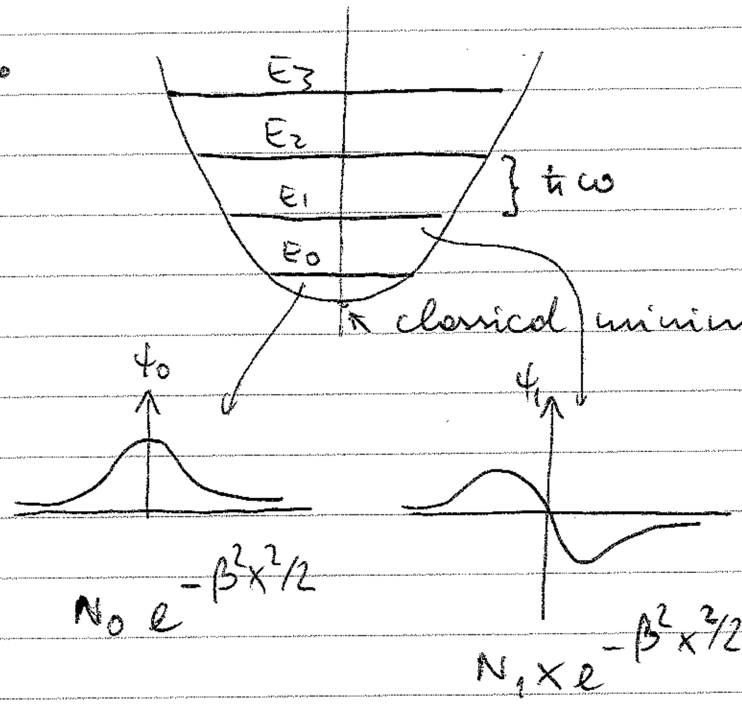
THE SIMPLE HARMONIC OSCILLATOR

- SIMPLEST AND MOST FUNDAMENTAL POTENTIAL IN ALL OF PHYSICS

$$V(x) = \frac{K}{2} x^2 = \frac{m}{2} \omega^2 x^2 = V(-x) \quad \text{(PARITY SYMM.)}$$

$$\boxed{\omega^2 = \frac{K}{m}}$$

- $E_n = \hbar\omega(n + \frac{1}{2})$ $\quad n = 0, 1, 2, 3, \ldots$ (QUANTISED ENERGY SPECTRUM)

- 

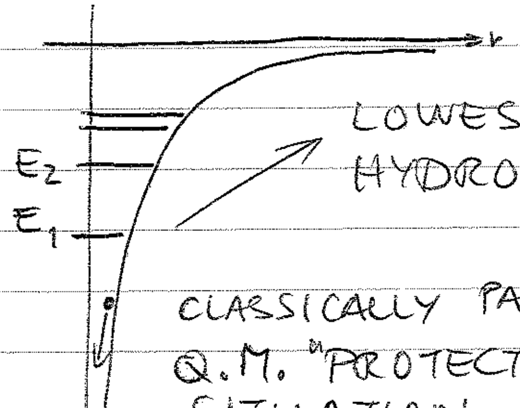
$$\boxed{\beta^2 = \frac{m\omega}{\hbar}}$$

SOLUTION OF TISE $\quad \hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{m}{2}\omega^2 x^2$

(see QMA, MT3)

- GROUNDSTATE OF Q.M. PROBLEM USUALLY LIES ABOVE CLASSICAL LOWEST ENERGY STATE!

COULOMB POTENTIAL $\quad \boxed{E_n = -\frac{m_e e^4}{8\epsilon_0^2 h^2} \frac{1}{n^2}}$



LOWEST ENERGY FOR e^- IN HYDROGEN ATOM IS FINITE

CLASSICALLY PARTICLE COULD HAVE $E = -\infty$!
Q.M. "PROTECTS" US FROM THIS SINGULAR SITUATION

<u>GOAL</u> • SOLVE SHO WITHOUT SOLVING DIFFERENTIAL EQUATION USING OPERATOR FORMALISM:

→ OPERATOR FORMALISM: <u>RAISING/LOWERING (LADDER) OPERATORS</u>

- SIMILAR TO OPERATORS FOUND IN THEORY OF ANGULAR MOMENTUM
- WIDELY USED IN QUANTUM FIELD THEORY PARTICLE PHYSICS → CREATE/ANNIHILATE PARTICLES

• <u>ILLUSTRATION</u> OF BRA-KET FORMALISM AND MATRIX MECHANICS:

$$H_{cl} = \frac{1}{2m} p_x^2 + \frac{m}{2}\omega^2 x^2$$

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

$$= \frac{1}{2m}(m\omega x + ip_x)(m\omega x - ip_x)$$

MAIN IDEA

$$b^2+c^2 = (b+ic)(b-ic)$$

$$= a\,a^* = |a|^2$$

$$a = b+ic$$

TRY THE SAME FOR $\hat{H} = \frac{1}{2m}\hat{p}_x^2 + \frac{1}{2}m\omega^2 x^2$

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

<u>INTRODUCE</u> $\beta^2 = \frac{m\omega}{\hbar}$

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

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

$$\xi \equiv \beta x : \hat{a} = \frac{1}{\sqrt{2}}\left(\xi + \frac{\partial}{\partial\xi}\right), \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\xi - \frac{\partial}{\partial\xi}\right)$$

IT IS EASY TO SHOW THAT

$$\boxed{[\hat{a}, \hat{a}^{+}] = 1}$$ (HOMEWORK)

$$\hat{a}\hat{a}^{+} = \frac{m\omega}{2\hbar} x^2 + \frac{1}{2m\omega\hbar}\hat{p}_x^2 + \underbrace{\frac{i}{2\hbar}\underbrace{[\hat{p}_x, x]}_{-i\hbar}}_{+\frac{1}{2}}$$

$$\hat{a}^{+}\hat{a} = \underbrace{\frac{m\omega}{2\hbar} x^2 + \frac{1}{2m\omega\hbar}\hat{p}_x^2}_{\text{WHAT WE WANT!}} - \frac{1}{2}$$

SO $\boxed{\hat{H} = \hbar\omega\left(\hat{a}^{+}\hat{a} + \frac{1}{2}\right)}$

$\hat{N} = \hat{a}^{+}\hat{a}$ IS OFTEN CALLED NUMBER OPERATOR

LADDER OPERATORS $\hat{a}, \hat{a}^{+}$

$$[\hat{H}, \hat{a}^{+}] = +\hbar\omega\hat{a}^{+} \Rightarrow \hat{H}\hat{a}^{+} = \hat{a}^{+}\hat{H} + \hbar\omega\hat{a}^{+}$$

$$[\hat{H}, \hat{a}] = -\hbar\omega\hat{a}$$

ASSUME $\hat{H}|E\rangle = E|E\rangle$ $\quad (\hat{H}\psi_E = E\psi_E)$

WHAT IS ENERGY EIGENVALUE OF $\hat{a}^{+}|E\rangle$?

$$\hat{H}(\hat{a}^{+}|E\rangle) = \hat{a}^{+}\hat{H}|E\rangle + \hbar\omega\hat{a}^{+}|E\rangle$$

$$= (E + \hbar\omega)\hat{a}^{+}|E\rangle$$

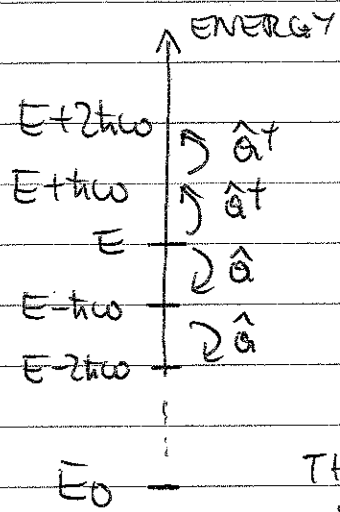
$\hat{a}^{+}$.. RAISING OPERATOR

ENERGY EIGEN VALUE OF

$\hat{a}^{+}|E\rangle$ IS $E + \hbar\omega$

SIMILARLY $\hat{a}$ ... LOWERING OPERATOR

ENERGY EIGENVALUE OF $\hat{a}|E\rangle$
IS $E - \hbar\omega$



LADDER OPERATORS

THERE MUST BE A LOWEST ENERGY EIGENVALUE!

WHY? $\hat{H}$ CONTAINS SQUARES OF HERMITIAN OPERATORS

$$\Rightarrow \langle \hat{H} \rangle \geq 0 \, !$$

SO FOR SOME LOWEST ENERGY EIGENVALUE E_0:

$$\boxed{\hat{a}|E_0\rangle = 0}$$

$$\Rightarrow 0 = \hbar\omega\, \hat{a}^\dagger \hat{a} |E_0\rangle = \left(\hat{H} - \tfrac{1}{2}\hbar\omega\right)|E_0\rangle$$

$$\Rightarrow \hat{H}|E_0\rangle = \frac{\hbar\omega}{2}|E_0\rangle$$

LOWEST ENERGY EIGENVALUE IS $\frac{\hbar\omega}{2} = E_0$

ACTING WITH $\hat{a}^\dagger$ ON $|E_0\rangle$ REPEATEDLY WE CREATE ALL OTHER EIGENSTATES
(UP TO PRECISE NORMALISATION FACTOR)

$\hat{a}^\dagger|E_0\rangle, \ (\hat{a}^\dagger)^2|E_0\rangle, \ \ldots$

SHORT HAND FOR $|E_n\rangle$

RENAME: $|E_n\rangle \rightarrow |n\rangle \leftrightarrow \psi_n(x)$

GROUND STATE

$$\hat{a}|0\rangle = 0 \Rightarrow \left(\sqrt{\frac{m\omega}{2\hbar}}\,x + \sqrt{\frac{\hbar}{2m\omega}}\frac{\partial}{\partial x}\right)\psi_0(x) = 0$$

$$\Rightarrow \left(\frac{m\omega x}{\hbar} + \frac{\partial}{\partial x}\right)\psi_0(x) = 0$$

$$\Rightarrow \boxed{\psi_0(x) = N_0\, e^{-\frac{m\omega x^2}{2\hbar}}}$$

ALL OTHER STATES ACT n-TIMES WITH

$$\hat{a}^\dagger = \left(\sqrt{\frac{m\omega}{2\hbar}}\,x - \sqrt{\frac{\hbar}{2m\omega}}\frac{\partial}{\partial x}\right)$$

ON $\psi_0(x)$

BEING CAREFUL WITH NORMALISATION ONE FINDS

a) $\psi_n(x) = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n\psi_0(x)$ OR $|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n|0\rangle$

b) $|n+1\rangle = \frac{1}{\sqrt{n+1}}\hat{a}^\dagger|n\rangle$

c) $|n-1\rangle = \frac{1}{\sqrt{n}}\hat{a}|n\rangle$

CHECK c): $\langle n-1|n-1\rangle = \frac{1}{n}\langle \hat{a}n|\hat{a}n\rangle$

$$= \frac{1}{n}\langle n|\underbrace{\hat{a}^\dagger\hat{a}}_{}|n\rangle$$

$$\hat{N} \equiv \frac{\hat{H}}{\hbar\omega} - \frac{1}{2} \qquad \hat{H}|n\rangle = E_n|n\rangle$$
$$= \hbar\omega(n+\tfrac{1}{2})|n\rangle$$

$$= \frac{1}{n}\langle n|(n+\tfrac{1}{2}-\tfrac{1}{2})|n\rangle = \frac{n}{n}\langle n|n\rangle = 1 \checkmark$$

NOTE

- $\hat{a}^{+}$ and $\hat{a}$ CAN BE USED TO CALCULATE ANY QUANTITIES WE WANT:

  ANY OBSERVABLE IS A FUNCTION OF x and $\hat{p}_x$, WHICH CAN BE EXPRESSED IN TERMS OF $\hat{a}$ AND $\hat{p}_x$

  E.G. $$x = \sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a} + \hat{a}^{+})$$

  $$\hat{p}_x = \sqrt{\frac{m\omega\hbar}{2}}\,\frac{1}{i}\,(\hat{a} - \hat{a}^{+})$$

- EXAMPLE CONSIDER THE ANHARMONIC OSCILLATOR WITH POTENTIAL

  $$V(x) = \frac{m\omega^2}{2}x^2 + \underline{\underline{\lambda x^4}}$$

  TIME-INDEPENDENT PERTURBATION THEORY THAT THE MODIFICATION OF ENERGY EIGENVALUES (TO FIRST ORDER) IS:

  $$E_n \rightarrow E_n + \langle n|\lambda x^4|n\rangle = E_n + \lambda\langle n|x^4|n\rangle$$

Q: CALCULATE CORRECTION TO GROUNDSTATE ENERGY E_0

$$\langle 0|x^4|0\rangle = \frac{\hbar^2}{4m^2\omega^2}\langle 0|(\hat{a}+\hat{a}^{+})^4|0\rangle$$

$$= \langle 0|\text{ many terms }|0\rangle$$

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SHO IN OPERATOR FORMALISM (SUMMARY)

$$\hat{H} = \hbar\omega\left(\hat{a}^{+}\hat{a} + \tfrac{1}{2}\right) \qquad \hat{H}|n\rangle = E_n|n\rangle,\ E_n = \hbar\omega(n+\tfrac{1}{2})$$

$$|n\rangle = \psi_n(x)$$

RAISING/LOWERING (LADDER) OPERATORS

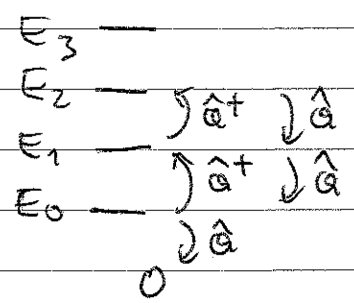
$$\psi_n(x) = \frac{1}{\sqrt{n!}}\left(\hat{a}^{+}\right)^{n}\psi_0(x)$$

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

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

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

$$\beta^2 = \frac{m\omega}{\hbar}$$



$$\hat{a}\,\psi_0(x) = 0$$

- MANY CALCULATIONS OF EXPECTATION VALUES CAN BE DONE ALGEBRAICALLY FOR S.H.O.

EX1 $\quad \Psi = \psi_n(x) \qquad \langle x\rangle,\ \langle x^2\rangle,\ \Delta x$

$$\langle x\rangle = \langle n|\hat{x}|n\rangle = \frac{1}{\sqrt{2}\beta}\langle n|\hat{a} + \hat{a}^{+}|n\rangle$$

$$= \frac{1}{\sqrt{2}\beta}\left(\sqrt{n}\,\langle n|n-1\rangle + \sqrt{n+1}\,\langle n|n+1\rangle\right) = 0$$

$$\hat{x}^2 = \frac{1}{2\beta^2}\,(\hat{a}+\hat{a}^\dagger)(\hat{a}+\hat{a}^\dagger) = \frac{\hbar}{2m\omega}(\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger 2})$$

$$(\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger 2})|n\rangle$$

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

$$= \sqrt{n(n-1)}\,|n-2\rangle + (n+1)|n\rangle + n|n\rangle + \sqrt{(n+1)(n+2)}\,|n+2\rangle$$

$$\langle\hat{x}^2\rangle = \frac{\hbar}{2m\omega}\Big[\sqrt{n(n-1)}\,\underbrace{\langle n|n-2\rangle}_{0} + (2n+1)\underbrace{\langle n|n\rangle}_{1} + \sqrt{(n+1)(n+2)}\,\underbrace{\langle n|n+2\rangle}_{0}\Big]$$

ORTHONORMALITY

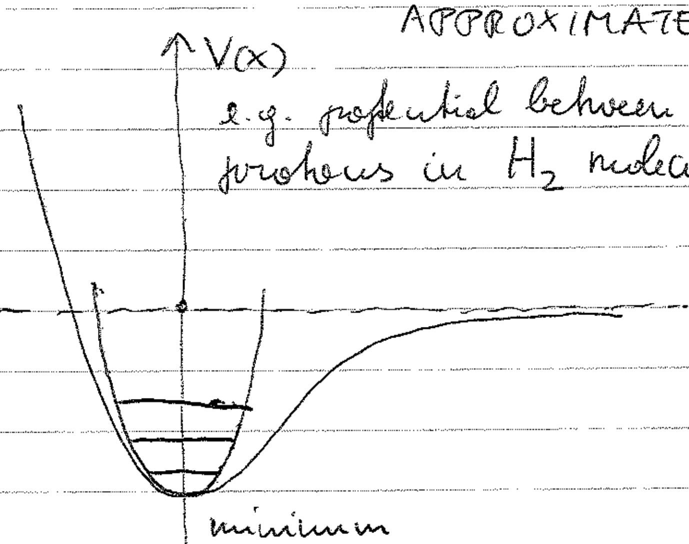
$$= \frac{\hbar}{m\omega}\left(n+\frac{1}{2}\right)$$

$$\Rightarrow \quad \Delta x = \sqrt{\frac{\hbar}{m\omega}\left(n+\frac{1}{2}\right)}$$

- THIS CAN BE GENERALISED TO GENERAL OPERATORS $F(\hat{x}, \hat{p}_x)$ WHICH ARE POLYNOMIALS OF $\hat{a}, \hat{a}^\dagger$

- <u>EX2</u> <u>ANHARMONIC OSCILLATOR</u>

MOTIVATION: GENERAL POTENTIALS WELL APPROXIMATED BY SHO



$$V(x) = V(0) + \frac{1}{2}V''(0)\,x^2 + \frac{1}{3!}V'''(0)\,x^3 + \frac{1}{4!}V'''(0)\,x^4 + \dots$$

CONSIDER $V(x) = \frac{m}{2}\omega^2 x^2 + \lambda x^4$

$\downarrow$ SHO — $\uparrow$ small parameter

Q: FIND CORRECTION TO GROUNDSTATE ENERGY

- FIRST ORDER TIME-INDEPENDENT PERTURBATION THEORY (DERIVED LATER IN COURSE)

$$\Delta E_0 = \langle 0 | \lambda x^4 | 0 \rangle = \lambda \langle 0 | x^4 | 0 \rangle$$

$$x^4 = \frac{\hbar^2}{4m^2\omega^2} (\hat{a} + \hat{a}^\dagger)^4$$

$$(\hat{a}+\hat{a}^\dagger)^4 = \hat{a}^4$$
$$+ \hat{a}^3\hat{a}^\dagger + \hat{a}^2\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger\hat{a}^2 + \hat{a}^\dagger\hat{a}^3$$
$$+ \hat{a}^2(\hat{a}^\dagger)^2 + \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\hat{a}\hat{a}^\dagger$$
$$+ \hat{a}\hat{a}^\dagger\hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}$$
$$+ \hat{a}(\hat{a}^\dagger)^3 + 3 \text{ terms} + (\hat{a}^\dagger)^4$$

e.g. $\langle 0 | \hat{a}^4 | 0 \rangle = 0$

$\langle 0 | \underbrace{(\hat{a}^\dagger)^4 | 0 \rangle}_{c|4\rangle} = 0$

- all terms with different number of $\hat{a}$ and $\hat{a}^\dagger$ operators vanish
- also $\hat{a}|0\rangle = 0$
- $\Rightarrow \langle 0 | \hat{a}^2(\hat{a}^\dagger)^2 + \hat{a}\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\hat{a}\hat{a}^\dagger | 0 \rangle$

$$\hat{a}^2 \hat{a}^{+2}|0\rangle = \hat{a}^2 \hat{a}^{+}|1\rangle = \sqrt{2}\,\hat{a}^2|2\rangle$$

$$= \sqrt{2}\sqrt{2}\;\hat{a}|1\rangle = 2|0\rangle$$

$$\hat{a}\,\hat{a}^{+}\hat{a}\,\hat{a}^{+}|0\rangle = \hat{a}\,\hat{a}^{+}\hat{a}|1\rangle = \hat{a}\,\hat{a}^{+}|0\rangle = |0\rangle$$

$$\hat{a}^{+}\hat{a}\,\hat{a}\,\hat{a}^{+}|0\rangle = 0$$

$$= \langle 0|2+1|0\rangle = 3$$

$$\boxed{\Delta E_0 = \frac{3\lambda\hbar^2}{4m^2\omega^2}}$$

EX3: SHO AND MATRIX Q.M.

MATRIX CORRESPONDING TO OPERATOR $\hat{O}$:

$$O_{mn} = \langle m|\hat{O}|n\rangle$$

$$H_{mn} = \langle m|\hat{H}|n\rangle = E_n\langle m|n\rangle = \hbar\omega(n+\tfrac{1}{2})\,\delta_{mn}$$

$$H = \hbar\omega \begin{array}{cc} & n=0,1,2 \\ m=0,1 & \begin{pmatrix} \frac{1}{2} & 0 & 0 & \cdots \\ 0 & \frac{3}{2} & 0 & \\ 0 & 0 & \frac{5}{2} & \\ \vdots & & & \ddots \end{pmatrix} \end{array}$$

$$\psi_0 \leftrightarrow u_{(0)} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \qquad \psi_1 \Leftrightarrow u_{(1)} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}$$

$$H\,u_{(n)} = E_n\,u_{(n)}$$ MATRIX EIGENVALUE EQN.

$$\hat{a} \rightarrow A_{mn} = \langle m|\hat{a}|n\rangle = \sqrt{n}\,\langle m|n-1\rangle$$

$$= \sqrt{n}\,\delta_{m,n-1}$$

$$A = \begin{array}{ll} & \quad n=0,1,\dots \\ m=0,1,\dots & \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \\ \vdots & \vdots & 0 & \sqrt{3} & \\ & & \vdots & 0 & \\ & & & & \ddots \end{pmatrix} \end{array}$$

NOT HERMITIAN

SIMILARLY

$$A^{+}_{mn} = \langle m|\hat{a}^{+}|n\rangle = \sqrt{n+1}\,\langle m|n+1\rangle$$

$$= \sqrt{n+1}\,\delta_{m,n+1}$$

$$A^{+} = \begin{pmatrix} 0 & & & & \\ \sqrt{1} & 0 & & & \\ 0 & \sqrt{2} & 0 & & \\ 0 & 0 & \sqrt{3} & 0 & \\ \vdots & \vdots & & & \ddots \end{pmatrix}$$

GENERAL OPERATORS CONTAIN PRODUCTS OF $\hat{a}$, $\hat{a}^{+}$

$$\dots + \hat{a}\hat{a}^{+}\hat{a}^{+}\hat{a} + \dots \quad \Longleftrightarrow \quad AA^{+}A^{+}A$$

GIVEN A GENERAL STATE

$$\psi = \sum_{n=0}^{\infty} c_n \psi_n \quad \Leftrightarrow \quad C = \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}$$

<u>ANY EXPECTATION VALUE CAN BE CALCULATED</u>

<u>FROM MATRIX</u> O_{mn}

$$\langle \hat{O} \rangle = \langle \psi | \hat{O} | \psi \rangle = \sum_{m,n} c_m^* O_{mn} c_n = C^\dagger O C$$