}|n\rangle, \ldots.\, \hat{a}^{+p}|n\rangle,$$

belonging to the eigenvalues, n+1, n+2, n+3,….., n+p,

Thus the eigenvalues are either zeo or positive integers: n = 0, 1, 2, 3, 4, .

The properties of $\hat{a}^+$ and $\hat{a}$

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

since $\langle 0|\hat{a}^+\hat{a}|0\rangle = 0$.

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

$$[\hat{n}, \hat{a}^+]|n\rangle = \hat{a}^+|n\rangle\,.$$

$$\hat{n}\hat{a}^+|n\rangle = \hat{a}^+\hat{n}|n\rangle + \hat{a}^+|n\rangle = (n+1)\hat{a}^+|n\rangle\,.$$

$\hat{a}^+|n\rangle$ is an eigenket of $\hat{n}$ with the eigenvalue (n + 1).

Then

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

Since

$$\langle n|\hat{a}\hat{a}^{+}|n\rangle = |c|^{2}\langle n+1|n+1\rangle = |c|^{2},$$

or

$$\langle n|\hat{a}^{+}\hat{a}+1|n\rangle = n+1 = |c|^{2},$$

or

$$|c| = \sqrt{n+1} .$$

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

$$[\hat{n},\hat{a}]|n\rangle = -\hat{a}|n\rangle .$$

$$\hat{n}\hat{a}|n\rangle = \hat{a}\hat{n}|n\rangle - \hat{a}|n\rangle = (n-1)\hat{a}|n\rangle .$$

$\hat{a}|n\rangle$ is an eigenket of $\hat{n}$ with the eigenvalue (n - 1)

Then

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

Since

$$\langle n|\hat{a}^{+}\hat{a}|n\rangle = |c|^{2}\langle n-1|n-1\rangle = |c|^{2} = n,$$

$$|c| = \sqrt{n} .$$

3. Basis $|n\rangle$ vectors in terms of $|0\rangle$

We use the relation

$$|1\rangle = \hat{a}^{+}|0\rangle,$$

$$|2\rangle = \frac{1}{\sqrt{2}}\hat{a}^+|1\rangle = \frac{1}{\sqrt{2!}}\left(\hat{a}^+\right)^2|0\rangle,$$

$$|3\rangle = \frac{1}{\sqrt{3}}\hat{a}^+|2\rangle = \frac{1}{\sqrt{3!}}\left(\hat{a}^+\right)^3|0\rangle,$$

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

The expression for $\hat{x}|n\rangle$ and $\hat{p}|n\rangle$

$$\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\hat{a}+\hat{a}^+\right)|n\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\sqrt{n+1}|n+1\rangle + \sqrt{n}|n-1\rangle\right)$$

$$\hat{p}|n\rangle = \sqrt{\frac{m\hbar\omega_0}{2}}i\left(\hat{a}^+-\hat{a}\right)|n\rangle = \sqrt{\frac{m\hbar\omega_0}{2}}i\left(\sqrt{n+1}|n+1\rangle - \sqrt{n}|n-1\rangle\right)$$

Therefore the matrix elements of $\hat{a}$, $\hat{a}^+$, $\hat{x}$, and $\hat{p}$ operators in the $\{|n\rangle\}$ representation are as follows.

$$\langle n'|\hat{a}|n\rangle = \sqrt{n}\delta_{n',n-1},$$

$$\langle n'|\hat{a}^+|n\rangle = \sqrt{n+1}\delta_{n',n+1},$$

$$\langle n'|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1}\right),$$

$$\langle n'|\hat{p}|n\rangle = i\sqrt{\frac{m\hbar\omega_0}{2}}\left(\sqrt{n+1}\delta_{n',n+1} - \sqrt{n}\delta_{n',n-1}\right),$$

$$\hat{H} = \hbar\omega\begin{pmatrix} 1/2 & 0 & \cdots & 0 & \cdots \\ 0 & 3/2 & & & \\ \vdots & & \ddots & & \\ 0 & & & (2n+1)/2 & \\ \vdots & & & & \ddots \end{pmatrix}$$

$$\hat{x} = \frac{1}{\sqrt{2}\beta}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix}$$

$$\hat{p} = \frac{m\omega_0}{\sqrt{2}i\beta}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ -\sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & -\sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & -\sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix}$$

$$\hat{a} = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ 0 & 0 & \sqrt{2} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \\ 0 & 0 & 0 & 0 & 0 & \\ & & \vdots & & & \end{pmatrix}$$

$$\hat{a}^{+} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \\ \sqrt{1} & 0 & 0 & 0 & 0 & \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix}$$

$$\hat{N} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \\ \sqrt{1} & 0 & 0 & 0 & 0 & \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ 0 & 0 & \sqrt{2} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \\ 0 & 0 & 0 & 0 & 0 & \\ & & \vdots & & & \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 0 & 0 & 0 & & & \\ 0 & 1 & 0 & 0 & & & \\ 0 & 0 & 2 & 0 & & & \\ 0 & 0 & 0 & 3 & & & \\ & & & & \ddots & & \\ & & & & & n & \\ & & & & & & \ddots \end{pmatrix}$$

4. Heisenberg's principle of uncertainty

Mean values and root-mean-square deviations of $\hat{x}$ and $\hat{p}$ in the state $|n\rangle$.

$$\langle n|\hat{x}|n\rangle = 0 .$$

$$\langle n|\hat{p}|n\rangle = 0 .$$

$$(\Delta x)^2 = \langle n|\hat{x}^2|n\rangle = \left(n + \frac{1}{2}\right)\frac{\hbar}{m\omega_0} .$$

$$(\Delta p)^2 = \langle n|\hat{p}^2|n\rangle = \left(n + \frac{1}{2}\right)m\hbar\omega_0 .$$

The product $\Delta x \Delta p$ is

$$\Delta x \Delta p = \left(n + \frac{1}{2}\right)\hbar \geq \frac{1}{2}\hbar \qquad \text{(Heisenberg's principle of uncertainty)}$$

Note that

$$\hat{x}^2 = \frac{\hbar}{2m\omega_0}\left(\hat{a}^+ + \hat{a}\right)\left(\hat{a}^+ + \hat{a}\right) = \frac{\hbar}{2m\omega_0}\left(\hat{a}^+\hat{a}^+ + \hat{a}\hat{a} + \hat{a}^+\hat{a} + \hat{a}\hat{a}^+\right)$$

$$\hat{p}^2 = \frac{m\hbar\omega_0}{2}\left(\hat{a}^+ - \hat{a}\right)\left(\hat{a}^+ - \hat{a}\right) = \frac{m\hbar\omega_0}{2}\left(\hat{a}^+\hat{a}^+ + \hat{a}\hat{a} - \hat{a}^+\hat{a} - \hat{a}\hat{a}^+\right)$$

and

$$\langle n|\left(\hat{a}^+\right)^2|n\rangle = 0$$

$$\langle n|\hat{a}^2|n\rangle = 0$$

$$\langle n|\hat{a}^+\hat{a} + \hat{a}\hat{a}^+|n\rangle = \langle n|2\hat{a}^+\hat{a} + 1|n\rangle = 2n + 1$$

5. Virial theorem

The mean potential energy is

$$\langle V\rangle = \frac{1}{2}m\omega^2\langle n|\hat{x}^2|n\rangle = \frac{1}{2}m\omega^2(\Delta x)^2 = \frac{1}{2}\varepsilon_n .$$

The mean kinetic energy is

$$\langle K\rangle = \frac{1}{2m}\langle n|\hat{p}^2|n\rangle = \frac{1}{2m}(\Delta p)^2 = \frac{1}{2}\varepsilon_n .$$

Thus we have

$$\langle V\rangle = \langle K\rangle .$$

(virial theorem)

6 Wave functions associated with the stationary state

We start with

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

We note that

$$\langle x|\hat{a}|0\rangle = 0 , \qquad \langle x|\frac{\beta}{\sqrt{2}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right)|0\rangle = 0$$

or

$$\frac{\beta}{\sqrt{2}}(x + \frac{\hbar}{m\omega_0}\frac{\partial}{\partial x})\langle x|0\rangle = 0 ,$$

$$\frac{1}{\sqrt{2}}(\beta x+\frac{1}{\beta}\frac{\partial}{\partial x})\langle x|0\rangle=0$$

We use new variable (dimensionless),

$$\xi=\beta x\ .$$

We have

$$|\xi\rangle=\frac{1}{\sqrt{\beta}}|x\rangle\ .$$

since

$$\langle\xi'|\xi''\rangle=\delta(\xi'-\xi'')=\delta(\beta(x'-x'')]=\frac{1}{\beta}\delta(x'-x'')=\frac{1}{\beta}\langle x'|x''\rangle\ .$$

Then we have

$$\frac{1}{\sqrt{2}}\left(\xi+\frac{\partial}{\partial\xi}\right)\varphi_0(\xi)=0\ ,$$

where

$$\varphi_0(\xi)=\langle\xi|0\rangle\ .$$

the solution of this differential equation for $\varphi_0(\xi)$ is obtained as

$$\varphi_0(\xi)=A_0e^{-\frac{\xi^2}{2}}$$

Normalization:

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

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

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

We note that

$$\varphi_0(x) = \langle x|0\rangle = \sqrt{\beta}\langle \xi|0\rangle = \sqrt{\beta}\pi^{-\frac{1}{4}}e^{-\frac{\xi^2}{2}} = \sqrt{\beta}\pi^{-\frac{1}{4}}e^{-\frac{\beta^2 x^2}{2}} = (\frac{\pi\hbar}{m\omega_0})^{-1/4}e^{-\frac{m\omega_0 x^2}{2\hbar}}$$

((**Note-1**))

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

where

$$\xi = \beta x, \qquad \beta = \sqrt{\frac{m\omega_0}{\hbar}}.$$

((**Note-2**))
The characteristic length is defined by

$$l = \sqrt{\frac{\hbar}{2m\omega_0}}$$

$$\varphi_0(x) = (\frac{\pi\hbar}{m\omega_0})^{-1/4}e^{-\frac{m\omega_0 x^2}{2\hbar}} = \frac{1}{(2\pi l^2)^{1/4}}e^{-\frac{x^2}{4l^2}} = \frac{1}{\sqrt{\sqrt{2\pi}l}}e^{-\frac{x^2}{4l^2}}$$

Note that the probability density is given by the Gaussian distribution function, as

$$|\varphi_0(x)|^2 = \frac{1}{\sqrt{2\pi}l}e^{-\frac{x^2}{2l^2}}.$$

with the standard deviation $\sigma = l$ (see the detail later).

((**Note**)) **Example**
S. Holzner, Quantum Physics for Dummies (John Wiley and Sons).

Suppose that we have a proton undergoing harmonic oscillation with $\omega = 4.58\times 10^{21}$ rad/s. The ground state energy of the proton, in MeV, is

$$E_0 = \frac{1}{2}\hbar\omega_0 = 1.51 \text{ MeV}.$$

The characteristic length *l* is

$$l=\sqrt{\frac{\hbar}{2m\omega_0}}=2.621\ \text{fm}$$

Here the mass of proton is $m=1.672621637\times10^{-24}$ g. The Dirac constant is $\hbar=1.054571628\times10^{-27}$ erg s. 1fm (femtmeters)= 10^{-15} m = 10^{-13} cm. 1THz=10^{12} Hz.

7. Wave functions $\varphi_n(\xi)=\langle\xi|n\rangle$ and $\varphi_n(x)=\langle x|n\rangle$

$$\varphi_n(\xi)=\langle\xi|n\rangle=\frac{1}{\sqrt{\beta}}\langle x|n\rangle=\frac{1}{\sqrt{\beta}}\varphi_n(x),$$

since

$$|\xi\rangle=\frac{1}{\sqrt{\beta}}|x\rangle,$$

with

$$\langle\xi|\xi'\rangle=\delta(\xi-\xi')=\delta(\beta(x-x'))=\frac{1}{\beta}\delta(x-x')=\frac{1}{\beta}\langle x|x'\rangle.$$

The wave function for the $|n\rangle$ state is given by

$$\begin{aligned}\varphi_n(x)=\langle x|n\rangle&=\frac{1}{\sqrt{n!}}\langle x|(\hat{a}^+)^n|0\rangle=\frac{1}{\sqrt{n!}}\frac{1}{\sqrt{2^n}}\beta^n\langle x|\left(\hat{x}-\frac{i\hat{p}}{m\omega_0}\right)^n|0\rangle\\&=\frac{1}{\sqrt{n!}}\frac{1}{\sqrt{2^n}}\beta^n\left(x-\frac{\hbar}{m\omega_0}\frac{\partial}{\partial x}\right)^n\varphi_0(x)\\&=\frac{1}{\sqrt{n!}}\frac{1}{\sqrt{2^n}}\left(\beta x-\frac{1}{\beta}\frac{\partial}{\partial x}\right)^n\varphi_0(x)\end{aligned}$$

((Note)) In general, one can use the formula,

$$\langle x|f(\hat{x},\hat{p})|n\rangle=f(x,\frac{\hbar}{i}\frac{\partial}{\partial x})\langle x|n\rangle.$$

Since

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

we have

$$\varphi_n(\xi) = \langle \xi | n \rangle = (2^n n!)^{-\frac{1}{2}} (\xi - \frac{\partial}{\partial \xi})^n \varphi_0(\xi) .$$

where

$$\xi = \beta x$$

Note that $\varphi_0(\xi) = \pi^{-\frac{1}{4}} e^{-\frac{\xi^2}{2}}$,

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

((**Note**))
Using the Mathematica, we can get the normalized wave function $\varphi_n(\xi)$

```
Clear["Global`"]; CR1 := (1/Sqrt[2] (ξ # - D[#, ξ]) &);
f0[ξ_] := Exp[-ξ^2 / 2];
ψ[n_, ξ_] := 1/Sqrt[Sqrt[π] n!] Nest[CR1, f0[ξ], n] //
  Simplify; Table[{n, ψ[n, ξ]}, {n, 0, 3}] //
 TableForm
```

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 $\frac{e^{-\frac{\xi^2}{2}}\,\xi\left(-3+2\,\xi^2\right)}{\sqrt{3}\,\pi^{1/4}}$

Using the operator identity

$$(\xi - \frac{\partial}{\partial \xi}) = -e^{\frac{\xi^2}{2}} \frac{\partial}{\partial \xi} e^{-\frac{\xi^2}{2}},$$

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

....
in general

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

or, for any function $\psi(\xi)$, we have

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

Then we obtain

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

Using the Hermite polynomial defined by

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

we have

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

((**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

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

8. Differential equation derived from the Hamiltonian

(a)

$$\hat{a}^+ = \frac{\beta}{\sqrt{2}} \left(\hat{x} - \frac{i\hat{p}}{m\omega_0} \right) \rightarrow \frac{1}{\sqrt{2}} \left(\xi - \frac{\partial}{\partial \xi} \right)$$

$$\hat{a} = \frac{\beta}{\sqrt{2}} \left(\hat{x} + \frac{i\hat{p}}{m\omega_0} \right) \rightarrow \frac{1}{\sqrt{2}} \left(\xi + \frac{\partial}{\partial \xi} \right)$$

$$\xi = \beta x$$

with

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}.$$

(b)

$$\left|\xi\right\rangle = \frac{1}{\sqrt{\beta}}\left|x\right\rangle,$$

and

$$\varphi_n(\xi) = \left\langle \xi \middle| n \right\rangle = \frac{1}{\sqrt{\beta}}\left\langle x \middle| n \right\rangle = \frac{1}{\sqrt{\beta}}\varphi_n(x).$$

(c)

$$\hat{H} = \hbar\omega_0\left(\hat{a}^+\hat{a} + \frac{1}{2}\hat{1}\right),$$

$$\hat{a}^+\hat{a}\left|n\right\rangle = n\left|n\right\rangle$$

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

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

$$\hat{a}^+\hat{a} = \frac{\beta^2}{2}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right)\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right),$$

$$\left\langle x\middle|\hat{a}^+\hat{a}\middle|n\right\rangle = n\left\langle x \middle| n\right\rangle,$$

Then we get

$$\frac{1}{2}\left(\xi - \frac{\partial}{\partial\xi}\right)\left(\xi + \frac{\partial}{\partial\xi}\right)\left\langle\xi\middle|n\right\rangle = n\left\langle\xi\middle|n\right\rangle$$

or

$$\left(\xi - \frac{\partial}{\partial\xi}\right)\left(\xi + \frac{\partial}{\partial\xi}\right)\varphi_n(\xi) = 2n\varphi_n(\xi)$$

$\varphi_n(\xi) = \left\langle\xi\middle|n\right\rangle$ satisfies the differential equation

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

When

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

we find that $H_n(\xi)$ satisfies

$$H_n''(\xi) - 2\xi H_n'(\xi) + 2nH_n(\xi) = 0.$$

where $H_n(\xi)$ is a Hermite polynomial.

(d)

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

$$\hat{a}^+ = \frac{\beta}{\sqrt{2}}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right),$$

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

or

$$\frac{\beta}{\sqrt{2}}(x - \frac{\hbar}{m\omega_0}\frac{\partial}{\partial x})\langle x|n\rangle = \sqrt{n+1}\langle x|n+1\rangle,$$

or

$$\frac{1}{\sqrt{2}}(\xi - \frac{\partial}{\partial \xi})\langle \xi|n\rangle = \sqrt{n+1}\langle \xi|n+1\rangle, \qquad \text{(Arfken p.826)}$$

(e)

Similarly we have

$$\frac{1}{\sqrt{2}}(\xi + \frac{\partial}{\partial \xi})\langle \xi|n\rangle = \sqrt{n}\langle \xi|n-1\rangle, \qquad \text{(Arfken p.826)}$$

from the relation, $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$

9. Mathematica-1

(a) Derivation of the differential equation from the relation

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

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

AN := 1/Sqrt[2] (ξ # + D[#, ξ]) &;

eq1 = CR[AN[ψ[ξ]]] == n ψ[ξ] // Simplify
```

$\psi[\xi] + 2\,n\,\psi[\xi] + \psi''[\xi] == \xi^2\,\psi[\xi]$

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

eq11 = eq1 /. rule1 // Simplify
```

$e^{-\frac{\xi^2}{2}}\,(2\,n\,H[\xi] - 2\,\xi\,H'[\xi] + H''[\xi]) == 0$

```
DSolve[eq11, H[ξ], ξ]
```

$\{\{H[\xi] \to C[1]\,\text{HermiteH}[n, \xi] + C[2]\,\text{Hypergeometric1F1}[-\frac{n}{2}, \frac{1}{2}, \xi^2]\}\}$

(b) 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	$2\,x$
2	$-2 + 4\,x^2$
3	$-12\,x + 8\,x^3$
4	$12 - 48\,x^2 + 16\,x^4$
5	$120\,x - 160\,x^3 + 32\,x^5$
6	$-120 + 720\,x^2 - 480\,x^4 + 64\,x^6$
7	$-1680\,x + 3360\,x^3 - 1344\,x^5 + 128\,x^7$
8	$1680 - 13\,440\,x^2 + 13\,440\,x^4 - 3584\,x^6 + 256\,x^8$
9	$30\,240\,x - 80\,640\,x^3 + 48\,384\,x^5 - 9216\,x^7 + 512\,x^9$
10	$-30\,240 + 302\,400\,x^2 - 403\,200\,x^4 + 161\,280\,x^6 - 23\,040\,x^8 + 1024\,x^{10}$

10. 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 $n = 0, 1, 2, \ldots$

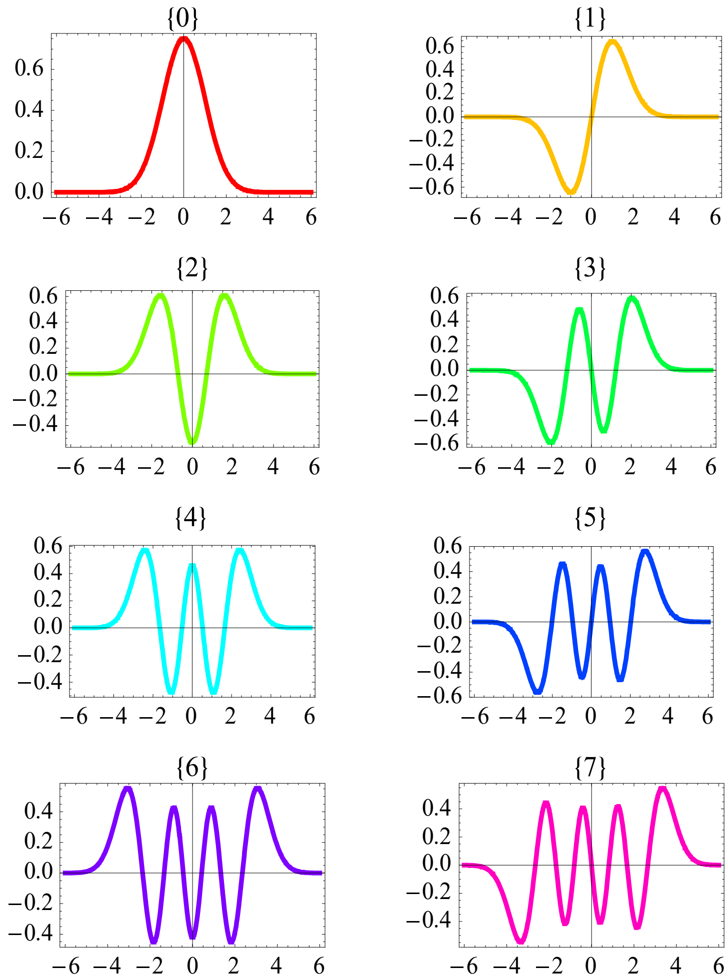


Fig. The plot of the wave function $\varphi_n(\xi)$ as a function of ξ. n – 0, 1, 2, 3, …., for the harmonic oscillator.

11. Mathematica-3

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

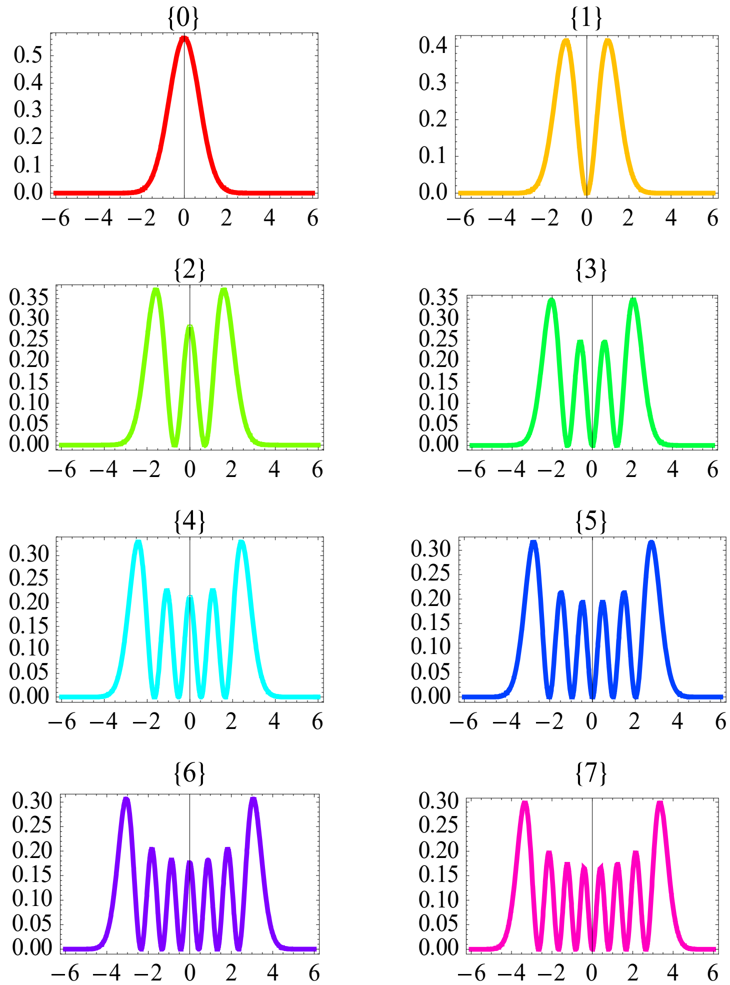


Fig. Plot of the probability $|\varphi_n(\xi)|^2$ as a function of ξ. n – 0, 1, 2, 3, …., for the harmonic oscillator. There are $(n + 1)$ peaks for the n state.

12. 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	$\left(-1+\xi^2\right)\chi[\xi] - 2\,\xi\,\chi'[\xi] + \chi''[\xi]$
3	$\xi\left(-3+\xi^2\right)\chi[\xi] - 3\left(-1+\xi^2\right)\chi'[\xi] + 3\,\xi\,\chi''[\xi] - \chi^{(3)}[\xi]$
4	$\left(3-6\,\xi^2+\xi^4\right)\chi[\xi] - 4\,\xi\left(-3+\xi^2\right)\chi'[\xi] - 6\,\chi''[\xi] + 6\,\xi^2\,\chi''[\xi] - 4\,\xi\,\chi^{(3)}[\xi] + \chi^{(4)}[\xi]$

13. Mathematica-5

$$\hat{a}^{+} = \frac{\beta}{\sqrt{2}}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right) \rightarrow \frac{1}{\sqrt{2}}\left(\xi - \frac{\partial}{\partial\xi}\right)$$

$$\hat{a} = \frac{\beta}{\sqrt{2}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right) \rightarrow \frac{1}{\sqrt{2}}\left(\xi + \frac{\partial}{\partial\xi}\right)$$

Creation and annihilation operators : differential form

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

AN := 1/Sqrt[2] (ξ # + D[#, ξ]) &
```

The wave function of the ground state

```
φ0[ξ_] := π^(-1/4) Exp[-ξ^2/2];
```

The properties of creation and annihilation operators

```
eq1 = AN[CR[ψ[ξ]]] - CR[AN[ψ[ξ]]] // Simplify
```

$\psi[\xi]$

```
eq2 = CR[AN[ψ[ξ]]] == n ψ[ξ] // Simplify
```

$\psi[\xi] + 2\,n\,\psi[\xi] + \psi''[\xi] == \xi^2\,\psi[\xi]$

```
srule = {ψ → (Exp[-#^2/2] H[#] &)}
```

$\left\{\psi \to \left(\mathrm{Exp}\left[-\frac{\#1^2}{2}\right] H[\#1]\ \&\right)\right\}$

Hermite differential equation

```
eq2 /. srule // Simplify
```

$$e^{-\frac{\xi^2}{2}} \left(2\, n\, H[\xi] - 2\, \xi\, H'[\xi] + H''[\xi]\right) == 0$$

```
AN[φ0[ξ]]
```

0

```
CR[φ0[ξ]]
```

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

```
AN[CR[CR[CR[φ0[ξ]]]]] /. srule // Simplify
```

$$\frac{e^{-\frac{\xi^2}{2}} \left(-3 + 6\, \xi^2\right)}{\pi^{1/4}}$$

```
CR[AN[CR[CR[φ0[ξ]]]]] /. srule // Simplify
```

$$\frac{e^{-\frac{\xi^2}{2}} \left(-2 + 4\, \xi^2\right)}{\pi^{1/4}}$$

The wave function of the n-th state

```
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. Parity of the wave function

$$\left|1\right\rangle = \hat{a}^{+}\left|0\right\rangle,$$

with

$$\hat{a}^{+} = \frac{\beta}{\sqrt{2}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right).$$

Noting that

$$\hat{\pi}\hat{x} = -\hat{x}\hat{\pi},$$

$$\hat{\pi}\hat{p} = -\hat{p}\hat{\pi},$$

we have the relation

$$\hat{\pi}\hat{a}^{+} = \frac{\beta}{\sqrt{2}}\hat{\pi}\left(\hat{x} - \frac{i}{m\omega_0}\hat{p}\right) = -\frac{\beta}{\sqrt{2}}\left(\hat{x} - \frac{i}{m\omega_0}\hat{p}\right)\hat{\pi} = -\hat{a}^{+}\hat{\pi}.$$

where $\hat{\pi}$ is the parity boperator. We note that

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

Since $\langle\xi|\hat{\pi}|0\rangle = \langle-\xi|0\rangle = \langle\xi|0\rangle$ (even function of $\varphi_0(\xi) = \pi^{-1/4}e^{-\xi^2/2}$), we have

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

$$\hat{\pi}|1\rangle = \hat{\pi}\frac{\hat{a}^+}{\sqrt{1}}|0\rangle = -\hat{a}^+\hat{\pi}|0\rangle = -\hat{a}^+|0\rangle = -|1\rangle$$

Then $|1\rangle$ must have an odd parity. Similarly

$$\hat{\pi}|2\rangle = \hat{\pi}\frac{\hat{a}^+}{\sqrt{2}}|1\rangle = -\frac{\hat{a}^+}{\sqrt{2}}\hat{\pi}|1\rangle = \frac{\hat{a}^+}{\sqrt{2}}|1\rangle = |2\rangle .$$

Then $|2\rangle$ must have an odd parity. In general, $|n\rangle$ has a $(-1)^n$ parity:

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

Since $\hat{\pi}|x\rangle = |-x\rangle$ or $\langle x|\hat{\pi} = \langle -x|$, we have

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

or

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

which means that $\langle x|n\rangle$ is an even function of *x* for even number and is an odd function of *x* for odd number.

15. Parity selection rule (even and odd parity operators)

We define a new operator as

$$\hat{\pi}^+\hat{A}_+\hat{\pi} = \hat{A}_+$$

for operator with even parity

$$\hat{\pi}^+\hat{A}_-\hat{\pi} = -\hat{A}_-$$

and for operator with odd parity.

So the operators $\hat{x}$ and $\hat{p}$ are odd parity operators:

$$\hat{\pi}^{+}\hat{x}\hat{\pi} = -\hat{x}, \quad \text{and} \qquad \hat{\pi}^{+}\hat{p}\hat{\pi} = -\hat{p}.$$

The operator $\hat{x}\hat{p}$ is the even parity'

$$\hat{\pi}^{+}\hat{x}\hat{p}\hat{\pi} = \hat{\pi}^{+}\hat{x}\hat{\pi}^{+}\hat{\pi}\hat{p}\hat{\pi} = \hat{x}\hat{p}.$$

In general,

$$\hat{\pi}^{+}\hat{x}^{k}\hat{p}^{\ell}\hat{\pi} = \hat{\pi}^{+}\hat{x}^{k}\hat{\pi}\hat{\pi}^{+}\hat{p}^{\ell}\hat{\pi} = (-1)^{k+\ell}\hat{x}^{k}\hat{p}^{\ell}$$

$\hat{x}^{k}\hat{p}^{\ell}$ is an even parity when $k+\ell$ =even and is an odd parity when $k+\ell$ =odd.

We now consider the matix element of the operators $\hat{A}_{+}$ and $\hat{A}_{-}$ with $\langle n|$ and $|m\rangle$, where

$$\hat{\pi}|n\rangle = (-1)^{n}|n\rangle, \qquad \hat{\pi}|m\rangle = (-1)^{m}|m\rangle.$$

The matrix element is given by

$$\langle n|\hat{A}_{+}|m\rangle = \langle n|\hat{\pi}^{+}\hat{A}_{+}\hat{\pi}|m\rangle = (-1)^{n+m}\langle n|\hat{A}_{+}|m\rangle$$

$\langle n|\hat{A}_{+}|m\rangle$ is equal to zero when $n+m=$ odd.

Similarly,

$$\langle n|\hat{A}_{-}|m\rangle = -\langle n|\hat{\pi}^{+}\hat{A}_{-}\hat{\pi}|m\rangle = (-1)^{n+m+1}\langle n|\hat{A}_{-}|m\rangle.$$

$\langle n|\hat{A}_{-}|m\rangle$ is equal to zero when $n+m=$ even.

16. Generating function

$$\exp(2\xi t - t^{2}) = \sum_{n=0}^{\infty}\frac{H_{n}(\xi)t^{n}}{n!}$$

((**Proof**))

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

$$\sum_{n=0}^{\infty}\frac{H_n(\xi)t^n}{n!} = \sum_{n=0}^{\infty}(-1)^n e^{\xi^2}\frac{\partial^n}{\partial\xi^n}e^{-\xi^2}\frac{t^n}{n!}$$

Taylor expansion:

$$e^{-(\xi-t)^2} = \sum_{n=0}^{\infty}\frac{t^n}{n!}\left[\frac{\partial^n}{\partial t^n}e^{-(\xi-t)^2}\right]_{t=0}$$

Note that $\frac{\partial}{\partial t}f(\xi-t) = -\frac{\partial}{\partial\xi}f(\xi-t)$. We put

$$X = \xi - t$$

$$\frac{\partial}{\partial t}f(\xi-t) = \frac{\partial X}{\partial t}\frac{\partial f(X)}{\partial X} = -\frac{\partial f(X)}{\partial X},$$

$$\frac{\partial}{\partial\xi}f(\xi-t) = \frac{\partial X}{\partial\xi}\frac{\partial f(X)}{\partial X} = \frac{\partial f(X)}{\partial X},$$

Then we have

$$\frac{\partial}{\partial t}f(\xi-t) = -\frac{\partial}{\partial\xi}f(\xi-t),$$

or more generally

$$\frac{\partial^n}{\partial t^n}f(\xi-t) = (-1)^n\frac{\partial^n}{\partial\xi^n}f(\xi-t),$$

$$e^{-(\xi-t)^2} = \sum_{n=0}^{\infty}\frac{t^n}{n!}(-1)^n\left[\frac{\partial^n}{\partial\xi^n}e^{-(\xi-t)^2}\right]_{t=0} = \sum_{n=0}^{\infty}\frac{t^n}{n!}(-1)^n\frac{\partial^n}{\partial\xi^n}e^{-\xi^2},$$

or

$$e^{-(\xi-t)^2}e^{\xi^2} = \sum_{n=0}^{\infty}\frac{t^n}{n!}(-1)^n e^{\xi^2}\frac{\partial^n}{\partial\xi^n}e^{-\xi^2},$$

or

$$\exp(-2\xi t + t^2) = \sum_{n=0}^{\infty} \frac{t^n}{n!}(-1)^n e^{\xi^2} \frac{\partial^n}{\partial \xi^n} e^{-\xi^2} = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(\xi)$$

17. Proof the generating function using the Baker-Hausdorff relation

$$F(t,x) = \langle x|\exp(\hat{a}^+ t)|0\rangle = \sum_{n=0}^{\infty} \frac{t^n}{n!}\langle x|(\hat{a}^+)^n|0\rangle = \sum_{n=0}^{\infty} \frac{t^n}{\sqrt{n!}}\langle x|n\rangle$$

((Lemma))

If the commutator of two operators $\hat{A}$ and $\hat{B}$ commute with each of them

$$[\hat{A},[\hat{A},\hat{B}]] = [\hat{B},[\hat{A},\hat{B}]] = 0$$

One has the identity

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-[\hat{A},\hat{B}]/2}$$

Now we assume that

$$\hat{A} = \frac{\beta t}{\sqrt{2}}\hat{x}, \qquad \hat{B} = -i\frac{\beta t}{\sqrt{2}}\frac{\hat{p}}{m\omega_o}$$

Note that

$$\hat{A} + \hat{B} = \frac{\beta t}{\sqrt{2}}(\hat{x} - \frac{i\hat{p}}{m\omega_o}) = \hat{a}^+ t$$

$$[\hat{A},\hat{B}] = [\frac{\beta t}{\sqrt{2}}\hat{x}, -i\frac{\beta t}{\sqrt{2}}\frac{\hat{p}}{m\omega_o}] = (\frac{\beta t}{\sqrt{2}})^2(\frac{-i}{m\omega_o})[\hat{x},\hat{p}] = \frac{t^2}{2}$$

$$e^{\hat{a}^+ t} = \exp[\frac{\beta t}{\sqrt{2}}(\hat{x} - \frac{i\hat{p}}{m\omega_0})]$$
$$= \exp(\frac{\beta t}{\sqrt{2}}\hat{x})\exp(-i\frac{\beta t}{\sqrt{2}}\frac{\hat{p}}{m\omega_o})\exp(-\frac{t^2}{4})$$

$$F(t,x) = \langle x|\exp(\hat{a}^{+}t)|0\rangle = \langle x|\exp(\frac{\beta t}{\sqrt{2}}\hat{x})\exp(-i\frac{\beta t}{\sqrt{2}}\frac{\hat{p}}{m\omega_o})\exp(-\frac{t^2}{4})|0\rangle$$
$$= \exp(-\frac{t^2}{4})\exp(\frac{\beta t}{\sqrt{2}}x)\langle x|\exp(-i\frac{\beta t}{\sqrt{2}}\frac{\hat{p}}{m\omega_o})|0\rangle$$
$$= \exp(-\frac{t^2}{4})\exp(\frac{\beta t}{\sqrt{2}}x)\left\langle x - \frac{t}{\sqrt{2}\beta}\middle|0\right\rangle$$

Note that the translation operator is defined by

$$\hat{T}_a = \exp(-\frac{i}{\hbar}\hat{p}a), \qquad \hat{T}a_x{}^{+}(a) = \exp(\frac{i}{\hbar}\hat{p}a),$$

$$\langle x|\hat{T}_a^{+}(a) = \langle x+a|,$$

with

$$a = -\frac{\beta t}{\sqrt{2}}\frac{\hbar}{m\omega_0} = -\frac{\beta t}{\sqrt{2}}\frac{1}{\beta^2} = -\frac{t}{\sqrt{2}\beta}.$$

Using the form of $\langle x|0\rangle$

$$F(t,x) = \exp(-\frac{t^2}{4})\exp(\frac{\beta t}{\sqrt{2}}x)\beta^{\frac{1}{2}}\pi^{-\frac{1}{4}}\exp[-\frac{1}{2}\beta^2(x-\frac{t}{\sqrt{2}\beta})^2]$$
$$= \beta^{\frac{1}{2}}\pi^{-\frac{1}{4}}\exp(-\frac{1}{2}\beta^2x^2 + \sqrt{2}t\beta x - \frac{1}{2}t^2)$$

Thus we have

$$F(t,x) = \sum_{n=0}^{\infty}\frac{t^n}{\sqrt{n!}}\varphi_n(x) = \beta^{\frac{1}{2}}\pi^{-\frac{1}{4}}\exp(-\frac{1}{2}\beta^2x^2 + \sqrt{2}t\beta x - \frac{1}{2}t^2),$$

Since

$$\varphi_n(\xi) = \beta^{-\frac{1}{2}}\varphi_n(x),$$

we have

$$\sum_{n=0}^{\infty}\frac{t^n}{\sqrt{n!}}\varphi_n(\xi) = \pi^{-\frac{1}{4}}\exp(-\frac{1}{2}\xi^2 + \sqrt{2}t\xi - \frac{1}{2}t^2) = K(t,x),$$

$K(t,x)$ is called the generating function of $\varphi_n(\xi)$.

Since

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

we get

$$\sum_{n=0}^{\infty} \frac{1}{n!} (\frac{t}{\sqrt{2}})^n H_n(\xi) = \exp(\sqrt{2}t\xi - \frac{1}{2}t^2).$$

When t is replaced by $\sqrt{2}t$, we have

$$\sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(\xi) = \exp(-t^2 + 2t\xi). \qquad \text{(generating function)}$$

18. 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

$$\begin{aligned} W_{class}(x)dx &= W_{class}(x)\omega x_M dt\sqrt{1-(\frac{x}{x_M})^2} \\ &= \frac{dt}{T} \\ &= \frac{\omega dt}{2\pi} \end{aligned}\ ,$$

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

$$\xi = \beta x,$$

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

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

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).

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

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

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

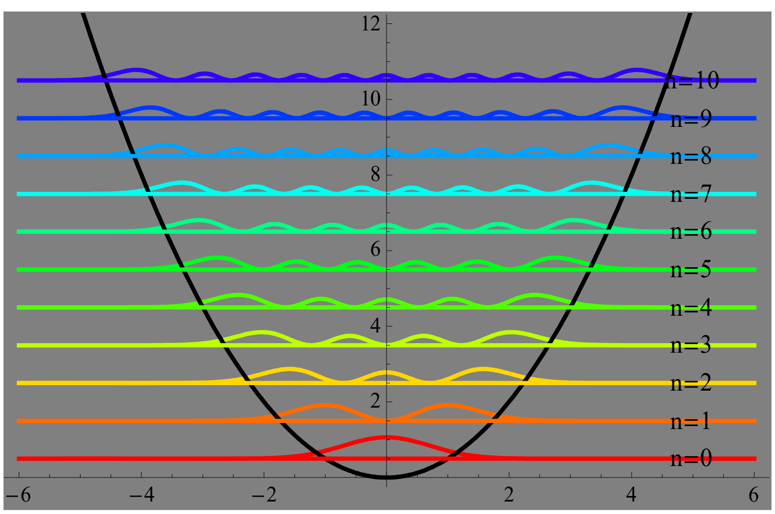
19. Mathematica-6

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

20. Mathematica-7



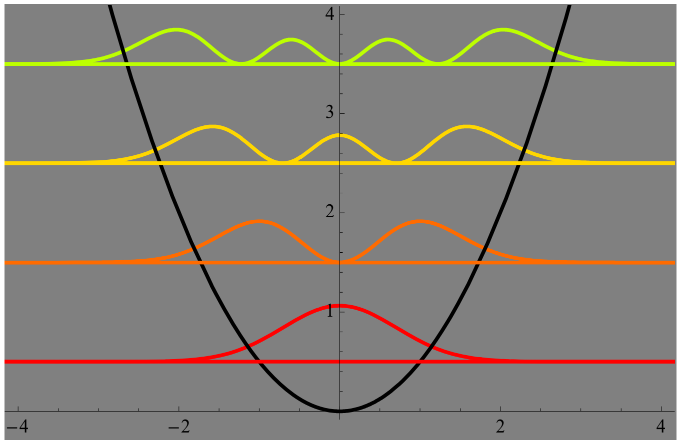


Fig. Energy eigenstate probability density function of the 1D harmonic oscillator. The horizontal axis is ξ $(=\beta x)$. The vertical axis is Energy E divided by $\hbar\omega$. The bottom line is at $E/\hbar\omega=(n+1/2)$ for the state n. The parabola denoted by black line is the potential energy $(=\xi^2/2)$. The wave functions penetrate into the regions that are not accessible according to the classical mechanics. The classical turning point is given by $\xi_M=\sqrt{2n+1}$.

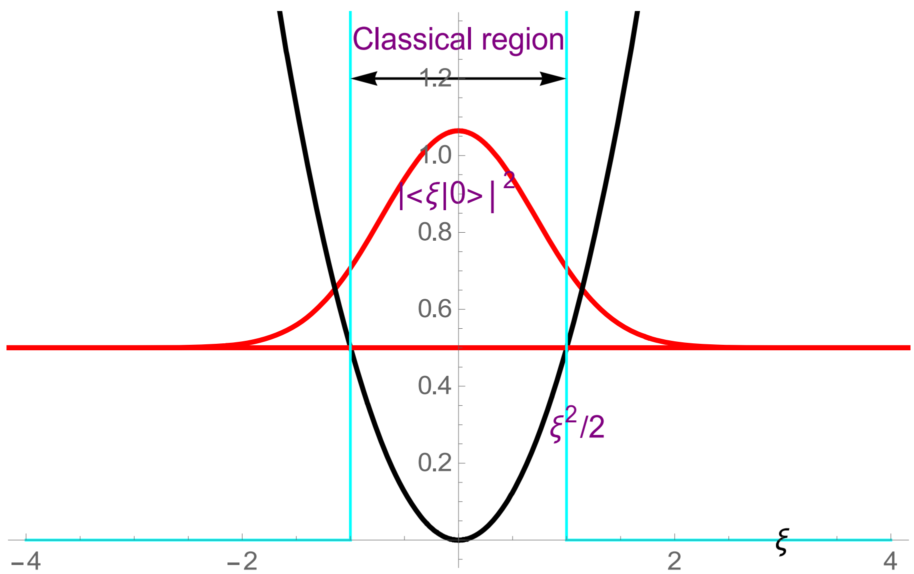
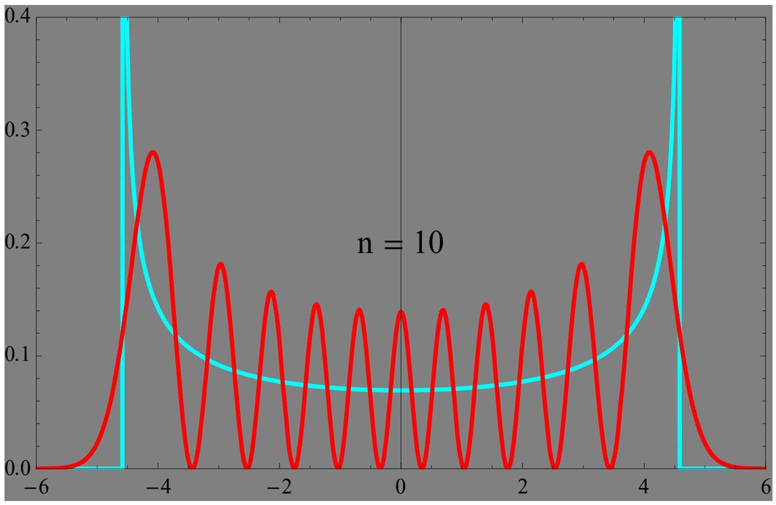


Fig. The ground state energy eigenstate probability density function of the 1D harmonic oscillator (denoted by $|\langle\xi|0\rangle|^2$ The horizontal axis is ξ $(=\beta x)$. The vertical axis is Energy E divided by $\hbar\omega$. The bottom line is at $E/\hbar\omega=1/2$ for the ground state. The parabola denoted by black line is the potential energy $(=\xi^2/2)$. The wave functions penetrate into the regions ($|\xi|>1$that are not accessible according to the classical mechanics. The classical turning point is given by $\xi_M = \pm\sqrt{2n+1} = \pm 1$ for $n = 0$.

21. Mathematica-8



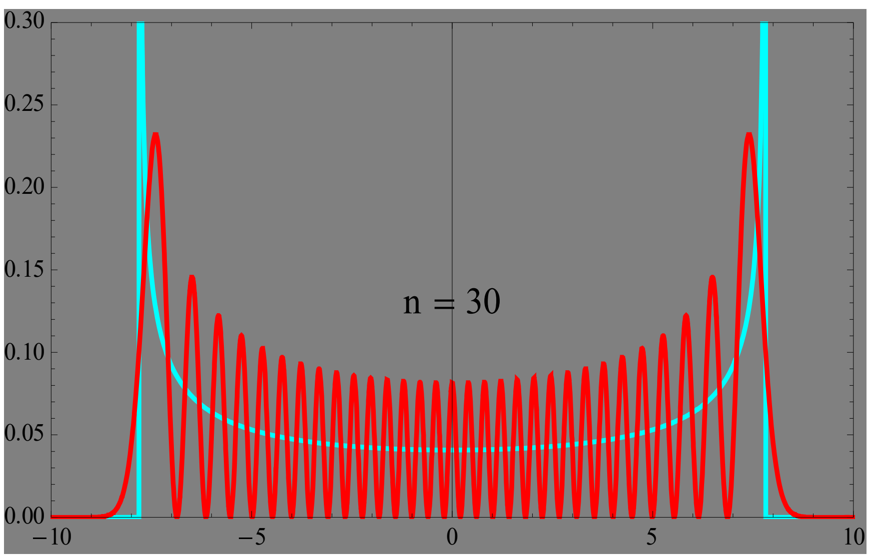


Fig. Probability density for the n = 30 state as a function of ξ. The classical probability distribution (denoted by blue line) peaks at the classical turning point. The region for $|\xi_M| > \sqrt{2n+1} = \sqrt{61} = 7.81$ is not allowed classically.

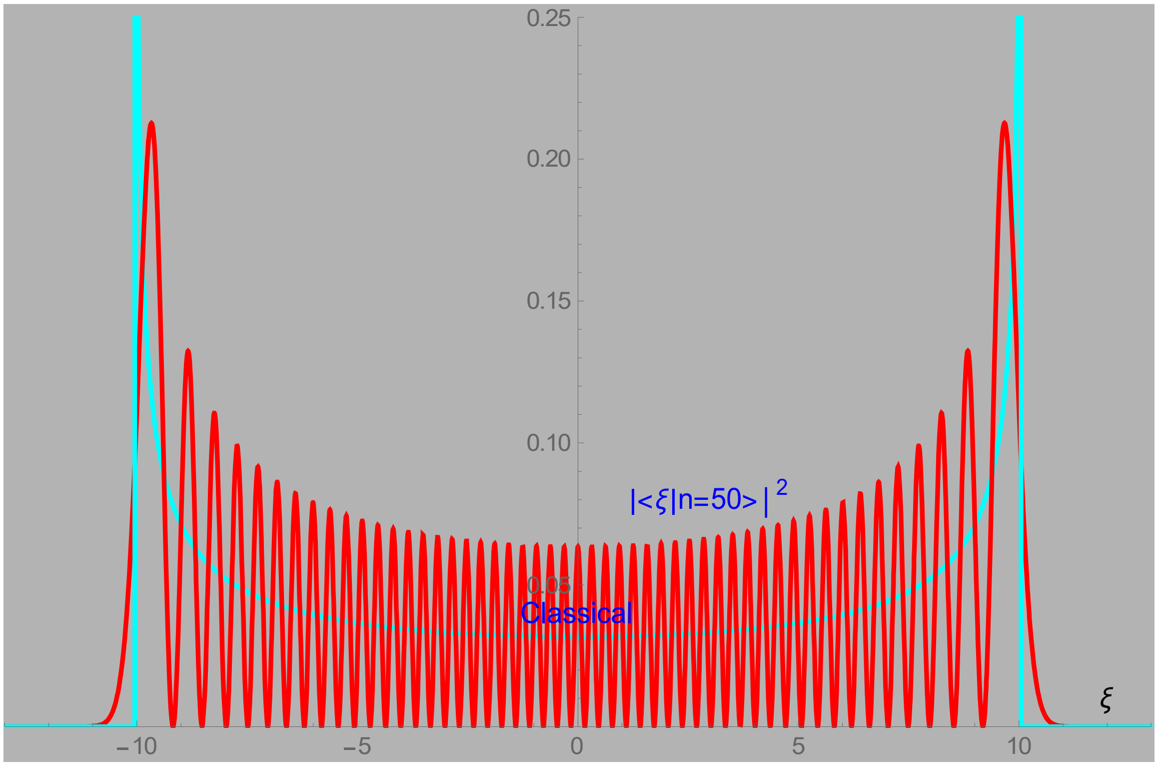


Fig. Probability density for the n = 50 state as a function of ξ. The classical probability distribution (denoted by blue line) peaks at the classical turning point. The region for $|\xi_M| > \sqrt{2n+1} = \sqrt{101} = 10.05$ is not allowed classically.

22. Differential equation (Series expansion method)

We start with the original differential equation for the simple harmonics.

$$\hat{H}|\psi\rangle = E|\psi\rangle,$$

or

$$[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_0{}^2x^2]\langle x|\psi\rangle = E|\psi\rangle.$$

We introduce

$$\xi = \beta x \qquad\qquad |x\rangle = \sqrt{\beta}|\xi\rangle$$

$$\langle\xi|\psi\rangle = \frac{1}{\sqrt{\beta}}\langle x|\psi\rangle$$

with

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}\,.$$

Then we get

$$[-\frac{\hbar^2}{2m}\beta^2\frac{d^2}{d\xi^2} + \frac{1}{2}m{\omega_0}^2\frac{\xi^2}{\beta^2}]\langle\xi|\psi\rangle = E\langle\xi|\psi\rangle$$

or

$$(\frac{d^2}{d\xi^2} - \xi^2)\langle\xi|\psi\rangle = -\frac{2mE}{\hbar^2\beta^2}\langle\xi|\psi\rangle = -\frac{2E}{\hbar\omega_0}\langle\xi|\psi\rangle$$

For simplicity we use

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

where

$$\varepsilon = \frac{E}{\hbar\omega_0}, \qquad \varphi(\xi) = \langle\xi|\psi\rangle\,.$$

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

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

from a physical point of view.

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

Now we set

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

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

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

((**Note**))

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

$$\begin{aligned}\frac{d^2}{d\xi^2}\varphi(\xi) &= -e^{-\frac{\xi^2}{2}} h(\xi) + \xi^2 e^{-\frac{\xi^2}{2}} h(\xi) - \xi e^{-\frac{\xi^2}{2}} \frac{d}{d\xi} h(\xi) \\ &\quad - \xi e^{-\frac{\xi^2}{2}} \frac{d}{d\xi} h(\xi) + e^{-\frac{\xi^2}{2}} \frac{d^2}{d\xi^2} h(\xi) \\ &= e^{-\frac{\xi^2}{2}} [-h(\xi) + \xi^2 h(\xi) - 2\xi\frac{d}{d\xi} h(\xi) + \frac{d^2}{d\xi^2} h(\xi)]\end{aligned}$$

Then we get

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

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

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

$h(\xi)$ 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 $a_0 \neq 0$.

[This expression is used by Cohen-Tannoudji et al. *Quantum Mechanics*, volume I and volume II (John Wiley & Sons, New York, 1977].

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

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

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

We note that

$$\sum_{m=0}^{\infty} a_{2m}(2m+p)(2m+p-1)\xi^{2m+p-2} = a_0 p(p-1)\xi^{p-2} + \sum_{m=1}^{\infty} a_{2m}(2m+p)(2m+p-1)\xi^{2m+p-2}$$

$$= a_0 p(p-1)\xi^{p-2} + \sum_{m=0}^{\infty} a_{2m+2}[2(m+1)+p][2(m+1)+p-1)\xi^{2(m+1)+p-2}$$

$$= a_0 p(p-1)\xi^{p-2} + \sum_{m=0}^{\infty} a_{2m+2}(2m+p+2)(2m+p+1)\xi^{2m+p}$$

Then Eq.(1) can be rewritten as

$$a_0 p(p-1)\xi^{p-2} + \sum_{m=0}^{\infty}[(2m+p+2)(2m+p+1)a_{2m+2} + (2\varepsilon - 1 - 4m - 2p)a_{2m}]\xi^{2m+p} = 0$$

The coefficient of ξ^{p-2} leads to

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

Then p = 0 or 1, since $a_0 \neq 0$.

....

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.

First we consider what happens when ε is not a half integer such that

$$2\varepsilon \neq 4m + 2p + 1 = 2(2m+p) + 1.$$

Then $a_{2m+2} \neq 0$, $a_{2m+4} \neq 0$,……. We note that

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

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

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

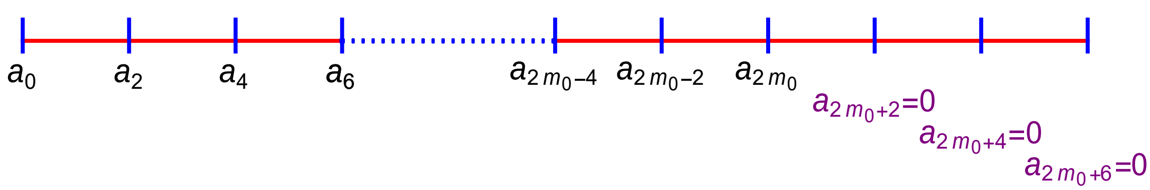
which become infinity when ξ tends to infinity. We must reject this solution. This solution makes no sense physically.

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

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

and

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



Thus we have

$$a_{2m_0+2}=-\frac{2\varepsilon-(4m_0+2p+1)}{(2m_0+p+1)(2m_0+p+2)}a_{2m0}=0,$$

where

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

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

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

where p = 0 or 1.

We consider the two cases.

(a) $p = 0$.

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

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) $p = 1$

$$a_{2m+2} = -\frac{2\varepsilon - (4m+3)}{(2m+2)(2m+3)} a_{2m} .$$

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

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

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

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

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

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

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

23. 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
```

$(-1+2\varepsilon)\, h[\xi] - 2\,\xi\, h'[\xi] + h''[\xi]$

```
Eq4=(-1+2 ε) h[ξ]-2 ξ h'[ξ]+h''[ξ]
```

$(-1+2\varepsilon)\, h[\xi] + h''[\xi] - 2\,\xi\, h'[\xi]$

$$f[x\_] := x^p \sum_{k=-2}^{2} a[2\,m + 2\,k]\, x^{2\,m+2\,k}$$

```
f[ξ] // Expand
```

$\xi^{2m+p}\, a[2m] + \xi^{-4+2m+p}\, a[-4+2m] + \xi^{-2+2m+p}\, a[-2+2m] + \xi^{2+2m+p}\, a[2+2m] + \xi^{4+2m+p}\, a[4+2m]$

```
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 :

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

```
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
```

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

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

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

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

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

24. Stationary wave function

Ground state ($n = 0$)

$\varepsilon = 1/2$

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

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

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

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

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

<u>$n = 1$ state</u>

$\varepsilon = 3/2$

$m_0 = 0, p = 1.$ $\{a_0 \neq 0\}$.

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

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

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

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

<u>$n = 2$ state</u>

$\varepsilon = 5/2$, or $E = \hbar\omega_0(2+\frac{1}{2})$

$m_0 = 1, p = 0.$ $\{a_0 \neq 0,\ a_2 \neq 0\}$

$$a_2 = -2a_0,$$

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

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

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

<u>$n = 3$ state</u>

$\varepsilon = 7/2$, or $E = \hbar\omega_0(3+\frac{1}{2})$

$m_0 = 1, p = 1.$ $\{a_0 \neq 0, a_2 \neq 0\}$,

$6a_2 + 4a_0 = 0$,

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

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

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

$n = 4$ state

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

$p = 0, m_0 = 2,$ $\{a_0 \neq 0, a_2 \neq 0, a_4 \neq 0\}$.

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

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

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

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

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

---

25 Characteristic length in the ground state

(a) Definition of the characteristic length

The operators $\hat{x}$ and $\hat{p}$ are defined by

$$\hat{x} = \frac{1}{\sqrt{2}\beta}\left(\hat{a} + \hat{a}^+\right) = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\hat{a} + \hat{a}^+\right),$$

$$\hat{p} = \frac{m\omega_0}{i\sqrt{2}\beta}(\hat{a} - \hat{a}^+),$$

with

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}} .$$

We now introduce a characteristic length *l*, given by

$$l = \sqrt{\frac{\hbar}{2m\omega_0}},$$

Then $\hat{x}$ and $\hat{p}$ can be rewritten as

$$\hat{x} = l(\hat{a} + \hat{a}^+),$$

$$\hat{p} = \frac{1}{i}\frac{\hbar}{2l}(\hat{a} - \hat{a}^+) = \frac{1}{i}\sigma_p(\hat{a} - \hat{a}^+),$$

where

$$\sigma_p = \frac{\hbar}{2l}.$$

We note that

$$\sigma_p l = \frac{\hbar}{2}.$$

We also note that

$$\hat{a} = \frac{\beta}{\sqrt{2}}(\hat{x} + \frac{i\hat{p}}{m\omega_0}) \Rightarrow \frac{1}{\sqrt{2}}(\xi + \frac{\partial}{\partial\xi}), \qquad \text{in the } |\xi\rangle \text{ representation}$$

$$\hat{a}^+ = \frac{\beta}{\sqrt{2}}(\hat{x} - \frac{i\hat{p}}{m\omega_0}) \Rightarrow \frac{1}{\sqrt{2}}(\xi - \frac{\partial}{\partial\xi}), \qquad \text{in the } |\xi\rangle \text{ representation}$$

where

$$\xi = \beta x. \qquad |\xi\rangle = \frac{1}{\sqrt{\beta}}|x\rangle .$$

(b) Property of the ground state

We start with

$$\hat{a}|0\rangle = \frac{\beta}{\sqrt{2}}(\hat{x} + \frac{i\hat{p}}{m\omega_0})|0\rangle = 0,$$

or

$$(x + \frac{\hbar}{m\omega_0}\frac{\partial}{\partial x})\langle x|0\rangle = 0.$$

Using $\xi = \beta x$ and $|x\rangle = \sqrt{\beta}|\xi\rangle$, we get

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

The solution of this differential equation is

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

The constant A can be deterimined from the normalization condition,

$$\langle 0|0\rangle = 1 = \int_{-\infty}^{\infty}\langle 0|\xi\rangle\langle \xi|0\rangle d\xi = |A|^2\int_{-\infty}^{\infty}\exp(-\xi^2)d\xi = |A|^2\sqrt{\pi},$$

or

$$A = \frac{1}{\pi^{1/4}}.$$

Then we get

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

or

$$\langle x|0\rangle = \sqrt{\beta}\langle \xi|0\rangle = \frac{1}{\pi^{1/4}}\sqrt{\frac{m\omega_0}{\hbar}}\exp(-\frac{m\omega_0 x^2}{2\hbar}).$$

Using the characteristic length l,

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

where

$$2l^2 = \frac{\hbar}{m\omega_0}, \quad \text{or} \quad l = \sqrt{\frac{\hbar}{2m\omega_0}}.$$

The probability is given by the normal distribution

$$P_0(x) = \left|\langle x|0\rangle\right|^2 = \frac{1}{\sqrt{2\pi}l}\exp(-\frac{x^2}{2l^2}),$$

with the standard deviation of the position

$$\sigma_x = l.$$

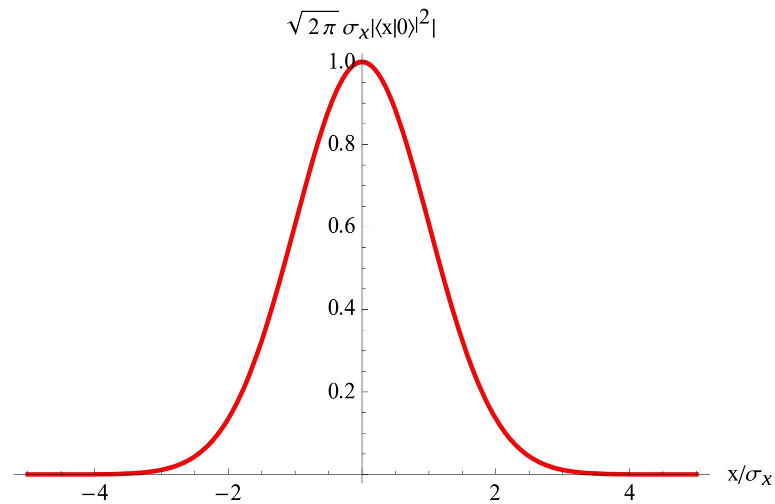


Fig. Normal distribution. $(2\pi)^{1/2}\sigma_x\left|\langle x|0\rangle\right|^2$ vs x/σ_x. $\sigma_x = l = \sqrt{\frac{\hbar}{2m\omega_0}}$

The momentum representation of the wave function can be derived from the Fourier transform as

$$\begin{aligned}\langle p|0\rangle &= \int \langle p|x\rangle\langle x|0\rangle dx \\ &= \frac{1}{\sqrt{2\pi\hbar}}\frac{1}{(2\pi l^2)^{1/4}}\int_{-\infty}^{\infty}\exp(-\frac{i}{\hbar}px)\exp(-\frac{x^2}{4l^2})dx \\ &= \frac{1}{\sqrt{2\pi\hbar}}\frac{1}{(2\pi l^2)^{1/4}}2l\sqrt{\pi}\exp(-\frac{l^2p^2}{\hbar^2}) \\ &= \frac{1}{(2\pi)^{1/4}\sqrt{\sigma_p}}\exp(-\frac{p^2}{4\sigma_p{}^2})\end{aligned}$$

where σ_p is the standard deviation of the linear momentum,

$$\sigma_p = \frac{\hbar}{2l}.$$

Then the probability is given by the normal distribution

$$\left|\langle p|0\rangle\right|^2 = \frac{1}{(2\pi)^{1/2}\sigma_p}\exp(-\frac{p^2}{2\sigma_p{}^2}).$$

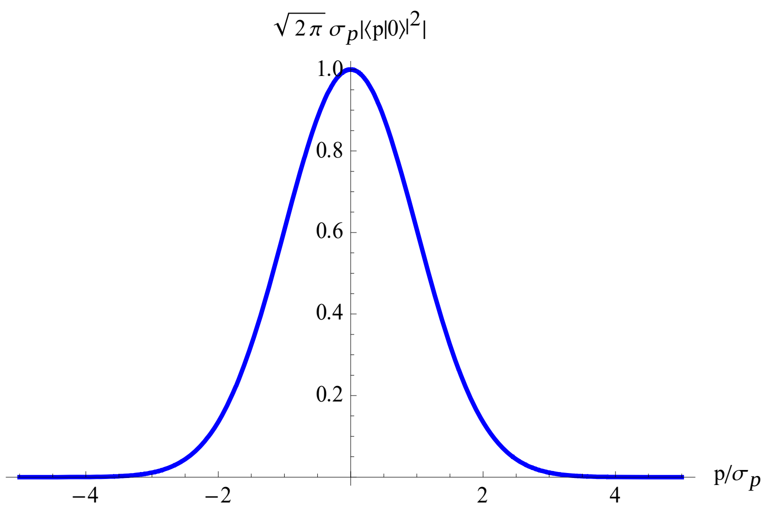


Fig. Normal distribution. $(2\pi)^{1/2}\sigma_p\left|\langle p|0\rangle\right|^2$ vs p/σ_p. $\sigma_p = \frac{\hbar}{2l}$.

We note that

$$\sigma_p\sigma_x = \frac{\hbar}{2l}l = \frac{\hbar}{2},$$

which is consistent with the Heisenberg uncertainty principle.

(c) Expectation and fluctuation

$$\langle n|\hat{x}|n\rangle = l\langle n|\hat{a}^+ + \hat{a}|n\rangle = 0$$

$$\begin{aligned}\langle n|\hat{x}^2|n\rangle &= l^2\langle n|(\hat{a}^+ + \hat{a})^2|n\rangle \\ &= l^2\langle n|\hat{a}^+\hat{a}^+ + \hat{a}\hat{a} + \hat{a}\hat{a}^+ + \hat{a}^+\hat{a}|n\rangle \\ &= l^2\langle n|2\hat{a}^+\hat{a} + \hat{1}|n\rangle \\ &= {\sigma_x}^2(2n+1) = l^2(2n+1)\end{aligned}$$

$$\langle n|\hat{p}|n\rangle = -i\sigma_p\langle n|\hat{a} - \hat{a}^+|n\rangle = 0$$

$$\begin{aligned}\langle n|\hat{p}^2|n\rangle &= -\sigma_p^2\langle n|(\hat{a} - \hat{a}^+)^2|n\rangle \\ &= -\sigma_p^2\langle n|\hat{a}^+\hat{a}^+ + \hat{a}\hat{a} - \hat{a}\hat{a}^+ - \hat{a}^+\hat{a}|n\rangle \\ &= \sigma_p^2\langle n|2\hat{a}^+\hat{a} + \hat{1}|n\rangle \\ &= \sigma_p^2(2n+1) = (2n+1)\frac{\hbar^2}{4l^2}\end{aligned}$$

since

$$\hat{p} = \frac{1}{i}\sigma_p(\hat{a} - \hat{a}^+), \qquad \hat{x} = l(\hat{a} + \hat{a}^+),$$

with

$$\sigma_p = \frac{\hbar}{2l}, \qquad \sigma_x = l.$$

Then we have the uncertainties of the position and momentum as

$$\Delta x = \sqrt{\langle n|\hat{x}^2|n\rangle} = l\sqrt{2n+1},$$

$$\Delta p = \sqrt{\langle n|\hat{p}^2|n\rangle} = \frac{\hbar}{2l}\sqrt{2n+1},$$

and the product $\Delta x\Delta p$ as

$$\Delta x\Delta p = \frac{\hbar}{2}(2n+1).$$

The expectation value of the Hamiltonian $\hat{H}$

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

is given by

$$\begin{aligned}
\langle n|\hat{H}|n\rangle &= \frac{1}{2m}(2n+1)\sigma_p^2 + \frac{1}{2} m\omega_0{}^2 \sigma_x{}^2 (2n+1) \\
&= (2n+1)[\frac{1}{2m}\sigma_p^2 + \frac{1}{2} m\omega_0{}^2 \sigma_x{}^2] \\
&= (2n+1)[\frac{\hbar^2}{2m}\frac{1}{4l^2} + \frac{1}{2} m\omega_0{}^2 l^2] \\
&= \frac{1}{2}\hbar\omega_0 (2n+1)
\end{aligned}$$

(d) Dynamics of oscillators

$$|\psi(t=0)\rangle = \sum_n a_n |n\rangle ,$$

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(t=0)\rangle = \sum_n a_n e^{-i\hat{H}t/\hbar} |n\rangle = \sum_n a_n e^{-i\omega_0 (n+1/2)t} |n\rangle .$$

We calculate the expectation;

$$\begin{aligned}
\langle \psi(t)|\hat{x}|\psi(t)\rangle &= \sum_{n,m} a_n{}^* e^{i\omega_0 (n+1/2)t} a_m e^{-i\omega_0 (m+1/2)t} \langle n|\hat{x}|m\rangle \\
&= \sum_{n,m} e^{i\omega_0 (n-m)t} a_n{}^* a_m \langle n|\hat{x}|m\rangle
\end{aligned}$$

Here we note that

$$\begin{aligned}
\langle n|\hat{x}|m\rangle &= l\langle n|\hat{a} + \hat{a}^+|m\rangle \\
&= l\sqrt{m}\langle n|m-1\rangle + l\sqrt{m+1}\langle n|m+1\rangle \\
&= l\sqrt{m}\delta_{n,m-1} + l\sqrt{m+1}\delta_{n,m+1}
\end{aligned}$$

since

$$\hat{x} = l\left(\hat{a} + \hat{a}^+\right).$$

Then we get

$$\langle\psi(t)|\hat{x}|\psi(t)\rangle = l\sum_{n,m} e^{i\omega_0(n-m)t} a_n{}^* a_m (\sqrt{m}\delta_{n,m-1} + \sqrt{m+1}\delta_{n,m+1})$$

$$= l\sum_n (e^{-i\omega_0 t}\sqrt{n+1} a_n{}^* a_{n+1} + e^{i\omega_0 t}\sqrt{n} a_n{}^* a_{n-1})$$

$$= l\sum_n \sqrt{n}(e^{-i\omega_0 t} a_{n-1}{}^* a_n + e^{i\omega_0 t} a_n{}^* a_{n-1})$$

We put

$$l\sqrt{n} a_{n-1}{}^* a_n = x_n e^{-i\phi_n} .$$

Then

$$\langle\psi(t)|\hat{x}|\psi(t)\rangle = \sum_n x_n (e^{-i\omega_0 t} e^{-i\phi_n} + e^{i\omega_0 t} e^{i\phi_n})$$

$$= 2\sum_n x_n \cos(\omega_0 t + \phi_n)$$

This is the sinusoidal oscillation with the angular frequency ω_0.

26. 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

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

27. Simple harmonics: momentum space

(a) Dimensionless variables: $\xi = \beta x$ and $\kappa = \frac{k}{\beta} = \frac{p}{\hbar \beta}$

$$\xi = \beta x, \qquad p = \hbar k, \qquad \kappa = \frac{k}{\beta} = \frac{p}{\hbar \beta}$$

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

(b) Transformation function: $\langle \xi | \kappa \rangle == \frac{1}{\sqrt{2\pi}} e^{i\kappa\xi}$

$$\langle x | p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}} ,$$

$$\langle x|k\rangle = \sqrt{\hbar}\langle x|p\rangle = \frac{1}{\sqrt{2\pi}}e^{ikx},$$

$$\langle x|p\rangle = \sqrt{\frac{\beta}{\hbar}}\langle \xi|k\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ipx}{\hbar}},$$

$$\langle \xi|\kappa\rangle = \frac{\sqrt{\hbar\beta}}{\sqrt{\beta}}\langle x|p\rangle = \sqrt{\hbar}\frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ipx}{\hbar}} = \frac{1}{\sqrt{2\pi}}e^{i\kappa\xi}.$$

(c) The Fourier transform; $\langle \kappa|n\rangle$

The Fourier transform is defined by

$$\varphi_n(\kappa) = \langle \kappa|n\rangle = \int \langle \kappa|\xi\rangle\langle \xi|n\rangle d\xi = \int \frac{1}{\sqrt{2\pi}}e^{-i\kappa\xi}\langle \xi|n\rangle d\xi.$$

So $\langle \kappa|n\rangle$ is the Fourier transform of $\langle \xi|n\rangle$ (dimensionless). We note that

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

(d) Creation operator $\hat{a}^+$ and annihilation operator $\hat{a}$

The creation operator and the annihilation operator are given by

$$\hat{a} = \frac{\beta}{\sqrt{2}}(x + \frac{i\hat{p}}{m\omega_0}) = \frac{1}{\sqrt{2}}(\hat{\xi} + i\hat{\kappa}),$$

$$\hat{a}^+ = \frac{\beta}{\sqrt{2}}(x - \frac{i\hat{p}}{m\omega_0}) = \frac{1}{\sqrt{2}}(\hat{\xi} - i\hat{\kappa}).$$

28. Relations $-i\frac{\partial}{\partial\xi}\langle \xi|n\rangle = \langle \xi|\hat{\kappa}|n\rangle$ and $i\frac{\partial}{\partial\kappa}\langle \kappa|n\rangle = \langle \kappa|\hat{\xi}|n\rangle$

(a) $$-i\frac{\partial}{\partial\xi}\langle \xi|n\rangle = \langle \xi|\hat{\kappa}|n\rangle$$

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

where

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

We now calculate

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

or

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

(b) $$i\frac{\partial}{\partial\kappa}\langle\kappa|n\rangle = \langle\kappa|\hat{\xi}|n\rangle$$

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

where

$$\langle\kappa|\xi\rangle = \langle\xi|\kappa\rangle^* = \frac{1}{\sqrt{2\pi}} e^{-i\kappa\xi}.$$

We now calculate

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

or

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

29. Fourier transform of $\langle\xi|n\rangle$

$$\langle\xi|0\rangle = \pi^{-\frac{1}{4}} e^{-\frac{\xi^2}{2}},$$

$$\langle\kappa|0\rangle = \int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi}}e^{-i\kappa\xi}\langle\xi|0\rangle d\xi = \int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi}}e^{-i\kappa\xi}\pi^{-\frac{1}{4}}e^{-\frac{\xi^2}{2}}d\xi .$$

Note that

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

Then we get

$$\langle\kappa|0\rangle = \frac{\pi^{-\frac{1}{4}}e^{-\frac{\kappa^2}{2}}}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2}(\xi+i\kappa)^2} d\xi = \pi^{-\frac{1}{4}}e^{-\frac{\kappa^2}{2}}.$$

where

$$\int_{-\infty}^{\infty} e^{-\frac{1}{2}(\xi+i\kappa)^2} d\xi = \sqrt{2\pi} .$$

So we have

$$\varphi_0(\kappa) = (-i)^0\varphi_0(\xi)|_{\xi=\kappa} = \varphi_0(\xi)|_{\xi=\kappa}.$$

In general we have the following relations.

$$\varphi_n(\kappa) = (-i)^n\varphi_n(\xi)|_{\xi=\kappa},$$

$$|\varphi_n(\kappa)|^2 = |\varphi_n(\xi)|^2|_{\xi=\kappa}.$$

We show that $\varphi_n(\kappa)$ satisfies the same differential equation for $\varphi_n(\xi)$.

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

with

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

Then we have

$$\frac{d^2\varphi_n(\kappa)}{d\kappa^2} = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}}(-\xi^2)e^{-i\kappa\xi}\varphi_n(\xi)d\xi \,. \qquad (1)$$

We note that $\varphi_n(\xi)$ satisfies the differential equation.

$$(\frac{d^2}{d\xi^2} - \xi^2 + 2n + 1)\varphi_n(\xi) = 0.$$

Taking the Fourier transform of this differential equation,

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

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

Then

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-i\kappa\xi}(\frac{d^2}{d\xi^2} - \xi^2 + 2n + 1)\varphi_n(\xi)d\xi = (\frac{d^2}{d\kappa^2} - \kappa^2 + 2n + 1)\varphi_n(\kappa) = 0$$

or

$$(\frac{d^2}{d\kappa^2} - \kappa^2 + 2n + 1)\varphi_n(\kappa) = 0 \, ,$$

$\varphi_n(\kappa)$ satisfies the same differential equation as $\varphi_n(\xi)$.

30 The form of the Fourier transform: $\langle\kappa|n\rangle$

Here we show that

$$\langle\kappa|n\rangle = (-i)^n \langle\xi|n\rangle|_{\xi=\kappa} \, .$$

In other words, the form of $\langle \kappa | n \rangle$ is essentially the same as the form of $\langle \xi | n \rangle$, except for the factor $(-i)^n$.

((**Proof**))

$$\begin{aligned}
\langle \xi | n \rangle &= \frac{1}{\sqrt{n!}} \langle \xi | (\hat{a}^+)^n | 0 \rangle \\
&= \frac{1}{\sqrt{2^n n!}} \langle \xi | (\hat{\xi} - i\hat{\kappa})^n | 0 \rangle \\
&= \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} (\xi - \frac{\partial}{\partial \xi})^n e^{-\xi^2/2}
\end{aligned}$$

Similarly,

$$\begin{aligned}
\langle \kappa | n \rangle &= \frac{1}{\sqrt{n!}} \langle \kappa | (\hat{a}^+)^n | 0 \rangle \\
&= \frac{1}{\sqrt{2^n n!}} \langle \kappa | (\hat{\xi} - i\hat{\kappa})^n | 0 \rangle \\
&= \frac{1}{\sqrt{2^n n!}} (i\frac{\partial}{\partial \kappa} - i\kappa)^n \langle \kappa | 0 \rangle \\
&= \frac{1}{\sqrt{2^n n!}} (-i)^n (\kappa - \frac{\partial}{\partial \kappa})^n \langle \kappa | 0 \rangle \\
&= (-i)^n \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} (\kappa - \frac{\partial}{\partial \kappa})^n e^{-\frac{\kappa^2}{2}} \\
&= (-i)^n \langle \xi | n \rangle |_{\xi = \kappa}
\end{aligned}$$

where

$$\langle \kappa | 0 \rangle = \pi^{-\frac{1}{4}} e^{-\frac{\kappa^2}{2}}$$

31. Mathematica-10

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

Prepend[
  Table[
   {n, FourierTransform[φ[n, ξ], ξ, κ, FourierParameters → {0, -1}],
     (-ⅈ)^n φ[n, κ]} // Simplify, {n, 0, 4}],
  {"n", "φ[n,κ]", "(-i)^nφ[n,ξ=κ]"}] // TableForm
```

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

32. Classical probability density in the κ spane

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

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

where

$$p_M = m x_M \omega .$$

Noting that

$$\frac{dp}{dt} = -p_M \omega \sin(\omega t).$$

the probability density is given by

$$W(p)dp = W(\kappa)d\kappa = \frac{dt}{T} = \frac{1}{T}\frac{dp}{p_M \omega |\sin(\omega t)|} = \frac{dp}{2\pi p_M |\sin(\omega t)|}.$$

Taking into account of the factor 2 for the probability correction, we have

$$W(\kappa)d\kappa = \frac{dp}{\pi\sqrt{{p_M}^2 - p^2}} = \frac{d\kappa}{\pi\sqrt{{\kappa_M}^2 - \kappa^2}},$$

where

$$\kappa_M = \sqrt{2n+1} .$$

Thus we get

$$W(\kappa) = \frac{1}{\pi\sqrt{(2n+1)-\kappa^2}} ,$$

which has the same form as

$$W(\kappa) = W(\xi)|_{\xi=\kappa}$$

33. Wave packet of simple harmonics

(L.I. Schiff, Quantum mechanics, p.67-68)

$$\begin{aligned}\langle x|\psi(t)\rangle &= \langle x|\exp(-\frac{i}{\hbar}\hat{H}t)|\psi(t=0)\rangle \\ &= \int \langle x|\exp(-\frac{i}{\hbar}\hat{H}t)|x'\rangle\langle x'|\psi(t=0)\rangle dx'\end{aligned}$$

We define the kernel $K(x,x',t)$ as

$$\begin{aligned}K(x,x',t) &= \langle x|\exp(-\frac{i}{\hbar}\hat{H}t)|x'\rangle \\ &= \sum_n \langle x|n\rangle \exp(-\frac{i}{\hbar}E_n t)\langle n|x'\rangle \\ &= \sum_n \exp(-\frac{i}{\hbar}E_n t)\varphi_n(x)\varphi_n^*(x')\end{aligned}$$

Note that

$$\xi = \beta x ,$$

with

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}} .$$

Then we have

$$\psi(x,t) = \sum_n \exp(-\frac{i}{\hbar}E_n t)\int dx'\varphi_n^*(x')\psi(x')\varphi_n(x).$$

We assume that

$$\psi(x) = \frac{\beta^{1/2}}{\pi^{1/4}}\exp[-\frac{1}{2}\beta^2(x-a)^2],$$

or

$$\varphi_n(\xi) = \langle \xi | n \rangle = \frac{1}{\sqrt{\beta}}\langle x | n \rangle = \frac{1}{\sqrt{\beta}}\varphi_n(x),$$

or

$$\varphi(\xi) = \frac{1}{\pi^{1/4}}\exp[-\frac{1}{2}(\xi-\xi_0)^2],$$

with

$$\xi_0 = \beta x_0 .$$

We need to calculate the integral defined by

$$\begin{aligned}
I &= \int dx'\varphi_n^*(x')\psi(x') \\
&= \int dx'\varphi_n^*(x')\frac{\beta^{1/2}}{\pi^{1/4}}\exp[-\frac{1}{2}\beta^2(x'-a)^2] \\
&= \int \frac{d\xi}{\beta}\beta^{1/2}\varphi_n^*(\xi)\frac{\beta^{1/2}}{\pi^{1/4}}\exp[-\frac{1}{2}(\xi-\xi_0)^2] \\
&= \frac{1}{\pi^{1/4}}\int d\xi\varphi_n^*(\xi)\exp[-\frac{1}{2}(\xi-\xi_0)^2]
\end{aligned}$$

Here

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

Then we get

$$I = \frac{1}{\pi^{1/4}}(\sqrt{\pi}2^n n!)^{-\frac{1}{2}}\int d\xi \exp(-\frac{\xi^2}{2})H_n(\xi)\exp[-\frac{1}{2}(\xi-\xi_0)^2]).$$

Here we use the generating function:

$$\exp(2s\xi - s^2) = \sum_{n=0}^{\infty} \frac{s^n}{n!} H_n(\xi)$$

Note that

$$\int_{-\infty}^{\infty} d\xi \exp(2s\xi - s^2)\exp(-\frac{\xi^2}{2})\exp[-\frac{1}{2}(\xi-\xi_0)^2] = \sum_{n=0}^{\infty}\int_{-\infty}^{\infty} d\xi \frac{s^n}{n!} H_n(\xi)\exp(-\frac{\xi^2}{2})\exp[-\frac{1}{2}(\xi-\xi_0)^2]$$
$$= \sum_{n=0}^{\infty}\int_{-\infty}^{\infty} d\xi \frac{s^n}{n!} H_n(\xi)\exp[-(\xi^2 - \xi_0\xi + \frac{1}{2}\xi_0^{\ 2})]$$

The left-hand side is

$$\int_{-\infty}^{\infty} d\xi \exp(2s\xi - s^2)\exp[-(\xi^2 - \xi_0\xi + \frac{1}{2}\xi_0^{\ 2})] = \pi^{1/2}\exp(s\xi_0 - \frac{\xi_0^{\ 2}}{4})$$
$$= \pi^{1/2}\exp(-\frac{\xi_0^{\ 2}}{4})\sum_{n=0}^{\infty}\frac{s^n \xi_0^{\ n}}{n!}$$

Thus we have

$$\pi^{1/2}\exp(-\frac{\xi_0^{\ 2}}{4})\sum_{n=0}^{\infty}\frac{s^n \xi_0^{\ n}}{n!} = \sum_{n=0}^{\infty}\int_{-\infty}^{\infty} d\xi \frac{s^n}{n!} H_n(\xi)\exp[-(\xi^2 - \xi_0\xi + \frac{1}{2}\xi_0^{\ 2})]$$

or

$$\pi^{1/2}\exp(-\frac{\xi_0^{\ 2}}{4})\xi_0^{\ n} = \int_{-\infty}^{\infty} d\xi H_n(\xi)\exp[-(\xi^2 - \xi_0\xi + \frac{1}{2}\xi_0^{\ 2})]$$

Then

$$I = (\sqrt{\pi}2^n n!)^{-\frac{1}{2}}\exp(-\frac{\xi_0^{\ 2}}{4})\xi_0^{\ n}$$

Then

$$\psi(x,t) = \sum_n \exp(-\frac{i}{\hbar}E_n t)(2^n n!)^{-\frac{1}{2}}\exp(-\frac{\xi_0^{\ 2}}{4})\xi_0^{\ n}\varphi_n(x)$$

Since

$$E_n = \hbar\omega_0(n+\frac{1}{2}),$$

or

$$\exp(-\frac{i}{\hbar}E_n t) = \exp(-\frac{i}{2}\omega_0 t - in\omega_0 t),$$

and

$$\psi(\xi,t) = \frac{1}{\sqrt{\beta}}\psi(x,t),$$

we get

$$\psi(\xi,t) = \sum_{n=0}^{\infty}(2^n n!)^{-\frac{1}{2}}\exp(-\frac{\xi_0^{\ 2}}{4})(\xi_0 e^{-i\omega_0 t})^n \exp(-\frac{i}{2}\omega_0 t)\varphi_n(\xi),$$

or

$$\psi(\xi,t) = \frac{1}{\pi^{1/4}}\sum_{n=0}^{\infty}(2^n n!)^{-1}\exp(-\frac{\xi_0^{\ 2}}{4})(\xi_0 e^{-i\omega_0 t})^n \exp(-\frac{i}{2}\omega_0 t)e^{-\frac{\xi^2}{2}}H_n(\xi)$$

$$= \frac{1}{\pi^{1/4}}\exp(-\frac{\xi_0^{\ 2}}{4} - \frac{i}{2}\omega_0 t - -\frac{\xi^2}{2})\sum_{n=0}^{\infty}\frac{1}{n!}(\frac{\xi_0 e^{-i\omega_0 t}}{2})^n H_n(\xi)$$

Using the generating function

$$\sum_{n=0}^{\infty}\frac{1}{n!}(\frac{\xi_0 e^{-i\omega_0 t}}{2})^n H_n(\xi) = \exp[-\frac{1}{4}\xi_0^{\ 2}e^{-2in\omega_0 t} + \xi_0 e^{-i\omega_0 t}\xi],$$

we have the final form

$$\psi(\xi,t) = \frac{1}{\pi^{1/4}}\exp(-\frac{\xi_0^{\ 2}}{4} - \frac{\xi^2}{2} - \frac{i}{2}\omega_0 t - \frac{1}{4}\xi_0^{\ 2}e^{-2i\omega_0 t} + \xi_0\xi e^{-i\omega_0 t})$$

$$\psi(\xi,t) = \frac{1}{\pi^{1/4}}\exp[-\frac{\xi_0^{\ 2}}{4} - \frac{\xi^2}{2} - \frac{i}{2}\omega_0 t - \frac{1}{4}\xi_0^{\ 2}(\cos 2\omega_0 t - i\sin 2\omega_0 t)$$

$$+ \xi_0\xi(\cos\omega_0 t - i\sin\omega_0 t)]$$

$$\left|\psi(\xi,t)\right|^2 = \frac{1}{\pi^{1/2}}\exp[-\frac{\xi_0^{\ 2}}{2} - \xi^2 - \frac{1}{2}\xi_0^{\ 2}\cos 2\omega_0 t + 2\xi_0\xi\cos\omega_0 t]$$

or

$$|\psi(\xi,t)|^2 = \frac{1}{\pi^{1/2}}\exp[-(\xi-\xi_0\cos\omega_0 t)^2]$$

$|\psi(\xi,t)|^2$ represents a wave packet that oscillates without change of shape about $\xi = 0$ with amplitude ξ_0 and angular frequency ω_0.

34. Mathematica-11

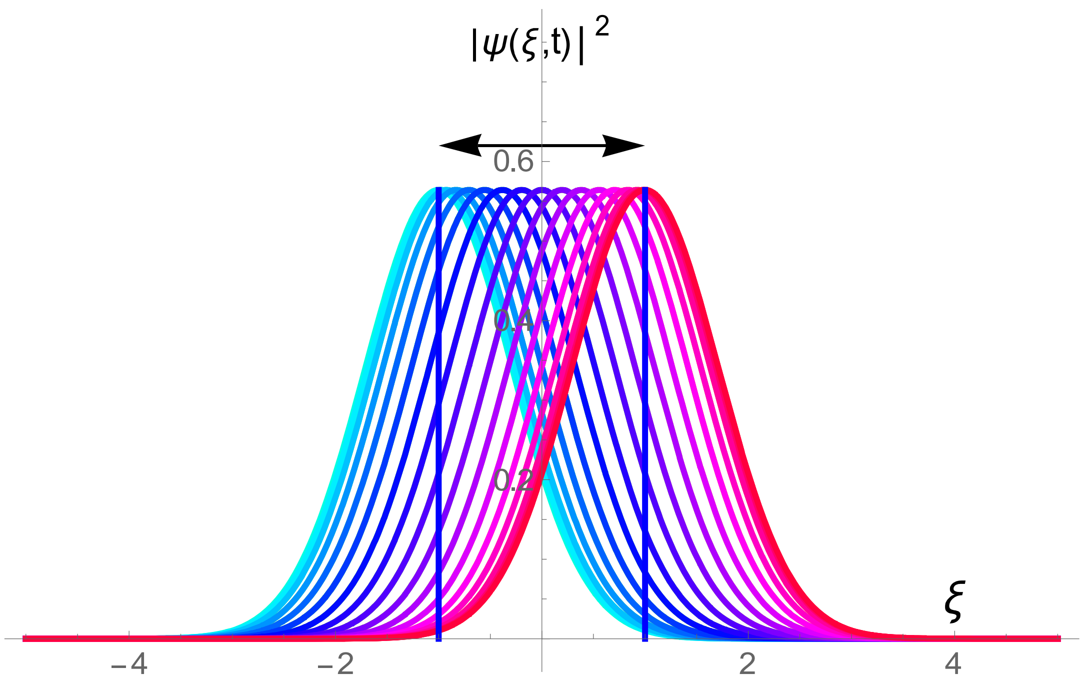

Fig. The time dependence of $|\psi(\xi,t)|^2 = \frac{1}{\pi^{1/2}}\exp[-(\xi-\xi_0\cos\omega_0 t)^2]$, where ξ_0=1. $T = 2\pi/\omega_0$. The peak shifts from ξ = 0 at t = 0 to ξ = 0 at t = T/4, ξ = ξ_0 at t = T/2, ξ = - ξ_0 at t = 3T/4, and ξ = 0 at t = T.

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35. Application of Schrӧdinger and Heisenberg pictures

Simple harmonics

$$\hat{U} = e^{-\frac{i}{\hbar}\hat{H}t}.$$

The operator in the Heisenberg picture is defined by

$$\hat{A}_H = \hat{U}^+ \hat{A}_s \hat{U} = e^{\frac{i}{\hbar}\hat{H}t} \hat{A}_s e^{-\frac{i}{\hbar}\hat{H}t},$$

where $\hat{H}$ is the Hamiltonian

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

Using the equation of Heisenberg picture, we obtain

$$\hat{x}_H = \hat{x}\cos\omega_0 t + \frac{1}{m\omega_0}\hat{p}\sin\omega_0 t,$$

and

$$\hat{p}_H = \hat{p}\cos\omega_0 t - m\omega_0 \hat{x}\sin\omega_0 t.$$

The matrix of $\hat{x}$ and $\hat{p}$ are given by

$$\hat{x} = \frac{1}{\sqrt{2}\beta}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix}$$

and

$$\hat{p} = \frac{m\omega_0}{\sqrt{2}i\beta}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ -\sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & -\sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & -\sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix}$$

((**Discussion**))

What are the expectation values $\langle\psi(t)|\hat{x}|\psi(t)\rangle$ and $\langle\psi(t)|\hat{p}|\psi(t)\rangle$?

$$\langle\psi(t)|\hat{x}|\psi(t)\rangle = \langle\psi(0)|\hat{x}_H|\psi(0)\rangle$$
$$= \langle\psi(0)|\hat{x}\cos\omega_0 t + \frac{1}{m\omega_0}\hat{p}\sin\omega_0 t|\psi(0)\rangle$$
$$= \langle\psi(0)|\hat{x}|\psi(0)\rangle\cos\omega_0 t + \frac{1}{m\omega_0}\langle\psi(0)|\hat{p}|\psi(0)\rangle\sin\omega_0 t$$

$$\langle\psi(t)|\hat{p}|\psi(t)\rangle = \langle\psi(0)|\hat{p}_H|\psi(0)\rangle$$
$$= \langle\psi(0)|\hat{p}\cos\omega_0 t - m\omega_0\hat{x}\sin\omega_0 t|\psi(0)\rangle$$
$$= \langle\psi(0)|\hat{p}|\psi(0)\rangle\cos\omega_0 t - m\omega_0\langle\psi(0)|\hat{x}|\psi(0)\rangle\sin\omega_0 t$$

Suppose that

(1) $$|\psi(0)\rangle = \frac{1}{\sqrt{6}}(|0\rangle + 2|1\rangle + |2\rangle)$$

we can calculate the matrix elements $\langle\psi(0)|\hat{x}|\psi(0)\rangle$ and $\langle\psi(0)|\hat{p}|\psi(0)\rangle$ as follows.

$$\langle\psi(0)|\hat{x}|\psi(0)\rangle = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{pmatrix} \frac{1}{\sqrt{2}\beta} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{pmatrix}$$
$$= \frac{1}{\sqrt{2}\beta}\frac{2}{3}(1+\sqrt{2})$$

$$\langle\psi(0)|\hat{p}|\psi(0)\rangle = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{pmatrix} \frac{m\omega_0}{\sqrt{2}\beta i} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{pmatrix} = 0$$

(2) $$|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$\langle\psi(0)|\hat{x}|\psi(0)\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \frac{1}{\sqrt{2}\beta} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}\beta}$$

$$\langle\psi(0)|\hat{p}|\psi(0)\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{pmatrix}\frac{1}{\sqrt{2}\beta}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix} = 0$$

$$\langle\psi(t)|\hat{x}|\psi(t)\rangle = \frac{1}{\sqrt{2}\beta}\cos\omega_0 t\,,$$

and

$$\langle\psi(t)|\hat{p}|\psi(t)\rangle = -\frac{m\omega_0}{\sqrt{2}\beta}\sin\omega_0 t\,.$$

36. Schrödinger picture

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}\frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) = \frac{1}{\sqrt{2}}\left(e^{-iE_0t/\hbar}|0\rangle + e^{-iE_1t/\hbar}|1\rangle\right) = \frac{1}{\sqrt{2}}\begin{pmatrix}e^{-iE_0t/\hbar}\\ e^{-iE_1t/\hbar}\end{pmatrix}$$

$$\langle\psi(t)| = \frac{1}{\sqrt{2}}\begin{pmatrix}e^{iE_0t/\hbar} & iE_1t/\hbar\end{pmatrix}$$

$$\begin{aligned}\langle\psi(t)|\hat{x}|\psi(t)\rangle &= \left(\frac{1}{\sqrt{2}}\right)^2\frac{1}{\sqrt{2}\beta}\begin{pmatrix}e^{iE_0t/\hbar} & iE_1t/\hbar\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}e^{-iE_0t/\hbar}\\ e^{-iE_1t/\hbar}\end{pmatrix}\\ &= \frac{1}{2}\frac{1}{\sqrt{2}\beta}\begin{pmatrix}e^{iE_0t/\hbar} & iE_1t/\hbar\end{pmatrix}\begin{pmatrix}e^{-iE_1t/\hbar}\\ e^{-iE_0t/\hbar}\end{pmatrix}\\ &= \frac{1}{2}\frac{1}{\sqrt{2}\beta}(e^{i\omega_0t} + e^{-i\omega_0t})\\ &= \frac{1}{\sqrt{2}\beta}\cos\omega_0 t\end{aligned}$$

$$\langle\psi(t)|\hat{p}|\psi(t)\rangle = \left(\frac{1}{\sqrt{2}}\right)^2 \frac{m\omega_0}{\sqrt{2}\beta i}\begin{pmatrix} e^{iE_0 t/\hbar} & e^{iE_1 t/\hbar}\end{pmatrix}\begin{pmatrix} 0 & 1 \\ -1 & 0\end{pmatrix}\begin{pmatrix} e^{-iE_0 t/\hbar} \\ e^{-iE_1 t/\hbar}\end{pmatrix}$$

$$= \frac{1}{2}\frac{m\omega_0}{\sqrt{2}\beta i}\begin{pmatrix} e^{iE_0 t/\hbar} & e^{iE_1 t/\hbar}\end{pmatrix}\begin{pmatrix} e^{-iE_1 t/\hbar} \\ -e^{-iE_0 t/\hbar}\end{pmatrix}$$

$$= \frac{1}{2}\frac{m\omega_0}{\sqrt{2}\beta i}(e^{-i\omega_0 t} - e^{i\omega_0 t})$$

$$= -\frac{m\omega_0}{\sqrt{2}\beta}\sin\omega_0 t$$

37. Sturm-Liouville problem of the simple harmonics

The Hamiltonian of the simple harmonics

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

The eigenvalue problem of the simple harmonics

$$\hat{H}|n\rangle = \varepsilon_n|n\rangle$$

with

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

Schrödinger equation

$$\langle x|\hat{H}|n\rangle = \varepsilon_n\langle x|n\rangle$$

$$\langle x|\frac{1}{2m}\hat{p}^2 + \frac{m\omega_0^2}{2}\hat{x}^2|n\rangle = \varepsilon_n\langle x|n\rangle$$

or

$$(-\frac{1}{2m}\frac{d^2}{dx^2} + \frac{m\omega_0^2}{2}x^2)\langle x|n\rangle = \varepsilon_n\langle x|n\rangle$$

$\xi = \beta x$, $\langle x|n\rangle = \sqrt{\beta}\langle\xi|n\rangle$, and $|\xi\rangle = \frac{1}{\sqrt{\beta}}|x\rangle$

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}.$$

We note that

$$\frac{d}{dx} = \frac{d\xi}{dx}\frac{d}{d\xi} = \beta\frac{d}{d\xi},$$

$$\frac{d^2}{dx^2} = \frac{d\xi}{dx}\frac{d}{d\xi}(\frac{d\xi}{dx}\frac{d}{d\xi}) = \beta\frac{d}{d\xi}(\beta\frac{d}{d\xi}) = \beta^2\frac{d^2}{d\xi^2},$$

$$(-\frac{\hbar^2}{2m}\beta^2\frac{d^2}{d\xi^2} + \frac{m\omega_0^2}{2}\frac{\xi^2}{\beta^2})\langle\xi|n\rangle = \hbar\omega_0(n+\frac{1}{2})\langle\xi|n\rangle,$$

$$(-\frac{\hbar\omega_0}{2}\frac{d^2}{d\xi^2} + \frac{\hbar\omega_0}{2}\xi^2)\langle\xi|n\rangle = \hbar\omega_0(n+\frac{1}{2})\langle\xi|n\rangle,$$

or

$$(\frac{d^2}{d\xi^2} - \xi^2 + 2n + 1)\varphi_n(\xi) = 0,$$

with

$$\langle\xi|n\rangle = \varphi_n(\xi).$$

We put

$$\varphi_n(\xi) = \exp(-\frac{\xi^2}{2})u_n(\xi),$$

with $u_n(\xi) = H_n(\xi)$: Hermite polynomials.

$$u_n''(\xi) - 2\xi u_n'(\xi) + 2nu_n(\xi) = 0, \qquad (1)$$

Sturm-Liouville type differential equation

38. Determination of the weight function $w(\xi)$

Eq.(1) × $w(\xi)$

$$w(\xi)u_n''(\xi) - 2\xi w(\xi)u_n'(\xi) + 2nw(\xi)u_n(\xi) = 0\,.$$

The weight function should be determined such that

$$w(\xi)u_n''(\xi) - 2\xi w(\xi)u_n'(\xi) = \frac{d}{d\xi}[w(\xi)u_n'(\xi)]\,,$$

or

$$,w'(\xi) = -2\xi w(\xi)$$

$$w(\xi) = \exp(-\xi^2)\,,$$

$$L[u_n] + 2n\exp(-\xi^2)u_n = 0\,,$$

with

$$L[u_n] = \frac{d}{d\xi}[\exp(-\xi^2)u_n'(\xi)].$$

((**Orthogonality**))

$$L[u_n] + 2n\exp(-\xi^2)u_n = 0\,,$$

$$L[u_m] + 2m\exp(-\xi^2)u_m = 0\,.$$

We show that

$$\int_{-\infty}^{\infty} u_m^* L[u_m] d\xi = \int_{-\infty}^{\infty} u_n L[u_m^*] d\xi\,,$$

$$\int_{-\infty}^{\infty} u_m^* L[u_m] d\xi = \int_{-\infty}^{\infty} u_m^* \frac{d}{d\xi}[\exp(-\xi^2)u_n'] d\xi = -\int_{-\infty}^{\infty} (u_m^*)' \exp(-\xi^2)u_n' \, d\xi$$
$$= \int_{-\infty}^{\infty} u_n \frac{d}{d\xi}[\exp(-\xi^2)u_m^{*\prime}] d\xi = \int_{-\infty}^{\infty} u_n L[u_m^*] d\xi$$

$$\int_{-\infty}^{\infty} u_m^* (-2n\exp(-\xi^2)u_n d\xi = \int_{-\infty}^{\infty} u_n (-2m\exp(-\xi^2)u_m^* d\xi$$

or

$$(n-m)\int_{-\infty}^{\infty} u_m^{\ *}\exp(-\xi^2)u_n d\xi = 0\,.$$

If $n \neq m$,

$$\int_{-\infty}^{\infty} u_m^{\ *}\exp(-\xi^2)u_n d\xi = 0\,.$$

39. Summary

Notations

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}$$

$$\xi = \beta x$$

annihilation and creation operators

$$\hat{a} = \frac{\beta}{\sqrt{2}}(\hat{x} + i\frac{\hat{p}}{m\omega_0})$$

$$\hat{a}^+ = \frac{\beta}{\sqrt{2}}(\hat{x} - i\frac{\hat{p}}{m\omega_0})$$

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

$$\hat{n} = \hat{a}^+\hat{a}$$

$$\hat{H} = \hbar\omega_0(\hat{n} + \frac{1}{2})$$

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

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

$$\hat{n}\,|\,n >= n\,|\,n>$$

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

$$[\widehat{N}, \hat{a}] = -\hat{a}$$

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

The parity operator

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

Corodinate and momentum operators

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

$$\hat{p} = \frac{m\omega_0}{i}(\frac{\hat{a} - \hat{a}^{+}}{\sqrt{2}\beta}).$$

Wave function

$$\varphi_n(\xi) =< \xi \,|\, x >= \frac{1}{\sqrt{\beta}} < x \,|\, n >= \frac{1}{\sqrt{\beta}}\varphi_n(x),$$

$$|\, \xi >= \frac{1}{\sqrt{\beta}} \,|\, x >,$$

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

with

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

using

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

and

$$\varphi_0(\xi) = (\pi)^{-\frac{1}{4}} e^{-\frac{\xi^2}{2}},$$

we have the final form of wave function using ther Hermite polynomials

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

Note that Hermite polynomials (definitions) is defined by

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

Normalization

$$\int_{-\infty}^{\infty} d\xi e^{-\xi^2} [H_n(\xi) H_m(\xi)] = \sqrt{\pi} 2^n n! \delta_{n,m}$$

Differential equation

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

The integral representation

$$H_n(\xi) = \frac{2^n}{\sqrt{\pi}} \int_{-\infty}^{\infty} (\xi + iu)^n e^{-u^2} du.$$

The generating function

$$\exp(-t^2 + 2t\xi) = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} t^n.$$

$$K(t,\xi) = \pi^{-1/4} \exp(-\frac{1}{2}\xi^2 + \sqrt{2}t\xi - -\frac{1}{2}t^2) = \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} \varphi_n(\xi) t^n.$$

The recursion relation

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

$$\frac{d}{d\xi} H_n(\xi) = 2n H_{n-1}(\xi).$$

Momentum space

$$\kappa = \frac{k}{\beta}$$

$$|\kappa> = \sqrt{\beta}\,|k>,$$

$$\varphi_n(k) = <k|n> = \frac{1}{\sqrt{\beta}} <\kappa|n> = \frac{1}{\sqrt{\beta}}\varphi_n(\kappa),$$

$$<x|k> = \frac{1}{\sqrt{2\pi}} e^{ikx},$$

$$\varphi_n(\kappa) = <\kappa|n> = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\kappa\xi} \varphi_n(\xi) d\xi,$$

$$\hat{H} = \hbar\omega \begin{pmatrix} 1/2 & 0 & \cdots & 0 & \cdots \\ 0 & 3/2 & & & \\ \vdots & & \ddots & & \\ 0 & & & (2n+1)/2 & \\ \vdots & & & & \ddots \end{pmatrix}$$

$$\hat{x} = \frac{1}{\sqrt{2}\beta} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix}$$

$$\hat{p} = \frac{m\omega_0}{\sqrt{2}i\beta} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ -\sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & -\sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & -\sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix}$$

$$\hat{a} = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ 0 & 0 & \sqrt{2} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \\ 0 & 0 & 0 & 0 & 0 & \\ & & \vdots & & & \end{pmatrix}$$

$$\hat{a}^+ = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \\ \sqrt{1} & 0 & 0 & 0 & 0 & \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix}$$

$$\hat{n} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \\ \sqrt{1} & 0 & 0 & 0 & 0 & \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ 0 & 0 & \sqrt{2} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \\ 0 & 0 & 0 & 0 & 0 & \\ & & \vdots & & & \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 0 & 0 & 0 & & & \\ 0 & 1 & 0 & 0 & & & \\ 0 & 0 & 2 & 0 & & & \\ 0 & 0 & 0 & 3 & & & \\ & & & & \ddots & & \\ & & & & & n & \\ & & & & & & \ddots \end{pmatrix}$$

40. The properties of the translation operator $\hat{T}(\lambda)$

The translation operator is given by

$$\hat{T}_\mu = \exp[-\frac{i}{\hbar}\hat{p}\mu],$$

where μ is the x co-ordinate. Using the relation

$$\hat{p} = i\frac{\hbar\beta}{\sqrt{2}}(\hat{a}^{+} - \hat{a}),$$

the translation operator can be rewritten as

$$\hat{T}_{\mu} = \hat{T}(\lambda) = \exp[-\lambda(\hat{a} - \hat{a}^{+})],$$

where

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}, \quad \lambda = \frac{\beta\mu}{\sqrt{2}} = \mu\sqrt{\frac{m\omega_0}{2\hbar}}.$$

Some properties of the translation operators are shown as follows.

(1)

$$\hat{T}(\lambda) = \exp(\lambda\hat{a}^{+} - \lambda\hat{a}) = \exp(-\frac{1}{2}\lambda^{2})\exp(\lambda\hat{a}^{+})\exp(-\lambda\hat{a}).$$

(2)

$$\hat{T}^{+}(\lambda) = \hat{T}(-\lambda) = \exp(-\lambda\hat{a}^{+} + \lambda\hat{a}) = \exp(-\frac{1}{2}\lambda^{2})\exp(-\lambda\hat{a}^{+})\exp(\lambda\hat{a}).$$

(3)

$$\hat{T}^{+}(\lambda)\hat{a}\hat{T}(\lambda) = \lambda\hat{1} + \hat{a}.$$

(4)

$$\hat{T}^{+}(\lambda)\hat{a}^{+}\hat{T}(\lambda) = \lambda\hat{1} + \hat{a}^{+}.$$

(5)

$$[\exp(\lambda\hat{a}^{+}), \hat{a}] = -\exp(\lambda\hat{a}^{+})\lambda.$$

(6)

$$[\exp(\lambda\hat{a}), \hat{a}^{+}] = \exp(\lambda\hat{a})\lambda.$$

(7)

$$\hat{T}^{+}(\lambda)\hat{n}\hat{T}(\lambda) = \hat{n} + \lambda^{2}\hat{1} + \lambda(\hat{a} + \hat{a}^{+}).$$

with

$$\hat{n} = \hat{a}^{+}\hat{a}$$

(8)

$$\hat{T}^{+}(\lambda)\hat{a}\hat{a}\hat{T}(\lambda) = \hat{a}\hat{a} + \lambda^{2}\hat{1} + 2\lambda\hat{a} = (\hat{a} + \lambda\hat{1})^{2}$$

(9)

$$\hat{T}^{+}(\lambda)\hat{a}^{+}\hat{a}^{+}\hat{T}(\lambda) = \hat{a}^{+}\hat{a}^{+} + \lambda^{2}\hat{1} + 2\lambda\hat{a}^{+} = (\hat{a}^{+} + \lambda\hat{1})^{2}$$

(10)

In general

$$\hat{T}^{+}(\lambda)f(\hat{a},\hat{a}^{+})\hat{T}(\lambda) = f(\hat{a} + \lambda\hat{1}, \hat{a}^{+} + \lambda\hat{1})$$

where f is any function of $\hat{a}$ and $\hat{a}^{+}$ with a power series expansion.

(11)

$$\hat{T}(\lambda_1)\hat{T}(\lambda_2) = \hat{T}(\lambda_2)\hat{T}(\lambda_1) = \hat{T}(\lambda_1 + \lambda_2)$$

41. Simple harmonics of charged particle in the presence of an electric field

Claude Cohen-Tannoudji, Bernard Diu, and Franck Laloë, *Quantum Mechanics volume I and volume II* (John Wiley & Sons, New York, 1977).

The one-dimensional harmonic oscillator consists of a particle of mass *m* having a potential energy. Assume, in addition, that this particle has a charge *q* that it is placed in a uniform electric field ε parallel to the *x* axis. What are its new stationary states and the corresponding energies.

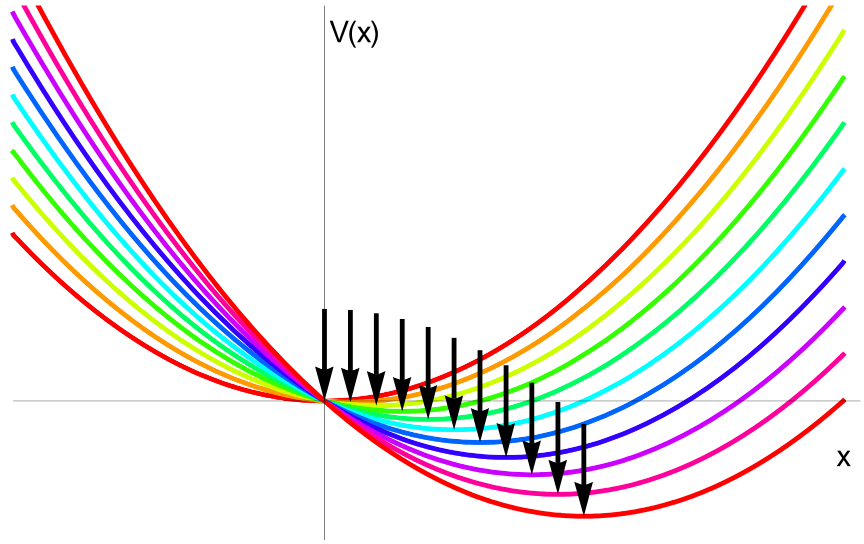

Fig. The potential energy $V(x) = \frac{1}{2} m\omega^2 x^2 - q\varepsilon x$. The potential takes a minimum at $x_0 = \mu = \frac{q\varepsilon}{m\omega_0{}^2}$. The minimum position of the potential energy shfts to the larger x as the electric field increases.

The Hamiltonian of a particle placed in a uniform electric field ε is given by

$$\hat{H}' = \hat{H}_0 - q\varepsilon\hat{x} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 - q\varepsilon\hat{x}$$

We find the eigenvalues and eigenkets of this Hamiltonian. To this end, we use the translation operator given by

$$\hat{T}_\mu = \hat{T}(\lambda) = \exp[-\lambda(\hat{a} - \hat{a}^+)],$$

with

$$\lambda = \frac{\beta\mu}{\sqrt{2}}. \qquad (\lambda \text{ is real})$$

The Hermite conjugate of $\hat{T}(\lambda)$ is given by

$$\hat{T}^+(\lambda) = \hat{T}(-\lambda) = \exp[\lambda(\hat{a} - \hat{a}^+)]$$

and

$$\hat{T}^{+}(\lambda)\hat{T}(\lambda) = \hat{1} \qquad \text{(unitary operator)}$$

The Hamiltonian $\hat{H}_0$ of the simple harmonics is given by

$$\hat{H}_0 = \frac{1}{2m}\hat{p}^2 + \frac{m\omega_0{}^2}{2}\hat{x}^2 = \hbar\omega_0(\hat{a}^{+}\hat{a} + \frac{1}{2}\hat{1}).$$

Under the translation operator $\hat{T}(\lambda)$, the Hamiltonian becomes

$$\hat{H}_{new} = \hat{T}(\lambda)\hat{H}_0\hat{T}^{+}(\lambda) = \hat{T}_\mu\hat{H}_0\hat{T}_\mu{}^{+} = \hat{T}_\mu(\frac{1}{2m}\hat{p}^2 + \frac{m\omega_0{}^2}{2}\hat{x}^2)\hat{T}_\mu{}^{+}.$$

Here we note that

$$\hat{T}_\mu\hat{p}\hat{T}_\mu{}^{+} = \hat{p}$$

$$\hat{T}_\mu\hat{p}^2\hat{T}_\mu{}^{+} = \hat{p}^2$$

$$\hat{T}_\mu\hat{x}\hat{T}_\mu{}^{+} = \hat{x} - \mu\hat{1}$$

$$\hat{T}_\mu\hat{x}^2\hat{T}_\mu{}^{+} = (\hat{x} - \mu\hat{1})^2 = \hat{x}^2 - 2\mu\hat{x} + \mu^2\hat{1}.$$

Then we have

$$\begin{aligned}
\hat{H}_{new} &= \hat{T}_\mu\hat{H}_0\hat{T}_\mu{}^{+} \\
&= \hat{T}_\mu(\frac{\hat{p}^2}{2m} + \frac{m\omega_0{}^2}{2}\hat{x}^2)\hat{T}_\mu{}^{+} \\
&= \frac{\hat{p}^2}{2m} + \frac{m\omega_0{}^2}{2}(\hat{x} - \mu\hat{1})^2 \\
&= \frac{\hat{p}^2}{2m} + \frac{m\omega_0{}^2}{2}\hat{x}^2 - m\omega_0{}^2\mu\hat{x} + \frac{m\omega_0{}^2}{2}\mu^2\hat{1}
\end{aligned}$$

Then the new Hamiltonian can be rewritten as

$$\hat{H}_{new} = (\hat{H}_0 - m\omega_0{}^2\mu\hat{x}) + \frac{m\omega_0{}^2}{2}\mu^2\hat{1} = \hat{H}' + \hbar\omega_0\lambda^2\hat{1}$$

where

$$\hat{H}' = \hat{H}_0 - m\omega_0{}^2\mu\hat{x}$$

and

$$\frac{m\omega_0{}^2}{2}\mu^2 = \frac{m\omega_0{}^2}{2}\frac{2\lambda^2}{\beta^2} = \frac{m\omega_0{}^2\lambda^2}{\beta^2} = m\omega_0{}^2\lambda^2\frac{\hbar}{m\omega_0} = \hbar\omega_0\lambda^2,$$

or

$$m\omega_0{}^2\mu = q\varepsilon .$$

42. The eigenstate and eigenket of $\hat{H}'$

Suppose that $|n\rangle$ is the eigenket of $\hat{H}_0$ with the wigenvalue $E_n = \hbar\omega_0(n+\frac{1}{2})$,

$$\hat{H}_0|n\rangle = \hbar\omega_0(n+\frac{1}{2})|n\rangle,$$

Then we have

$$\hat{H}_0|n\rangle = \hat{T}^+(\lambda)\hat{H}_{new}\hat{T}(\lambda)|n\rangle = \hbar\omega_0(n+\frac{1}{2})|n\rangle$$

or

$$\hat{H}_{new}\hat{T}(\lambda)|n\rangle = \hbar\omega_0(n+\frac{1}{2})\hat{T}(\lambda)|n\rangle$$

implying that $\hat{T}(\lambda)|n\rangle$ is the eigenket of $\hat{H}_{new}$ with the eigenvalue $\hbar\omega_0(n+\frac{1}{2})$. Because of the commutation relation,

$$[\hat{H}_{new}, \hat{H}'] = 0$$

it is concluded that the eigenket of $\hat{H}'$ is the same as that of $\hat{H}_{new}$,

$$\hat{H}'\hat{T}(\lambda)|n\rangle = (\hat{H}_{new} - \hbar\omega_0\lambda^2\hat{1})\hat{T}(\lambda)|n\rangle = [\hbar\omega_0(n+\frac{1}{2}) - \hbar\omega_0\lambda^2)\hat{T}(\lambda)|n\rangle \qquad (2)$$

with the energy eigenvalue of $\hat{H}'$ given by

$$E_n' = \hbar\omega_0 (n + \frac{1}{2}) - \hbar\omega_0 \lambda^2$$

The $|x\rangle$ representation of the eigenket $\hat{T}(\lambda)|n\rangle$ is

$$\langle x|\hat{T}(\lambda)|n\rangle = \langle x|\hat{T}(\mu)|n\rangle = \langle x - \mu|n\rangle = \left\langle x - \sqrt{\frac{2\hbar}{m\omega_0}}\lambda \middle| n \right\rangle$$

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APPENDIX-I

A1. The property of generating function

We now show that

$$g(\xi,t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(\xi) = \exp(-t^2 + 2t\xi).$$

using the recursion formula of the Hermite polynomials.

(a) Recusion formula

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

$$\frac{d}{d\xi} H_n(\xi) = 2nH_{n-1}(\xi),$$

$$H_{2n}(0) = (-1)^n \frac{(2n)!}{n!},$$

$$H_{2n+1}(0) = 0,$$

$$\int_{-\infty}^{\infty} d\xi e^{-\xi^2} [H_n(\xi) H_m(\xi)] = \sqrt{\pi} 2^n n! \delta_{n,m} .$$

(b) Differential equation

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

The integral representation

$$H_n(\xi) = \frac{2^n}{\sqrt{\pi}} \int_{-\infty}^{\infty} (\xi + iu)^n e^{-u^2} du .$$

$$g(\xi,t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(\xi) ,$$

$$\frac{\partial g(\xi,t)}{\partial \xi} = \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{\partial H_n(\xi)}{\partial \xi} = \sum_{n=0}^{\infty} \frac{t^n}{n!} 2n H_{n-1}(\xi)$$
$$= \sum_{n=0}^{\infty} \frac{2}{(n-1)!} H_{n-1}(\xi) t t^{n-1} = 2t \sum_{n=0}^{\infty} \frac{1}{(n-1)!} H_{n-1}(\xi) t^{n-1} = 2t g(\xi,t)$$

$$\int \frac{\partial g}{g} = 2t \int d\xi ,$$

$$\ln[g(\xi,t)] = 2t\xi + \ln[g(\xi,t=0)], \qquad (1)$$

$$g(\xi = 0,t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(0) .$$

We use the relations

$$H_{2n}(0) = (-1)^n \frac{(2n)!}{n!},$$

$$H_{2n+1}(0) = 0,$$

$$g(\xi = 0, t) = \sum_{m=0}^{\infty} \frac{t^{2m}}{(2m)!} H_{2m}(0) = \sum_{m=0}^{\infty} \frac{t^{2m}}{(2m)!} (-1)^m \frac{(2m)!}{m!} = \sum_{m=0}^{\infty} \frac{(-t^2)^m}{m!} = \exp(-t^2),$$

From Eq.(1),

$$\ln[g(\xi,t)] = 2t\xi - t^2.$$

Thus we have

$$g(\xi,t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(\xi) = \exp(2t\xi - t^2).$$

((Generating function))

A2. **Normalization**

$$I = \int_{-\infty}^{\infty} \exp(-\xi^2)\exp(2t\xi - t^2)\exp(2s\xi - s^2) d\xi$$

$$= \sum_{m.n=0}^{\infty} \frac{t^n}{n!} \frac{s^m}{m!} \int_{-\infty}^{\infty} \exp(-\xi^2) H_n(\xi) H_m(\xi) d\xi$$

Here we use

$$\int_{-\infty}^{\infty} \exp(-\xi^2) H_n(\xi) H_m(\xi) d\xi = \delta_{n,m} \int_{-\infty}^{\infty} \exp(-\xi^2)[H_n(\xi)]^2 d\xi.$$

Then

$$I = \sum_{m.n=0}^{\infty} \frac{t^n}{n!} \frac{s^m}{m!} \delta_{n,m} \int_{-\infty}^{\infty} \exp(-\xi^2)[H_n(\xi)]^2 d\xi = \sum_{n=0}^{\infty} \frac{(ts)^n}{(n!)^2} \int_{-\infty}^{\infty} \exp(-\xi^2)[H_n(\xi)]^2 d\xi.$$

The left-hand side:
Noting that

$$\xi^2 + s^2 + t^2 - 2t\xi - 2s\xi = (\xi - s - t)^2 - 2st,$$

$$I = \int_{-\infty}^{\infty} \exp[-(\xi - s - t)^2] \exp(2st) d\xi = \sqrt{\pi}\exp(2st) = \sqrt{\pi} \sum_{n=0}^{\infty} \frac{(2st)^n}{n!},$$

Coefficient of $(st)^n$

$$\int_{-\infty}^{\infty} \exp(-\xi^2)[H_n(\xi)]^2 d\xi = \sqrt{\pi}\, 2^n n!$$

or

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

A3. Recursion relation

(a)

$$g(\xi, t) = \exp(2\xi t - t^2) = \sum_{n=0}^{\infty} \frac{H_n(\xi) t^n}{n!}. \qquad (1)$$

$$\frac{\partial g}{\partial \xi} = 2t \exp(2\xi t - t^2) = \sum_{n=0}^{\infty} \frac{H_n'(\xi) t^n}{n!}. \qquad (2)$$

$$\frac{\partial^2 g}{\partial \xi^2} = 4t^2 \exp(2\xi t - t^2) = \sum_{n=0}^{\infty} \frac{H_n''(\xi) t^n}{n!}. \qquad (3)$$

Eq.(3)-2ξ x Eq(2):

$$\sum_{n=0}^{\infty} \frac{[H_n''(\xi) - 2\xi H_n'(\xi)] t^n}{n!} = (4t^2 - 4\xi t) \exp(2\xi t - t^2), \qquad (4)$$

On the other hand,

$$\frac{\partial g}{\partial t} = (2\xi - 2t) \exp(2\xi t - t^2),$$

or

$$\begin{aligned} 2t \frac{\partial g}{\partial t} &= (4\xi t - 4t^2) \exp(2\xi t - t^2) \\ &= \sum_{n=0}^{\infty} \frac{H_n(\xi) t^{n-1}}{n!} 2nt = \sum_{n=0}^{\infty} \frac{2n H_n(\xi) t^n}{n!}, \end{aligned} \qquad (5)$$

From Eqs.(4) and (5)

$$\sum_{n=0}^{\infty} \frac{[H_n''(\xi) - 2\xi H_n'(\xi) + 2n H_n(\xi)] t^n}{n!} = 0.$$

In fact, $H_n(\xi)$ satisfies the Hermite differential equation.

(b)
We show that

$$H_n'(\xi) = 2nH_{n-1}(\xi),$$

$$\frac{\partial g}{\partial \xi} = 2t\exp(2\xi t - t^2) = \sum_{n=0}^{\infty} \frac{H_n'(\xi)t^n}{n!},$$

or

$$\frac{\partial g}{\partial \xi} = 2t\exp(2\xi t - t^2) = 2t\sum_{n=0}^{\infty} \frac{H_n(\xi)t^n}{n!} = \sum_{n=0}^{\infty} \frac{2(n+1)H_n(\xi)t^{n+1}}{(n+1)!} = \sum_{n=0}^{\infty} \frac{2nH_{n-1}(\xi)t^n}{n!}.$$

Thus we have the reloation, $H_n'(\xi) = 2nH_{n-1}(\xi)$.

(b)

$$\frac{\partial g}{\partial t} = (2\xi - 2t)\exp(2\xi t - t^2) = \sum_{n=0}^{\infty} \frac{H_n(\xi)t^{n-1}}{(n-1)!}.$$

A4. Matrix of Hermitian (Arefken)

Table[{n,HermiteH[n,ξ]},{n,0,10}]//TableForm

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	$-30240 + 302400\xi^2 - 403200\xi^4 + 161280\xi^6 - 23040\xi^8 + 1024\xi^{10}$

These functions cane be written using the matrix

$$
\begin{pmatrix} H_0(\xi) \\ H_1(\xi) \\ H_2(\xi) \\ H_3(\xi) \\ H_4(\xi) \\ H_5(\xi) \\ H_6(\xi) \\ H_7(\xi) \\ H8(\xi) \\ H_9(\xi) \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -2 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -12 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 \\ 12 & 0 & -48 & 0 & 16 & 0 & 0 & 0 & 0 & 0 \\ 0 & 120 & 0 & -160 & 0 & 32 & 0 & 0 & 0 & 0 \\ -120 & 0 & 720 & 0 & -480 & 0 & 64 & 0 & 0 & 0 \\ 0 & -1680 & 0 & 3360 & 0 & -1344 & 0 & 128 & 0 & 0 \\ 1680 & 0 & -13440 & 0 & 13440 & 0 & -3584 & 0 & 256 & 0 \\ 0 & 30240 & 0 & -80640 & 0 & 48384 & 0 & -9216 & 0 & 512 \end{pmatrix} \begin{pmatrix} 1 \\ \xi \\ \xi^2 \\ \xi^3 \\ \xi^4 \\ \xi^5 \\ \xi^6 \\ \xi^7 \\ \xi^8 \\ \xi 9 \end{pmatrix}
$$

This can be written as follows using the inverse matrix.

$$
\begin{pmatrix} 1 \\ \xi \\ \xi^2 \\ \xi^3 \\ \xi^4 \\ \xi^5 \\ \xi^6 \\ \xi^7 \\ \xi^8 \\ \xi 9 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1/2 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3/4 & 0 & 1/8 & 0 & 0 & 0 & 0 & 0 & 0 \\ 3/4 & 0 & 3/4 & 0 & 1/16 & 0 & 0 & 0 & 0 & 0 \\ 0 & 15/8 & 0 & 5/8 & 0 & 1/32 & 0 & 0 & 0 & 0 \\ 15/8 & 0 & 45/16 & 0 & 15/32 & 0 & 1/64 & 0 & 0 & 0 \\ 0 & 105/16 & 0 & 105/32 & 0 & 21/644 & 0 & 1/128 & 0 & 0 \\ 105/16 & 0 & 105/8 & 0 & 105/32 & 0 & 7/32 & 0 & 1/256 & 0 \\ 0 & 945/32 & 0 & 315/16 & 0 & 189/64 & 0 & 9/64 & 0 & 1/512 \end{pmatrix} 1/ \begin{pmatrix} H_0(\xi) \\ H_1(\xi) \\ H_2(\xi) \\ H_3(\xi) \\ H_4(\xi) \\ H_5(\xi) \\ H_6(\xi) \\ H_7(\xi) \\ H8(\xi) \\ H_9(\xi) \end{pmatrix}
$$

The wave function of the simple harmonics

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

or

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

$$\begin{pmatrix} H_0(\xi) \\ H_1(\xi) \\ H_2(\xi) \\ H_3(\xi) \\ H_4(\xi) \\ H_5(\xi) \\ H_6(\xi) \\ H_7(\xi) \\ H_8(\xi) \\ H_9(\xi) \end{pmatrix} = \pi^{1/4} e^{\xi^2/2} \begin{pmatrix} \varphi_0(\xi) \\ \sqrt{2}\varphi_1(\xi) \\ 2\sqrt{2}\varphi_2(\xi) \\ 4\sqrt{3}\varphi_3(\xi) \\ 8\sqrt{6}\varphi_4(\xi) \\ 16\sqrt{15}\varphi_5(\xi) \\ 96\sqrt{5}\varphi_6(\xi) \\ 96\sqrt{70}\varphi_7(\xi) \\ 384\sqrt{70}\varphi_8(\xi) \\ 2304\sqrt{35}\varphi_9(\xi) \end{pmatrix}$$

Now we consider the wave function given by

$$\langle \xi | \psi \rangle = \frac{1}{\sqrt{2}}[\langle \xi | 1 \rangle + \langle \xi | 2 \rangle] = \frac{1}{\sqrt{2}}[\frac{1}{\left(2\sqrt{\pi}\right)^{1/2}} e^{-\xi^2/2} H_1(\xi) + \frac{1}{\left(2^2 2! \sqrt{\pi}\right)^{1/2}} e^{-\xi^2/2} H_2(\xi)]$$

$$=$$

$$= \frac{1}{\sqrt{2}} e^{-\xi^2/2} \frac{1}{\left(2\sqrt{\pi}\right)^{1/2}} [H_1(\xi) + \frac{1}{2} H_2(\xi)] = \frac{1}{2} e^{-\xi^2/2} \frac{1}{\left(\sqrt{\pi}\right)^{1/2}} [2\xi + 2\xi^2 - 1]$$

APPENDIX-B

$$(\hat{a} + \hat{a}^+)^2 = (\hat{a})^2 + \hat{a}\hat{a}^+ + \hat{a}^+\hat{a} + (\hat{a}^+)^2$$

$$(\hat{a} + \hat{a}^+)^3 = (\hat{a})^3 + (\hat{a})^2\hat{a}^+ + \hat{a}\hat{a}^+\hat{a} + \hat{a}(\hat{a}^+)^2 + \hat{a}^+(\hat{a})^2 + \hat{a}^+\hat{a}\hat{a}^+ + (\hat{a}^+)^2\hat{a} + (\hat{a}^+)^3$$

$$\begin{aligned}(\hat{a} + \hat{a}^+)^4 = {} & (\hat{a})^4 + (\hat{a})^3\hat{a}^+ + (\hat{a})^2\hat{a}^+\hat{a} + (\hat{a}^2)^2(\hat{a}^+)^2 + \hat{a}\hat{a}^+(\hat{a})^2 + \hat{a}\hat{a}^+\hat{a}\hat{a}^+ \\ & + \hat{a}\hat{a}^+\hat{a}^+\hat{a} + \hat{a}(\hat{a}^+)^3 + \hat{a}^+(\hat{a})^3 + \hat{a}^+(\hat{a})^2\hat{a}^+ + \hat{a}^+\hat{a}\hat{a}^+\hat{a} + \hat{a}^+\hat{a}(\hat{a}^+)^2 \\ & + (\hat{a}^+)^2(\hat{a})^2 + (\hat{a}^+)^2\hat{a}\hat{a}^+ + (\hat{a}^+)^3\hat{a} + (\hat{a}^+)^4\end{aligned}$$

$$\begin{aligned}(\hat{a} + \hat{a}^+)^2 |n\rangle = {} & \sqrt{n(n-1)}|n-2\rangle + (2n+1)|n\rangle \\ & + \sqrt{(n+1)(n+2)}|n+2\rangle\end{aligned}$$

$$\begin{aligned}(\hat{a} + \hat{a}^+)^3 |n\rangle = {} & \sqrt{n(n-1)(n-2)}|n-3\rangle + 3n\sqrt{n}|n-1\rangle + 3\sqrt{n+1}(n+1)|n+1\rangle \\ & + \sqrt{(n+1)(n+2)(n+3)}|n+3\rangle\end{aligned}$$

APPENDIX-C
Commutation relations

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

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

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

4. $[\hat{a},(\hat{a}^{+})^{n}]=n(\hat{a}^{+})^{n-1}$, $\qquad [\hat{a}, f(\hat{a}^{+})]=nf'(\hat{a}^{+})$

5. $[\hat{a}^{+},(\hat{a})^{2}]=-2\hat{a}$

6. $[\hat{a}^{+},(\hat{a})^{3}]=-3(\hat{a})^{2}$

7. $[\hat{a}^{+},(\hat{a})^{n}]=-n(\hat{a})^{n-1}$, $\qquad [\hat{a}^{+}, f(\hat{a})]=-nf'(\hat{a})$

8. $[(\hat{a})^{2},(\hat{a}^{+})^{2}]=2(\hat{a}^{+}\hat{a}+\hat{a}\hat{a}^{+})=2(2\hat{a}^{+}\hat{a}+\hat{1})$

9. $[(\hat{a}^{+})^{2},(\hat{a})^{2}]=-2(\hat{a}^{+}\hat{a}+\hat{a}\hat{a}^{+})=2(2\hat{a}^{+}\hat{a}+\hat{1})$

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

APPENDIX-D
Problems and solutions of simple harmonics

J.J. Sakurai and J. Napolitano, *Modern Quantum Mechanics*, second edition (Addison-Wesley, New York, 2011).

Problem Sakurai ((2-6))

Consider a particle in one dimension whose Hamiltonian is given by

$$H=\frac{\hat{p}^{2}}{2m}+V(\hat{x}).$$

By calculating $[[\hat{H},\hat{x}],\hat{x}]$, prove

$$\sum_{a'}\left|\langle a''|\hat{x}|a'\rangle\right|^{2}(E_{a'}-E_{a''})=\frac{\hbar^{2}}{2m}$$

whose $|a'\rangle$ is an energy eigenket with eigenvalue $E_{a'}$.

((**Solution**))

$$[[\hat{H},\hat{x}],\hat{x}] = [[\frac{\hat{p}^2}{2m},\hat{x}],\hat{x}] + [[V(\hat{x}),\hat{x}],\hat{x}]$$
$$= [[\frac{\hat{p}^2}{2m},\hat{x}],\hat{x}]$$
$$= [-i\hbar\frac{\partial}{\partial\hat{p}}\left(\frac{\hat{p}^2}{2m}\right),\hat{x}]$$
$$= [-i\hbar\frac{\hat{p}}{m},\hat{x}]$$
$$= i\hbar\frac{1}{m}[\hat{x},\hat{p}] = (i\hbar)^2\frac{1}{m}\hat{1} = -\frac{\hbar^2}{m}\hat{1}$$

Then

$$\langle a''|[[\hat{H},\hat{x}],\hat{x}]|a''\rangle = -\frac{\hbar^2}{m}\hat{1} \qquad (1)$$

On the other hand

$$\langle a''|[[\hat{H},\hat{x}],\hat{x}]|a''\rangle = \langle a''|[\hat{H},\hat{x}]\hat{x}|a''\rangle - \langle a''|\hat{x}[\hat{H},\hat{x}]|a''\rangle$$
$$= \sum_{a'}\{\langle a''|[\hat{H},\hat{x}]|a'\rangle\langle a'|\hat{x}|a''\rangle - \langle a''|\hat{x}|a'\rangle\langle a'|[\hat{H},\hat{x}]|a''\rangle\}$$
$$= \sum_{a'}\{(E_{a''}-E_{a'})\langle a''|\hat{x}|a'\rangle\langle a'|\hat{x}|a''\rangle - (E_{a'}-E_{a''})\langle a''|\hat{x}|a'\rangle\langle a'|\hat{x}|a''\rangle\}$$
$$= -2\sum_{a'}(E_{a'}-E_{a''})|\langle a''|\hat{x}|a'\rangle|^2$$

(2)

Combining Eqs. (1) and (2), we obtain

$$\sum_{a'}|\langle a''|\hat{x}|a'\rangle|^2(E_{a'}-E_{a''}) = \frac{\hbar^2}{2m} \quad (3)$$

Problem Sakurai ((2-7))

Consider a particle in one dimension whose Hamiltonian is given by

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x}) .$$

By calculating $[\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{p}}, H]$, obtain

$$\frac{d}{dt}\langle \hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{p}} \rangle = \left\langle \frac{\hat{\boldsymbol{p}}^2}{m} \right\rangle - \langle \hat{\boldsymbol{r}} \cdot \nabla V(\hat{\boldsymbol{r}}) \rangle$$

In order for us to identify the preceding relation with the quantum-mechanical analogue of the virial theorem, it is essential that the left-hand side vanish. Under what condition would this happen?

((**Solution**))

$$\begin{aligned}
[\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{p}}, H] &= \left[\sum_i \hat{x}_i \hat{p}_i , \frac{1}{2m} \sum_l \hat{p}_j^2 + V(\hat{\boldsymbol{r}}) \right] \\
&= \sum_i \left(\left[\hat{x}_i \hat{p}_i , \frac{1}{2m} \sum_l \hat{p}_j^2 \right] + [\hat{x}_i \hat{p}_i , V(\hat{\boldsymbol{r}})] \right) \\
&= \sum_i \left(\left[\hat{x}_i , \frac{1}{2m} \sum_l \hat{p}_j^2 \right] \hat{p}_i + \hat{x}_i [\hat{p}_i , V(\hat{\boldsymbol{r}})] \right) \\
&= i\hbar \sum_i \left\{ \left(\frac{\partial}{\partial \hat{p}_i} \frac{1}{2m} \hat{p}_i^2 \right) \hat{p}_i - \hat{x}_i \frac{\partial V(\hat{\boldsymbol{r}})}{\partial \hat{x}_i} \right\} \\
&= i\hbar \sum_i \left(\frac{1}{m} \hat{p}_i^2 - \hat{x}_i \frac{\partial V(\hat{\boldsymbol{r}})}{\partial \hat{x}_i} \right)
\end{aligned}$$

Then

$$\frac{d}{dt}\langle \psi(t) | \hat{A} | \psi(t) \rangle = -\frac{i}{\hbar} \langle \psi(t) | [\hat{A}, \hat{H}] | \psi(t) \rangle$$

When $\hat{A} = \hat{\mathbf{r}} \cdot \hat{\mathbf{p}}$

$$\frac{d}{dt}\langle \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} \rangle = -\frac{i}{\hbar} \langle [\hat{\mathbf{r}} \cdot \hat{\mathbf{p}}, \hat{H}] \rangle = \left\langle \frac{\hat{\mathbf{p}}^2}{m} \right\rangle - \langle \hat{\mathbf{r}} \cdot \nabla V(\hat{\mathbf{r}}) \rangle$$

When $\frac{d}{dt}\langle \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} \rangle = 0$,

$$\left\langle \frac{\hat{\mathbf{p}}^2}{m} \right\rangle - \langle \hat{\mathbf{r}} \cdot \nabla V(\hat{\mathbf{r}}) \rangle = 0 .$$

Since $\hat{T} = \frac{1}{2m}\hat{\mathbf{p}}^2$ (kinetic energy),

$$2\langle \hat{T} \rangle - \langle \hat{\mathbf{r}} \cdot \nabla V(\hat{\mathbf{r}}) \rangle = 0 , \qquad \text{(virial theorem)}$$

We now consider the following case.

$$\begin{aligned}
\langle \hat{\mathbf{r}} \cdot \hat{\boldsymbol{p}} \rangle &= \langle \varphi_n(t) | \hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{p}} | \varphi_n(t) \rangle \\
&= \langle \varphi_n | e^{\frac{i}{\hbar}\hat{H}t} \hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{p}} e^{-\frac{i}{\hbar}\hat{H}t} | \varphi_n \rangle \\
&= e^{\frac{i}{\hbar}\varepsilon_n t} \langle \varphi_n | \hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{p}} | \varphi_n \rangle e^{-\frac{i}{\hbar}\varepsilon_n t} \\
&= \langle \varphi_n | \hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{p}} | \varphi_n \rangle
\end{aligned}$$

which is independent of t. Therefore $\frac{d}{dt}\langle \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} \rangle = 0$.

Problem Sakurai 2-11

Using the one-dimensional simple harmonic oscillator as an example, illustrate the difference between the Heisenberg picture and the Schrodinger picture. Discuss in particular how (a) the dynamic variables x and p and (b) the most general state vector evolves with time in each of the two pictures.

((**Solution**))

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

a. variables x and p

Schrödinger picture => no change

Heisenberg picture

$$\frac{d\hat{x}_H(t)}{dt} = \frac{1}{i\hbar}\left[\hat{x}_H(t), \hat{H}\right] = \frac{1}{m}\hat{p}_H(t)$$
$$\frac{d\hat{p}_H(t)}{dt} = \frac{1}{i\hbar}\left[\hat{p}_H(t), \hat{H}\right] = -m\omega^2 \hat{x}_H(t)$$

$$\hat{x}_H(t) = \hat{x}\cos\omega t + \left(\frac{\hat{p}}{m\omega}\right)\sin\omega t$$
$$\hat{p}_H(t) = -m\omega\hat{x}\sin\omega t + \hat{p}\cos\omega t$$

b. state vector

Heisenberg picture => no change

Schrödinger picture

$$|\psi(t)\rangle = \exp\left(-\frac{i\hat{H}}{\hbar}t\right)|\psi(t=0)\rangle$$

with

$$|\psi(t=0)\rangle = \sum_n c_n|n\rangle,\ c_n = \langle n|\psi(t=0)\rangle$$

$$|\psi(t)\rangle = \sum_n c_n e^{-\frac{i}{\hbar}E_n t}|n\rangle$$
$$= \sum_n c_n e^{-i\omega(n+\frac{1}{2})}|n\rangle$$
$$= \begin{pmatrix} c_0 e^{-i\frac{1}{2}\omega} \\ c_1 e^{-i\frac{3}{2}\omega} \\ \vdots \\ \vdots \end{pmatrix}$$

with

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

Problem Sakurai ((2-12))

Consider a particle subject to a one-dimensional simple harmonic oscillator potential. Suppose that at $t = 0$ the state vector is given by

$$\exp\left(-\frac{i\hat{p}a}{\hbar}\right)|0\rangle$$

where $\hat{p}$ is the momentum operator and a is some number with dimension of length. Using the Heisenberg picture, evaluate the expectation value $\langle x \rangle$ for $t \geq 0$.

((**Solution**))
In the Heisenberg picture

$$\hat{x}_H(t) = \hat{x}\cos\omega t + \frac{\hat{p}}{m\omega}\sin\omega t$$

Using

$$\exp\left(\frac{i\hat{p}a}{\hbar}\right)\hat{x}\exp\left(-\frac{i\hat{p}a}{\hbar}\right) = \hat{x} + a\hat{1}$$

$$\exp\left(\frac{i\hat{p}a}{\hbar}\right)\hat{p}\exp\left(-\frac{i\hat{p}a}{\hbar}\right) = \hat{p}$$

Note

$$\left[\hat{x}, \exp\left(\frac{i\hat{p}a}{\hbar}\right)\right] = i\hbar\frac{\partial}{\partial\hat{p}}\exp\left(\frac{i\hat{p}a}{\hbar}\right) = i\hbar\left(\frac{ia}{\hbar}\right)\exp\left(\frac{i\hat{p}a}{\hbar}\right) = -a\exp\left(\frac{i\hat{p}a}{\hbar}\right)$$

$$\exp\left(\frac{i\hat{p}a}{\hbar}\right)\hat{x} - \hat{x}\exp\left(\frac{i\hat{p}a}{\hbar}\right) = a\exp\left(\frac{i\hat{p}a}{\hbar}\right)$$

$$\begin{aligned}
\langle x_H(t)\rangle &= \langle 0|\exp\left(\frac{i\hat{p}a}{\hbar}\right)\hat{x}_H(t)\exp\left(-\frac{i\hat{p}a}{\hbar}\right)|0\rangle \\
&= \cos\omega t\langle 0|\exp\left(\frac{i\hat{p}a}{\hbar}\right)\hat{x}\exp\left(-\frac{i\hat{p}a}{\hbar}\right)|0\rangle \\
&\quad + \frac{1}{m\omega}\sin\omega t\langle 0|\exp\left(\frac{i\hat{p}a}{\hbar}\right)\hat{p}\exp\left(-\frac{i\hat{p}a}{\hbar}\right)|0\rangle \\
&= \cos\omega t\langle 0|(\hat{x} + a\hat{1})|0\rangle + \frac{1}{m\omega}\sin\omega t\langle 0|\hat{p}|0\rangle \\
&= a\cos\omega t
\end{aligned}$$

where

$$\langle 0|\hat{x}|0\rangle = 0, \qquad \langle 0|\hat{p}|0\rangle = 0.$$

At $t = 0$, the wave function is given by

$$\langle x|\psi(0)\rangle = \langle x|\exp\left(-\frac{i\hat{p}a}{\hbar}\right)|0\rangle$$

Problem Sakurai ((2-13))

a. Write down the wave function (in coordinate space) for the state specified in Problem 2.12 at $t = 0$. You may use

$$\langle x'|0\rangle \pi^{-\frac{1}{4}} x_0^{-\frac{1}{2}} \exp[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2], \text{ with } x_0 = \sqrt{\frac{\hbar}{m\omega_0}}.$$

b. Obtain a simple expression for the probability that the state is found in the ground state at $t = 0$. Does this probability change for $t>0$?

---

a.

$$\begin{aligned}\langle x'|\exp\left(-\frac{i\hat{p}a}{\hbar}\right)|0\rangle &= \langle x'|\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{ia}{\hbar}\right)^n \hat{p}^n|0\rangle \\ &= \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{ia}{\hbar}\right)^n \langle x'|\hat{p}^n|0\rangle \\ &= \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{ia}{\hbar}\right)^n \left(\frac{\hbar}{i}\right)^n \frac{\partial^n}{\partial x'^n}\langle x'|0\rangle \\ &= \pi^{-\frac{1}{4}} x_0^{-\frac{1}{2}} \exp\left[-\frac{1}{2}\left(\frac{x'-a}{x_0}\right)^2\right]\end{aligned}$$

$$(\langle x'|\hat{p} = \langle x'|\frac{\hbar}{i}\frac{\partial}{\partial x'} = \frac{\hbar}{i}\langle x'|\frac{\partial}{\partial x'})$$

b.

$$\begin{aligned}\langle 0|\exp\left(-\frac{i\hat{p}a}{\hbar}\right)|0\rangle &= \int dx'\langle 0|x'\rangle\langle x'|\exp\left(-\frac{i\hat{p}a}{\hbar}\right) \\ &= \pi^{-\frac{1}{4}} x_0^{-\frac{1}{2}} \int dx' \exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right] \pi^{-\frac{1}{4}} x_0^{-\frac{1}{2}} \exp\left[-\frac{1}{2}\left(\frac{x'-a}{x_0}\right)^2\right] \\ &= \pi^{-\frac{1}{2}} x_0^{-1} \exp\left(-\frac{a^2}{4x_0^2}\right)\int dx' \exp[-(\frac{x'-\frac{1}{2}a}{x_0})^2] \\ &= \exp\left(-\frac{a^2}{4x_0^2}\right)\end{aligned}$$

Therefore the probability is given by

$$P(t=0) = \left|\langle 0|\exp\left(-\frac{i\hat{p}a}{2x_0^2}\right)|0\rangle\right|^2 = \exp\left(-\frac{a^2}{2x_0^2}\right)$$

$$P(t) = \left|\langle 0|\exp\left(-\frac{i\hat{H}}{\hbar}t\right)\exp\left(-\frac{i\hat{p}a}{2x_0^2}\right)|0\rangle\right|^2$$

$$= \left|\exp\left(-\frac{i\omega t}{2}\right)\langle 0|\exp\left(-\frac{i\hat{p}a}{2x_0^2}\right)|0\rangle\right|^2 = P(t=0)$$

invariant

Problem Sakurai ((2-13))

Consider a one-dimensional simple harmonic oscillator.

a. Using

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{i\hat{p}}{m\omega}), \qquad \hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} - \frac{i\hat{p}}{m\omega})$$

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

evaluate $\langle m|\hat{x}|n\rangle$, $\langle m|\hat{p}|n\rangle$, $\langle m|\{\hat{x},\hat{p}\}|n\rangle$, $\langle m|\hat{x}^2|n\rangle$, and $\langle m|\hat{p}^2|n\rangle$.

b. Check that the virial theorem holds for the expectation values of the kinetic and the potential energy taken with respect to an energy eigenstate.

---

a.

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^+\right)$$

$$\hat{p} = -i\sqrt{\frac{m\hbar\omega}{2}}\left(\hat{a} - \hat{a}^+\right)$$

$$\langle m|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\langle m|\hat{a}|n\rangle + \langle m|\hat{a}^+|n\rangle\right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right)$$

$$\langle m|\hat{p}|n\rangle = -i\sqrt{\frac{m\hbar\omega}{2}}\left(\langle m|\hat{a}|n\rangle - \langle m|\hat{a}^{+}|n\rangle\right)$$
$$= -i\sqrt{\frac{m\hbar\omega}{2}}\left(\sqrt{n}\delta_{m,n-1} - \sqrt{n+1}\delta_{m,n+1}\right)$$

$$\{\hat{x},\hat{p}\} = \sqrt{\frac{\hbar}{2m\omega}}\left(-i\sqrt{\frac{m\hbar\omega}{2}}\right)\{\hat{a}+\hat{a}^{+},\hat{a}-\hat{a}^{+}\}$$
$$= -\frac{i\hbar}{2}\{\hat{a}+\hat{a}^{+},\hat{a}-\hat{a}^{+}\}$$
$$= -\frac{i\hbar}{2}\{(\hat{a}+\hat{a}^{+})(\hat{a}-\hat{a}^{+}) + (\hat{a}-\hat{a}^{+})(\hat{a}+\hat{a}^{+})\}$$
$$= -\frac{i\hbar}{2}\left(\hat{a}^{2} - \hat{a}\hat{a}^{+} + \hat{a}^{+}\hat{a} - \hat{a}^{+^{2}} + \hat{a}^{2} + \hat{a}\hat{a}^{+} - \hat{a}^{+}\hat{a} - a^{+^{2}}\right)$$
$$= -i\hbar\left(\hat{a}^{2} - \hat{a}^{+^{2}}\right)$$

$$\langle m|\{\hat{x},\hat{p}\}|n\rangle = -i\hbar\left(\langle m|\hat{a}^{2}|n\rangle - \langle m|\hat{a}^{+^{2}}|n\rangle\right)$$
$$= -i\hbar\{\sqrt{n(n-1)}\delta_{m,n-2} - \sqrt{(n+1)(n+2)}\delta_{m,n+2}\}$$

$$\langle m|x^{2}|n\rangle = \frac{\hbar}{2m\omega}\langle m|\hat{a}^{2} + \hat{a}\hat{a}^{+} + \hat{a}^{+}\hat{a} + \hat{a}^{+^{2}}|n\rangle$$
$$= \frac{\hbar}{2m\omega}\langle m|\hat{a}^{2} + \hat{a}^{+^{2}} + (2\hat{a}^{+}\hat{a}+1)|n\rangle$$
$$= \frac{\hbar}{2m\omega}\{\sqrt{n(n+1)}\delta_{m,n-2} + \sqrt{(n+1)(n+2)}\delta_{m,n+2} + (2n+1)\delta_{m,n}\}$$

$$\langle m|\hat{p}^{2}|n\rangle = -\frac{m\hbar\omega}{2}\langle m|\hat{a}^{2} - \hat{a}\hat{a}^{+} - \hat{a}^{+}\hat{a} + \hat{a}^{+^{2}}|n\rangle$$
$$= -\frac{m\hbar\omega}{2}\{\sqrt{n(n+1)}\delta_{m,n-2} + \sqrt{(n+1)(n+2)}\delta_{m,n+2} - (2n+1)\delta_{m,n}\}$$

b.

$$\langle n|\frac{\hat{p}^{2}}{m}|n\rangle = \hbar\omega\left(n+\frac{1}{2}\right)$$

Then

$$\langle n|\hat{x}\frac{dV}{d\hat{x}}|n\rangle = \langle n|\hat{x}\frac{d}{d\hat{x}}\left(\frac{1}{2}m\omega^{2}\hat{x}^{2}\right)|n\rangle = m\omega^{2}\langle n|\hat{x}^{2}|n\rangle = \hbar\omega\left(n+\frac{1}{2}\right)$$

$$\langle n|\frac{\hat{p}^2}{m}|n\rangle = \langle n|\hat{x}\frac{dV}{d\hat{x}}|n\rangle,$$

showing that the virial theorem holds.

Note

$$\left\langle \frac{\hat{p}^2}{2m} \right\rangle = \left\langle \frac{1}{2} m\omega^2 \hat{x}^2 \right\rangle$$

The kinetic energy is equal to the potential energy

Problem Sakurai ((2-14))
a. Using

$$\langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp(\frac{ip'x'}{\hbar}) \qquad \text{(one dimension)}$$

Prove

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

b. Consider a one-dimensional harmonic oscillator. Starting with the Schrödinger equation for the state vector, derive the Schrödinger equation for the momentum-space wave function. (Make sure to distinguish the operator $\hat{p}$ from the eigenvalue p'.) Can you guess the energy eigenfunctions in momentum space?

((**Solution**))

$$
\begin{aligned}
\langle p'|x|\alpha\rangle &= \int dx' \langle p'|x|x'\rangle\langle x'|\alpha\rangle \\
&= \int dx'x'\langle p'|x'\rangle\langle x'|\alpha\rangle \\
&= \int dx'x'\left(\frac{1}{\sqrt{2\pi\hbar}}\exp\left(\frac{-ipx'}{\hbar}\right)\right)\langle x'|\alpha\rangle \\
&= \int dx' i\hbar\frac{\partial}{\partial p'}\left(\frac{1}{\sqrt{2\pi\hbar}}\exp\left(\frac{-ipx'}{\hbar}\right)\right)\langle x'|\alpha\rangle \\
&= i\hbar\frac{\partial}{\partial p'}\int dx'\langle p'|x'\rangle\langle x'|\alpha\rangle \\
&= i\hbar\frac{\partial}{\partial p'}\langle p'|\alpha\rangle
\end{aligned}
$$

b.

$$
i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle
$$

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\langle p'|\psi(t)\rangle &= \langle p'|\frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2|\psi(t)\rangle \\
&= \frac{1}{2m}p'^2\langle p'|\psi(t)\rangle + \frac{1}{2}m\omega^2(i\hbar)^2\frac{\partial^2}{\partial p'^2}\langle p'|\psi(t)\rangle
\end{aligned}
$$

Therefore

$$
i\hbar\frac{\partial}{\partial t}\langle p'|\psi(t)\rangle = -\frac{1}{2}m\omega^2\hbar^2\frac{\partial^2}{\partial p'^2}\langle p'|\psi(t)\rangle + \frac{1}{2m}p'^2\langle p'|\psi(t)\rangle
$$

Suppose that

$$
|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi(t=0)\rangle = e^{-\frac{i}{\hbar}E_n t}|n\rangle,
$$

we have

$$
E_n\langle p'|n\rangle = -\frac{1}{2}m\omega^2\hbar^2\frac{\partial^2}{\partial p'^2}\langle p'|n\rangle + \frac{1}{2m}p'^2\langle p'|n\rangle.
$$

Here note that the Schrödinger equation in the position space is

$$
E_n\langle x'|n\rangle = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x'^2}\langle x'|n\rangle + \frac{1}{2}m\omega^2 x'^2\langle x'|n\rangle.
$$

The eigenfunction in momentum space is

$$\langle p'|n\rangle = (2^n n!)^{-\frac{1}{2}} \left(\frac{1}{m\omega\hbar\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{1}{2}\zeta^2\right) H_n(\zeta)$$

with

$$\zeta = \frac{p'}{\sqrt{m\omega\hbar}} .$$

Problem Sakurai ((2-15))

Consider a function, known as the correlation function, defined by

$$C(t) = \langle \hat{x}_H(t)\hat{x}_H(0)\rangle ,$$

where $\hat{x}_H(t)$ is the position operator in the Heisenberg picture. Evaluate the correlation function explicitly for the ground state of a one-dimensional simple harmonic oscillator.

((**Solution**))
For the 1D harmonic oscillator (Heisenberg picture)

$$\hat{x}_H(t) = \hat{x}\cos\omega_0 t + \frac{1}{m\omega_0}\hat{p}\sin\omega_0 t .$$

$$\begin{aligned} C(t) &= \langle 0|\hat{x}_H(t)\hat{x}_H(0)|0\rangle \\ &= \langle 0|\hat{x}^2\cos\omega_0 t + \frac{1}{m\omega_0}\hat{p}\hat{x}\sin\omega_0 t|0\rangle \\ &= \cos\omega_0 t\langle 0|\hat{x}^2|0\rangle + \frac{\sin\omega t}{m\omega}\langle 0|\hat{p}\hat{x}|0\rangle \\ &= \cos\omega_0 t\frac{\hbar}{2m\omega_0} + \frac{\sin\omega_0 t}{m\omega_0}\left(-\frac{i\hbar}{2}\right) \\ &= \frac{\hbar}{2m\omega_0}e^{-i\omega_0 t} \end{aligned}$$

where we use

$$\hat{p}\hat{x} = -\frac{i\hbar}{2}(\hat{a}^2 - \hat{a}^{+2} - \hat{a}^+\hat{a} + \hat{a}\hat{a}^+)$$

$$\langle 0|\hat{p}\hat{x}|0\rangle = -\frac{i\hbar}{2}$$

$$\langle 0|\hat{x}^2|0\rangle = \frac{\hbar}{2m\omega_0}.$$

Problem Sakurai ((2-16))

Consider again a one-dimensional simple harmonic oscillator. Do the following algebraically, that is, without using wave functions.

a. Construct a linear combination of $|0\rangle$ and $|1\rangle$ such that $\langle x\rangle$ is as large as possible.

b. Suppose the oscillator is in the state constructed in (a) at $t = 0$. What is the state vector for t>0 in the Schrödinger picture? Evaluate the expectation value $\langle x\rangle$ as a function of time t for t>0 using (i) the Schrödinger picture and (ii) the Heisenberg picture.

c. Evaluate $\langle(\Delta x)^2\rangle$ as a function of time using either picture.

((**Solution**))

a.

In Schrödinger picture

$$|\alpha\rangle = c_0|0\rangle + c_1|1\rangle$$

$$\begin{aligned}\langle\hat{x}\rangle &= \langle\alpha|\hat{x}|\alpha\rangle \\ &= |c_0|^2\langle 0|\hat{x}|0\rangle + |c_1|^2\langle 1|\hat{x}|1\rangle + c_0^*c_1\langle 0|\hat{x}|1\rangle + c_0c_1^*\langle 1|\hat{x}|0\rangle \\ &= \sqrt{\frac{\hbar}{2m\omega}}(c_0^*c_1 + c_0c_1^*)\end{aligned}$$

$$c_0 \equiv r_0e^{i\theta_0},\ c_1 \equiv r_1e^{i\theta_1}$$

or using the matrix,

$$\langle\alpha|\hat{x}|\alpha\rangle = \frac{1}{\sqrt{2}\beta}\begin{pmatrix} c_0^* & c_1^*\end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0\end{pmatrix}\begin{pmatrix} c_0 \\ c_1\end{pmatrix} = \sqrt{\frac{\hbar}{2m\omega}}(c_0^*c_1 + c_0c_1^*)$$

$$|c_0|^2 + |c_1|^2 = 1 \qquad \Rightarrow \qquad r_0^2 + r_1^2 = 1$$

(r_i, θ_i: real numbers) $\qquad r_0 = \cos\phi$, $r_1 = \sin\phi$,

$$
\begin{aligned}
\langle x \rangle &= \sqrt{\frac{\hbar}{2m\omega}} r_0 r_1 \left[e^{i(\theta_1-\theta_0)} + e^{-i(\theta_1-\theta_0)} \right] \\
&= \sqrt{\frac{\hbar}{2m\omega}} 2 r_0 r_1 \cos(\theta_0 - \theta_1) \\
&= \sqrt{\frac{\hbar}{2m\omega}} \sin(2\phi) \cos(\theta_0 - \theta_1)
\end{aligned}
$$

The maximum of $\langle x \rangle$ is given when

$$
\sin(2\phi) = 1, \ \cos(\theta_0 - \theta_1) = 1
$$

$$
\phi = \frac{\pi}{4}, \qquad r_0 = r_1 = \frac{1}{\sqrt{2}}
$$

$$
|\alpha\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)
$$

b.

$$
\begin{aligned}
|\alpha(t)\rangle &= \exp\left(-\frac{iH}{\hbar}t\right)|\alpha(t=0)\rangle \\
&= \exp\left(-\frac{iH}{\hbar}t\right)\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\
&= \frac{1}{\sqrt{2}} e^{-\frac{1}{2}i\omega t}|0\rangle + \frac{1}{\sqrt{2}} e^{-\frac{3}{2}i\omega t}|1\rangle
\end{aligned}
$$

$$
\begin{aligned}
\langle \hat{x} \rangle &= \langle \alpha(t)|\hat{x}|\alpha(t)\rangle \\
&= \frac{1}{2}\left(e^{-i\omega t}\langle 0|\hat{x}|1\rangle + e^{i\omega t}\langle 1|\hat{x}|0\rangle\right) \\
&= \sqrt{\frac{\hbar}{2m\omega}} \cos\omega t
\end{aligned}
$$

In the Heisenberg picture

$$\begin{aligned}\langle x\rangle &= \langle\alpha(0)|\hat{x}_H|\alpha(0)\rangle \\ &= \langle\alpha|(\hat{x}\cos\omega t + \frac{\hat{p}}{m\omega}\sin\omega t)|\alpha\rangle \\ &= (\frac{1}{\sqrt{2}}\langle 0| + \frac{1}{\sqrt{2}}\langle 1|)(\hat{x}\cos\omega t + \frac{\hat{p}}{m\omega}\sin\omega t)(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle) \\ &= \sqrt{\frac{\hbar}{2m\omega}}\cos\omega t\end{aligned}$$

Note:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^+) \qquad \hat{x}^2 = \frac{\hbar}{2m\omega}(\hat{a}+\hat{a}^+)^2 = \frac{\hbar}{2m\omega}(\hat{a}^2 + \hat{a}^{+2} + 2\hat{a}^+\hat{a} + \hat{1})$$

$$\begin{cases}\langle 0|\hat{x}|1\rangle \neq 0 \\ \langle 1|\hat{x}|0\rangle \neq 0 \\ \langle 0|\hat{x}|0\rangle = 0 \\ \langle 1|\hat{x}|1\rangle = 0\end{cases} \qquad \begin{cases}\langle 0|\hat{x}^2|1\rangle = 0 \\ \langle 1|\hat{x}^2|0\rangle = 0 \\ \langle 0|\hat{x}^2|0\rangle \neq 0 \\ \langle 1|\hat{x}^2|1\rangle \neq 0\end{cases}$$

c.
In Schrödinger picture, we calculate

$$\begin{aligned}\langle(\Delta x)^2\rangle &= \langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2 \\ &= \frac{\hbar}{m\omega} - \frac{\hbar}{2m\omega}\cos^2\omega t \\ &= \frac{\hbar}{m\omega} - \frac{\hbar}{2m\omega}(1-\sin^2\omega t) \\ &= \frac{\hbar}{2m\omega}(1+\sin^2\omega t)\end{aligned}$$

$$\begin{aligned}\langle\alpha(t)|\hat{x}^2|\alpha(t)\rangle &= \frac{1}{2}(e^{\frac{1}{2}i\omega t}\langle 0| + e^{\frac{3}{2}i\omega t}\langle 1|)\hat{x}^2(e^{-\frac{1}{2}i\omega t}|0\rangle + e^{-\frac{3}{2}i\omega t}|1\rangle) \\ &= \frac{1}{2}\left(\langle 0|\hat{x}^2|0\rangle + \langle 1|\hat{x}^2|1\rangle + e^{-i\omega t}\langle 0|\hat{x}^2|1\rangle + e^{i\omega t}\langle 1|\hat{x}^2|0\rangle\right) \\ &= \frac{1}{2}(\langle 0|\hat{x}^2|0\rangle + \langle 1|\hat{x}^2|1\rangle) \\ &= \frac{1}{2}\frac{\hbar}{2m\omega}(1+3) = \frac{\hbar}{m\omega}\end{aligned}$$

Problem Sakurai ((**2-17**))

17. Show for the one-dimensional simple harmonic oscillator

$$\langle 0|\exp(ik\hat{x})|0\rangle = \exp[-k^2\langle 0|\hat{x}^2|0\rangle/2],$$

where $\hat{x}$ is the position operator.

$$\begin{aligned}\langle 0|e^{ik\hat{x}}|0\rangle &= \int dx'\langle 0|x'\rangle\langle x'|e^{ik\hat{x}}|0\rangle \\ &= \int dx' e^{ikx'}|\langle x'|0\rangle|^2 \\ &= \int dx' e^{ikx'}\frac{1}{\pi^{1/2}x_0}\exp(-\frac{x'^2}{x_0^2}) \\ &= \int dx'\frac{1}{\pi^{1/2}x_0}\exp[-\frac{1}{x_0^2}(x'-\frac{ikx_0}{2})^2-\frac{k^2}{4}x_0^2] \\ &= \exp(-\frac{k^2}{4}x_0^2) \\ &= \exp(-\frac{k^2\langle 0|\hat{x}^2|0\rangle}{2})\end{aligned}$$

where

$$\langle 0|\hat{x}^2|0\rangle = \frac{\hbar}{2m\omega} = \frac{x_0}{2}$$

$$\langle x'|0\rangle = \frac{1}{\pi^{1/4}x_0^{1/2}}\exp(-\frac{x'^2}{2x_0^2})$$

APPENDIX-E
Problems and solutions of simple harmonics

Claude Cohen-Tannoudji, Bernard Diu, and Franck Laloë, *Quantum Mechanics*, volume I and volume II (John Wiley & Sons, New York, 1977).

Problem 5-8 ((Cohen-Tannoudji))

The evolution operator $\hat{U}(t,0)$ of a one-dimensional harmonic oscillator is written :

$$\hat{U}(t,0) = \exp(-\frac{i\hat{H}t}{\hbar})$$

with

$$\hat{H} = \hbar\omega(\hat{a}^{+}\hat{a} + \frac{1}{2}\hat{1})$$

(a) Consider the operators

$$\hat{a}_H(t) = \hat{U}^{+}(t)\hat{a}\hat{U}(t), \qquad \hat{a}_H{}^{+}(t) = \hat{U}^{+}(t)\hat{a}^{+}\hat{U}(t)$$

By calculating their action on the eigenkets $|n\rangle$ of $\hat{H}$, find the expression for $\hat{a}_H(t)$ and $\hat{a}_H{}^{+}(t)$ in terms of $\hat{a}$ and $\hat{a}^{+}$.

(b) Calculate the operator $\hat{x}_H(t)$ and $\hat{p}_H(t)$ obtained from $\hat{x}$ and $\hat{p}$ by the unitary transformation:

$$\hat{x}_H(t) = \hat{U}^{+}(t,0)\hat{x}\hat{U}(t,0), \qquad \hat{p}_H(t) = \hat{U}^{+}(t,0)\hat{p}\hat{U}(t,0).$$

How can the relations so obtained be interpreted?

(c) Show that $\hat{U}^{+}(\frac{\pi}{2\omega},0)|x\rangle$ is an eigenvector of $\hat{p}$ and specify its eigenvalue. Similarly, establish that $\hat{U}^{+}(\frac{\pi}{2\omega},0)|p\rangle$ is an eigenvector of $\hat{x}$.

(d) At $t = 0$, the wave function of the oscillator is $\psi(x,0)$. How can one obtain from $\psi(x,0)$ the wave function of the oscillator at all subsequent times $t_q = \frac{q\pi}{2\omega}$ (where q is a positive integer).

(e) Choose for $\psi(x,0)$ the wave function $\langle x|n\rangle$ associated with a stationary state. From the preceding question derive the relation which must exist between $\langle x|n\rangle$ and its Fourier transform $\langle p|n\rangle$.

(f) Describe qualitatively the evolution of the wave function in the following cases:

(i) $\psi(x,0) = e^{ikx}$, where k, real is given.

(ii) $\psi(x,0) = e^{-\rho x}$, where ρ is real and positive.

(iii) $$\psi(x,0) = \begin{cases} = \frac{1}{\sqrt{a}} & (|x| \le \frac{a}{2} \\ = 0 & (everywhere, else) \end{cases}$$

(iv) $\psi(x,0) = e^{-\rho^2 x^2}$, where ρ is real.

((**Solution**))

$$\hat{U}(t) = \exp(-\frac{i}{\hbar}\hat{H}t), \qquad \hat{U}^+(t) = \exp(\frac{i}{\hbar}\hat{H}t)$$

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

Heisenberg picture:

$$\langle\psi_H|\hat{a}_H|\psi_H\rangle = \langle\psi_s(t)|\hat{a}|\psi_s(t)\rangle$$

where the relation between the Heisenberg picture and Schrodinger picture is given by

$$|\psi_s(t)\rangle = \hat{U}(t)|\psi_H\rangle$$

Then we have

$$\langle\psi_H|\hat{a}_H(t)|\psi_H\rangle = \langle\psi_H|\hat{U}^+(t)\hat{a}\hat{U}(t)|\psi_H\rangle$$

or

$$\hat{a}_H(t) = \hat{U}^+(t)\hat{a}\hat{U}(t)$$

(a)

$$\begin{aligned}
\hat{a}_H(t)|n\rangle &= \hat{U}^+(t)\hat{a}\hat{U}(t)|n\rangle \\
&= \exp(-\frac{i}{\hbar}\varepsilon_n t)\hat{U}^+(t)\hat{a}|n\rangle \\
&= \exp(-\frac{i}{\hbar}\varepsilon_n t)\sqrt{n}\hat{U}^+(t)|n-1\rangle \\
&= \exp[-\frac{i}{\hbar}(\varepsilon_n - \varepsilon_{n-1})t]\sqrt{n}|n-1\rangle \\
&= e^{-i\omega t}\sqrt{n}|n-1\rangle
\end{aligned}$$

where

$$\hat{U}(t)|n\rangle = \exp(-\frac{i}{\hbar}\varepsilon_n t)|n\rangle$$

Noting that

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

we get

$$\hat{a}_H(t)|n\rangle = e^{-i\omega t}\sqrt{n}|n-1\rangle = e^{-i\omega t}\hat{a}|n\rangle$$

Similarly

$$\begin{aligned}\hat{a}_H{}^+(t)|n\rangle &= \hat{U}^+(t)\hat{a}^+\hat{U}(t)|n\rangle \\ &= \exp(-\frac{i}{\hbar}\varepsilon_n t)\hat{U}^+(t)\hat{a}^+|n\rangle \\ &= \exp(-\frac{i}{\hbar}\varepsilon_n t)\sqrt{n+1}\hat{U}^+(t)|n+1\rangle \\ &= \exp[-\frac{i}{\hbar}(\varepsilon_n - \varepsilon_{n+1})t]\sqrt{n+1}|n+1\rangle \\ &= e^{i\omega t}\sqrt{n+1}|n+1\rangle\end{aligned}$$

where

$$\hat{U}(t)|n\rangle = \exp(-\frac{i}{\hbar}\varepsilon_n t)|n\rangle$$

Noting that

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

we get

$$\hat{a}_H{}^+(t)|n\rangle = e^{i\omega t}\sqrt{n+1}|n+1\rangle = e^{i\omega t}\hat{a}^+|n\rangle$$

(b) Noting that

$$\hat{a}_H(t) = \sum_n \hat{a}_H(t)|n\rangle\langle n| = e^{-i\omega t}\sum_n \hat{a}|n\rangle\langle n| = e^{-i\omega t}\hat{a}$$

$$\hat{a}_H{}^+(t) = \sum_n \hat{a}_H{}^+(t)|n\rangle\langle n| = e^{i\omega t}\sum_n \hat{a}^+|n\rangle\langle n| = e^{i\omega t}\hat{a}^+$$

we have

$$\hat{x}_H(t) = \sqrt{\frac{\hbar}{2m\omega}}[\hat{a}_H(t) + \hat{a}_H{}^+(t)]$$
$$= \frac{1}{\sqrt{2}\beta}[\hat{a}_H(t) + \hat{a}_H{}^+(t)]$$
$$= \frac{1}{\sqrt{2}\beta}(e^{i\omega t}\hat{a}^+ + e^{-i\omega t}\hat{a})$$

where

$$\beta = \sqrt{\frac{m\omega}{\hbar}},$$

Similarly, we get

$$\hat{p}_H(t) = \frac{1}{\sqrt{2}\beta}\frac{m\omega}{i}[\hat{a}_H(t) - \hat{a}_H{}^+(t)]$$
$$= i\frac{m\omega}{\sqrt{2}\beta}(e^{i\omega t}\hat{a}^+ - e^{-i\omega t}\hat{a})$$

$$\frac{d}{dt}\hat{p}_H(t) = -\frac{1}{\sqrt{2}\beta}m\omega^2(e^{i\omega t}\hat{a}^+ + e^{-i\omega t}\hat{a}) = -m\omega^2 x_H(t)$$

which is the equation of motion for the simple harmonics.

(c)

$$\hat{p}_H(t) = i\frac{m\omega}{\sqrt{2}\beta}(e^{i\omega t}\hat{a}^+ - e^{-i\omega t}\hat{a}) = i\sqrt{\frac{m\hbar\omega}{2}}(e^{i\omega t}\hat{a}^+ - e^{-i\omega t}\hat{a})$$

When $t = \frac{\pi}{2\omega}$, we have

$$\hat{p}_H(t = \frac{\pi}{2\omega}) = i\sqrt{\frac{m\hbar\omega}{2}}(e^{i\frac{\pi}{2}}\hat{a}^+ - e^{-i\frac{\pi}{2}}\hat{a}) = -\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^+ + \hat{a}) = -m\omega\hat{x}$$

$$\hat{x}_H(t = \frac{\pi}{2\omega}) = \frac{1}{\sqrt{2}\beta}(e^{i\frac{\pi}{2}}\hat{a}^+ + e^{-i\frac{\pi}{2}}\hat{a}) = \sqrt{\frac{\hbar}{2m\omega}}(i\hat{a}^+ - i\hat{a}) = \frac{1}{m\omega}\hat{p}$$

From these relations

$$\hat{p}_H(t=\frac{\pi}{2\omega})=\hat{U}^+(\frac{\pi}{2\omega})\hat{p}\hat{U}(\frac{\pi}{2\omega})=-m\omega\hat{x}$$

$$\hat{x}_H(t=\frac{\pi}{2\omega})=\hat{U}^+(\frac{\pi}{2\omega})\hat{x}\hat{U}(\frac{\pi}{2\omega})=\frac{1}{m\omega}\hat{p}$$

we get

$$\hat{p}\hat{U}^+(\frac{\pi}{2\omega})=m\omega\hat{U}^+(\frac{\pi}{2\omega})\hat{x}\hat{U}(\frac{\pi}{2\omega})\hat{U}^+(\frac{\pi}{2\omega})$$
$$=m\omega\hat{U}^+(\frac{\pi}{2\omega})\hat{x}$$

$$\hat{x}\hat{U}^+(\frac{\pi}{2\omega})=-\frac{1}{m\omega}\hat{U}^+(\frac{\pi}{2\omega})\hat{p}\hat{U}(\frac{\pi}{2\omega})\hat{U}^+(\frac{\pi}{2\omega})$$
$$=-\frac{1}{m\omega}\hat{U}^+(\frac{\pi}{2\omega})\hat{p}$$

Therefore

$$\hat{p}\hat{U}^+(\frac{\pi}{2\omega})|x\rangle=m\omega\hat{U}^+(\frac{\pi}{2\omega})\hat{x}|x\rangle=m\omega x\hat{U}^+(\frac{\pi}{2\omega})|x\rangle$$

$\hat{U}^+(\frac{\pi}{2\omega})|x\rangle$ is the eigenket of $\hat{p}$ with the eigenvalue $m\omega x$

and

$$\hat{x}\hat{U}^+(\frac{\pi}{2\omega})|p\rangle=-\frac{1}{m\omega}\hat{U}^+(\frac{\pi}{2\omega})\hat{p}|p\rangle=-\frac{p}{m\omega}\hat{U}^+(\frac{\pi}{2\omega})|p\rangle$$

$\hat{U}^+(\frac{\pi}{2\omega})|p\rangle$ is the eigenket of $\hat{x}$ with the eigenvalue $-\frac{p}{m\omega}$.

(d) At $t = 0$, the wave function of the oscillator is $|\psi(0)\rangle$

$$|\psi(t)\rangle=\hat{U}(t)|\psi(0)\rangle.$$

Then the wave function is given by

$$\langle x|\psi(t)\rangle = \langle x|\hat{U}(t)|\psi(0)\rangle$$
$$= \int \langle x|\hat{U}(t)|x'\rangle dx' \langle x'|\psi(0)\rangle$$
$$= \int \langle x|\hat{U}(t)|x'\rangle dx' \psi(x',0)$$

We now calculate

$$\langle x|\hat{U}(t=\frac{q\pi}{2\omega})|x'\rangle$$

When $t=\frac{q\pi}{2\omega}$, we have

$$\hat{U}^{+}(\frac{q\pi}{2\omega})\hat{p}\hat{U}(\frac{q\pi}{2\omega}) = i\sqrt{\frac{m\hbar\omega}{2}}(e^{iq\frac{\pi}{2}}\hat{a}^{+} - e^{-iq\frac{\pi}{2}}\hat{a})$$
$$= i\sqrt{\frac{m\hbar\omega}{2}}e^{iq\frac{\pi}{2}}[\hat{a}^{+} - (-1)^{q}\hat{a}]$$

$$\hat{U}^{+}(\frac{q\pi}{2\omega})\hat{x}\hat{U}(\frac{q\pi}{2\omega}) = \sqrt{\frac{\hbar}{2m\omega}}e^{iq\frac{\pi}{2}}[\hat{a}^{+} + (-1)^{q}\hat{a}]$$

(i) For $q = 1$

$$\hat{U}^{+}(\frac{q\pi}{2\omega})\hat{p}\hat{U}(\frac{q\pi}{2\omega}) = -\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^{+} + \hat{a}) = -m\omega\hat{x}$$

$$\hat{U}^{+}(\frac{q\pi}{2\omega})\hat{x}\hat{U}(\frac{q\pi}{2\omega}) = i\sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^{+} - \hat{a}) = \frac{\hat{p}}{m\omega}$$

Thus we have

$$\hat{p}\hat{U}^{+}(\frac{q\pi}{2\omega})|x\rangle = m\omega x\hat{U}^{+}(\frac{q\pi}{2\omega})|x\rangle$$

which means that $\hat{U}^{+}(\frac{q\pi}{2\omega})|x\rangle$ is the eigenket of $\hat{p}$ with the eigenvalue $m\omega x$.

$$\hat{U}^{+}(\frac{q\pi}{2\omega})|x\rangle = |p = m\omega x\rangle$$

(ii) For $q = 2$

$$\hat{U}^+(\frac{q\pi}{2\omega})\hat{p}\hat{U}(\frac{q\pi}{2\omega}) = -i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^+ - \hat{a}) = -\hat{p}$$

$$\hat{U}^+(\frac{q\pi}{2\omega})\hat{x}\hat{U}(\frac{q\pi}{2\omega}) = -\sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^+ + \hat{a}) = -\hat{x}$$

Thus

$$\hat{x}\hat{U}^+(\frac{q\pi}{2\omega})|x\rangle = -x\hat{U}^+(\frac{q\pi}{2\omega})|x\rangle$$

which means that $\hat{U}^+(\frac{q\pi}{2\omega})|x\rangle$ is the eigenket of $\hat{x}$ with the eigenvalue (-*x*).

$$\hat{U}^+(\frac{q\pi}{2\omega})|x\rangle = |-x\rangle$$

(iii) For $q = 3$

$$\hat{U}^+(\frac{q\pi}{2\omega})\hat{p}\hat{U}(\frac{q\pi}{2\omega}) = \sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^+ + \hat{a}) = m\omega\hat{x}$$

$$\hat{U}^+(\frac{q\pi}{2\omega})\hat{x}\hat{U}(\frac{q\pi}{2\omega}) = -i\sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^+ - \hat{a}) = -\frac{\hat{p}}{m\omega}$$

$$\hat{p}\hat{U}^+(\frac{q\pi}{2\omega})|x\rangle = -m\omega x\hat{U}^+(\frac{q\pi}{2\omega})|x\rangle$$

which means that $\hat{U}^+(\frac{q\pi}{2\omega})|x\rangle$ is the eigenket of $\hat{p}$ with the eigenvalue $-m\omega x$.

$$\hat{U}^+(\frac{q\pi}{2\omega})|x\rangle = |p = -m\omega x\rangle$$

(iv) For $q = 4$

$$\hat{U}^+(\frac{q\pi}{2\omega})\hat{p}\hat{U}(\frac{q\pi}{2\omega}) = i\sqrt{\frac{m\hbar\omega}{2}}(\hat{a}^+ - \hat{a}) = \hat{p}$$

$$\hat{U}^+(\frac{q\pi}{2\omega})\hat{x}\hat{U}(\frac{q\pi}{2\omega}) = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^+ + \hat{a}) = \hat{x}$$

Thus

$$\hat{x}\hat{U}^{+}(\frac{q\pi}{2\omega})\left|x\right\rangle = x\hat{U}^{+}(\frac{q\pi}{2\omega})\left|x\right\rangle$$

which means that $\hat{U}^{+}(\frac{q\pi}{2\omega})\left|x\right\rangle$ is the eigenket of $\hat{x}$ with the eigenvalue x.

$$\hat{U}^{+}(\frac{q\pi}{2\omega})\left|x\right\rangle = \left|x\right\rangle$$

Here we note that

$$\hat{a}^{+} + \hat{a} = \sqrt{\frac{2m\omega}{\hbar}}\hat{x},$$

$$\hat{a}^{+} - \hat{a} = -i\sqrt{\frac{2}{m\hbar\omega}}\hat{p}$$

From the above discusion, we have a repeated pattern for $q = 4n+k$ (n; interger, q = 0, 1, 2, 3).

(i) For $q = 4n + 1$

$$\begin{aligned}\left\langle x\right|\hat{U}(\frac{q\pi}{2\omega})\left|\psi(0)\right\rangle &= \int \left\langle x\right|\hat{U}(\frac{q\pi}{2\omega})\left|x'\right\rangle dx'\psi(x',0)\\ &= \int \left\langle p = m\omega x\right|\left.x'\right\rangle\left\langle x'\right|\left.\psi(0)\right\rangle dx'\\ &= \left\langle p = m\omega x\right|\left.\psi(0)\right\rangle\end{aligned}$$

(ii) For $q = 4n + 2$

$$\begin{aligned}\left\langle x\right|\hat{U}(\frac{q\pi}{2\omega})\left|\psi(0)\right\rangle &= \int \left\langle x\right|\hat{U}(\frac{q\pi}{2\omega})\left|x'\right\rangle dx'\psi(x',0)\\ &= \int \left\langle -x\right|\left.x'\right\rangle\left\langle x'\right|\left.\psi(0)\right\rangle dx'\\ &= \int \delta(x'+x)\left\langle x'\right|\left.\psi(0)\right\rangle dx'\\ &= \left\langle -x\right|\left.\psi(0)\right\rangle\end{aligned}$$

(iii) For $q = 4n + 3$

$$\langle x|\hat{U}(\frac{q\pi}{2\omega})|\psi(0)\rangle = \int \langle x|\hat{U}(\frac{q\pi}{2\omega})|x'\rangle dx'\psi(x',0)$$

$$= \int \langle p=-m\omega x|x'\rangle\langle x'|\psi(0)\rangle dx'$$

$$= \langle p=-m\omega x|\psi(0)\rangle$$

(iv) For $q = 4n+4$

$$\langle x|\hat{U}(\frac{q\pi}{2\omega})|\psi(0)\rangle = \int \langle x|\hat{U}(\frac{q\pi}{2\omega})|x'\rangle dx'\psi(x',0)$$

$$= \int \langle x|x'\rangle\langle x'|\psi(0)\rangle dx'$$

$$= \int \delta(x'-x)\langle x'|\psi(0)\rangle dx'$$

$$= \langle x|\psi(0)\rangle$$

(e)

$$\psi(x,0) = \langle x|n\rangle$$

(i) For $q = 4n+1$

$$\left\langle x\middle|\psi(t=\frac{q\pi}{2\omega}\right\rangle = \langle p=m\omega x|n\rangle$$

(ii) For $q = 4n+2$

$$\left\langle x\middle|\psi(t=\frac{q\pi}{2\omega}\right\rangle = \langle -x|n\rangle$$

(iii) For $q = 4n+3$

$$\left\langle x\middle|\psi(t=\frac{q\pi}{2\omega}\right\rangle = \langle p=-m\omega x|n\rangle$$

(iv) For $q = 4n+4$

$$\left\langle x\middle|\psi(t=\frac{q\pi}{2\omega}\right\rangle = \langle x|n\rangle$$

(f)

(i)

$$\langle x|\psi(0)\rangle = e^{ikx}$$

$$\begin{aligned}\langle p|\psi(0)\rangle &= \int \langle p|x\rangle dx \langle x|\psi(0)\rangle \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int dx e^{-\frac{i}{\hbar}px} e^{ikx} \\ &= \frac{1}{\sqrt{2\pi\hbar}} \delta\left(\frac{p-\hbar k}{\hbar}\right) = \frac{1}{\sqrt{2\pi\hbar}} \hbar\delta(p-\hbar k)\end{aligned}$$

(ii)

$\langle x|\psi(0)\rangle = e^{-\rho x}$ for $x>0$, and 0 otherwise

$$\begin{aligned}\langle p|\psi(0)\rangle &= \int \langle p|x\rangle dx \langle x|\psi(0)\rangle \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int dx e^{-\frac{i}{\hbar}px} e^{\rho x} \\ &= \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{\rho - \frac{i}{\hbar} p}\end{aligned}$$

(iii)

$\langle x|\psi(0)\rangle = \frac{1}{\sqrt{a}}$ only for $|x| < \frac{a}{2}$.

$$\begin{aligned}\langle p|\psi(0)\rangle &= \int_{-a/2}^{a/2} \langle p|x\rangle dx \langle x|\psi(0)\rangle \\ &= \frac{1}{\sqrt{2\pi\hbar a}} 2\int_0^{a/2} \cos\left(\frac{px}{\hbar}\right) e dx \\ &= \frac{1}{\sqrt{2\pi\hbar}} \frac{\sin\left(\frac{ap}{2\hbar}\right)}{\frac{p}{2\hbar}}\end{aligned}$$

(iv)

$$\langle x|\psi(0)\rangle = e^{-\rho^2 x^2}$$

$$\langle p|\psi(0)\rangle = \int \langle p|x\rangle dx \langle x|\psi(0)\rangle$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int dx e^{-\frac{i}{\hbar}px} e^{-\rho^2 x^2}$$

$$= \frac{1}{2\sqrt{2\hbar}} \frac{e^{-\frac{p^2}{4\hbar^2\rho^2}}}{\rho} [1 - iErfi(\frac{p}{2\hbar\rho})]$$

APPENDIX-F
Heisenberg's picture for simple harmonics

The Hamilonian of the simple harmonics is given by

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

(a) **Relation between the the Hesenberg's picture and Schrödinger picture**

$$\hat{x}_H(t) = \exp(\frac{i}{\hbar}\hat{H}t)\hat{x}\exp(\frac{i}{\hbar}\hat{H}t)$$

$$\hat{p}_H(t) = \exp(\frac{i}{\hbar}\hat{H}t)\hat{p}\exp(\frac{i}{\hbar}\hat{H}t)$$

$$\hat{a}_H(t) = \exp(\frac{i}{\hbar}\hat{H}t)\hat{a}\exp(\frac{i}{\hbar}\hat{H}t)$$

$$\hat{a}_H{}^+(t) = \exp(\frac{i}{\hbar}\hat{H}t)\hat{a}^+\exp(\frac{i}{\hbar}\hat{H}t)$$

(b) **Heisenberg's equation of motion**:

$$\frac{d}{dt}\hat{x}_H(t) = \frac{i}{\hbar}[\hat{H}, \hat{x}_H(t)] = \exp(\frac{i}{\hbar}\hat{H}t)\frac{i}{\hbar}[\hat{H}, \hat{x}]\exp(\frac{i}{\hbar}\hat{H}t) = \frac{1}{m}\hat{p}_H(t) ,$$

$$\frac{d}{dt}\hat{p}_H(t) = \frac{i}{\hbar}[\hat{H}, \hat{p}_H(t)] = -m\omega_0{}^2\hat{x}_H$$

$$\frac{d}{dt}\hat{a}_H(t) = \frac{i}{\hbar}[\hat{H}, \hat{a}_H(t)] = -i\omega_0\hat{a}_H(t)$$

$$\frac{d}{dt}\hat{a}_H{}^+(t) = \frac{i}{\hbar}[\hat{H}, \hat{a}_H{}^+(t)] = i\omega_0 \hat{a}_H{}^+(t)$$

where

$$[\hat{H}, \hat{x}] = \frac{1}{2m}[\hat{p}^2, \hat{x}] = -\frac{1}{2m}[\hat{x}, \hat{p}^2] = -\frac{1}{2m} i\hbar \frac{\partial}{\partial \hat{p}} \hat{p}^2 = -\frac{1}{2m} i\hbar 2\hat{p} = -\frac{i\hbar}{m}\hat{p} ,$$

$$[\hat{H}, \hat{p}] = \frac{1}{2} m\omega_0^2 [\hat{x}^2, \hat{p}] = -\frac{1}{2} m\omega_0^2 [\hat{p}, \hat{x}^2] = -\frac{1}{2} m\omega_0^2 \frac{\hbar}{i} \frac{\partial}{\partial \hat{x}} \hat{x}^2 = -\frac{1}{2} m\omega_0^2 \frac{\hbar}{i} 2\hat{x} = i\hbar m\omega_0^2 \hat{x}$$

,

$$[\hat{H}, \hat{a}] = \hbar\omega_0 [\hat{a}^+\hat{a} + \frac{1}{2}\hat{1}, \hat{a}] = -\hbar\omega_0 \hat{a} ,$$

$$[\hat{H}, \hat{a}^+] = \hbar\omega_0 [\hat{a}^+\hat{a} + \frac{1}{2}\hat{1}, \hat{a}^+] = \hbar\omega_0 \hat{a}^+$$

$$\hat{a}_H(t) = \exp(-i\omega_0 t)\hat{a}_H(0)$$

or

$$x_H(t) + \frac{i}{m\omega_0}\hat{p}_H(t) = \exp(-i\omega_0 t)[\hat{x}_H(0) + \frac{i}{m\omega_0}\hat{p}_H(0)]$$

$$\hat{a}_H{}^+(t) = \exp(i\omega_0 t)\hat{a}_H{}^+(0)$$

or

$$x_H(t) - \frac{i}{m\omega_0}\hat{p}_H(t) = \exp(i\omega_0 t)[\hat{x}_H(0) - \frac{i}{m\omega_0}\hat{p}_H(0)]$$

Then from the above two equations, we get

$$x_H(t) = \cos(\omega_0 t)\hat{x}_H(0) + \frac{\hat{p}_H(0)}{m\omega_0}\sin(\omega_0 t)$$
$$= \cos(\omega_0 t)\hat{x} + \frac{\hat{p}}{m\omega_0}\sin(\omega_0 t),$$

$$p_H(t) = -m\omega_0 \sin(\omega_0 t)\hat{x}_H(0) + \hat{p}_H(0)\cos(\omega_0 t)$$
$$= -m\omega_0 \sin(\omega_0 t)\hat{x} + \hat{p}\cos(\omega_0 t)$$

These are the same as the classical equation of motion.

(c). Approach from the Baker-Hausdorff lemma

The operators of the Heisenberg picture can be obtained from those of the Schrodinger picture by using the Baker-Hausdorff lemma.

$$\hat{x}_H(t) = \exp(\frac{i}{\hbar}\hat{H}t)\hat{x}\exp(\frac{i}{\hbar}\hat{H}t)$$

We use the Baker-Hausdorff lemma

$$\exp(i\lambda\hat{G})\hat{A}\exp(-i\lambda\hat{G}) = \hat{A} + i\lambda[\hat{G},\hat{A}] + \frac{(i\lambda)^2}{2!}[G,[\hat{G},\hat{A}]] + \frac{(i\lambda)^3}{3!}[\hat{G},[\hat{G},[\hat{G},\hat{A}]]]$$

When $\lambda = \frac{t}{\hbar}$, $\hat{G} = \hat{H}$, $\hat{A} = \hat{x}$

$$\exp(i\frac{t}{\hbar}\hat{H})\hat{x}\exp(-i\frac{t}{\hbar}\hat{H}) = \hat{x} + i\frac{t}{\hbar}[\hat{H},\hat{x}] + \frac{(i)^2}{2!}\left(\frac{t}{\hbar}\right)^2[\hat{H},[\hat{H},\hat{x}]$$
$$+ \frac{(i)^3}{3!}\left(\frac{t}{\hbar}\right)^3[\hat{H},[\hat{H},[\hat{H},\hat{x}]] + \frac{(i)^4}{4!}\left(\frac{t}{\hbar}\right)^4[\hat{H},[\hat{H},[\hat{H},[\hat{H},\hat{x}]]]....$$

where

$$[\hat{H},\hat{x}] = -\frac{i\hbar}{m}\hat{p}, \qquad [\hat{H},\hat{p}] = i\hbar m{\omega_0}^2\hat{x}$$

$$[\hat{H},[\hat{H},\hat{x}]] = [\frac{1}{2}m{\omega_0}^2\hat{x}^2, -\frac{i\hbar}{m}\hat{p}] = \hbar^2{\omega_0}^2\hat{x},$$

$$[\hat{H},[\hat{H},[\hat{H},\hat{x}]]] = [\hat{H},\hbar^2{\omega_0}^2\hat{x}] = \hbar^2{\omega_0}^2[\hat{H},\hat{x}] = -\frac{i\hbar^3{\omega_0}^2}{m}\hat{p}$$

$$[\hat{H},[\hat{H},[\hat{H},[\hat{H},\hat{x}]]]] = [\hat{H},-\frac{i\hbar^3{\omega_0}^2}{m}\hat{p}] = -\frac{i\hbar^3{\omega_0}^2}{m}(i\hbar m{\omega_0}^2)\hat{x} = \hbar^4{\omega_0}^4\hat{x}$$

$$[H,[\hat{H},[\hat{H},[\hat{H},[\hat{H},\hat{x}]]]]] = [\hat{H},\hbar^4{\omega_0}^4\hat{x}] = \hbar^4{\omega_0}^4(-\frac{i\hbar}{m}\hat{p}) = -\frac{i\hbar^5{\omega_0}^4}{m}\hat{p}$$

Then we get

$$\begin{aligned}
\exp(i\frac{t}{\hbar}\hat{H})\hat{x}\exp(-i\frac{t}{\hbar}\hat{H}) &= \hat{x} + i\frac{t}{\hbar}(-\frac{i\hbar}{m}\hat{p}) + \frac{(i)^2}{2!}\left(\frac{t}{\hbar}\right)^2(\hbar^2{\omega_0}^2\hat{x}) \\
&+ \frac{(i)^3}{3!}\left(\frac{t}{\hbar}\right)^3(-\frac{i\hbar^3{\omega_0}^2}{m}\hat{p}) + \frac{(i)^4}{4!}\left(\frac{t}{\hbar}\right)^4(\hbar^4{\omega_0}^4\hat{x}) + \frac{(i)^5}{5!}\left(\frac{t}{\hbar}\right)^5(-\frac{i\hbar^5{\omega_0}^4}{m}\hat{p}) + \\
&= \hat{x} + \frac{\hat{p}}{m\omega_0}(\omega_0 t) - \frac{1}{2!}(\omega_0 t)^2\hat{x} - \frac{1}{3!}(\omega_0 t)^3\frac{\hat{p}}{m\omega_0} + \frac{1}{4!}(\omega_0 t)^4\hat{x} + \frac{1}{5!}(\omega_0 t)^5\frac{\hat{p}}{m\omega_0} + ... \\
&= [1 - \frac{1}{2!}(\omega_0 t)^2 + \frac{1}{4!}(\omega_0 t)^4 + ...]\hat{x} + [\omega_0 t - -\frac{1}{3!}(\omega_0 t)^3 + \frac{1}{5!}(\omega_0 t)^5 + ...]\frac{\hat{p}}{m\omega_0} \\
&= \cos(\omega_0 t)\hat{x} + \frac{\hat{p}}{m\omega_0}\sin(\omega_0 t)
\end{aligned}$$

Since

$$\begin{aligned}
\hat{p}_H(t) &= m\frac{d}{dt}\hat{x}_H(t) \\
&= m[-\omega_0\sin(\omega_0 t)\hat{x} + \frac{\hat{p}}{m\omega_0}\omega_0\cos(\omega_0 t)] \\
&= -m\omega_0\sin(\omega_0 t)\hat{x} + \hat{p}\cos(\omega_0 t)]
\end{aligned}$$