* Lecture 12 *

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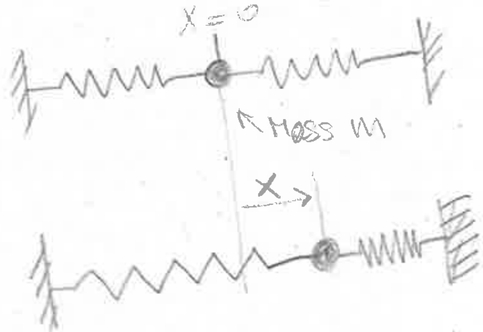
– THE HARMONIC OSCILLATOR (HO) –

HO is the single quantum system more important in QM.

Equilibrium:

Displacement:



The classical equation is:

$$m\frac{d^2x}{dt^2} = -Kx, \quad 0 < K = \text{spring constant}$$

Def: $\omega_0^2 \equiv \frac{K}{m} \Rightarrow K = m\omega_0^2$ and

$$\Rightarrow \boxed{\frac{d^2x}{dt^2} + \omega_0^2 x = 0}$$

Multiplying this eq. by $\frac{dx}{dt}$ we obtain

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

but $\frac{1}{2}\frac{d}{dt}(x^2) = x\dot{x}$ and $\frac{1}{2}\frac{d}{dt}(\dot{x}^2) = \dot{x}\ddot{x} \Rightarrow$

$$\Rightarrow \frac{d}{dt}\left[\frac{1}{2}(\dot{x}^2 + \omega_0^2 x^2)\right] = 0$$

Therefore the quantity

$$\frac{E}{m} \equiv \frac{1}{2}\dot{x}^2 + \frac{\omega_0^2}{2}x^2$$

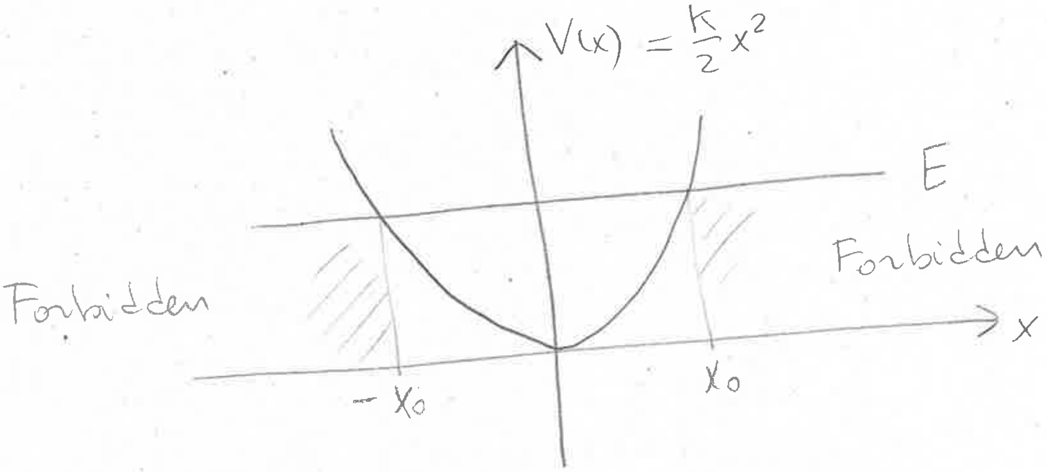
is a costant of motion : $\frac{dE}{dt} = 0$

$$E = \underbrace{\frac{1}{2}m\dot{x}^2}_{\text{Kinetic energy}} + \underbrace{\frac{K}{2}x^2}_{\text{potential energy } V(x)}$$

The TURNING POINTS $\pm x_0$ are found by imposing the zero-velocity condition:

$$E = V(x_0) = \frac{K}{2}x_0^2 \Rightarrow x_0 = \pm \frac{2E}{K}$$

$$= \pm \frac{2E}{m\omega_0^2}$$



In quantum mechanics,

$$E \to E(\hat{p},\hat{x}) \equiv \hat{H} = \frac{\hat{p}^2}{2m} + \frac{K}{2}\hat{x}^2$$

$$= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{K}{2}\hat{x}^2$$

For $-x_0 \leq x \leq x_0$, we have $E \geq V(x)$ and

$$\hat{H} u(x) = E u(x) \qquad (SE)$$

becomes:

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

where $$k^2(x) \equiv \frac{2m}{\hbar^2}\left(E - \frac{Kx^2}{2}\right) \geq 0$$

$\Rightarrow u(x)$ is oscillating

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

and SE becomes:

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

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

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

and, approximately: $$q(x) \underset{x^2 \gg x_0^2}{\simeq} \frac{mK}{\hbar^2} x^2$$

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

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

$$\equiv \beta^4 x^2$$

Then, noticing that:

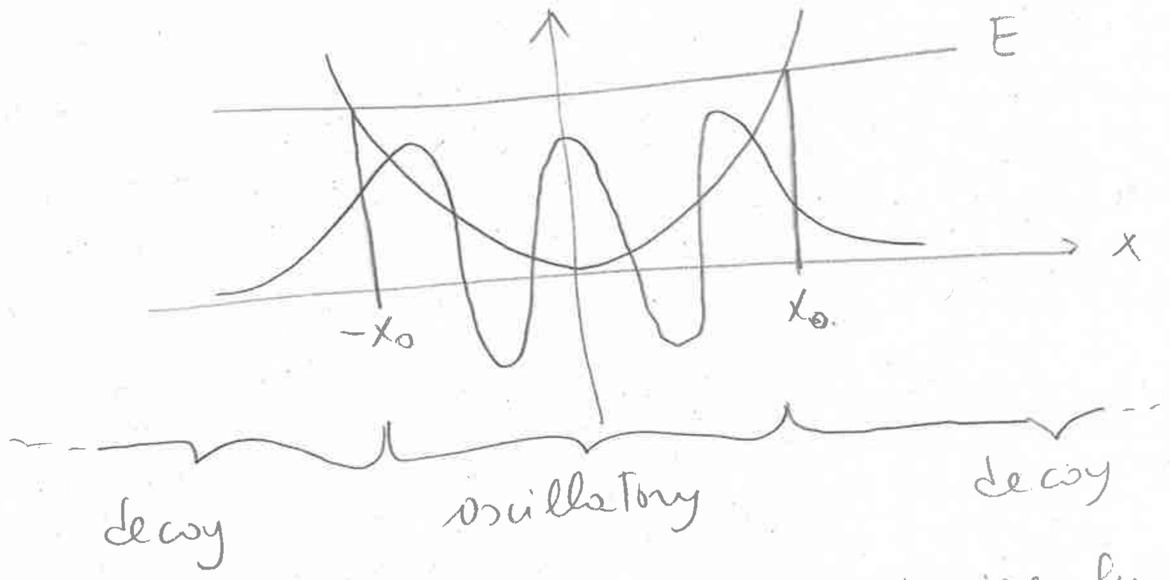
$$\frac{d}{dx} \underbrace{e^{\pm \frac{\beta^2 x^2}{2}}}_{=f(x)} = \pm \beta x e^{\pm \frac{\beta^2 x^2}{2}} \Rightarrow \frac{d^2}{dx^2} e^{\pm \frac{\beta^2 x^2}{2}} = \pm \beta^2 f + \beta^4 x^2 f$$

$$\simeq \beta^4 x^2 f \quad \text{if } x^2 \gg x_0^2$$

Therefore, asymptotically:

$$u(x) \sim \exp\left[\pm\left(\frac{m\omega_0}{\hbar}\right)\frac{x^2}{2}\right]$$

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:

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

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:

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

and

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

$\hat{a}$ = ANNIHILATION (OR DISTRUCTION) OPERATOR

$\hat{a}^+$ = CREATION OPERATOR

$\hat{N} \equiv \hat{a}^+\hat{a}$ = NUMBER OPERATOR

Therefore

$$\boxed{\hat{H} = \hbar\omega_0\left(\hat{N} + \frac{1}{2}\right)} \qquad (1.5)$$

Also note that $\frac{1}{2} = \frac{[\hat{a},\hat{a}^+]}{2} = \frac{\hat{a}\hat{a}^+}{2} - \frac{\hat{a}^+\hat{a}}{2} \Rightarrow$

$$\Rightarrow \hat{H} = \frac{\hbar\omega_0}{2}\left(\hat{a}^+\hat{a} + \hat{a}\hat{a}^+\right)$$ ← symmetric form.

From (1.5) ⇒ eigenfunctions of $\hat{H}$ = eigenfunctions of $\hat{N}$.

let :

$$\hat{N}u_n(x) = \lambda_n u_n(x)$$

and consider

$$\begin{aligned}
\hat{N}(\hat{a}u_n) &= (a^+a)a\,u_n \\
&= (\underbrace{a^+a - aa^+}_{=-1} + aa^+)a\,u_n \\
&= (aa^+ - 1)a\,u_n \\
&= a(a^+a - 1)u_n \\
&= \hat{a}(\hat{N} - 1)u_n = \hat{a}(\lambda_n - 1)u_n \\
&= (\lambda_n - 1)(\hat{a}u_n)
\end{aligned}$$

CAVEAT: here and hereafter we will often omit the "hat" to mark operators

Therefore, if u_n is an eigenfunction of $\hat{N}$ with eigenvalue λ_n, then "$\hat{a} u_n$" is an eigenfunction with eigenvalue $\lambda_n - 1$:

In a similar way, one can show that:

$$\boxed{\hat{N}(\hat{a}^+ u_n) = (\lambda_n + 1)(\hat{a}^+ u_n)} \quad (1.6)$$

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:

$$\hat{N} u_{n_-} = \overbrace{(\lambda_n - 1)}^{\equiv \lambda_{n_-}} u_{n_-} \qquad \text{with } u_{n_-} = \hat{a} u_n$$

$$\hat{N} u_{n_+} = \underbrace{(\lambda_n + 1)}_{\equiv \lambda_{n_+}} u_{n_+} \qquad \text{with } u_{n_+} = \hat{a}^+ u_n$$

$$\hat{N} u_n = \lambda_n u_n$$

By definition,

$$\langle \hat{N} \rangle_\psi = \int \psi^* (\hat{N} \psi) dq$$

$$= \int \psi^* \hat{a}^+ (\hat{a} \psi) dq$$

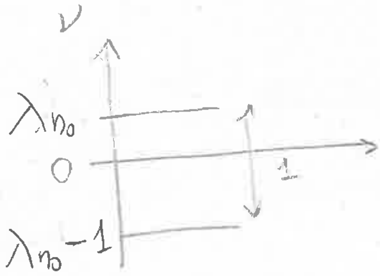
$$= \int (\hat{a} \psi)^* (\hat{a} \psi) dq = \| \hat{a} \psi \|^2 \geq 0$$

Therefore:

$$\langle \hat{N} \rangle_{n} = \int u_n^* (\hat{N} u_n) dq = \lambda_n \int |u_n|^2 dq \geq 0 \Rightarrow \lambda_n \geq 0 \ \forall n$$

Let $n = n_0$ the minimum value of n for which

$$\lambda_{n_0} \geq 0 \quad \text{but} \quad \lambda_{n_0} - 1 < 0$$



For this value we have

$$\hat{N} u_{n_0} = \lambda_{n_0} u_{n_0}$$

but also $\hat{N}(\hat{a} u_{n_0}) = \underbrace{(\lambda_{n_0} - 1)}_{<0}(\hat{a} u_{n_0})$

But $\lambda_{n_0} - 1 < 0$, cannot belong to the spectrum of $\hat{N}$, therefore it must be

$$\boxed{\hat{a} u_{n_0} = 0}$$

However, if this is true, then

$$\hat{N} u_{n_0} = \begin{cases} \hat{a}^{+}(\hat{a} u_{n_0}) = 0 \\ \lambda_{n_0} u_{n_0} \end{cases} \Rightarrow \boxed{\lambda_{n_0} = 0}$$

By convention, we put $n_0 = 0$ and we write

$$\begin{cases} \hat{a} u_0 = 0 \\ \lambda_0 = 0 \end{cases}$$

Now we can apply (1.6) to calculate

$$\hat{N}(\hat{a}^{+}u_0) = (\lambda_0+1)(a^{+}u_0)$$
$$= 1\cdot a^{+}u_0 \quad \Rightarrow a^{+}u_0 \propto u_1$$

Similarly, since

$$\hat{N}\hat{a}^{+} = a^{+}(a a^{+})$$
$$= a^{+}(\underbrace{a a^{+} - a^{+}a}_{=1} + \hat{N})$$
$$= a^{+} + a^{+}N$$

Then $\quad \hat{N}a^{+2} = (Na^{+})a^{+}$

$$= a^{+2} + a^{+}(Na^{+})$$
$$= a^{+2} + a^{+}(a^{+} + a^{+}N)$$
$$= 2a^{+2} + a^{+2}N$$

Therefore $\quad \hat{N}(a^{+2}u_0) = 2(a^{+2}u_0) \quad \Rightarrow a^{+2}u_0 \propto u_2$

and so on. Suppose that $u_n(x)$ are normalized:

$$\int u_n^{*} u_n \, dx = 1$$

Then, if I write

$$\hat{a}u_n = c\, u_{n-1}$$

I have: $\quad \int (\hat{a}u_n)^{*}(\hat{a}u_n)\,dx = |c|^2 \underbrace{\int |u_{n-1}|^2 dx}_{=1 \text{ by hypothesis}}$

$$|c|^2 = \int u_n^* \underbrace{\hat{a}^+\hat{a} u_n}_{= n u_n} dx = n\int |u_n|^2 dx = n$$

$\Rightarrow \quad c = \sqrt{n}$

So:

$$\boxed{\hat{a} u_n = \sqrt{n}\, u_{n-1}}$$

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

Similarly, if

$$\hat{a}^+ u_n = d\, u_{n+1}$$

then

$$\int (a^+ u_n)^* (a^+ u_n)\, dx = |d|^2$$

$$\Leftrightarrow \quad \int u_n^* a a^+ u_n\, dx = |d|^2$$

$$\Leftrightarrow \quad |d|^2 = \int u_n^* (\overbrace{a a^+ - a^+ a}^{=1} + \hat{N}) u_n\, dx$$

$$= (1+n) \quad \Rightarrow \quad |d| = \sqrt{n+1}$$

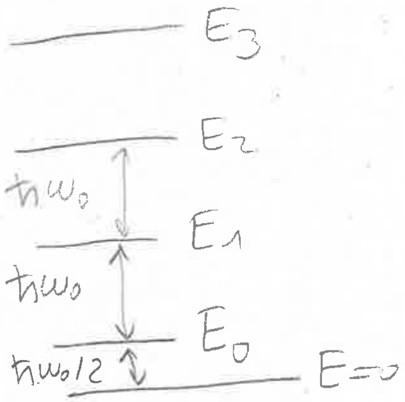
and

$$\boxed{\hat{a}^+ u_n = \sqrt{n+1}\, u_{n+1}}$$

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.

n	E_n
⋮	
3	$\frac{7}{2}\hbar\omega_0$
2	$\frac{5}{2}\hbar\omega_0$
1	$\frac{3}{2}\hbar\omega_0$
0	$\frac{1}{2}\hbar\omega_0$



— Eigenfunctions —

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

$$\Rightarrow \begin{cases} \hat{a} = \frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right) \\ \hat{a}^+ = \frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right) \end{cases} \qquad (1.10)$$

Then $\hat{H}u = Eu \iff \hbar\omega_0(\hat{a}^+\hat{a} + \frac{1}{2})u = Eu$

becomes $\quad (2a^+a + 1)u = \frac{2E}{\hbar\omega_0} u \qquad (2.10)$

but $\quad 2a^+a\,u = \left(\xi - \frac{d}{d\xi}\right)\left(\xi + \frac{d}{d\xi}\right)u$

$$= \left(\xi - \frac{d}{d\xi}\right)(\xi u + u')$$

$$= \xi^2 u + \cancel{\xi u'} - u - \cancel{\xi u'} - u''$$

and $(2a^\dagger a + 1)u = -u'' \cancel{-u} + \xi^2 u \cancel{+u}$

Therefore

$$(2.10) \Rightarrow -u'' + \xi^2 u - \frac{2E}{\hbar\omega_0} u = 0$$

$$\Leftrightarrow \boxed{u'' + \left(\frac{2E}{\hbar\omega_0} - \xi^2\right) u = 0} \qquad (1.11)$$

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

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

If we try: $\boxed{u_0(\xi) = A_0 e^{-\xi^2/2}} \Rightarrow$

$$\Rightarrow \frac{du_0}{d\xi} = -\xi u_0 \Rightarrow \frac{d^2 u}{d\xi^2} = -u_0 - \xi \frac{du_0}{d\xi}$$

$$= -u_0 + \xi^2 u_0$$

$$\Leftrightarrow u_0'' + (1 - \xi^2) u_0 = 0$$

The normalization requires

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

and $\boxed{u_0(\xi) = \frac{1}{\pi^{1/4}} \exp\left(-\frac{\xi^2}{2}\right)}$ (2.11)

In Terms of x, we have:

$$u_0(x) = B_0\, e^{-(\beta^2 x^2)/2}$$

and
$$1 = \int_{-\infty}^{\infty} |u_0(x)|^2 dx = \frac{B_0^2}{\beta}\int_{-\infty}^{\infty} e^{-\xi^2} d\xi = \frac{B_0^2\sqrt{\pi}}{\beta} \Rightarrow$$

$$\Rightarrow \boxed{u_0(x) = \left(\frac{\beta^2}{\pi}\right)^{1/4} \exp\left(-\frac{\beta^2 x^2}{2}\right)} \qquad (1.12)$$

The other eigenfunctions are found applying $\hat{a}^+$ repeatedly:

$$u_n = \frac{1}{\sqrt{n}} a^+ u_{n-1}$$

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

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

$$- - - - - - -$$

$$= \frac{1}{\sqrt{n(n-2)\cdots(n-p)}} (a^+)^p u_{n-p} \qquad \text{I stop in } n=p$$

So:
$$\boxed{u_n = \frac{(a^+)^n}{\sqrt{n!}} u_0} \qquad (2.12)$$

$$= A_n\left(\xi - \frac{d}{d\xi}\right)^n e^{-\xi^2/2}$$

Clearly: for

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

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

$$= 2 e^{-\xi^2/2}\left(\xi^2 - 1 + \xi^2\right)$$

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In general:

$$\boxed{\left(\xi - \frac{d}{d\xi}\right)^n e^{-\xi^2/2} = H_n(\xi) e^{-\xi^2/2}},$$

where:

$H_n(\xi) =$ <u>Hermite polynomials</u>

They are solution of the equation:

$$H_n'' - 2\xi H_n' + 2n H_n = 0$$

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

$$u_n(x) = B_n H_n(\beta x) \exp\left(-\frac{\beta^2 x^2}{2}\right)$$

$$I_n = \int u_n^*(x) u_m(x)\, dx$$

$$= B_n B_m \underbrace{\int H_n(\beta x) H_m(\beta x) e^{-x^2\beta^2} dx}$$

$$= \text{Grad \& Ryz? } 7.374$$

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

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

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

Therefore:

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