Harmonic Oscillator Redux ~~Part II~~

- Let's use operator math, inspired by Hilbert space approach to QM, to solve harm. osc.

- We did it before in position space, but this is easier

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

$$\omega = \sqrt{\frac{k}{m}}$$

- Start with $[x,p] = i\hbar$

- Define "ladder operators"

$$a = \frac{1}{\sqrt{2}}\left(\beta x + \frac{i}{\hbar\beta}p\right)$$

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

with $\beta = \left(\frac{m\omega}{\hbar}\right)^{1/2}$ $\quad \omega = \sqrt{\frac{k}{m}}$

- Notice

$$a \neq a^{\dagger} \quad (\text{not Hermitian})$$

since x & p are Hermitian

Obvious $aa^{\dagger} - a^{\dagger}a = -(a^{\dagger}a - aa^{\dagger})$

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

Proof:

Using $[x, x] = 0 \quad [p, p] = 0 \quad [x, p] = i\hbar$

$$[a, a^{\dagger}] = \frac{1}{2}\left[\beta x, \frac{-i}{\hbar\beta} p\right] + \frac{1}{2}\left[\frac{i}{\hbar\beta} p, \beta x\right]$$

$$= \frac{-i}{2\hbar} i\hbar + \frac{i}{2\hbar}(-i\hbar)$$

$$= 1$$

Define $N = a^\dagger a$. Don't know what N does yet. Just an op.

Then $\underline{H = \hbar\omega\left(N + \frac{1}{2}\right)}$

Proof:

$$N = a^\dagger a = \frac{1}{2}\left(\beta x - \frac{i}{\hbar\beta}p\right)\left(\beta x + \frac{i}{\hbar\beta}p\right)$$

$$= \frac{1}{2}\left[\beta^2 x^2 + \frac{1}{(\hbar\beta)^2}p^2 + \beta\left(\frac{i}{\hbar\beta}\right)(xp - px)\right]$$

$$= \frac{1}{2}\left[\frac{m\omega}{\hbar}x^2 + \frac{1}{\hbar m\omega}p^2 + \frac{i}{\hbar}(i\hbar)\right]$$

$$= \frac{1}{\hbar\omega}\left[\frac{1}{2}kx^2 + \frac{1}{2m}p^2 - \frac{1}{2}\hbar\omega\right]$$

So $$= \frac{1}{\hbar\omega}\left[H - \frac{1}{2}\hbar\omega\right]$$

$$\Rightarrow H = \hbar\omega\left(N + \frac{1}{2}\right) \checkmark$$

Thus, if we can find eigenvectors of N, we know eigenvectors of H & eigenvalues trivially related

$$N|\psi_i\rangle = n_i|\psi_i\rangle \Rightarrow H|\psi_i\rangle = \hbar\omega\left(n_i + \frac{1}{2}\right)|\psi_i\rangle$$

$$Na = a(N-1) \quad , \quad Na^+ = a^+(N+1)$$

Proof: (Goal is to move N across a or a^+)

$$Na = a^+aa = aa^+a + [a^+, a]a$$

$$= aN + (-1)a = a(N-1)$$

$$Na^+ = a^+aa^+ = a^+a^+a + a^+[a, a^+]$$

$$= a^+N + a^+(+1) = a^+(N+1)$$

What is meaning?

Let $N|\psi_i\rangle = n_i|\psi_i\rangle$

Now act N on $a|\psi_i\rangle$ & $a^+|\psi_i\rangle$:

$$Na|\psi_i\rangle = a(N-1)|\psi_i\rangle = (n_i-1)a|\psi_i\rangle$$

$$Na^+|\psi_i\rangle = a^+(N+1)|\psi_i\rangle = (n_i+1)a^+|\psi_i\rangle$$

~~Relationship between~~

- So $a|\psi_i\rangle$ & $a^\dagger|\psi_i\rangle$ are eigenvectors of N with eigenvalues $(n_i - 1)$, $(n_i + 1)$.

- Thus for any state $|\psi_i\rangle$ we get a ladder of eigenvectors

eigenvector	$a^2\|\psi_i\rangle$	$a\|\psi_i\rangle$	$\|\psi_i\rangle$	$a^\dagger\|\psi_i\rangle$	$(a^\dagger)^2\|\psi_i$
e.v.	$n_i - 2$	$n_i - 1$	n_i	$n_i + 1$	$n_i + 2$

- It is reasonable that ladder goes up to $E = \infty$, but we know there must be some minimum-energy state of the H.O.

- Is it possible to tell from the Hilbert space formalism that this is ~~is~~ the case, without resorting to making arguments about solutions to the dif. eq in position space?

- Yes & it is principle of positive norm - one of ingredients built into $\mathcal{H}$

- Let $N|\psi_i\rangle = n_i|\psi_i\rangle$, Let $|\psi_i^-\rangle = a|\psi_i\rangle$

  then what is $\langle\psi_i^-|\psi_i^-\rangle$, if $\langle\psi_i|\psi_i\rangle = 1$?

$$\langle\psi_i^-|\psi_i^-\rangle = \langle a\psi_i|a\psi_i\rangle = \langle\psi_i|a^\dagger a|\psi_i\rangle = \langle\psi_i|N|\psi_i\rangle = n_i$$

- If $n_i > 0$ this is fine. (I think the null state is technically in $\mathcal{H}$, but this seems to be just a question of definitions.)

- But what if $n_i < 0$? Then norm of $|\psi_i^-\rangle$ would be negative, & this violates principle that $\mathcal{H}$ ~~has~~ is composed of states with positive norm. ~~So $|\psi_i^-\rangle$ does not always exist in $\mathcal{H}$~~.

- That's all we needed to define states. Apply a repeatedly, & eventually we will get one of two cases:

  a) Successive n_i will go from positive to neg. w/out including 0. But that would be a contradiction of positive norm. ~~$a|\psi_i\rangle$ would be~~ ~~neither state exists but gives us a state with both properties~~es.

That is actually just ~~a~~ not possible.
Might be easier to see in function space.

x & $\frac{d}{dx}$ operators take $f(x) \to g(x)$, and

$g^*(x)g(x) \geq 0$ for all x. So this is indeed

impossible to get $\langle \psi^- | \psi^- \rangle < 0$.

b) The sequence $n_i, n_i - 1, n_i - 2, \ldots$ will include

0. Call the state $|0\rangle$ for which $N|0\rangle = n_0|0\rangle$
$= 0|0\rangle = 0$

what is $a|0\rangle$?

- Then $\langle a0 | a0 \rangle = \langle 0 | a^\dagger a | 0 \rangle = 0$

$\Rightarrow$ $a|0\rangle$ is null vector: $a|0\rangle = 0$

And $a(a|0\rangle) = 0$ also $\Rightarrow$ No states lower than $|0\rangle$

- Ladder begins with $|0\rangle$ & can be built up

from there: $|0\rangle, a^\dagger|0\rangle, (a^\dagger)^2|0\rangle, \ldots$

- All eigenstates of N are in ladders of this form.

Same for H since $[H, N] = 0$, b/c $H = \hbar\omega(N + \frac{1}{2})$

* - So we have our energy spectrum

- How many ladders are there?
- This amounts to asking how many states meeting description of $|0\rangle$ there are, i.e. is $|0\rangle$ degenerate? Will return to this
- First, normalize

$$\langle a^+ \psi_i | a^+ \psi_i \rangle = \langle \psi_i | a a^+ | \psi_i \rangle = \langle \psi_i | (a^+ a + 1) | \psi_i \rangle = n_i + 1$$

define $|n\rangle$ as the normalized state with $N|n\rangle = n|n\rangle$

- So, let's normalize $|n\rangle$ to 1.

we know these are non-negative integers by above arguments.

$$\langle 0 | 0 \rangle = 1$$

$$\langle a^+ 0 | a^+ 0 \rangle = 1$$

$$\langle a^+ 1 | a^+ 1 \rangle = 2 \Rightarrow a^+ |1\rangle = \sqrt{2}\, |2\rangle$$

$$\langle a^+ 2 | a^+ 2 \rangle = 3 \Rightarrow a^+ |2\rangle = \sqrt{3}\, |3\rangle$$

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

- These states are normalized eigenvectors of H, with $E_n = (n+\frac{1}{2})\hbar\omega$
- They are orthogonal, since they are eigenstates of a Hermitian operator with different eigenvalues

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

  & similar analysis leads to

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

- Check that these equations are consistent:

$$\sqrt{n} = \langle n-1|a|n\rangle = \left(\langle n-1|a|n\rangle\right)^* \quad (\text{since } \sqrt{n} \text{ real})$$

$$= \langle n|a^+|n-1\rangle = \sqrt{n} \;\checkmark$$

Harmonic Oscillator Redux, Part II

- We have found the energy spectrum for the H.O.

- Let's find the wavefunctions, i.e. $\langle x | n \rangle$, the projection of e.s. onto the position space basis

$\mathcal{O}|\psi\rangle$?

expand in basis - $|\psi\rangle = \sum_n c_n |\psi_n\rangle$

e.g. eigenstates of some operator.

Parity, H, position, etc.

~~Finite dim space~~

$\underbrace{\langle\psi_n|\mathcal{O}|\psi\rangle}_{\substack{\text{matrix when} \\ \text{collected over} \\ n}}$

~~describes~~ action of operator described by a matrix which takes expansion coefficients as input & gives other coefficients as output

What does "a" & "a^+" operators do?

Using energy eigenstate basis:

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

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

$$a = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 & 0 & \cdots \end{pmatrix} \quad \begin{matrix} |0\rangle \\ |1\rangle \\ |2\rangle \\ \vdots \end{matrix}$$

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Using position space basis

$\langle x | a | \psi \rangle$

what are coefficients for expansion in pos space?

$\psi(x)$

$\Updownarrow$

$\langle x | \psi \rangle = \psi(x)$

How do we represent action of $a = \frac{1}{\sqrt{2}}\left(\beta x + \frac{i}{\hbar\beta} p\right)$ in this basis?

$$\langle x | p | \psi \rangle = -i\hbar \frac{d}{dx} \psi(x) \iff \langle x | p = -i\hbar \frac{d}{dx} \langle x |$$

Could break down onto grid & write a matrix, but more convenient to write algebraic expression for transformation of coef in $\to$ coef. out

~~- Apart from proving that there is only one ladder, we have found~~

~~- We have found energy spectrum for H.O.~~

~~- Lets find wave functions, i.e.~~ $\cancel{\langle x|n\rangle}$ ~~projection of e.s. onto position space basis.~~

- Lets examine $\langle x|0\rangle = \varphi_0(x)$

$$0 = \langle x|a|0\rangle = \langle x|\frac{1}{\sqrt{2}}\left(\beta X + \frac{i}{\hbar\beta}P\right)|0\rangle$$

$$= \frac{1}{\sqrt{2}}\left(\beta x + \frac{i}{\hbar\beta}\left(-i\hbar\frac{d}{dx}\right)\right)\langle x|0\rangle$$

~~Recall~~ $\cancel{\psi(x)=\langle x|\psi\rangle,\ \langle x|P|\psi\rangle = -i\hbar\frac{d}{dx}\psi(x) \Leftrightarrow \langle x|P = -i\hbar\frac{d}{dx}\langle x|}$ ~~from~~

So

$$\left(\beta x + \frac{1}{\beta}\frac{d}{dx}\right)\varphi_0(x) = 0$$

This eqn has a unique solution, up to normalization:

$$\varphi_0(x) = \left(\frac{\beta}{\sqrt{\pi}}\right)^{1/2} e^{-\frac{1}{2}\beta^2 x^2} = \left(\frac{\beta}{\sqrt{\pi}}\right)^{1/2} e^{-\frac{1}{2}z^2}, \quad z = \beta x$$

It matches g.s. w.f. we found before, solving Sch. in pos. space.

- Since there is only one solution required for pos space requirements for $|0\rangle$, we have answered the degeneracy question. There is only one ladder + each eigen energy is non-degenerate.

- To construct higher w.f.s, we can use pos. space representation of $a^\dagger$

$$\langle x | a | \psi \rangle = \frac{1}{\sqrt{2}}\left(\beta x + \frac{1}{\beta}\frac{d}{dx}\right)\langle x | \psi \rangle \quad (x \,\&\, \tfrac{d}{dx} \text{ passes thru } \langle x|)$$

$$= \frac{1}{\sqrt{2}}\left(z + \frac{d}{dz}\right)\psi(x)$$

Similarly,

$$\langle x | a^\dagger | \psi \rangle = \frac{1}{\sqrt{2}}\left(z - \frac{d}{dz}\right)\psi(x)$$

(This is how a + $a^\dagger$ act in position space)

- A nice check on these formulae is to verify the pos-space reps of the operators satisfy the right commutation relations

$$\langle x | [a, a^\dagger] |\psi\rangle = \frac{1}{2}\left(z + \frac{d}{dz}\right)\left(z - \frac{d}{dz}\right)\psi(z) - \frac{1}{2}\left(z - \frac{d}{dz}\right)\left(z + \frac{d}{dz}\right)\psi(z)$$

z^2 + $\frac{d^2}{dz^2}$ die obviously

$$= -\frac{1}{2} z \frac{d}{dz}\psi + \frac{1}{2}\frac{d}{dz} z\psi - \frac{1}{2} z\frac{d}{dz}\psi + \frac{1}{2}\frac{d}{dz} z\psi$$

$$= \frac{d}{dz} z\psi - z\frac{d}{dz}\psi$$

$$= \psi + z\frac{d}{dz}\psi - z\frac{d}{dz}\psi$$

$$= 1 \cdot \psi(x)$$

So $[a, a^\dagger] = 1$ as expected

Now use ladder op to get $\varphi_1(x)$

$$|1\rangle = a^+|0\rangle :$$

$$\varphi_1(x) = \langle x|1\rangle = \langle x|a^+|0\rangle$$

$$= \frac{1}{\sqrt{2}}\left(z - \frac{d}{dz}\right)\left(\frac{\beta}{\sqrt{\pi}}\right)^{1/2} e^{-z^2/2}$$

$$= \left[\frac{\beta}{\sqrt{\pi}\cdot 2}\right]^{1/2} \cdot 2z\, e^{-z^2/2}$$

which ~~is~~ matches what we had before

$$\varphi_2(x) = \langle x|2\rangle = \langle x|\frac{a^+}{\sqrt{2}}|1\rangle = \ldots$$

Can generalize:

$$\varphi_n = \langle x|n\rangle = \left[\frac{\beta}{\sqrt{\pi}\, 2^n n!}\right]^{1/2} H_n(z)\, e^{-z^2/2}, \quad z = \beta x,$$

$$H_n(z) = e^{z^2}(-1)^n \frac{d^n}{dz^n} e^{-z^2}$$

More ~~simplified~~ compact form than we wrote before

E1 Transition

$d = \vec{\mathcal{E}} \cdot q\vec{r}$ ← location of charge

$\quad = \mathcal{E} q x$ for $\vec{\mathcal{E}} = \mathcal{E}\hat{x}$

$$P_{exc} \propto |\langle e | d | g \rangle|^2 \propto |\langle e | x | g \rangle|^2$$

Harm osc.:

- Could use pos. space basis
- But let's use φ_n basis

$\beta = \left(\frac{m\omega}{\hbar}\right)^{1/2}$

$\omega = \sqrt{\frac{k}{m}}$

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

$$p = (\ldots)(a - a^{+})$$

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

$\Rightarrow$ Dipole transition selection rule for H.O.:

$$\Delta n = \pm 1$$

- But anharm allows $\Delta n > 1$