

End Matrix Solution of H-O, a + 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. showed  $p_{nm} = \frac{m}{i\hbar} x_{nm} (E_m - E_n)$

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

$\therefore x_{nn} = 0, p_{nn} = 0$  and  $\begin{cases} x_{nm} \\ p_{nm} \end{cases} = 0$  if  $E_n = E_m$

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

$E_m - E_n = \pm i\hbar\omega$   $\omega = (k/m)^{1/2}$

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

4. combs of connected states, block diag. of  $\mathbf{H}, \mathbf{x}, \mathbf{p}, \mathbf{x}^2, \mathbf{p}^2$   $E_n^{(i)} = \hbar\omega n + \epsilon_i$

5. lowest index must exist because lowest E must exist. Call this index 0

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

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

<p>from phase choice</p> <p><math>x_{01} = +i(km)^{-1/2} p_{01}</math></p>
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Today

6. Recursion Relationship  $|x_{nn+1}|^2$  in terms of  $|x_{nn-1}|^2$   
 $\Downarrow$   
 general matrix elements  $|x_{nn+1}|^2, |p_{nn+1}|^2$

7. general  $\mathbf{x}$  and  $\mathbf{p}$  elements

8. only blocks correspond to  $\epsilon_i = \frac{1}{2}\hbar\omega$

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



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

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

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

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

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

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

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

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


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

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

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

recursion  
relation

thus

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

general  
result

7. Magnitudes and Phases for  $x_{nn\pm 1}$  and  $p_{nn\pm 1}$

verify phase consistency and Hermiticity for  $\mathbf{x}$  and  $\mathbf{p}$

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

one self-consistent set is

$\mathbf{x}$  real and positive

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

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

AND

$\mathbf{p}$  imaginary w/sign flip for up vs. down

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

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

This is the usual phase convention

8. Possible existence of noncommunicating blocks along diagonal of  $\mathbf{H}$ ,  $\mathbf{x}$ ,  $\mathbf{p}$

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

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

This result implies

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

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 of  $k, \mu, \omega$  and also  $\hbar$ .

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

$$\tilde{x} \equiv \left(\frac{m\omega}{\hbar}\right)^{1/2} x \quad \tilde{p} \equiv (\hbar m\omega)^{-1/2} p$$

dimensionless  $\uparrow$   $\uparrow$  regular

$$\tilde{x}^2 = \left(\frac{\hbar}{m\omega}\right) x^2 \quad \tilde{p}^2 = \hbar m\omega p^2$$

We choose these factors to make everything come out dimensionless.

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

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

from results for  $\mathbf{x}, \mathbf{p}, \mathbf{H}$

$$\begin{aligned} x_{mn} &= 2^{-1/2} \left[ (n+1)^{1/2} \delta_{mn+1} + n^{1/2} \delta_{mn-1} \right] \\ \tilde{p}_{mn} &= 2^{-1/2} i \left[ (n+1)^{1/2} \delta_{mn+1} - n^{1/2} \delta_{mn-1} \right] \\ H_{mn} &= (n + 1/2) \delta_{mn} \end{aligned}$$

square root of larger q.n.

note the negative sign

Kronecker -  $\delta$ 's specify selection rules for nonzero matrix elements

now define something new  $\mathbf{a}, \mathbf{a}^\dagger$  to clean things up even more!

$$\begin{aligned} \mathbf{a} &= 2^{-1/2}(\underline{\mathbf{x}} + i\underline{\mathbf{p}}) \\ \mathbf{a}^\dagger &= 2^{-1/2}(\underline{\mathbf{x}} - i\underline{\mathbf{p}}) \end{aligned} \quad \rightarrow \quad \begin{aligned} \underline{\mathbf{x}} &= 2^{-1/2}(\mathbf{a} + \mathbf{a}^\dagger) \\ \underline{\mathbf{p}} &= 2^{-1/2}i(\mathbf{a}^\dagger - \mathbf{a}) \end{aligned}$$

Let's examine the matrix elements of  $\mathbf{a}$  and  $\mathbf{a}^\dagger$

$$\begin{aligned} a_{mn} &= \left[ 2^{-1/2} \underline{x}_{mn} + 2^{-1/2} i \underline{p}_{mn} \right] \\ &= \left[ \underbrace{\frac{1}{2}(n+1)^{1/2} \delta_{mn+1}}_{\underline{x}} - \underbrace{\frac{1}{2}(n+1)^{1/2} \delta_{mn+1}}_{i\underline{p}} + \underbrace{\frac{1}{2}n^{1/2} \delta_{mn-1}}_{\underline{x}} + \underbrace{\frac{1}{2}n^{1/2} \delta_{mn-1}}_{i\underline{p}} \right] \end{aligned}$$

group according to "selection rule"      cancel      add

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

first index is one smaller than second

$$a_{mn} = \langle \mathbf{m} | \mathbf{a} | \mathbf{n} \rangle$$

row      column  
 $n^{1/2} |n-1\rangle$

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

similarly

$$\boxed{a^\dagger_{mn} = (n+1)^{1/2} \delta_{mn+1}}$$

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

$$\mathbf{a}^\dagger = \begin{matrix} & 0 & 1 & 2 & 3 & 4 \\ \begin{matrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{matrix} & \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 1^{1/2} & 0 & 0 & 0 & 0 \\ 0 & 2^{1/2} & 0 & 0 & 0 \\ 0 & 0 & 3^{1/2} & 0 & 0 \\ 0 & 0 & 0 & 4^{1/2} & 0 \end{pmatrix} \end{matrix}$$

square root of integers always only one step below main diagonal.  $\mathbf{a}$ ,  $\mathbf{a}^\dagger$  are obviously not Hermitian

e.g.  $\langle 3|\mathbf{a}^\dagger|2\rangle = 3^{1/2}$

$\mathbf{a}^\dagger$  raises

$$\mathbf{a} = \begin{pmatrix} 0 & 1^{1/2} & 0 & 0 & 0 \\ 0 & 0 & 2^{1/2} & 0 & 0 \\ 0 & 0 & 0 & 3^{1/2} & 0 \\ 0 & 0 & 0 & 0 & 4^{1/2} \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

square root of integers always only one step above main diagonal

e.g.  $\langle 3|\mathbf{a}|4\rangle = 4^{1/2}$

$\mathbf{a}$  lowers

What is so great about  $\mathbf{a}$ ,  $\mathbf{a}^\dagger$ ?

$\mathbf{a}|n\rangle = n^{1/2}|n-1\rangle$       annihilates 1 quantum  
 $\mathbf{a}^\dagger|n\rangle = (n+1)^{1/2}|n+1\rangle$       creates 1 quantum  
 $|n\rangle = [n!]^{-1/2}(\mathbf{a}^\dagger)^n|0\rangle$       generate any state from lowest one  $|0\rangle$

↑ needed to normalize. Each application of  $\mathbf{a}^\dagger$  gives next integer. Do it n times, get n!

more tricks: look at  $\mathbf{a}\mathbf{a}^\dagger$  and  $\mathbf{a}^\dagger\mathbf{a}$

is  $\mathbf{a}\mathbf{a}^\dagger$  Hermitian?

$[(AB)^\dagger = B^\dagger A^\dagger]$  definition of hermitian

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

$\therefore \mathbf{a}\mathbf{a}^\dagger$  and  $\mathbf{a}^\dagger\mathbf{a}$  are Hermitian — to what “observable” quantity do they correspond? We will see that one of these is the “number operator.”

$$\begin{aligned} \mathbf{a}\mathbf{a}^\dagger &= \frac{1}{2} \left( \tilde{\mathbf{x}} + i\tilde{\mathbf{p}} \right) \left( \tilde{\mathbf{x}} - i\tilde{\mathbf{p}} \right) = \frac{1}{2} \left( \tilde{\mathbf{x}}^2 + i\tilde{\mathbf{p}}\tilde{\mathbf{x}} - i\tilde{\mathbf{x}}\tilde{\mathbf{p}} + \tilde{\mathbf{p}}^2 \right) \\ &= \frac{1}{2} \left( \tilde{\mathbf{x}}^2 + \tilde{\mathbf{p}}^2 - \underbrace{i[\tilde{\mathbf{x}}, \tilde{\mathbf{p}}]}_{i} \right) = \frac{1}{2} \left( \tilde{\mathbf{x}}^2 + \tilde{\mathbf{p}}^2 + 1 \right) \end{aligned}$$

$$\text{similarly } \mathbf{a}^\dagger\mathbf{a} = \frac{1}{2} \left( \tilde{\mathbf{x}}^2 + \tilde{\mathbf{p}}^2 - 1 \right)$$

$$\left. \begin{aligned} \therefore \tilde{\mathbf{H}} &= \frac{1}{2} \left( \mathbf{a}^\dagger\mathbf{a} + \mathbf{a}\mathbf{a}^\dagger \right) \quad \text{and} \quad \left[ \mathbf{a}, \mathbf{a}^\dagger \right] = 1 \\ \tilde{\mathbf{H}} &= \mathbf{a}^\dagger\mathbf{a} + 1/2 \quad \text{number operator} + 1/2 \end{aligned} \right\} \text{simple form for } \tilde{\mathbf{H}}$$

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

↑ # of quanta

$$\mathbf{a}^\dagger\mathbf{a}|n\rangle = n|n\rangle \quad \mathbf{a}^\dagger\mathbf{a} \text{ is "number operator"}$$

$$\left[ \mathbf{a}\mathbf{a}^\dagger|n\rangle = (n+1)|n\rangle \right] \quad \text{not as useful}$$

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.



# 5.73 Lecture #13

What about  $X^3$ ?

$$\begin{aligned}
 X^3 &= \left(\frac{m\omega}{\hbar}\right)^{-3/2} \tilde{X}^3 \\
 \tilde{X}^3 &= (2^{-3/2})(\mathbf{a} + \mathbf{a}^\dagger)^3 \\
 &= (2^{-3/2}) \left[ \mathbf{a}^3 + (\mathbf{a}^\dagger \mathbf{a} \mathbf{a} + \mathbf{a} \mathbf{a}^\dagger \mathbf{a} + \mathbf{a} \mathbf{a} \mathbf{a}^\dagger) + (\mathbf{a} \mathbf{a}^\dagger \mathbf{a}^\dagger + \mathbf{a}^\dagger \mathbf{a} \mathbf{a}^\dagger + \mathbf{a}^\dagger \mathbf{a}^\dagger \mathbf{a}) + \mathbf{a}^{\dagger 3} \right] \\
 \Delta n &= \quad \quad -3, \quad \quad -1, \quad \quad +1, \quad \quad (+3)
 \end{aligned}$$

(# of † minus # of non-†)

When you multiply this out, preserve the order of  $\mathbf{a}$  and  $\mathbf{a}^\dagger$  factors.

Simplify each group using commutation properties so that it has form

$$\begin{array}{ccc}
 \mathbf{a}[\mathbf{a}^\dagger \mathbf{a}]|n\rangle & \text{or} & \mathbf{a}^\dagger[\mathbf{a}^\dagger \mathbf{a}]|n\rangle \\
 \Downarrow & & \Downarrow \\
 n^{1/2}n|n-1\rangle & & (n+1)^{1/2}n|n+1\rangle
 \end{array}$$

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

$$\begin{aligned}
 \mathbf{a}^\dagger \mathbf{a} \mathbf{a} &= \mathbf{a} \mathbf{a}^\dagger \mathbf{a} - \underbrace{\mathbf{a} \mathbf{a}^\dagger \mathbf{a} + \mathbf{a}^\dagger \mathbf{a} \mathbf{a}}_{[\mathbf{a}^\dagger, \mathbf{a}] \mathbf{a} = -\mathbf{a}} = \mathbf{a} \mathbf{a}^\dagger \mathbf{a} - \mathbf{a} \\
 \mathbf{a} \mathbf{a} \mathbf{a}^\dagger &= \mathbf{a} \mathbf{a}^\dagger \mathbf{a} - \underbrace{\mathbf{a} \mathbf{a}^\dagger \mathbf{a} + \mathbf{a} \mathbf{a} \mathbf{a}^\dagger}_{\mathbf{a}[\mathbf{a}, \mathbf{a}^\dagger] = \mathbf{a}} = \mathbf{a} \mathbf{a}^\dagger \mathbf{a} + \mathbf{a} \\
 [\mathbf{a}^\dagger \mathbf{a} \mathbf{a} + \mathbf{a} \mathbf{a}^\dagger \mathbf{a} + \mathbf{a} \mathbf{a} \mathbf{a}^\dagger] &= 3\mathbf{a} \mathbf{a}^\dagger \mathbf{a}
 \end{aligned}$$

add and subtract term needed to reverse order

try to put everthing into  $\mathbf{a} \mathbf{a}^\dagger \mathbf{a}$  order

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

$$\begin{aligned}
 \mathbf{a} \mathbf{a}^\dagger \mathbf{a}^\dagger &= \mathbf{a}^\dagger \mathbf{a} \mathbf{a}^\dagger - \underbrace{\mathbf{a}^\dagger \mathbf{a} \mathbf{a}^\dagger + \mathbf{a} \mathbf{a}^\dagger \mathbf{a}^\dagger}_{[\mathbf{a}, \mathbf{a}^\dagger] \mathbf{a}^\dagger = \mathbf{a}^\dagger} = \mathbf{a}^\dagger \mathbf{a} \mathbf{a}^\dagger + \mathbf{a}^\dagger \\
 \mathbf{a}^\dagger \mathbf{a} \mathbf{a}^\dagger &= \mathbf{a}^\dagger \mathbf{a}^\dagger \mathbf{a} - \underbrace{\mathbf{a}^\dagger \mathbf{a}^\dagger \mathbf{a} + \mathbf{a}^\dagger \mathbf{a} \mathbf{a}^\dagger}_{\mathbf{a}^\dagger[\mathbf{a}, \mathbf{a}^\dagger] = \mathbf{a}^\dagger} = \mathbf{a}^\dagger \mathbf{a}^\dagger \mathbf{a} + \mathbf{a}^\dagger \\
 [\mathbf{a} \mathbf{a}^\dagger \mathbf{a}^\dagger + \mathbf{a}^\dagger \mathbf{a} \mathbf{a}^\dagger + \mathbf{a}^\dagger \mathbf{a}^\dagger \mathbf{a}] &= 3\mathbf{a}^\dagger \mathbf{a}^\dagger \mathbf{a} + 3\mathbf{a}^\dagger
 \end{aligned}$$

$\Delta n = \pm 3$

$$\mathbf{a}^3 |n\rangle = [n(n-1)(n-2)]^{1/2} |n-3\rangle$$

$$\mathbf{a}^{\dagger 3} |n\rangle = [(n+1)(n+2)(n+3)]^{1/2} |n+3\rangle$$

$\Delta n = \pm 1$

$$[\mathbf{a}^\dagger \mathbf{a} \mathbf{a} + \mathbf{a} \mathbf{a}^\dagger \mathbf{a} + \mathbf{a} \mathbf{a} \mathbf{a}^\dagger] |n\rangle = 3(n^{3/2}) |n-1\rangle$$

$$[\mathbf{a} \mathbf{a}^\dagger \mathbf{a}^\dagger + \mathbf{a}^\dagger \mathbf{a} \mathbf{a}^\dagger + \mathbf{a}^\dagger \mathbf{a}^\dagger \mathbf{a}] |n\rangle = 3[(n+1)^{1/2} n |n+1\rangle + (n+1)^{1/2} |n+1\rangle]$$

$$= 3(n+1)^{1/2} (n+1) |n+1\rangle$$

$$= 3(n+1)^{3/2} |n+1\rangle$$

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

“Second Quantization”

$$\mathbf{x}_{mn}^3 = \left(\frac{\hbar}{2m\omega}\right)^{3/2} \left[ \begin{array}{l} \delta_{mn+3} ((n+1)(n+2)(n+3))^{1/2} \quad \leftarrow \text{same as } |n+3\rangle\langle n| \\ + \delta_{mn+1} 3(n+1)^{3/2} \quad \leftarrow |n+1\rangle\langle n| \\ + \delta_{mn-1} 3n^{3/2} \quad \leftarrow |n\rangle\langle n-1| \\ + \delta_{mn-3} (n(n-1)(n-2))^{1/2} \quad \leftarrow |n\rangle\langle n-3| \end{array} \right]$$

simple!  $\mathbf{x}^3$  is arranged into four separate terms, each with its own explicit selection rule.

\*  $V(x) = \frac{1}{2} kx^2 + \underbrace{ax^3 + bx^4}_{\text{anharmonic terms} \rightarrow \text{perturbation theory}}$

- \* IR transition intensities  $\propto |\langle n|x|n+1\rangle|^2$
- \* Survival and transfer probabilities of initially prepared pure harmonic oscillator non-eigenstate in anharmonic potential.
- \* Expectation values of any function of  $x$  and  $p$ .

## 5.73 Lecture #13

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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  $\langle \Delta x \rangle^2 = [\langle x^2 \rangle - \langle x \rangle^2]$

$$x^2 = \frac{\hbar}{m\omega} \tilde{x} = \frac{\hbar}{m\omega} \left[ \frac{1}{2} (\mathbf{a} + \mathbf{a}^\dagger)^2 \right]$$

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

pure numbers in [ ]