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End of Matrix Solution of H-O, and Feel the Power of the a and a[†] Operators

1. starting from
$$\mathbf{H} = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}k\mathbf{x}^2$$
 and $[\mathbf{x},\mathbf{p}] = i\hbar$

2. we showed
$$p_{nm} = \frac{m}{i\hbar} x_{nm} (E_m - E_n)$$

 $x_{nm} = \frac{i}{\hbar k} p_{nm} (E_m - E_n)$
 $\therefore x_{nn} = 0, p_{nn} = 0 \text{ and } \begin{cases} x_{nm} \\ p_{nm} \end{cases} = 0 \text{ if } E_n = E_m$
3. $x_{nm}^2 = -\frac{1}{km} p_{nm}^2$
 $E_m - E_n = \pm \hbar \omega \qquad \omega = (k/m)^{1/2}$

 \therefore the only non-zero **x** and **p** elements are between states whose *E*'s differ by $\pm \hbar \omega$

- 4. combs of connected states, "block diagonalization" of **H**, **x**, **p**, **x**², **p**²: $E_n^{(i)} = \hbar \omega n + \varepsilon_i$
- 5. lowest index must exist because lowest *E* must exist. Call this index 0

$$|x_{01}|^{2} = \frac{\hbar}{2} (km)^{-1/2}$$
 from arbitrary (but almost universally chosen) phase choice
$$|p_{01}|^{2} = \frac{\hbar}{2} (km)^{+1/2}$$

$$x_{01} = +i(km)^{-1/2} p_{01}$$

Today

- 6. Recursion Relationship: $|x_{nn+1}|^2$ in terms of $|x_{nn-1}|^2$ general matrix elements $|x_{nn+1}|^2$, $|p_{nn+1}|^2$
- 7. general **x** and **p** elements
- 8. the only blocks of **H** correspond to $\varepsilon_i = \frac{1}{2}\hbar\omega$

We are ready to derive a powerful, compact, and intuitive algebra:

Dimensionless \mathbf{x} , \mathbf{p} , \mathbf{H} and \mathbf{a} (annihilation) and \mathbf{a}^{\dagger} (creation) operators.

constant offset for block *i*

phase ambiguity: we can specify absolute phase of \mathbf{x} or \mathbf{p} BUT NOT BOTH because that would affect the value of $[\mathbf{x},\mathbf{p}]$

BY CONVENTION:

matrix elements of **x** are REAL **p** are IMAGINARY try $x_{01} = +i(km)^{-1/2} p_{01}$ and plug 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! check for self-consistency of seemingly arbitrary phase choices at every opportunity: *Hermiticity $(\mathbf{A}^{\dagger} = \mathbf{A}, A_{ij}^* = A_{ji})$ $* | | |^2 \ge 0$ for any A_{ij}

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

start again with general equation derived in part #3 of Lecture #12 using the phase choice that worked

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

c.c. of both sides
index decreasing
$$x_{n+1n} = -i(km)^{-1/2} p_{n+1n}$$

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

now the arbitrary part of the phase ambiguity in the relationship between ${\bf x}$ and ${\bf p}$ is eliminated

Apply this to the general term in $[\mathbf{x},\mathbf{p}] \Rightarrow$ algebra

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

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

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

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

thus

general result

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

7. <u>Magnitudes and Phases for x_{nn+1} and p_{nn+1} </u>

verify phase consistency and Hermiticity for \boldsymbol{x} and \boldsymbol{p}

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

one self-consistent set is
matrix elements
of **x** real and
positive
$$\begin{bmatrix} x_{nn+1} = +(n+1)^{1/2} \left(\frac{\hbar}{2(km)^{1/2}}\right)^{1/2} = +x_{n+1n} \\ x_{nn-1} = +(n)^{1/2} \left(\frac{\hbar}{2(km)^{1/2}}\right)^{1/2} = +x_{nn-1} \\ Kmn \\ kmn \\ matrix elements
of p imaginary
with sign flip for
up vs. down
$$\begin{bmatrix} p_{nn+1} = -i(n+1)^{1/2} \left(\frac{\hbar(km)^{1/2}}{2}\right)^{1/2} = -p_{n+1n} \\ p_{nn-1} = +i(n)^{1/2} \left(\frac{\hbar(km)^{1/2}}{2}\right)^{1/2} = -p_{n-1n} \\ \end{bmatrix}$$$$

This is the usual phase convention

Phase is a recurrent problem in matrix mechanics because we never look at wavefunctions or evaluate integrals explicitly.

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

you show that $H_{nm} = (n+1/2)\hbar \left(\frac{k}{m}\right)^{1/2} \delta_{nm}$ (note that \mathbf{x}^2 and \mathbf{p}^2 have non-zero $\Delta n = \pm 2$ elements but $\frac{1}{2}k\mathbf{x}^2 + \frac{\mathbf{p}^2}{2m}$ has cancelling contributions in $\Delta n = \pm 2$ locations)

This result implies

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

End of repetition from Lecture #12

Creation and Annihilation Operators (CTDL pages 488-508)

- * Dimensionless operators
- * simple operator algebra rather than complicated real algebra
- * matrices arranged according to "selection rules"
- * matrix elements calculated by extremely simple rules
- * automatic generation of any basis function by repeated operations on lowest (nodeless) basis state

Get rid of system-specific factors k, μ , ω and also \hbar .

$$\omega = (k/m)^{1/2}$$

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

$$\mathbf{p} = (\hbar m\omega)^{-1/2} \mathbf{p}$$

$$\mathbf{p} = (\hbar m\omega)^{-1/2} \mathbf{p}$$

$$\mathbf{H} = \frac{1}{\hbar\omega} \mathbf{H} = \frac{1}{2} \left(\mathbf{x}^{2} + \mathbf{p}^{2}\right)$$

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

$$\frac{1}{2} k \left(\frac{\hbar}{m\omega}\right) = \frac{1}{2} \hbar \omega \left(\mathbf{x}^{2} + \mathbf{p}^{2}\right)$$

$$\frac{1}{2} \frac{1}{2} k \left(\frac{\hbar}{m\omega}\right) = \frac{1}{2} \hbar \omega \left(\mathbf{x}^{2} + \mathbf{p}^{2}\right)$$

$$\frac{1}{2} \frac{1}{2} k \left(\frac{\hbar}{m\omega}\right) = \frac{1}{2} \hbar \omega \left(\mathbf{x}^{2} + \mathbf{p}^{2}\right)$$

$$\frac{1}{2m} (\hbar m\omega) = \frac{1}{2} \hbar \omega$$

$$\left[\mathbf{x}, \mathbf{p}\right] = \left(\frac{m\omega}{\hbar} \frac{1}{\hbar m\omega}\right)^{1/2} \left[\mathbf{x}, \mathbf{p}\right] = \frac{1}{\hbar} (i\hbar) = i$$
dimensionless
from results for $\mathbf{x}, \mathbf{p}, \mathbf{H}$

$$x_{mn} = 2^{-1/2} \left[(n+1)^{1/2} \delta_{mn+1} + n^{1/2} \delta_{mn-1} \right]$$

$$p_{mn} = 2^{-1/2} i \left[(n+1)^{1/2} \delta_{mn+1} - n^{1/2} \delta_{mn-1} \right]$$

$$H_{mn} = (n+1/2) \delta_{mn}$$
have the negative sign

Kronecker – δ 's specify selection rules for all nonzero matrix elements

Now define something new: use \mathbf{a} , \mathbf{a}^{\dagger} to clean things up even more!



Let's examine the matrix elements of **a** and \mathbf{a}^{\dagger} now plug in *m n* matrix elements of **x** and **p** from previous page

$$a_{mn} = \begin{bmatrix} 2^{-1/2} \mathbf{x}_{mn} + 2^{-1/2} i \mathbf{p}_{mn} \end{bmatrix}$$
$$= \begin{bmatrix} \frac{1}{2} (n+1)^{1/2} \delta_{mn+1} - \frac{1}{2} (n+1)^{1/2} \delta_{mn+1} + \frac{1}{2} n^{1/2} \delta_{mn-1} + \frac{1}{2} n^{1/2} \delta_{mn-1} \end{bmatrix}$$
$$\mathbf{x}_{mn} = \begin{bmatrix} \mathbf{x}_{mn} + \mathbf{x}_{mn} + \mathbf{x}_{mn} \end{bmatrix}$$

group terms according to "selection rule"

two terms cancel

two terms add

 $a_{mn} = n^{1/2} \delta_{mn-1}$

the first (left) index is <u>one smaller</u> than the second (right)

$$a_{mn} = \langle m | \mathbf{a} | \mathbf{n} \rangle = n^{1/2}$$
row
$$n^{1/2} | n - 1 \rangle$$

similarly

$$a_{mn}^{\dagger} = \left(n+1\right)^{1/2} \delta_{mn+1}$$

 ${\boldsymbol{a}}$ is lowering or "annihilation" operator

$$a_{mn}^{\dagger} = \left\langle m \middle| \mathbf{a}^{\dagger} \middle| n \right\rangle = (n+1)^{1/2}$$

the first index is one larger than the second \mathbf{a}^{\dagger} is a "creation" operator



needed to normalize. Each application of \mathbf{a}' gives the next larger integer. Do it *n* times on $|0\rangle$, get $n! |n\rangle$.

More tricks: look at $\,\,aa^{\dagger}\,and\,\,a^{\dagger}a$

is **aa**[†] Hermitian?

$$\left(\mathbf{a}\mathbf{a}^{\dagger}\right)^{\dagger}=\mathbf{a}^{\dagger\dagger}\mathbf{a}^{\dagger}=\mathbf{a}\mathbf{a}^{\dagger}$$

∴ **aa**[†] and **a**[†]**a** are Hermitian — to what "observable" quantity do they correspond? We will see that one of these is called the "number operator."

 $[(AB)^{\dagger} = B^{\dagger}A^{\dagger}]$ definition of Hermitian

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

similarly $\mathbf{a}^{\dagger}\mathbf{a} = \frac{1}{2} \left(\mathbf{x}^{2} + \mathbf{p}^{2} - 1 \right)$ $\therefore \mathbf{H} = \frac{1}{2} \left(\mathbf{a}^{\dagger}\mathbf{a} + \mathbf{a}\mathbf{a}^{\dagger} \right) \text{ and } \left[\mathbf{a}, \mathbf{a}^{\dagger} \right] = 1$ $\mathbf{H} = \mathbf{a}^{\dagger}\mathbf{a} + 1/2$ simple form for \mathbf{H}

H is the number operator + 1/2

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

$$\mathbf{A}^{\dagger} \mathbf{a} | n \rangle = n | n \rangle$$

$$\mathbf{a}^{\dagger} \mathbf{a} | n \rangle = n | n \rangle$$

$$\mathbf{a}^{\dagger} \mathbf{a} \text{ is "number operator"}$$

$$\begin{bmatrix} \mathbf{a} \mathbf{a}^{\dagger} | n \rangle = (n+1) | n \rangle \end{bmatrix} \text{ not as useful}$$

What have we done? We have exposed all of the "symmetry" and universality of the H–O basis set. We can now trivially work out what the matrix for any $\mathbf{x}^n \mathbf{p}^m$ operator looks like and organize it according to selection rules.

What about \mathbf{x}^{3} ?

$$\mathbf{x}^{3} = \left(\frac{m\omega}{\hbar}\right)^{-3/2} \mathbf{x}^{3}$$
When you multiply this out,
preserve the order of **a** and **a**[†]
factors.

$$\mathbf{x}^{3} = (2^{-3/2})(\mathbf{a} + \mathbf{a}^{\dagger})^{3}$$

$$= (2^{-3/2})[\mathbf{a}^{3} + (\mathbf{a}^{\dagger}\mathbf{a}\mathbf{a} + \mathbf{a}\mathbf{a}^{\dagger}\mathbf{a} + \mathbf{a}\mathbf{a}\mathbf{a}^{\dagger} + \mathbf{a}^{\dagger}\mathbf{a}\mathbf{a}^{\dagger} + \mathbf{a}^{\dagger}\mathbf{a}^{\dagger}\mathbf{a}) + \mathbf{a}^{\dagger^{3}}]$$

$$\Delta n = -3, \quad -1, \quad +1, \quad (\# \text{ of } \dagger \text{ minus} \# \text{ of non-}\dagger)$$

Simplify each group using commutation properties so that it has form

NONLECTURE: Simplify the $\Delta n = -1$ terms.

$$a^{\dagger}aa = aa^{\dagger}a \underbrace{-aa^{\dagger}a + a^{\dagger}aa}_{[a^{\dagger}, a]a = -a} = aa^{\dagger}a - a$$
$$aaa^{\dagger} = aa^{\dagger}a \underbrace{-aa^{\dagger}a + aaa^{\dagger}}_{a[a, a^{\dagger}]=a} = aa^{\dagger}a + a$$
$$\begin{bmatrix} a^{\dagger}aa + aa^{\dagger}a + aaa^{\dagger} \end{bmatrix} = 3aa^{\dagger}a$$

add and subtract the term needed to reverse order

try to put everthing into **aa[†]a** order

NONLECTURE: Simplify the $\Delta n = +1$ terms.

$$\mathbf{a}\mathbf{a}^{\dagger}\mathbf{a}^{\dagger} = \mathbf{a}^{\dagger}\mathbf{a}\mathbf{a}^{\dagger} - \mathbf{a}^{\dagger}\mathbf{a}\mathbf{a}^{\dagger} + \mathbf{a}\mathbf{a}^{\dagger}\mathbf{a}^{\dagger} = \mathbf{a}^{\dagger}\mathbf{a}\mathbf{a}^{\dagger} + \mathbf{a}^{\dagger}$$
$$\begin{bmatrix} \mathbf{a},\mathbf{a}^{\dagger} \end{bmatrix} \mathbf{a}^{\dagger} = \mathbf{a}^{\dagger}$$
$$\begin{bmatrix} \mathbf{a},\mathbf{a}^{\dagger} \end{bmatrix} \mathbf{a}^{\dagger} = \mathbf{a}^{\dagger}$$
$$\mathbf{a}^{\dagger}\mathbf{a}\mathbf{a}^{\dagger} = \mathbf{a}^{\dagger}\mathbf{a}^{\dagger}\mathbf{a} - \mathbf{a}^{\dagger}\mathbf{a}^{\dagger}\mathbf{a} + \mathbf{a}^{\dagger}\mathbf{a}\mathbf{a}^{\dagger} = \mathbf{a}^{\dagger}\mathbf{a}^{\dagger}\mathbf{a} + \mathbf{a}^{\dagger}$$
$$\mathbf{a}^{\dagger}\begin{bmatrix} \mathbf{a},\mathbf{a}^{\dagger} \end{bmatrix} = \mathbf{a}^{\dagger}$$
$$\begin{bmatrix} \mathbf{a}\mathbf{a}^{\dagger}\mathbf{a}^{\dagger} + \mathbf{a}^{\dagger}\mathbf{a}\mathbf{a}^{\dagger} + \mathbf{a}^{\dagger}\mathbf{a}^{\dagger}\mathbf{a} \end{bmatrix} = 3\mathbf{a}^{\dagger}\mathbf{a}^{\dagger}\mathbf{a} + 3\mathbf{a}^{\dagger}$$

no need to do matrix multiplication. Just play with \mathbf{a} , \mathbf{a}^{\dagger} and the $[\mathbf{a}, \mathbf{a}^{\dagger}]$ commutation rule and the $\mathbf{a}^{\dagger}\mathbf{a}$ number operator

"Second Quantization"

$$\mathbf{x}_{nn}^{3} = \left(\frac{\hbar}{2m\omega}\right)^{3/2} \begin{bmatrix} \delta_{nn+3} ((n+1)(n+2)(n+3))^{1/2} \\ + \delta_{nn+1} 3(n+1)^{3/2} & |n+1\rangle\langle n| \\ + \delta_{nn-1} 3n^{3/2} & |n\rangle\langle n-1| \\ + \delta_{nn-3} (n(n-1)(n-2))^{1/2} \end{bmatrix}$$
 simple! \mathbf{x}^{3} is arranged into four separate terms, each with its own explicit selection rule. same as $|n\rangle\langle n-3|$
 $V(x) = \frac{1}{2}k\mathbf{x}^{2} + a\mathbf{x}^{3} + b\mathbf{x}^{4}$ anharmonic terms \rightarrow perturbation theory

- * IR transition intensities $\propto |\langle n | \mathbf{x} | n + 1 \rangle|^2$

*

- * Survival and transfer probabilities of initially prepared pure harmonic oscillator non-eigenstate in an anharmonic potential.
- * Expectation values of any function of **x** and **p**.

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Universality: all k,m (system-specific) constants are removed until we put them back in at the end of the calculation.

e.g., What is
$$\langle \Delta x \rangle^2 = \left[\langle x^2 \rangle - \langle x \rangle^2 \right]$$

 $\mathbf{x}^2 = \frac{\hbar}{m\omega} \frac{x}{\omega} = \frac{\hbar}{m\omega} \left[\frac{1}{2} (\mathbf{a} + \mathbf{a}^{\dagger})^2 \right]$ [pure numbers in []
 $\langle \Delta x \rangle^2 = \frac{\hbar}{2m\omega} \left[\langle (\mathbf{a} + \mathbf{a}^{\dagger})^2 \rangle - \langle \mathbf{a} + \mathbf{a}^{\dagger} \rangle^2 \right]$?

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