THE HARMONIC OSCILLATOR (HO)

HO is the single quantum system most important in QM.

Equilibrium:

Displacement:

The classical equation is:

\[ m \ddot{x} = -kx, \quad 0 < k = \text{spring constant} \]

Def:

\[ \omega_0^2 = \frac{k}{m} \Rightarrow k = MW_0^2 \quad \text{and} \]

\[ \Rightarrow \quad \ddot{x} + \omega_0^2 x = 0 \]

Multiplying this eq. by \( \frac{dx}{dt} \) we obtain:

\[ \dot{x} \ddot{x} + \omega_0^2 x \dot{x} = 0 \]

but

\[ \frac{1}{2} \frac{d}{dt}(x^2) = \dot{x} \dot{x} \quad \text{and} \quad \frac{1}{2} \frac{d}{dt}(\dot{x}^2) = \dot{x} \ddot{x} \Rightarrow \]

\[ \Rightarrow \quad \frac{d}{dt} \left[ \frac{1}{2} (\dot{x}^2 + \omega_0^2 x^2) \right] = 0 \]
Therefore, the quantity

\[ \frac{E}{m} = \frac{1}{2} \dot{x}^2 + \frac{k}{2} x^2 \]

is a constant of motion: \( \frac{dE}{dt} = 0 \)

\[ E = \frac{1}{2} m \dot{x}^2 + \frac{k}{2} x^2 \]

- Kinetic energy
- Potential energy \( V(x) \)

The turning points \( \pm x_0 \) are found by imposing the zero-velocity condition:

\[ E = V(x_0) = \frac{k}{2} x_0^2 \]

\[ x_0 = \pm \frac{2E}{k} \]

\[ E = \frac{k}{2m} \frac{d^2}{dx^2} + \frac{k}{2} x^2 \]

In quantum mechanics,

\[ E \rightarrow E(\hat{p}, \hat{x}) = \hat{A} = \frac{\hat{p}^2}{2m} + \frac{k}{2} \hat{x}^2 \]

\[ = - \frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{k}{2} x^2 \]
For $-x_0 \leq x \leq x_0$, we have $E \geq V(x)$ and

$$\hat{U}(x) = Eu(x) \quad (SE)$$

becomes:

$$U''(x) = -k^2(x)U(x)$$

while

$$k^2(x) = \frac{2m}{\hbar^2} \left( E - \frac{kx^2}{2} \right) \geq 0$$

$\Rightarrow U(x)$ is oscillating.

In the classically forbidden region: $x^2 > x_0^2$, $E < kx^2/2$

and SE becomes:

$$U''(x) = q^2(x)U(x)$$

while

$$q^2(x) = \frac{2m}{\hbar^2} \left( \frac{kx^2}{2} - E \right) > 0$$

For $x^2 \gg x_0^2$, $\frac{kx^2}{2}$ is arbitrarily big with respect to $E$

and, approximately:

$$q(x) \approx \frac{m \omega_0}{\hbar} \frac{x^2}{x^2} \approx \left( \frac{m \omega_0}{\hbar} \right)^2 x^2$$

Define: $\beta^2 = \frac{m \omega_0}{\hbar}$

Then, noticing that:

$$\frac{1}{2} \frac{d}{dx} \left( \pm \beta^2 x^2 \right) = \pm \beta x \frac{d}{dx} \left( \pm \beta^2 x^2 \right) = \pm \beta^2 f + \beta^4 x^2 f$$

$$= f(x)$$

if $x^2 \gg x_0^2$
Therefore, asymptotically:

\[ U(x) \sim \exp \left[ \pm \left( \frac{mw_0}{\hbar} \right)^{\frac{1}{2}} x^2 \right] \]

The + solution is not normalizable and, therefore, is discarded. The expected behavior is therefore:

Let us find eigenvalues \( E_n \) and eigenfunctions \( U_n(x) \) using an algebraic method. Let us DEFINE the new operators:

\[ \hat{a} = \frac{\beta}{\sqrt{2}} \left( \hat{x} + i \frac{\hat{p}}{mw_0} \right); \quad \hat{a}^+ = \frac{\beta}{\sqrt{2}} \left( \hat{x} - i \frac{\hat{p}}{mw_0} \right); \quad \beta^2 = \frac{mw_0}{\hbar} \]

where we used \( \hat{x} = \hat{x}^+ \) and \( \hat{p} = \hat{p}^+ \).

From \( [\hat{x}, \hat{p}] = i \hbar \) it follows that \( [\hat{a}, \hat{a}^+] = 1 \).

From inversion:

\[ \hat{x} = \frac{\hat{a} + \hat{a}^+}{\sqrt{2} \beta}; \quad \hat{p} = -i mw_0 \frac{\hat{a} - \hat{a}^+}{\sqrt{2} \beta} \]
\[ \hat{H} = \frac{\hat{p}^2}{2m} + \frac{\hbar}{2} \hat{x}^2 = \hbar \omega_0 \left( \hat{\alpha}^+ \hat{\alpha} + \frac{1}{2} \right) \]

\( \hat{\alpha} = \text{ANNIHILATION (OR DISTRUCTION) OPERATOR} \)
\( \hat{\alpha}^+ = \text{CREATION OPERATOR} \)
\( \hat{N} = \hat{\alpha}^+ \hat{\alpha} = \text{NUMBER OPERATOR} \)

Therefore
\[ \hat{H} = \hbar \omega_0 \left( \hat{N} + \frac{1}{2} \right) \]  
(1.5)

Also note that
\[ \frac{1}{\pi} = \frac{[\hat{\alpha}, \hat{\alpha}^+]}{\hbar} = \frac{\hat{\alpha}^+ \hat{\alpha} - \hat{\alpha} \hat{\alpha}^+}{\hbar} \implies \]
\[ \hat{H} = \frac{\hbar \omega_0}{2} (\hat{\alpha}^+ \hat{\alpha} + \hat{\alpha} \hat{\alpha}^+) \text{ Symmetric form.} \]

From (1.5) \( \Rightarrow \) eigenfunctions of \( \hat{H} = \) eigenfunctions of \( \hat{N} \):

let: \( \hat{N} u_n(x) = \lambda_n u_n(x) \)

and consider
\[ \hat{N} (\hat{\alpha} u_n) = (\hat{\alpha}^+ \hat{\alpha}) u_n \]
\[ = (\hat{\alpha}^+ \hat{\alpha} - \hat{\alpha} \hat{\alpha}^+) u_n \]
\[ = -(\hat{\alpha}^+ \hat{\alpha} - 1) u_n \]
\[ = (\hat{\alpha}^+ - 1) u_n \]
\[ = \hat{\alpha} \hat{N} u_n = \hat{\alpha} (\lambda_n - 1) u_n \]
\[ = (\lambda_n - 1) \hat{\alpha} u_n \]

\( \text{(CAVEAT: here and henceforth we will often omit the "hat" to mark operators) } \)
Therefore, if \( u_n \) is an eigenfunction of \( \hat{N} \) with eigenvalue \( \lambda_n \), then \( \hat{a}^+ u_n \) is an eigenfunction with eigenvalue \( \lambda_{n-1} \):

\[
\hat{N} (\hat{a}^+ u_n) = (\lambda_{n+1}) (\hat{a}^+ u_n) \tag{1.6}
\]

In a similar way, one can show that:

\[
\hat{N} \left( \hat{a}^+ u_n \right) = (\lambda_{n+1}) (\hat{a}^+ u_n)
\]

Since both \( \lambda_{n-1} \) and \( \lambda_{n+1} \) must belong to the spectrum of \( \hat{N} \), there exist 2 values of \( n \), say \( n_- \) and \( n_+ \), such that:

\[
\hat{N} u_{n_-} = \left( \lambda_{n-1} \right) u_{n_-} \quad \text{with} \quad u_{n_-} = \hat{a} u_n
\]

\[
\hat{N} u_{n_+} = \left( \lambda_{n+1} \right) u_{n_+} \quad \text{with} \quad u_{n_+} = \hat{a}^+ u_n
\]

\[
\hat{N} u_n = \lambda_n u_n
\]

By definition,

\[
\langle \hat{N} \rangle_q = \int q^* (\hat{N} q) dq = \int q^* \hat{a}^* (\hat{a} q) dq
\]

\[
= \int (\hat{a} q)^* (\hat{a} q) dq = \| \hat{a} q \|^2 \geq 0
\]

Therefore:

\[
\langle \hat{N} \rangle_{n_+} = \int u_{n_+}^* (\hat{N} u_{n_+}) dq = \lambda_{n_+} \int |u_{n_+}|^2 dq \geq 0 \Rightarrow \lambda_{n_+} \geq 0 \quad \forall n_+
\]
Let \( n = n_0 \) the minimum value of \( n \) for which \( \lambda_{n_0} \geq 0 \) but \( \lambda_{n_0} - 1 < 0 \).

![Diagram]

For this value we have
\[
\hat{N}U_{n_0} = \lambda_{n_0} U_{n_0}
\]
but also \( \hat{N}(\hat{\lambda}U_{n_0}) = (\lambda_{n_0} - 1)(\hat{\lambda}U_{n_0}) < 0 \).

But \( \lambda_{n_0} - 1 < 0 \), cannot belong to the spectrum of \( \hat{N} \), therefore it must be \( \hat{\lambda}U_{n_0} = 0 \).

However, if this is true, then
\[
\hat{N}U_{n_0} = \begin{cases} 
\hat{\lambda}^2 U_{n_0} & 0 \\
\lambda_{n_0} U_{n_0} &
\end{cases} \Rightarrow \lambda_{n_0} = 0
\]

By convention, we put \( n_0 = 0 \) and we write
\[
\begin{cases} 
\hat{\lambda}U_0 = 0 \\
\lambda_0 = 0
\end{cases}
\]
Now we can apply (1.6) to calculate
\[ \hat{N}(\hat{a}^+ u_0) = (\chi_{\alpha+\epsilon}) (\lambda^+ u_0) \]
\[ = 1 - \hat{a}^+ u_0 \Leftrightarrow \hat{a}^+ u_0 \text{ does not cross } U_2 \]

Similarly, since
\[ \hat{N} \hat{a}^+ = a^+(a a^+) \]
\[ = a^+ (a a^+ - a^+ a + \hat{N}) \]
\[ = e^+ a^+ a + \hat{N} \]
\[ = a^+ + a^+ N \]

Then
\[ \hat{N} a^+ = (N a^+) a^+ \]
\[ = a^+ (a a^+ - a^+ a + \hat{N}) \]
\[ = a^+ (a a^+ - a^+ a + \hat{N}) \]
\[ = 2 a^+ a + a^+ N \]

Therefore
\[ \hat{N}(a^2 u_0) = 2(\hat{a}^2 u_0) \Leftrightarrow \hat{a}^2 u_0 \text{ does not cross } U_2 \]

and so on. Suppose that \( u_n(x) \) are normalized,
\[ \int u_n^* u_n \, dx = 1 \]

Then, if I write
\[ \hat{a}^n = c u_{n-1} \]

I have:
\[ \int (\hat{a}^n)^* (\hat{a}^n) \, dx = 1 c^2 \int |u_{n-1}|^2 \, dx \]
\[ = 1 \text{ by hypothesis} \]
\[ l^2 = \int u_n^{*} \hat{a}^{+} a u_n dx = n \int u_n^{*} u_n dx = n \]

\[ \Rightarrow \hat{a} u_n = \sqrt{n} \ u_{n-1} \]

So:

This is consistent with \( \hat{a} u_0 = 0 \)

Similarly, if \( \hat{a}^{+} u_n = d u_{n+1} \)

Then

\[ \int (a^{+} u_n)^{*} (a^{+} u_n) dx = l d l^2 \]

\[ \Rightarrow \int u_n^{*} a a^{+} u_n dx = l d l^2 \]

\[ \Rightarrow l d l^2 = \int u_n^{*} (a^{+} a a^{+} a + \vec{n}) u_n dx \]

\[ = (1+n) \Rightarrow l d l = \sqrt{n+1} \]

And

\[ \hat{a}^{+} u_n = \sqrt{n+1} u_{n+1} \]

If we know \( u_0 \), we can calculate ALL the eigenstates. So, let us find \( u_0 \):
The spectrum of the HO is made like this.

<table>
<thead>
<tr>
<th>n</th>
<th>En</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$\frac{1}{2}t_w \omega_0$</td>
</tr>
<tr>
<td>1</td>
<td>$\frac{3}{2}t_w \omega_0$</td>
</tr>
<tr>
<td>2</td>
<td>$\frac{5}{2}t_w \omega_0$</td>
</tr>
<tr>
<td>3</td>
<td>$\frac{7}{2}t_w \omega_0$</td>
</tr>
</tbody>
</table>

$E_0 \quad E_1 \quad E_2 \quad E_3$

--- Eigenfunctions ---

Define $\xi^2 \equiv \frac{m \omega_0}{\hbar} x^2 \equiv \beta^2 x^2$ \(\Rightarrow\)

\[
\begin{align*}
\hat{a} &= \frac{1}{\sqrt{2}} \left( \xi + \frac{1}{\xi} \right) \\
\hat{a}^+ &= \frac{1}{\sqrt{2}} \left( \xi - \frac{1}{\xi} \right)
\end{align*}
\]  \hspace{1cm} (1.10)

Then $\hat{H} \Psi = E \Psi \Leftrightarrow \hbar \omega_0 (\hat{a}^+ \hat{a} + \frac{1}{2}) \Psi = E \Psi$

becomes

\[
(\hat{a} \hat{a}^+ + 1) \Psi = \frac{2E}{\hbar \omega_0} \Psi \quad \text{(2.10)}
\]

but $\hat{a}^+ \hat{a} \Psi = (\xi - \frac{1}{\xi})(\xi + \frac{1}{\xi}) \Psi$

$= (3 - \frac{1}{\xi^2})(\xi \Psi + \Psi)$
\[ \frac{\partial^2 u}{\partial t^2} u + \nabla^2 u - u \nabla^2 u = 0 \]

\[ (2a^2 + 1) u = -u'' + u + 5^2 u + u \]

Therefore

\[ (2.10) \Rightarrow -u'' + 5^2 u - \frac{2E}{\hbar \omega_0} u = 0 \]

\[ \Rightarrow \quad \left( -u'' + \left( \frac{2E}{\hbar \omega_0} - 5^2 \right) \right) u = 0 \]

In the ground state \( E = E_0 = \frac{\hbar \omega_0}{2} \) \( \Rightarrow \)

\[ \Rightarrow \frac{d^2 u_0}{d \xi^2} + (1 - 5^2) u_0 = 0 \]

If we try: \( u_0(\xi) = A_0 e^{-\frac{\xi^2}{2}} \)

\[ \Rightarrow \frac{d u_0}{d \xi} = -\xi u_0 \quad \Rightarrow \frac{d^2 u_0}{d \xi^2} = -u_0 - 5 \frac{d u_0}{d \xi} \]

\[ = -u_0 + 5^2 u_0 \]

\[ \Rightarrow u_0'' + (1 - 5^2) u_0 = 0 \]

The normalization requires:

\[ 1 = \int |u_0|^2 d\xi = A_0^2 \int_{-\infty}^{\infty} e^{-\frac{\xi^2}{2}} d\xi = \sqrt{\pi} A_0^2 \quad \Rightarrow \quad A_0 = \frac{1}{\pi^{1/4}} \]

and

\[ u_0(\xi) = \frac{1}{\pi^{1/4}} \exp \left( -\frac{\xi^2}{2} \right) \quad (2.11) \]
In terms of $x$, we have:

$$U_0(x) = B_0 \ e^{-\beta x^2/2}$$

and

$$1 = \int_{-\infty}^{\infty} |U_0(x)|^2 \ dx = \frac{B_0^2}{\beta} \int_{-\infty}^{\infty} e^{-\frac{\beta x^2}{2}} \ dx = \frac{B_0^2 \sqrt{\pi}}{\beta}$$

$$\Rightarrow \ U_0(x) = \left( \frac{\beta}{\pi} \right)^{1/4} \exp \left( -\frac{\beta x^2}{2} \right) \quad (1.17)$$

The other eigenfunctions are found applying $a^+$ successively:

$$U_n = \frac{1}{\sqrt{n}} \ a^+ U_{n-1}$$

$$= \frac{1}{\sqrt{n}} \ a^+ \left( \frac{1}{\sqrt{n-1}} \ a^+ U_{n-2} \right)$$

$$= \frac{1}{\sqrt{n(n-1)}} \ (a^+)^2 U_{n-2}$$

$$= \frac{1}{\sqrt{n(n-1)\cdots(n-p)}} \ (a^+)^p U_{n-p} \quad \text{for } p \leq n$$

So:

$$U_n = \left( \frac{a^+}{\sqrt{n!}} \right)^n \ U_0$$

$$= A n \left( \frac{1}{\frac{d}{d\xi}} \right)^n e^{-\frac{\xi^2}{2}} \quad (2.12)$$
Clearly: for

\[ n=1 \quad \left( \xi - \frac{d}{d\xi} \right) e^{-\xi^2/2} = 2\xi e^{-\xi^2/2} \]

\[ n=2 \quad \left( \xi - \frac{d}{d\xi} \right)^2 = 2 \left( \xi - \frac{d}{d\xi} \right) (\xi e^{-\xi^2/2}) = 2 e^{-\xi^2/2} \left( \xi^2 - 1 + \xi^2 \right) \]

In general:

\[ \left( \xi - \frac{d}{d\xi} \right)^n e^{-\xi^2/2} = -H_n(\xi) e^{-\xi^2/2} \]

where:

\[ H_n(\xi) = \text{Hermite polynomials} \]

They are solution of the equation:

\[ H''_n - 2\xi H'_n + 2nH_n = 0 \]

So

\[ \begin{cases} 
 U_n(\xi) = A_n H_n(\xi) e^{-\xi^2/2} \\
 E_n = \hbar \omega_0 \left( n + \frac{1}{2} \right) 
\end{cases} \]

or

\[ U_n(x) = B_n H_n(\beta x) \exp\left( -\frac{\beta^2 x^2}{2} \right) \]
\[ I_n = \int u_n^*(x) u_m(x) \, dx \]

\[ = B_n B_m \int H_n(\beta x) H_m(\beta x) e^{-x^2 \beta^2} \, dx \]

\[ = \text{Constant} \quad 7.374 \]

\[ = \delta_{nm} \frac{1}{\beta} 2^n n! \sqrt{\pi} \]

\[ = \delta_{nm} \frac{B_n^2 2^n n! \sqrt{\pi}}{\beta} \]

\[ \Rightarrow \quad \text{Choose} \quad B_n = \sqrt{\frac{\beta^2}{\pi}} \frac{1}{\sqrt{2^n n!}} \]

Therefore:

\[ u_n(x) = \frac{\beta}{\sqrt{2^n n! \pi}} H_n(\beta x) \exp\left(-\frac{\beta^2 x^2}{2}\right) \]