Matrix Solution of Harmonic Oscillator

Last time:

$$* \quad \mathbf{T}^{\dagger}\mathbf{A}^{\phi}\mathbf{T} = \begin{pmatrix} a_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & a_N \end{pmatrix}$$

$$* \quad \text{eigenbasis } |i\rangle = \begin{pmatrix} T_{1i} \\ \vdots \\ T_{Ni} \end{pmatrix}_{\phi} \qquad i-\text{th column of } \mathbf{T}$$

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

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

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

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

NO WAVEFUNCTIONS, NO INTEGRALS, ALL MAGIC!

Outline of steps:

1. Assumptions

   * $\mathbf{H} = \dfrac{\mathbf{p}^2}{2m} + \dfrac{k\mathbf{x}^2}{2}$

   * eigen basis exists for **H**

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

   * $\hat{x}$ and $\hat{p}$ are Hermitian (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**
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 $p_{nn\pm1}$
7. Magnitudes and phases for $x_{nn\pm1}$ and $p_{nn\pm1}$
8. Possibility of noncommunicating blocks along diagonal of **H, x, p** eliminated

See CTDL pages 488-500 for similar treatment. IN MORE ELEGANT NOTATION

You will never use this methodology - only the results!

1. <u>recall assumptions</u>
2. **x** and **p** matrix elements derived from Comm. Rules

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

** $[\mathbf{x},\mathbf{p}] = i\hbar$ $\quad \rightarrow [\mathbf{x},\mathrm{H}] = \dfrac{\mathbf{p}}{2\mathrm{m}} 2i\hbar = \dfrac{i\hbar}{\mathrm{m}}\mathbf{p}$

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

take matrix elements of both sides, insert completeness between **x** and **H**

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

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

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

but we know that some basis set must exist where **H** is diagonal. Use it implicitly:

$\therefore$ replace $\mathrm{H}_{\ell\mathrm{m}}$ by $\mathrm{E_m}\delta_{\mathrm{m}\ell}$

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

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

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

similarly for

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

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

3. solve for x_{nm} in terms of 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 RHS: $\frac{m}{i\hbar} x_{nm}^2 (E_m - E_n) = \frac{i}{\hbar k} p_{nm}^2 (E_m - E_n)$

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

* If $E_n \neq E_m$ $\boxed{x_{nm}^2 = -\frac{1}{km} p_{nm}^2}$

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

↑ THERE IS A PHASE AMBIGUITY HERE!

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

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

Either

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

OR

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

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 indices differ by ±1.

4. <u>**x, p, H** are block diagonalized</u>

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

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

could be another set

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

(↑ all n)

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

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

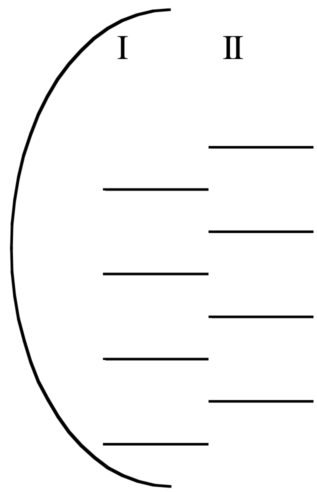
$$E_1^{(1)} = E_0^{(1)} + \hbar\omega$$

etc.

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

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

etc.



interleaved but noncommunicating?

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.

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

$[\mathbf{x},\mathbf{p}] = i\hbar$ is a diagonal matrix

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

$$i\hbar = \left(x_{nn+1}p_{n+1n} - p_{nn+1}x_{n+1n}\right) + \left(x_{nn-1}p_{n-1n} - p_{nn-1}x_{n-1n}\right)$$

must be equal

These are the only surviving nonzero terms in the sum over ℓ!

but there must be a lowest E_i because

$E = T + V$ and $T \geq 0$, $E \geq V_{min}$

let n = 0 be lowest index

$$p_{0,-1} = x_{0,-1} = 0$$

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

used Hermiticity here

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

previously $x_{nm} = \pm i(km)^{-1/2}\,p_{nm}$ (note that the same symbol is used for mass and basis state index)

we must make phase choices so that **x** and **p** are Hermitian phase ambiguity: we can specify absolute phase of **x** or **p** BUT NOT BOTH because that would affect value of [**x**,**p**]

BY CONVENTION:

matrix elements of **x** are REAL
p are IMAGINARY

try $x_{01} = +i(km)^{-1/2} p_{01}$ and eliminate p_{01} by plugging this into
$x_{01} p_{01}^{*} - p_{01} x_{01}^{*} = i\hbar$

get
$$|x_{01}|^2 = \frac{\hbar}{2}(km)^{-1/2}$$
$$|p_{01}|^2 = \frac{\hbar}{2}(km)^{+1/2}$$

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

two things that must be checked for self-consistency of seemingly arbitrary phase choices at every opportunity:
* Hermiticity
* $|\quad|^2 \geq 0$

6. Recursion Relation for $|x_{ii+1}|^2$

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

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

index going up

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

c.c. of both sides

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

index going down

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

now the arbitrary part of the phase ambiguity in the relationship between **x** and **p** is eliminated

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

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NONLECTURE : from four terms in [**x**,**p**] = i$\hbar$

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

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

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

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

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

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

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

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

$$|x_{nn+1}|^2 = \frac{\hbar(\mathrm{km})^{-1/2}}{2} + |x_{nn-1}|^2$$

recursion relation

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

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

thus

$$|x_{nn+1}|^2 = (n+1)\frac{\hbar}{2}(\mathrm{km})^{-1/2}$$

$$|p_{nn+1}|^2 = (n+1)\frac{\hbar}{2}(\mathrm{km})^{+1/2}$$

general result

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

verify phase consistency and hermiticity for **x** and **p**

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

one self-consistent set is

x real and positive

$$x_{nn+1} = +(n+1)^{1/2}\left(\frac{\hbar}{2(\text{km})^{1/2}}\right)^{1/2} = +x_{n+1n}$$

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

AND

p imaginary with sign flip for up vs. down

$$p_{nn+1} = -i(n+1)^{1/2}\left(\frac{\hbar(\text{km})^{1/2}}{2}\right)^{1/2} = -p_{n+1n}$$

$$p_{nn-1} = +i(n)^{1/2}\left(\frac{\hbar(\text{km})^{1/2}}{2}\right)^{1/2} = -p_{n-1n}$$

Note that nonzero matrix elements of x and p are always ∝ [larger quantum number]$^{1/2}$
This is the usual phase convention
Must be careful about phase choices because one never really looks at wavefunctions, operators, or integrals

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

you show that $H_{nm} = (n + \mathbf{1/2})\hbar\left(\frac{k}{m}\right)^{1/2}\delta_{nm}$

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

This result implies

* all of the possibly independent blocks in **x**, **p**, **H** are identical
* $\varepsilon_i = (1/2)\hbar\omega$ for all i
* degeneracy of all E_n? all E_n must have same degeneracy, but can't prove that it is 1.