Harmonic oscillator.

Most important basic system both in classical and quantum physics.* Here we will introduce the basics of the quantum harmonic oscillator.

Till now we have considered quantum systems which are discrete so the Hilbert space was finite and we could treat it entirely through linear algebra.

The harmonic oscillator is a continuous system with infinite dimensional Hilbert space.

Nevertheless we can essentially treat this system by using an algebraic formalism.

Plan of these notes.

1. Harmonic oscillator Hamiltonian.
2. Creation and annihilation operator
3. Algebraic diagonalisation of Hamiltonian.
4. Eigenstates in position representation.

* For example the electromagnetic field is an infinite collection of harmonic oscillators

1 Harmonic oscillator Hamiltonian

The classical harmonic oscillator is an elastic spring . The energy of a mass attached to the spring is contributed by the

Kinetic energy $\frac{1}{2} m v^2 = \frac{p^2}{2m}$ (with $p = mv$)

and the potential energy $\frac{1}{2} k x^2$ (Force $= -kx$).

So the total energy or Hamiltonian is

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

(Note here x = position of mass measured from equilibrium position.)

Classical equations of motion:

$$\begin{cases} p = m\dot{x} \\ \dot{p} = -kx \end{cases}$$

or perhaps in more familiar form $m\ddot{x} = -kx$.

Solution $x(t) = A\cos\omega t + B\sin\omega t$

$p(t) = m\dot{x}(t) = -A\omega\sin\omega t + B\omega\cos\omega t$

and replacing $\cos\omega t$ & $\sin\omega t$ in $m\ddot{x} = -kx$

we find $-m\omega^2 = -k \Rightarrow \boxed{\omega = \sqrt{\frac{k}{m}}}$.

frequency of oscillation.

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Now let us turn to the quantum formalism.

a) The state of the system is described by "vectors" in the Hilbert space $\underbrace{L^2(\mathbb{R})} = \mathcal{H}$

$$\text{functions } \psi : \mathbb{R} \to \mathbb{C}$$
$$x \mapsto \psi(x) \in \mathbb{C}$$

such that $\int_{-\infty}^{+\infty} dx\, |\psi(x)|^2 = 1$.

(or finite $< \infty$)

So "state vectors" are now square integrable wave fcts

In Dirac's notation $\psi(x) = \langle x | \psi \rangle$.

b) Observables position and momentum $\hat{x}$ and $\hat{p}$ are now "operators" (or infinite dimensional matrices) acting on functions of $L^2(\mathbb{R})$ (or vectors of Hilbert space).

The correspondence principle says:

$$\begin{cases} (\hat{x}\psi)(x) = x\,\psi(x) \\ (\hat{p}\psi)(x) = -i\hbar \dfrac{\partial}{\partial x}\psi(x) \end{cases}$$

How can we understand the second relation? Apply the relation to a plane wave $\psi(x) = e^{+i\frac{2\pi x}{\lambda}}$ with wave length λ. We find $\hat{p}\psi = \frac{2\pi\hbar}{\lambda}\psi$ so the associated momentum is $\frac{2\pi\hbar}{\lambda} = \frac{h}{\lambda}$ (since $\hbar = \frac{h}{2\pi}$).

This is compatible with the De Broglie relation giving wavelength $\frac{h}{p} = \lambda$ to a particle of momentum p.

c) Now simply apply the correspondence principle to the Hamiltonian of the harmonic oscillator and we get the <u>quantum hamiltonian of the harm osc</u>:

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2} K \hat{x}^2$$

Note that introducing the frequency $\omega = \sqrt{\frac{K}{m}}$ we have $K = m\omega^2$ and the Hamiltonian is usually defined as

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

This is an operator acting on functions of $L^2(\mathbb{R}^3)$.

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

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + \frac{1}{2}m\omega^2 x^2 \psi(x)$$

$$= \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right)\psi(x).$$

A differential operator ...

d) Commutation relation of position and momentum.

In fact $\hat{x}$ and $\hat{p}$ satisfy an algebraic relation (the commutation relation) which will allow us to basically use algebra instead of analysis with differential operators to solve this system.

The commutator between two operators or matrices A & B is by definition $[A, B] \equiv AB - BA$.

$$\boxed{\text{We have} \quad [\hat{x}, \hat{p}] = i\hbar}$$

Proof: $[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x}$

apply this on a state ψ:

$$(\hat{x}\hat{p} - \hat{p}\hat{x})\psi = \hat{x}(\hat{p}\psi) - \hat{p}(\hat{x}\psi)$$

This is a function of $x \in \mathbb{R}$:

$$x\left(-i\hbar\frac{\partial}{\partial x}\psi\right)(x) - \underbrace{\left(-i\hbar\frac{\partial}{\partial x}\right)(x\psi(x))}_{\left(-i\hbar\psi(x) - i\hbar x\frac{\partial\psi}{\partial x}\right)}$$

$$= -i\hbar \cancel{x\frac{\partial\psi}{\partial x}} + i\hbar\psi(x) + i\hbar \cancel{x\frac{\partial\psi}{\partial x}}$$

$$= \underbrace{i\hbar\psi(x)}_{(i\hbar \mathbb{1})\psi}. \qquad \left(i\hbar \text{ times "identity"}\right).$$

In other words we showed that

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

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

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2 Creation and annihilation operators.

Now we introduce an algebraic formalism that plays a very important role in quantum theory (and can be extended much beyond the harmonic oscillator).

In particular this formalism is at the basis of the quantum description of the modes of the electromagnetic field.

Since $\hbar\omega$ has units of energy $= J.s.\frac{1}{s} = J$.

its a good idea to write down:

$$\hat{H} = \hbar\omega \left(\frac{\hat{p}^2}{2m\hbar\omega} + \frac{m\omega}{2\hbar} \hat{x}^2 \right)$$

Then we try to factorize this "degree two pol expression" but with a "little" extra term due to non commutation of $\hat{x}$ & $\hat{p}$:

$$\hat{H} = \hbar\omega\left(\frac{\hat{p}}{\sqrt{2m\hbar\omega}} + i\sqrt{\frac{m\omega}{2\hbar}}\,\hat{x}\right)\left(\frac{\hat{p}}{\sqrt{2m\hbar\omega}} - i\sqrt{\frac{m\omega}{2\hbar}}\,\hat{x}\right)$$

$$-\hbar\omega\, i\sqrt{\frac{m\omega}{2\hbar}}\frac{1}{\sqrt{2m\hbar\omega}}\underbrace{\left(\hat{x}\hat{p} - \hat{p}\hat{x}\right)}_{i\hbar}.$$

So we find:

$$\hat{H} = \hbar\omega\left(\frac{\hat{p}}{\sqrt{2m\hbar\omega}} + i\sqrt{\frac{m\omega}{2\hbar}}\,\hat{x}\right)\left(\frac{\hat{p}}{\sqrt{2m\hbar\omega}} - i\sqrt{\frac{m\omega}{2\hbar}}\,\hat{x}\right) + \frac{\hbar\omega}{2}.$$

This suggest to define

$$\begin{cases} a = \dfrac{\hat{p}}{\sqrt{2m\hbar\omega}} - i\sqrt{\dfrac{m\omega}{2\hbar}}\,\hat{x} \\[2ex] a^{+} = \dfrac{\hat{p}}{\sqrt{2m\hbar\omega}} + i\sqrt{\dfrac{m\omega}{2\hbar}}\,\hat{x} \end{cases}$$

(Note we can show $\hat{p}^{+} = \hat{p}$ as it should for an observable)

$$\Rightarrow \boxed{\hat{H} = \hbar\omega\left(a^{+}a + \frac{1}{2}\right)}$$

The operators a & a^+ are called annihilation and creation operators for reasons that will become clear later on.

Their commutation relation follows from the basic relation $[\hat{x}, \hat{p}] = i\hbar$. An easy exercise shows that

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

Proof: write down $[a, a^+] = a a^+ - a^+ a$ and replace a & a^+ by their definitions and use $[\hat{x}, \hat{p}] = i\hbar$.

Remark: In fact a & a^+ are first order differential operators

$$\begin{cases} a = \dfrac{1}{\sqrt{2m\hbar\omega}}\left(-i\hbar\dfrac{\partial}{\partial x}\right) - i\sqrt{\dfrac{m\omega}{2\hbar}}\, x. \\[2ex] a^+ = \dfrac{1}{2m\hbar\omega}\left(-i\hbar\dfrac{\partial}{\partial x}\right) + i\sqrt{\dfrac{m\omega}{2\hbar}}\, x. \end{cases}$$

3 Diagonalisation of $\hat{H}$ and interpretation of a & a^+:

We seek eigenvalues and eigenvectors of $\hat{H}$. So we solve: $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$ or

equivalently

$$a^+ a\,|\psi_n\rangle = \left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right)|\psi_n\rangle.$$

We thus want eigenvectors and eigenvalues of $a^+ a$.

We define

$$N \equiv a^+ a.$$

and look at $[N, a]$ and $[N, a^+]$.

$$[N, a] = Na - aN = a^+ a^2 - a a^+ a$$

since $aa^+ - a^+a = 1$.

$$= a^+ a^2 - (1 + a^+ a)a = -a$$

$$\Rightarrow \boxed{[N, a] = -a}.$$

$$[N, a^+] = Na^+ - a^+ N = a^+ \underbrace{a a^+}_{1 + a^+ a} - (a^+)^2 a = a^+$$

$$\Rightarrow \boxed{[N, a^+] = a^+}$$

From the algebra $[N, a] = -a$ & $[N, a^+] = a^+$ we can deduce the spectrum of $a^+a = N$. Indeed

let $N|\psi_m\rangle = \mu_m|\psi_m\rangle$ (here $\mu_m = \frac{E_m}{\hbar\omega} - \frac{1}{2}$)

$$\Rightarrow \underbrace{aN}_{}|\psi_m\rangle = \mu_m a|\psi_m\rangle$$

$Na + a$ since $[N, a] = -a$ i.e $Na - aN = -a$

$$\Rightarrow N(a|\psi_m\rangle) = (\mu_m - 1)a|\psi_m\rangle.$$

- in words if $|\psi_m\rangle$ has e.v μ_m then $a|\psi_m\rangle$ has e.v $\mu_m - 1$, similarly $a^2|\psi_m\rangle$ has e.v $\mu_m - 2$, ... So the op a is a ladder operator which lowers the energy by one unit

- Similarly $N|\psi_m\rangle = \mu_m|\psi_m\rangle \Rightarrow a^+N|\psi_m\rangle = \mu_m a^+|\psi_m\rangle$

$$\Rightarrow N a^+|\psi_m\rangle = (\mu_m + 1)a^+|\psi_m\rangle$$

$$N(a^+)^2|\psi_m\rangle = (\mu_m + 2)(a^+)^2|\psi_m\rangle, \quad \ldots$$

and a^+ is a ladder operator that raises the energy by one unit.

Finally $N = a^\dagger a$ is a positive semi def operator.

Indeed $\langle\psi|N|\psi\rangle = \langle\psi|a^\dagger a|\psi\rangle = \| a|\psi\rangle \|^2 \geq 0.$

Thus all eigenvalues must be ≥ 0, The

only way is to have μ_n integer and also

$$a|\psi_0\rangle = 0 \cdot |\psi_0\rangle = 0 .$$

Otherwise the ladder op a would send us to negative energy states, (impossible).

In summary $a^\dagger a \, |\psi_n\rangle = n|\psi_n\rangle \quad n = 0, 1, 2 \dots$

$\uparrow$ integer eigenvalue

The standard notation adopted is $|\psi_n\rangle = |n\rangle$.

$$\Rightarrow \quad a^\dagger a|n\rangle = n|n\rangle = \left(\frac{E_n}{\hbar\omega} - \frac{1}{2}\right)|n\rangle$$

$$\Rightarrow \quad \boxed{E_n = \hbar\omega\left(n + \frac{1}{2}\right)}$$

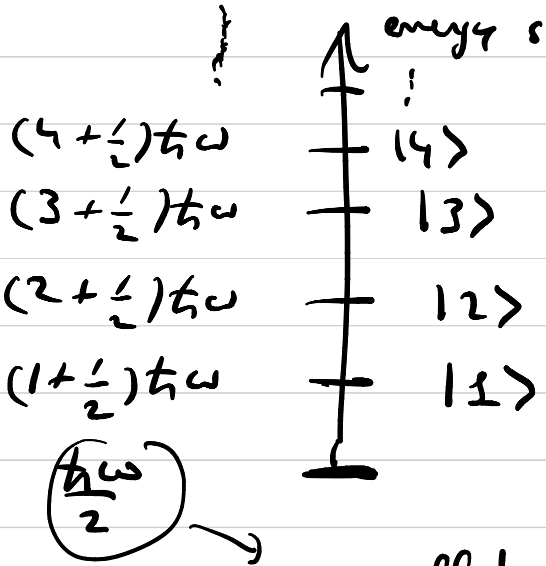
Summarizing:

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

$$\underset{\substack{\uparrow \\ \text{eigenvectors}}}{\hat{H}\,|n\rangle} = \underbrace{\hbar\omega\left(n+\frac{1}{2}\right)}_{\text{eigenvalues.}}|n\rangle \;;\; n = 0, 1, 2, 3\ldots$$

$N = a^\dagger a$ is a "number operator" which counts the number of excitations in state $|n\rangle$

energy spectrum of the harmonic oscillator,



is an infinite ladder

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

so called ground state $|0\rangle$ has zero excitations

Ladder ops $a^\dagger|n\rangle \sim |n+1\rangle$ and $a|n\rangle \sim |n-1\rangle$.

Correct normalisation: $a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$ and $a|n\rangle = \sqrt{n}\,|n\rangle$

Indeed this is implied by $\langle n|a^\dagger a|n\rangle = n$ and $\langle n|a a^\dagger|n\rangle = n+1$.

Parenthesis

Important example of quantum harmonic oscillator in nature:

Each mode of the free electromagnetic field in vaccuum is an harmonic oscillator. For a mode of wave length λ and frequence ω with $2\pi\omega = \frac{c}{\lambda}$ i.e $\omega = ck$ (with $k = \frac{2\pi}{\lambda}$ the wave number):

The Hamiltonian of the mode ω_k is:

$$\hat{H}_k = \hbar\omega_k \left(a_k^+ a_k + \tfrac{1}{2}\right) = \left(\begin{array}{l}\text{energy of a photon } \hbar\omega_k \text{ times} \\ \text{number of photons } + \\ \text{"vaccuum energy" term}\end{array}\right).$$

For a set of many modes (say in some wave guide):

$$\hat{H} = \sum_k \hbar\omega_k \left(a_k^+ a_k + \tfrac{1}{2}\right).$$

This is not the whole story because we should introduce a polarization index so for each mode we have two polarizations:

$$\hat{H} = \sum_{k,\lambda} \hbar\omega_k \left(a_{k,\lambda}^+ a_{k,\lambda} + \tfrac{1}{2}\right)$$ where λ is binary index.

4 States in Position Representation.

The eigenstates $|n\rangle$ can be represented in the "position basis"

i.e we want to compute $\psi_n(x) = \langle x | n \rangle$ to get

a better intuition of these states.

Recall $a|0\rangle = 0$ and $|n\rangle = \frac{a^\dagger}{\sqrt{n}}|n-1\rangle$.

This is enough to obtain the position representation. Indeed

$a|0\rangle = 0$ with $a = \frac{1}{\sqrt{2m\hbar\omega}}\left(-i\hbar\frac{\partial}{\partial x}\right) - i\sqrt{\frac{m\omega}{2\hbar}}\, x$ means:

$$\frac{1}{\sqrt{2m\hbar\omega}}\left(-i\hbar\frac{\partial}{\partial x}\right)\psi_0(x) - i\sqrt{\frac{m\omega}{2\hbar}}\, x\, \psi_0(x) = 0.$$

$$\Rightarrow \quad \psi_0'(x) = -m\omega x\, \psi_0(x).$$

$$\Rightarrow \quad \psi_0(x) = C.\exp\left(-\frac{1}{2}m\omega x^2\right)$$

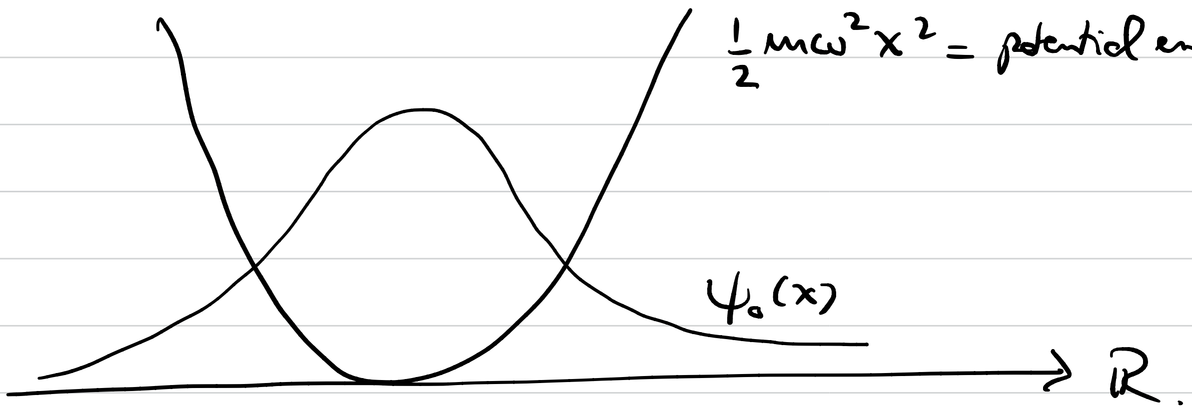
$\int dx\, e^{-\frac{1}{2}m\omega x^2} = 1.$ $= \sqrt{\frac{1}{m\omega}}\underbrace{\int dx\, e^{-\frac{1}{2}x^2}}_{=\sqrt{2\pi}}$

and C is found from the normalisation condition: $\int dx\, |\psi_0(x)|^2 = 1$

$\rightarrow \quad C = \sqrt{\frac{m\omega}{2\pi}}$

so $$\boxed{\psi_0(x) = \sqrt{\frac{m\omega}{2\pi}}\exp\left(-\frac{1}{2}m\omega x^2\right)}$$

This is the ground state wave fct of the Harmonic osc.



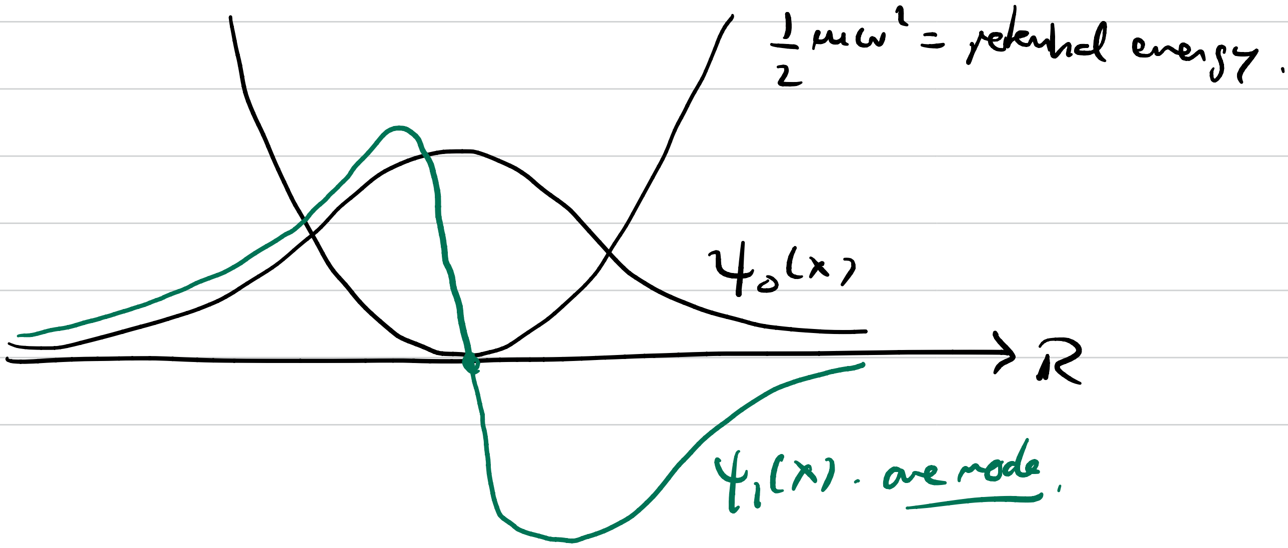
First excited state:

$$|1\rangle = a^\dagger |0\rangle \quad \text{with} \quad a^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}\left(-i\hbar\frac{\partial}{\partial x}\right) - i\sqrt{\frac{m\omega}{2\hbar}}\, x$$

implies $$\psi_1(x) = \frac{1}{\sqrt{2m\hbar\omega}}(-i\hbar)\,\psi_0'(x) - i\sqrt{\frac{m\omega}{2\hbar}}\,\underbrace{x\,\psi_0(x)}_{\propto\, \psi_0'(x)}$$

$$\propto \psi_0'(x)$$

$\propto x\,\psi_0(x)$ also.

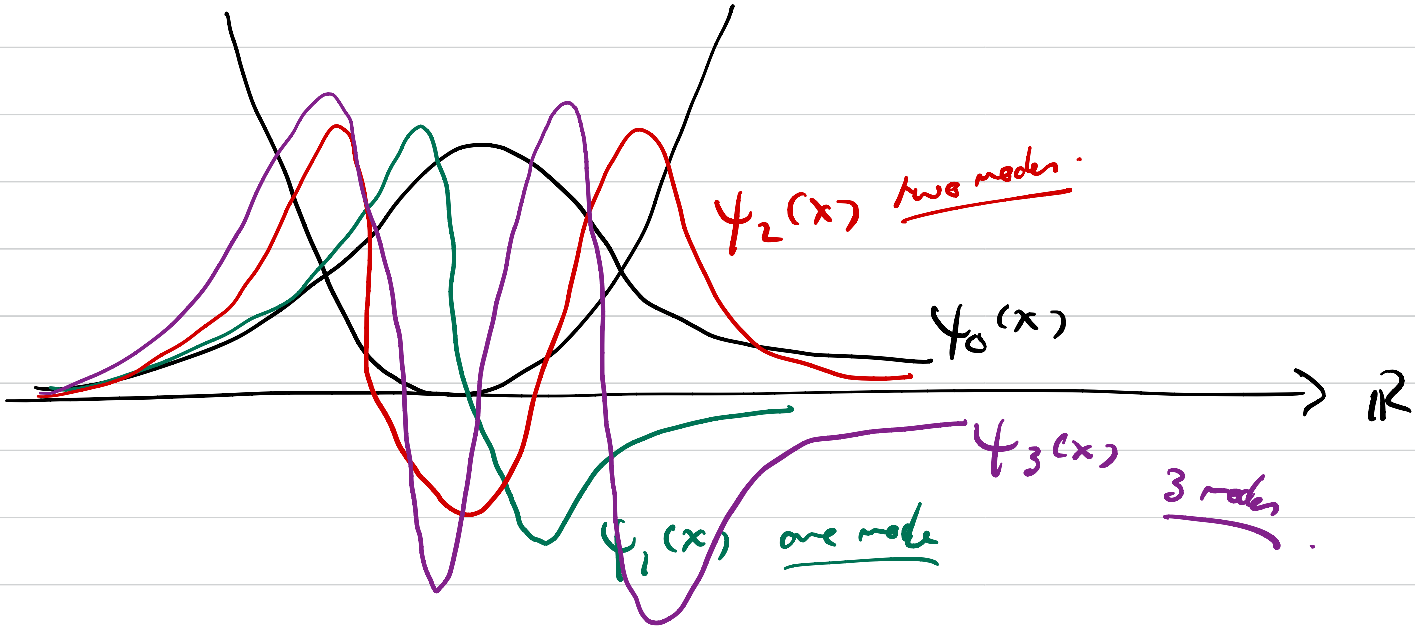


Higher excited states:

One can iterate $|n\rangle = \frac{a^\dagger}{\sqrt{n}}|n-1\rangle$

and find $\psi_n(x) \propto$ (polynomial of degree n)$\cdot\psi_0(x)$

this polynomial can be computed "explicitly" and is called the Hermite polynomial $H_n(x)$.



- The number of nodes corresponds to excitation level.
  Ground state → No node
  First exc state → one node
  Second exc state → two nodes ...
- This rule is valid more generally for one dimensional probls. (but in higher dim things get more complicated).