Matrix Solution of Harmonic Oscillator

Last time:

$$* \ \mathbf{T}^{\dagger}\mathbf{A}^{\phi}\mathbf{T} = \begin{pmatrix} a_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & a_N \end{pmatrix}_{\psi}$$ transformation to the diagonal form of **A**

$$* \text{ eigenbasis } |i\rangle = \begin{pmatrix} \mathrm{T}^{\dagger}_{1i} \\ \vdots \\ \mathrm{T}^{\dagger}_{Ni} \end{pmatrix}_{\phi}$$ $i-th$ column of $\mathbf{T}^{\dagger}$ eigenbasis for **A**

* matrix representation of a function of a matrix is given by $\mathbf{T}f\left(\mathbf{T}^{\dagger}\mathbf{x}\mathbf{T}\right)\mathbf{T}^{\dagger}$

$$\text{e.g. } f(x) = \mathbf{x}^N = \mathbf{T}\overbrace{(\mathbf{T}^{\dagger}\mathbf{x}\mathbf{T})(\mathbf{T}^{\dagger}\mathbf{x}\mathbf{T})\ldots}^{\text{N diagonal terms}}\mathbf{T}^{\dagger} = \mathbf{T}\tilde{\mathbf{x}}^N\mathbf{T}^{\dagger} = \mathbf{x}^N$$

* Discrete Variable Representation: Matrix representation for *any* 1-D problem

Matrix version of numerical integration — works even for repulsive V(x) via addition of an infinite well

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TODAY: Harmonic Oscillator: Derive all matrix elements of **x**, **p**, **H** from the [**x,p**] commutation rule and the definition of **H**.

Example of how one can get matrix results entirely from commutation rule definitions (e.g. we will soon see this for an angular momentum: $\mathbf{J}^2$, $\mathbf{J}_x$, $\mathbf{J}_y$, $\mathbf{J}_z$, and the Wigner-Eckart Theorem)

NO WAVEFUNCTIONS, NO INTEGRALS, ALL MAGIC!

Outline of steps:

1. Assumptions
   - $* \ \mathbf{H} = \dfrac{\mathbf{p}^2}{2m} + \dfrac{k\mathbf{x}^2}{2}$ Specific Model
   - * eigen-basis exists for **H**
   - $* \ \left[\hat{x},\hat{p}\right] = i\hbar$ **Central postulate of QM**
   - * $\hat{x}$ and $\hat{p}$ are Hermitian (they have real expectation values)
2. x_{nm} and p_{nm} in terms of $(E_n - E_m)$
3. x_{nm} in terms of p_{nm}
4. Block Diagonalize **x, p, H** matrices (this is the most difficult step to understand)
5. Lowest quantum number must exist (call it 0) → explicit values for $|x_{01}|^2$ and $|p_{01}|^2$
6. Recursion relationship for $x_{nn\pm1}$ and $p_{nn\pm1}$ (x_{nn+1} from x_{n-1n}…)
7. Magnitudes and phases for $x_{nn\pm1}$ and $p_{nn\pm1}$
8. Possibility of noncommunicating blocks along diagonal of **H, x, p**?

See CTDL pages 488-500 for similar treatment. IN MORE
You will never use this methodology - only the results! ELEGANT NOTATION

Enjoy this!

1. recall assumptions
2. **x** and **p** matrix elements are derived here from Commutation Rules: x_{nm} and p_{nm} in terms of $E_n - E_m$

$$[\mathbf{x},\mathbf{H}] = \left[\mathbf{x}, \frac{\mathbf{p}^2}{2m} + \frac{1}{2}k\mathbf{x}^2\right] = \frac{1}{2m}\left[\mathbf{x},\mathbf{p}^2\right] = \frac{1}{2m}\left(\mathbf{p}\underbrace{[\mathbf{x},\mathbf{p}]}_{i\hbar} + \underbrace{[\mathbf{x},\mathbf{p}]}_{i\hbar}\mathbf{p}\right) = \frac{2i\hbar}{2m}\mathbf{p}$$

$$** \; \boxed{[\mathbf{x},\mathbf{p}] = i\hbar} \qquad \rightarrow [\mathbf{x},\mathrm{H}] = \frac{\mathbf{p}}{2\mathrm{m}}2i\hbar = \frac{i\hbar}{\mathrm{m}}\mathbf{p}$$

$$\mathbf{p} = \left(\frac{\mathrm{m}}{i\hbar}\right)[\mathbf{x},\mathbf{H}]$$

Take n,m matrix elements of both sides, insert completeness operator, $\sum_\ell |\ell\rangle\langle\ell|$, between **x** and **H**.

$$p_{nm} = \left(\frac{m}{i\hbar}\right)\sum_\ell \left(x_{n\ell}H_{\ell m} - H_{n\ell}x_{\ell m}\right).$$

Similarly, starting from $[\mathbf{p},\mathbf{H}] = \left[\mathbf{p},\frac{1}{2}k\mathbf{x}^2\right] = -i\hbar k\mathbf{x}$

rearrange and solve for x_{nm}

$$x_{nm} = \frac{i}{k\hbar}\sum_\ell \left(p_{n\ell}H_{\ell m} - H_{n\ell}p_{\ell m}\right).$$

But we know that some basis set of functions (the "harmonic oscillator eigenbasis") must exist in which **H** is diagonal. Use it implicitly: $\therefore$ replace $H_{\ell m}$ by $E_m\delta_{m\ell}$. This kills the sum over ℓ.

$$p_{nm} = \left(\frac{m}{ih}\right)\left(x_{nm}E_m - E_n x_{nm}\right)$$

$$p_{nm} = \left(\frac{m}{i\hbar}\right)x_{nm}\left(E_m - E_n\right)$$

so for the special case of $n = m$, $p_{nn} = 0$

(but, in addition, $p_{nn} = 0$ if **H** for the harmonic oscillator has a <u>degenerate</u> eigenvalue, then $p_{nm} = 0$ if $E_n = E_m$)

similarly for the x_{nm} equation

$$x_{nm} = \frac{i}{\hbar k}p_{nm}\left(E_m - E_n\right)$$

$\therefore$ $x_{nn} = 0$ (and $x_{nm} = 0$ if $E_n = E_m$)

Updated 8/13/20 8:23 AM

3. solve for the non-zero x_{nm} in terms of the non-zero p_{nm}

multiply the x_{nm} equation by p_{nm}
multiply the p_{nm} equation by x_{nm}

The LHSs of both resulting equations are equal

equate RHSs: $\frac{\mathrm{m}}{\mathrm{i}\hbar} x_{nm}^2 (E_m - E_n) = \frac{i}{\hbar k} p_{nm}^2 (E_m - E_n)$

* If $E_n = E_m$ (degeneracy) – then we already know that $x_{nm} = 0$, $p_{nm} = 0$

* If $E_n \neq E_m$ then we can divide by $(E_m - E_n)$ and rearrange

$$\boxed{x_{nm}^2 = -\frac{1}{km} p_{nm}^2}$$

$$x_{nm} = \pm i(km)^{-1/2} p_{nm}$$

THERE IS A PHASE AMBIGUITY HERE!

Need to find out what phase choice is consistent with other requirements

Earlier we derived $\quad p_{nm} = \frac{m}{i\hbar} x_{nm} (E_m - E_n)$

plug in new result for x_{nm} $\quad p_{nm} = \frac{m}{i\hbar} \left(\pm i (km)^{-1/2}\right) p_{nm} (E_m - E_n)$

Thus either:

* $\quad p_{nm} \neq 0$ AND $E_m - E_n = \pm\hbar (k/m)^{1/2} \equiv \pm\hbar\omega$!!

(Why is it OK to divide thru by p_{nm}?)

OR

when $E_m \neq E_n \pm \hbar\omega$

* $\quad p_{nm} = 0 \Rightarrow x_{nm} = 0$

This is the most difficult but most crucial point in the logic.

The *only* non-zero off-diagonal matrix elements of **x** and **p** involve eigenfunctions of **H** that have energies differing by exactly $\hbar\omega$!
A "selection rule"! The only nonzero matrix elements of **x** and **p** are those where the indices for each non-zero x_{nm} and p_{nm} differ by ±1.

Updated 8/13/20 8:23 AM

4. <u>**x, p, H** are block "diagonalized"</u> within this set one finds all of the non-zero elements of **x** and **p**.

In what sense? There is a set of eigenstates of **H** that have energies that fall onto a comb of evenly spaced $E_n^{(1)}$ values:

$$E_n^{(1)} = n(\hbar\omega) + \varepsilon_1$$

But there could be another set:

$$E_n^{(2)} = n(\hbar\omega) + \varepsilon_2 \qquad \text{where } \varepsilon_2 - \varepsilon_1 \neq n\hbar\omega$$

for all n

Set II $E_0^{(2)}$ is lowest

$$E_1^{(2)} = E_0^{(2)} + \hbar\omega$$

But within each set, there must be a lowest energy level

Set I $E_0^{(1)}$ is lowest

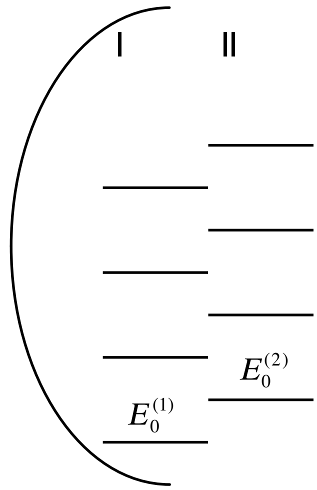
$$E_1^{(1)} = E_0^{(1)} + \hbar\omega$$

etc.

Set I $E_0^{(2)}$ is lowest

$$E_1^{(2)} = E_0^{(2)} + \hbar\omega$$

etc.



possibly interleaved but are they non-communicating?

Since **x** and **p** have nonzero elements only within communicating sets for **H**, thus **x**, **p**, **H** are block diagonalized into sets I, II, etc.

$$\mathbf{H},\mathbf{x},\mathbf{p} = \left(\begin{array}{c|c|c|c} \mathrm{I} & 0 & 0 & 0 \\ \hline 0 & \mathrm{II} & 0 & 0 \\ \hline 0 & 0 & \mathrm{III} & 0 \\ \hline 0 & 0 & 0 & \ddots \end{array}\right)$$

We will eventually show that all of these blocks along the diagonal are identical (and that each energy level is nondegenerate). If **x, p** are "block diagonal", then $\mathbf{x}^2$, $\mathbf{p}^2$ are similarly block diagonal.

Updated 8/13/20 8:23 AM

5. <u>A lowest index must exist within each block. Call it 0</u>.

[**x**,**p**] = i$\hbar$ is a diagonal matrix: i$\hbar\mathbb{1}$

$$\sum_{\ell}\left(x_{n\ell}p_{\ell m}-p_{n\ell}x_{\ell m}\right)=i\hbar\delta_{nm}$$ because [**x**,**p**] = i$\hbar\mathbb{1}$

$(\mathbf{xp})_{nm}$ $(\mathbf{px})_{nm}$

$$i\hbar=\left(\underbrace{x_{nn+1}p_{n+1n}}_{\text{indices must be equal}}-p_{nn+1}x_{n+1n}\right)+\left(x_{nn-1}p_{n-1n}-p_{nn-1}x_{n-1n}\right)$$

These are the only surviving nonzero terms in the sum over ℓ. because we showed that the ***x,p*** matrix elements are non-zero only between states with E different by $\pm\hbar\omega$. This is the basis for the indexing of the basis states within a block.

There *must* be a lowest E_i because, classically,

E = T + V and T ≥ 0, E ≥ V_{min}.

Let n = 0 be the lowest allowed index (this is an arbitrary choice of labels).

$p_{0,-1} = x_{0,-1} = 0$ (–1 is not an allowed index.)

$$\boxed{x_{01}p_{10}-p_{01}x_{10}=i\hbar}$$

used Hermiticity here

x,**p** are Hermitian $\left(\mathbf{A}=\mathbf{A}^{\dagger}\right)$ thus $x_{01}p_{01}^{*}-p_{01}x_{01}^{*}=i\hbar$

we are going to insert this into the above $x_{01}p_{10}$ equation

previously $x_{nm}=\pm i\left(km\right)^{-1/2}p_{nm}$

$x_{01}=\pm i\left(km\right)^{-1/2}p_{01}$

(note that the same symbol is used for mass and one of the basis state indices)

We must make phase choices so that both **x** and **p** are Hermitian.

Phase ambiguity: we are free to specify the absolute phase of **x** or **p** BUT NOT BOTH because that would affect the value of [**x**,**p**]

BY CONVENTION:

all non-zero matrix elements of **x** are REAL
all non-zero matrix elements of **p** are IMAGINARY

try $x_{01} = +i\left(km\right)^{-1/2} p_{01}$ and eliminate p_{01} by plugging this value of x_{01} into $x_{01}p_{01}^* - p_{01}x_{01}^* = i\hbar$: we get $i(km)^{-1/2}\left|p_{01}\right|^2 + i(km)^{-1/2}\left|p_{01}\right|^2 = i\hbar$

thus

$$\left|x_{01}\right|^2 = \frac{\hbar}{2}\left(km\right)^{-1/2}$$

$$\left|p_{01}\right|^2 = \frac{\hbar}{2}\left(km\right)^{+1/2} \quad !!!$$

[If we had chosen $x_{01} = -i\left(km\right)^{-1/2} p_{01}$ we would have obtained $\underbrace{\left|x_{01}\right|^2}_{\geq 0} = -\frac{\hbar}{2}\left(km\right)^{1/2}$ which is impossible!]

There are two things that must be checked for self-consistency of seemingly arbitrary phase choices at every opportunity:

* Hermiticity

* $\left| \qquad \right|^{\mathbf{2}} \geq \mathbf{0}$.

6. <u>Recursion Relation for $\left|x_{n,n+1}\right|^2$</u>

Start again with the general equation derived in part #3 above using the phase choice that worked in part #5 above

$$\underbrace{x_{nn+1}}_{\uparrow} = i(km)^{-1/2}\underbrace{p_{nn+1}}_{\uparrow}$$

index increasing by 1

Hermiticity of **x** and **p**

$$x_{n+1n}^* = i\left(km\right)^{-1/2} p_{n+1n}^*$$

c.c. of both sides

$$\underbrace{x_{n+1n}}_{\uparrow} = -i(km)^{-1/2}\underbrace{p_{n+1n}}_{\uparrow}$$

index decreasing by 1

Updated 8/13/20 8:23 AM

$$\therefore \quad x_{nn\pm1} = \pm i(km)^{-1/2}\, p_{nn\pm1}$$

these 3 choices of ± go together

Now the arbitrary part of the phase ambiguity in the relationship between **x** and **p** has been eliminated

Apply this to the general term in [**x**,**p**] ⇒ requires a lot of algebra

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NONLECTURE : evaluation of the four non-zero terms in [**x**,**p**] = i$\hbar$, given here:

$$x_{nn+1}p_{n+1n} = x_{nn+1}p^{*}_{nn+1} = x_{nn+1}\left(-\frac{(km)^{1/2}}{i}x^{*}_{nn+1}\right)$$

$$= \left|x_{nn+1}\right|^2\left(+i(km)^{1/2}\right)$$

$$-p_{nn+1}x_{n+1n} = -\left(\frac{(km)^{1/2}}{i}x_{nn+1}\right)\left(x^{*}_{nn+1}\right) = \left|x_{nn+1}\right|^2\left(+i(km)^{1/2}\right)$$

$$x_{nn-1}p_{n-1n} = x_{nn-1}p^{*}_{nn-1} = x_{nn-1}\left(+\frac{(km)^{1/2}}{i}x^{*}_{nn-1}\right)$$

$$= \left|x_{nn-1}\right|^2\left(-i(km)^{1/2}\right)$$

$$-p_{nn-1}x_{n-1n} = -\left(-\frac{(km)^{1/2}}{i}x_{nn-1}\right)\left(x^{*}_{nn-1}\right) = \left|x_{nn-1}\right|^2\left(-i(km)^{1/2}\right)$$

Combine the 4 terms in [**x**,**p**] = i$\hbar$ to get

$$i\hbar = 2i(km)^{1/2}\left[\left|x_{nn+1}\right|^2 - \left|x_{nn-1}\right|^2\right]$$

$$\left|x_{nn+1}\right|^2 = \frac{\hbar(km)^{-1/2}}{2} + \left|x_{nn-1}\right|^2 \qquad \text{recursion relation}$$

OK to reverse indices in $\left|\;\right|^2$

$$\text{but } \left|x_{01}\right|^2 = \left|x_{10}\right|^2 = \frac{\hbar}{2}(km)^{-1/2}$$

$$\left|x_{n+1n}\right|^2 \leftarrow \left|x_{nn+1}\right|^2$$

Each step-up in quantum number produces another additive term: $\frac{\hbar}{2}(km)^{-1/2}$

thus

$$\boxed{\begin{aligned}\left|x_{nn+1}\right|^2 &= (n+1)\frac{\hbar}{2}(km)^{-1/2}\\ \left|p_{nn+1}\right|^2 &= (n+1)\frac{\hbar}{2}(km)^{+1/2}\end{aligned}}$$

general result

Updated 8/13/20 8:23 AM

7. Magnitudes and Phases for $x_{nn\pm1}$ and $p_{nn\pm1}$

Verify phase consistency and Hermiticity for **x** and **p.**

In part #3 we derived $x_{nn\pm1} = \pm i(km)^{-1/2} p_{nn\pm1}$

one self-consistent set is

x real and positive

$$\begin{cases} x_{nn+1} = +(n+1)^{1/2}\left(\dfrac{\hbar}{2(km)^{1/2}}\right)^{1/2} = +x_{n+1n} \\ x_{nn-1} = +(n)^{1/2}\left(\dfrac{\hbar}{2(km)^{1/2}}\right)^{1/2} = +x_{nn-1} \end{cases}$$

AND

p imaginary with sign flip for up vs. down

$$\begin{cases} p_{nn+1} = -i(n+1)^{1/2}\left(\dfrac{\hbar(km)^{1/2}}{2}\right)^{1/2} = -p_{n+1n} \\ p_{nn-1} = +i(n)^{1/2}\left(\dfrac{\hbar(km)^{1/2}}{2}\right)^{1/2} = -p_{n-1n} \end{cases}$$

Note that nonzero matrix elements of x and p are always ∝ to the SQRT of the larger quantum number.
This is the usual phase convention: $x_{nn\pm1}$ real and positive, $p_{nn+1} = -p_{n+1n}$ imaginary.
Must be careful about phase choices because in the matrix form of QM one never really looks at wavefunctions, operators, or integrals

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8. Possible existence of noncommunicating blocks along the diagonal of **H, x, p**

You show that $H_{nm} = (n+1/2)\hbar\left(\dfrac{k}{m}\right)^{1/2}\delta_{nm}$ from definition of **H**

$$\left(\begin{array}{l}\text{Note that } \mathbf{x}^2 \text{ and } \mathbf{p}^2 \text{ have nonzero } \Delta\text{n}=\pm 2 \text{ elements but} \\ \dfrac{1}{2}k\mathbf{x}^2 + \dfrac{\mathbf{p}^2}{2m} \text{ has cancelling contributions in the } \Delta\text{n}=+2 \text{ and } \Delta\text{n} = -2 \text{ locations}\end{array}\right)$$

This result implies

* all of the possibly independent blocks in **x**, **p**, **H** are identical because they all start from the same lowest energy
* $E^{(i)}_n = n\hbar\omega + \varepsilon_i$ where $\varepsilon_i = (1/2)\hbar\omega$ for all i
* degeneracy of all E_n? All E_n must have the same degeneracy, but I can't prove that this degeneracy is 1. Are there parallel non-communicating universes?

Updated 8/13/20 8:23 AM