Lec 21 To wrap up time evolution, read S&N 2.2.5.

Our first elementary solution to a QM problem in 1D (other than free particle).

- Particle in a quadratic potential:

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

Let's go back to Ehrenfest's theorem:

$$m\frac{d^2\langle x\rangle}{dt^2} = -\langle \nabla V(x)\rangle = -\left\langle \frac{d}{dx}\left(\frac{m\omega^2 x^2}{2}\right)\right\rangle$$

$$\Rightarrow m\frac{d^2\langle x\rangle}{dt^2} = -m\omega^2\langle x\rangle = \text{"F"}$$

"F" = force

$$\frac{d^2\langle x\rangle}{dt^2} + \omega^2\langle x\rangle = 0 \Rightarrow \langle x\rangle = A\cos(\omega t) + B\sin(\omega t)$$

oscillatory sol.

Spring analogy

$$\text{"F"} = -m\omega^2\langle x\rangle \quad \text{if } \omega^2 = \frac{k}{m} \Rightarrow \boxed{F = -k\langle x\rangle}$$

Harmonic oscillator

* Bound State
* Discrete Spectrum

Let's learn about the energy of this system and find a solution:

$$E = \langle H \rangle_\psi = \frac{\langle p^2 \rangle}{2m} + \frac{m\omega^2}{2}\langle x^2 \rangle$$

$$\geq \frac{\Delta p^2}{2m} + \frac{m\omega^2}{2}\Delta x^2$$

because $\langle A^2 \rangle = (\Delta A)^2 + \langle A \rangle^2 \geq (\Delta A)^2$

Now let's saturate the uncertainty relation:

$$\Delta p \geq \frac{\hbar}{2}\frac{1}{\Delta x}$$

$$\langle H \rangle \geq \frac{\hbar^2}{8m}\frac{1}{(\Delta x)^2} + \frac{m\omega^2}{2}(\Delta x)^2 \geq \frac{\hbar\omega}{2}$$

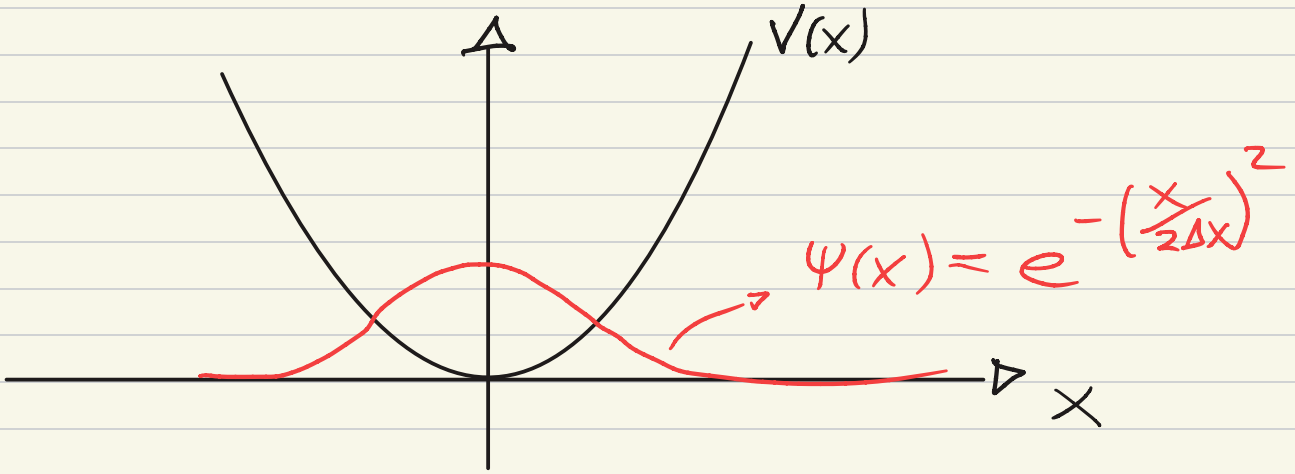
AM-GM inequality: $a + b \geq 2\sqrt{ab}$

Saturate this bound if $\langle x \rangle = 0$; $\langle p \rangle = 0$; and

$$(\Delta x)^2 = \frac{\hbar}{2m\omega}$$

one type of solution is a gaussian

$$\langle x|\psi \rangle = \psi(x) \propto e^{-m\omega x^2/2\hbar} = e^{-\frac{1}{4}\left(\frac{x}{\Delta x}\right)^2}$$



There is a nicer language for this problem. Currently, our $\hat{H}$ mixes canonical pair: $\hat{x}$, $\hat{p}$, both hermitian. It is a sum of squares. For reasons that will soon be evident, we define:

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right) \; ; \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)$$

Calculate:

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

$$a^\dagger a = \frac{m\omega}{2\hbar}\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} + \frac{i}{m\omega}\overbrace{(\hat{x}\hat{p} - \hat{p}\hat{x})}\right)$$

$$= \frac{m\omega}{2\hbar}\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega^2} - \frac{\hbar}{m\omega}\mathbb{1}\right) = \frac{\hat{H}}{\omega\hbar} - \frac{1}{2}\mathbb{1}$$

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

Also calculate $[\hat{a}, \hat{a}^\dagger] = \mathbb{1}$.

We call $\hat{N} = \hat{a}^\dagger\hat{a}$ the <u>number</u> operator.

Is it hermitian? Note that $\hat{H} = \omega\hbar\left(\hat{N} + 1/2\right)$

$\hat{N}$ clearly commutes w/ $\hat{H}$ so they can share an eigenbasis. Call it $|n\rangle$:

$$\hat{N}|n\rangle = n|n\rangle \Rightarrow E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega$$

Not clear yet what n or $\hat{N}$ are.
To see the beautiful structure behind them, act $\hat{N}$ on the states $a^\dagger|n\rangle$ and $a|n\rangle$:

$$\hat{N}\,\underbrace{a^\dagger|n\rangle}_{|n+1\rangle} = \left([\hat{N},\hat{a}^\dagger] + \hat{a}^\dagger\hat{N}\right)|n\rangle$$
$$= \hat{a}^\dagger|n\rangle + \hat{a}^\dagger n|n\rangle$$
$$= (n+1)\,\hat{a}^\dagger|n\rangle$$

$$\hat{N}\,\underbrace{a|n\rangle}_{|n-1\rangle} = \left([\hat{N},\hat{a}] + \hat{a}\hat{N}\right)|n\rangle$$
$$= \left(-\hat{a} + \hat{a}n\right)|n\rangle$$
$$= (n-1)\,\hat{a}|n\rangle.$$

$[\hat{N},\hat{a}^\dagger] = \hat{a}^\dagger$

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

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

The states $\hat{a}^\dagger|n\rangle$ and $\hat{a}|n\rangle$ are still eigenstates of $\hat{N}$ (and also of $\hat{H}$), except eigenvalues have been raised and lowered by one unit.

We call $\hat{a}$ → annihilation operator
$\hat{a}^\dagger$ → creation operator

* Are they hermitian? unitary? Invertible?

Let's first look at the states and fix their normalization.

Given that spectrum is discrete:

$$N|n+1\rangle = (n+1)|n+1\rangle \quad \longleftrightarrow \quad \hat{N}a^\dagger|n\rangle = (n+1)a^\dagger|n\rangle$$

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

$$\Rightarrow \quad a|n\rangle = c|n-1\rangle$$

Norm of $a|n\rangle$ is

$$\langle n|a^\dagger a|n\rangle = \langle n|\hat{N}|n\rangle = n$$

$$\text{and} = \langle n-1|c^* c|n-1\rangle = |c|^2$$

$$\Rightarrow \quad \boxed{a|n\rangle = \sqrt{n}\,|n-1\rangle}$$

and

$$a^\dagger|n\rangle = d|n+1\rangle$$

$$\Rightarrow \quad \langle n|aa^\dagger|n\rangle = |d|^2\langle n+1|n+1\rangle = |d|^2$$

$$= \langle n|\hat{N} - [a^\dagger, a]|n\rangle = \langle n|\hat{N} + 1|n\rangle = n+1$$

$$\Rightarrow \quad \boxed{a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle}$$

We recover $\hat{N}$: $\quad a^\dagger(a|n\rangle) = a^\dagger\sqrt{n}\,|n-1\rangle$

$$= \sqrt{n}\sqrt{(n-1)+1}\,|n\rangle$$

$$= n|n\rangle = \hat{N}|n\rangle \checkmark$$

Note that

$$\||n\rangle\| \geq 0 \quad \Rightarrow \quad n \geq 0.$$

$n=0$ is special because

$$a|n=0\rangle = 0 \quad \rightarrow \text{Full Annihilation}$$

When $n=0$: $\hat{H}|0\rangle = \omega\hbar\left(\overset{0}{\cancel{n}} + \frac{1}{2}\right)|0\rangle$

In general
$$\begin{cases} |1\rangle = a^\dagger|0\rangle \\ |2\rangle = \frac{a^\dagger a^\dagger}{\sqrt{2}}|0\rangle \\ |n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle \end{cases}$$

Note also:

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

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

You can also derive:

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a+a^\dagger) \qquad p = i\sqrt{\frac{m\omega\hbar}{2}}(a^\dagger - a)$$

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

units: $\left[\frac{\hbar}{2m\omega}\right] = \frac{J\cdot s}{kg\,Hz} = \frac{m^2}{s^2}\cdot s^2 = m^2$.

$$\langle n|\hat{x}^2|n\rangle = \frac{\hbar}{2m\omega}\langle a^2 + a^{\dagger 2} + aa^\dagger\, a^\dagger a\rangle_n$$

$$= \frac{\hbar}{2m\omega}\left((n+1) + n\right) = x_0^2\left(n+\frac{1}{2}\right)$$

↳ see next.

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

$$\langle n|\hat{p}^2|n\rangle = \frac{\hbar m\omega}{2}\langle aa^\dagger + a^\dagger a - a^2 - a^{\dagger 2}\rangle = \frac{\hbar^2}{x_0^2}(n+1/2)$$

$\frac{\hbar^2}{2x_0^2}$

Dec 2.5:

Finding our first wavefunction:

$$\langle x|\underbrace{a|0\rangle}_{=0} = \sqrt{\frac{m\omega}{2\hbar}}\langle x|\left(\hat{x} + \frac{i\hat{p}}{m\omega}\right)|0\rangle = 0$$

$$\langle x|\hat{x}|0\rangle + \frac{i}{m\omega}\underbrace{\langle x|\hat{p}|0\rangle}_{-i\hbar\frac{d}{dx}\langle x|0\rangle} = 0$$

$$\Rightarrow \quad x\psi_0(x) + \frac{\hbar}{m\omega}\frac{d}{dx}\psi(x) = 0 \qquad \text{define } \boxed{x_0 = \sqrt{\frac{\hbar}{m\omega}}}$$

$$\Rightarrow \quad \boxed{\frac{d\psi_0(x)}{dx} = -\frac{x}{x_0^2}\psi(x)}$$

$$\rightarrow \int_{\psi_0(x')}^{\psi_0(x)} \frac{d\psi_0(x)}{\psi_0(x)} = -\int^{x'} \frac{x}{x_0^2}dx$$

$$\rightarrow \ln\left(\psi_0(x)/\psi_0(x'_0)\right) = -\frac{x'^2}{2x_0^2} + C$$

$$\Rightarrow \quad \psi_0(x') = \sqrt{N}\exp\left(-x'^2/2x_0^2\right)$$

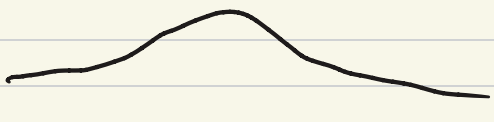
Normalization fixed by $\int_{-\infty}^{\infty} dx' |\psi_0(x')|^2 = 1$

$$\Rightarrow \int_{-\infty}^{\infty} e^{-x'^2/x_0^2}\,dx' = x_0\int_{-\infty}^{\infty} e^{-u^2}\,du = \sqrt{\pi}\,x_0 = 1/N$$

$$u = x'/\sqrt{2}x_0$$

$$\Rightarrow \text{Ground State Wavefunction:}$$

$$\psi_0(x) = \left(\frac{1}{\pi x_0^2}\right)^{1/4} e^{-x^2/2x_0^2}$$



For excited states:

$$\psi_1(x) = \langle x|1\rangle = \langle x|a^\dagger|0\rangle$$

$$a^\dagger = \sqrt{\frac{1}{2x_0}}\left(\hat{x} - i\frac{x_0^2}{\hbar}\hat{p}\right)$$

$$\psi_1(x) = \sqrt{\frac{1}{2x_0}}\left(x - x_0^2\frac{d}{dx}\right)\psi_0(x)$$

$$= \sqrt{\frac{1}{2x_0}}\frac{1}{\sqrt{x_0}}\frac{1}{\pi^{1/4}}\left(x - x_0^2\left(-\frac{x}{x_0^2}\right)\right)\psi_0(x)$$

$$= \left(\frac{1}{4\pi}\right)^{1/4}\frac{2x}{x_0}e^{-x^2/2x_0^2}$$

$$\psi_2(x) = \langle x|2\rangle = \langle x|a^\dagger|1\rangle$$

$$\psi_n(x) = \langle x|\frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle =$$

Recursive. Closed analytical solution //

Operator Method: Done!

S&N 2.5.2

Solving TISE: Sakurai's $u_E(x) = \psi(x)$.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x) + \frac{1}{2}m\omega^2x^2\psi_n(x) = E_n\psi_n(x)$$

Make it dimensionless: $y = x/x_0$; $x_0 = \sqrt{\hbar/m\omega}$

$$\varepsilon = 2E_n/\hbar\omega$$

$$\frac{d^2}{dy^2}\psi_n(y) + (\varepsilon - y^2)\psi_n(y) = 0$$

Solve the easier version

$$\frac{d^2}{dy^2}\psi(y) = y^2\psi(y) \rightarrow \psi(y) \sim e^{\pm y^2/2}$$

The $-$ sign has the right behavior but also the exponential envelope appears, which is nice. So we solve for:

$$\tilde{\psi}(y) = \psi(y)e^{+y^2/2} \quad \text{s.t.} \quad \psi(y) = \tilde{\psi}(y)e^{-y^2/2}$$

$$\Rightarrow \frac{d^2\tilde{\psi}}{dy^2} - 2y\frac{d\tilde{\psi}}{dy} + (\varepsilon - 1)\tilde{\psi} = 0$$

Now, write $\tilde{\psi}$ as a series. Use ansatz

$$\tilde{\psi}(y) = \sum_{j=0}^{\infty} c_j y^j \quad \text{Power series.}$$

Plugging into diff. eq. gives:

$$\sum_{j=0}^{\infty}\left[(j+1)(j+2)c_{j+2} - (2j+1-\varepsilon)c_j\right]y^j = 0$$

True for all values of y:

$$(j+1)(j+2)\,c_{j+2} = (2j+1-\varepsilon)\,c_j$$

Recursion relation. For large j: $c_{j+2} \sim \frac{c_j}{(j/2)}$

Continuing to apply this logic:

$$c_{j+2} = \frac{c_j}{j/2} = \frac{c_{j-2}}{\frac{j}{2}\left(\frac{j}{2}-1\right)} = \frac{c_{j-4}}{\frac{j}{2}\left(\frac{j}{2}-1\right)\left(\frac{j}{2}-2\right)} \rightarrow \frac{\text{const}}{\left(\frac{j}{2}\right)!}$$

This is bad though because:

$$\tilde{\psi}(y) = \text{const} \times \underbrace{\sum_j y^j/(j/2)!}_{\sum_n y^{2n}/n!} = \to e^{y^2}$$

and so $\psi \sim \tilde{\psi} e^{-y^2/2} \to O(1)$ and not exp. suppressed.

Resolution: Series is finite

Recall

$$c_{j+2} = \frac{(2j+1-\varepsilon)}{(j+1)(j+2)} c_j .$$

If for some j we get $\boxed{2j+1=\varepsilon}$

then series terminates, so:

$$\varepsilon = \frac{2E_n}{\omega\hbar} = 2j+1 \Rightarrow E_n = \omega\hbar\,(j+1/2)$$

Same index!

If n is even:

$\begin{cases} c_0, c_2, c_4, \ldots, c_n \text{ finite} \\ c_1, c_3, c_5, \ldots, \text{ must vanish!} \end{cases}$

If n is odd:

$\begin{cases} c_0, c_2, \ldots \text{ must vanish} \\ c_1, c_3, \ldots, c_n \text{ finite} \end{cases}$

Must be that $\boxed{\psi(-x) = (-1)^n \psi_n(x)}$

Solutions have definite parity.

$$\psi_0(y) = c_0 \, e^{-y^2/2}$$

$$\psi_1(y) = c_1 \, y \, e^{-y^2/2}$$

Now we imposed a constraint on ε:

$$\frac{d^2 \tilde{\psi}_n}{dy^2} - 2y \frac{d\tilde{\psi}_n}{dy} + 2n \tilde{\psi}_n = 0$$

$$\tilde{\psi}_n(y) = \text{const} \times y^n + \dots \text{ lower order.}$$

↳ Hermite polynomials.

In physics, one fixes:

$$H_n(y) = 2^n y^n + \text{lower order.}$$

Recall

$$c_{n-2} = -\frac{n(n-1)}{4} c_n$$

$$c_{n-2k} = (-1)^k \frac{n!}{(n-2k)!} \frac{2^n}{4^k k!}$$

↳ generate H_n

Solutions are finally:

$$\psi_n(x) = C_n H_n\left(x/x_0\right) e^{-x^2/2x_0^2}$$

BTW:

$$\int_{-\infty}^{\infty} H_n^*(x) H_m e^{-x^2} dx = \sqrt{\pi} \, 2^n n! \, \delta_{nm}$$