WILLIAM & MARY

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QUANTUM MECHANICS I NOTES

09/22/2023

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CHAPTER 2
MATRIX MECHANICS AND OPERATORS

Matrix representation of operators

Reminder: An operator is a mathematical entitie used to represent physical processes that result in the change of the quantum state; in general

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$$\tilde{A}|\psi\rangle = |\phi\rangle$$

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$$\tilde{A}|\psi\rangle = \boxed{a}|\psi\rangle$$

Eigenvalue

in $\tilde{A}|\psi\rangle = a|\psi\rangle$

the eigenvalue represents the possible measured values of the $\tilde{A}$ operator

$$\hat{J}_z|+z\rangle = \frac{\hbar}{2}|+z\rangle$$

↑

spin up.

let's recall the representation of a two spin state $\pm\frac{\hbar}{2}$

$$|\psi\rangle = |+z\rangle\underbrace{\langle +z|\psi\rangle}_{C_+} + |-z\rangle\underbrace{\langle -z|\psi\rangle}_{C_-}$$

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$$\hat{\tilde{A}}\left[|+z\rangle\langle +z|\psi\rangle + |-z\rangle\langle -z|\psi\rangle\right] = |+z\rangle\langle +z|\phi\rangle + |-z\rangle\langle -z|\phi\rangle$$

①

$$\tilde{A}\left[|+z\rangle\langle+z|\psi\rangle + |-z\rangle\langle-z|\psi\rangle\right] = |+z\rangle\langle+z|\phi\rangle + |-z\rangle\langle-z|\phi\rangle$$

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let's multiply by $\langle+z|$ in both sides of equation

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$$\langle+z|\tilde{A}|+z\rangle\langle+z|\psi\rangle + \langle+z|\hat{A}|-z\rangle\langle-z|\psi\rangle = \langle+z|\phi\rangle \quad (a)$$

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Note: in general $\underline{\langle a_i|\hat{A}|a_j\rangle \neq \tilde{A}\langle a_i|a_j\rangle} \leftarrow$ really important

(b)

①

$$\hat{A}\left[|+z\rangle\langle+z|\psi\rangle + |-z\rangle\langle-z|\psi\rangle\right] = |+z\rangle\langle+z|\phi\rangle + |-z\rangle\langle-z|\phi\rangle$$

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Now, insted of $\langle+z|$ let's multiply ① by $\langle-z|$

$$\langle-z|\hat{A}|+z\rangle\langle+z|\psi\rangle + \langle-z|\hat{A}|-z\rangle\langle-z|\psi\rangle = \langle-z|\phi\rangle \quad (b)$$

We can summarize this sistem of two equations into a Matrix equation

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$$\underbrace{\begin{pmatrix} \langle +z|\tilde{\hat{A}}|+z\rangle & \langle +z|\tilde{\hat{A}}|-z\rangle \\ \langle -z|\tilde{\hat{A}}|+z\rangle & \langle -z|\tilde{\hat{A}}|-z\rangle \end{pmatrix}}_{\tilde{\hat{A}} \rightarrow 2\times 2 \text{ Matrix}} \underbrace{\begin{pmatrix} \langle +z|\psi\rangle \\ \langle -z|\psi\rangle \end{pmatrix}}_{\text{Column Vector}} = \underbrace{\begin{pmatrix} \langle +z|\phi\rangle \\ \langle -z|\phi\rangle \end{pmatrix}}_{\text{Column Vector}}.$$

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$$\tilde{A} \xrightarrow[\text{z basis}]{} \begin{pmatrix} \langle +z|\tilde{A}|+z\rangle & \langle +z|\tilde{A}|-z\rangle \\ \langle -z|\tilde{A}|+z\rangle & \langle -z|\tilde{A}|-z\rangle \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

$$A_{ij} = \langle i|\tilde{A}|j\rangle$$

with $|1\rangle = |+z\rangle$

$|2\rangle = |-z\rangle$

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we know Now the Matrix representation of an operator $\tilde{\hat{A}}$ in the $|\pm z\rangle$ basis ; so in general:

in a Space of N basis elements

we know Now the Matrix representation of an operator $\tilde{A}$ in the $|\pm z\rangle$ basis; so in general:- in a Space of N basis elements

$$\tilde{A}_{ij} \longrightarrow \langle i|\tilde{A}|j\rangle$$

Matrix of
$N \times N$

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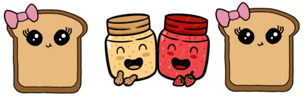

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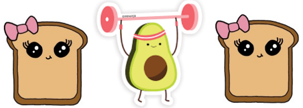

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Matrix of NxN

All kets

$$\begin{array}{cc} & \begin{array}{cccc}|1\rangle & |2\rangle & \cdots & |N\rangle\end{array} \\ \begin{array}{c}\langle 1| \\ \langle 2| \\ \vdots \\ \langle N|\end{array} & \left(\begin{array}{cccc} \quad & \quad & \quad & \quad \\ & & & \\ & & & \\ & & & \end{array}\right)\end{array}$$

all bras

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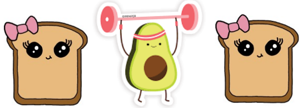

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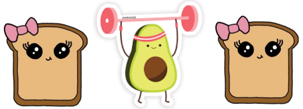

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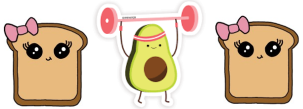

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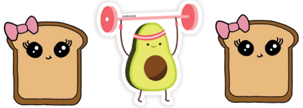

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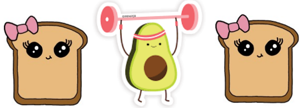

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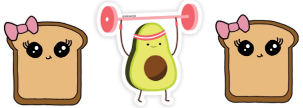

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\vdots & \vdots & & \ddots & \vdots \\
\langle N| & \langle N|\tilde{A}|1\rangle & \langle N|\tilde{A}|2\rangle & \cdots & \langle N|\tilde{A}|N\rangle
\end{array}$$

All kets

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Example Rotation operator $\hat{J}_z$ in the z basis

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$$\hat{J}_z \xrightarrow[z\,\text{basis}]{} \begin{array}{c|cc} & |+z\rangle & |-z\rangle \\ \hline \langle +z| & & \\ \langle -z| & & \end{array}$$

Example Rotation operator $\hat{J}_z$ in the z basis

$$\hat{J}_z \xrightarrow[z\,\text{basis}]{} \begin{array}{cc} & \begin{array}{cc} |+z\rangle & \qquad\qquad |-z\rangle \end{array} \\ \begin{array}{c} \langle +z| \\ \\ \langle -z| \end{array} & \begin{pmatrix} \langle +z|\,\hat{J}_z\,|+z\rangle & \qquad\qquad \\ & \\ & \end{pmatrix} \end{array}$$

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$$\hat{J}_z \xrightarrow[\text{z basis}]{} \begin{array}{c|cc} & |+z\rangle & |-z\rangle \\ \hline \langle +z| & \langle +z|\hat{J}_z|+z\rangle & \langle +z|\hat{J}_z|-z\rangle \\ \langle -z| & \langle -z|\hat{J}_z|+z\rangle & \langle -z|J_z|-z\rangle \end{array}$$

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$$\hat{J}_z\, |\pm z\rangle = \pm\frac{\hbar}{2}$$

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$$\begin{pmatrix} \frac{\hbar}{2}\langle +z|+z\rangle & -\frac{\hbar}{2}\langle +z|-z\rangle \\ \frac{\hbar}{2}\langle -z|+z\rangle & -\frac{\hbar}{2}\langle -z|-z\rangle \end{pmatrix}$$

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$$\hat{J}_z |\pm z\rangle = \pm\frac{\hbar}{2}$$

$$\Downarrow$$

$$\begin{pmatrix} \frac{\hbar}{2}\langle +z|+z\rangle & -\frac{\hbar}{2}\langle +z|-z\rangle \\ \frac{\hbar}{2}\langle -z|+z\rangle & -\frac{\hbar}{2}\langle -z|-z\rangle \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \xrightarrow[\text{zbasis}]{} \hat{J}_z$$

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$$\begin{pmatrix} \frac{\hbar}{2}\langle +z|+z\rangle & -\frac{\hbar}{2}\langle +z|-z\rangle \\ \frac{\hbar}{2}\langle -z|+z\rangle & \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \rightarrow \hat{J}_z$$

What is the matrix representation of the $\hat{P}_+$ and $\hat{P}_-$ operators in the z basis?

$$\hat{P}_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \hat{P}_- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

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$$\hat{J}_z \xrightarrow[z\text{ basis}]{} \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix} - \frac{\hbar}{2}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}$$

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$$\boxed{\hat{J}_z = \frac{\hbar}{2}\hat{P}_+ - \frac{\hbar}{2}\hat{P}_-}$$

$\hat{P}_+ = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}$ and $\hat{P}_- = \begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}$

$$\hat{J}_z \xrightarrow[\text{z basis}]{} \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix} - \frac{\hbar}{2}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}$$

$$\boxed{\hat{J}_z = \frac{\hbar}{2}\hat{P}_+ - \frac{\hbar}{2}\hat{P}_-}$$

☺

Somethin important to know about "Sandwiches"

$\langle i|\hat{A}^\dagger|j\rangle = \langle j|\hat{A}|i\rangle^*$ or we can say that the elements of the Matrix $A^\dagger_{ij} = A^*_{ji}$

Expectaction Values of an operator; For a two spin state $|\psi\rangle = |+z\rangle\langle +z|\psi\rangle + |-z\rangle\langle -z|\psi\rangle$

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it can be shown that

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it can be shown that

$$\langle S_z\rangle = \underbrace{(\langle\psi|+z\rangle, \langle\psi|-z\rangle)}_{\text{Row vector}} \frac{\hbar}{2} \underbrace{\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}}_{2\times2\text{ Matrix}} \begin{pmatrix}\langle+z|\psi\rangle\\ \langle-z|\psi\rangle\end{pmatrix}$$

← Column Vector

Expectation Values of an operator; For a two spin state $|\psi\rangle = |+z\rangle\langle+z|\psi\rangle + |-z\rangle\langle-z|\psi\rangle$

then $\langle S_z\rangle = \left(\frac{\hbar}{2}\right)|\langle+z|\psi\rangle|^2 + \left(-\frac{\hbar}{2}\right)|\langle-z|\psi\rangle|^2$

it can be shown that

$$\langle S_z\rangle = \overbrace{\underbrace{(\langle\psi|+z\rangle, \langle\psi|-z\rangle)}_{\substack{\text{Row vector}\\ \langle\psi|}} \frac{\hbar}{2} \underbrace{\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}}_{\substack{2\times2\text{ Matrix}\\ \hat{J}_z}} \underbrace{\begin{pmatrix}\langle+z|\psi\rangle\\ \langle-z|\psi\rangle\end{pmatrix}}_{\substack{\text{Column Vector}\\ |\psi\rangle}}}$$

$$\langle S_z\rangle = \langle\psi|\hat{J}_z|\psi\rangle$$

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$$= \Big[\langle +z|\psi\rangle^* \langle +z| + \langle -z|\psi\rangle^* \langle -z|\Big] \Big[\frac{\hbar}{2}|+z\rangle\langle +z|\psi\rangle + \left(-\frac{\hbar}{2}\right)|-z\rangle\langle -z|\psi\rangle\Big]$$

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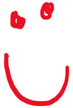
$$= \frac{\hbar}{2} \left|\langle +z|\psi\rangle\right|^2 + \left(-\frac{\hbar}{2}\right) \left|\langle -z|\psi\rangle\right|^2$$



$$\langle S_z \rangle = \frac{\hbar}{2}\langle +z|\psi\rangle^* \langle +z|\psi\rangle + \left(-\frac{\hbar}{2}\right)\langle -z|\psi\rangle^* \langle -z|\psi\rangle$$

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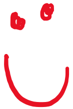
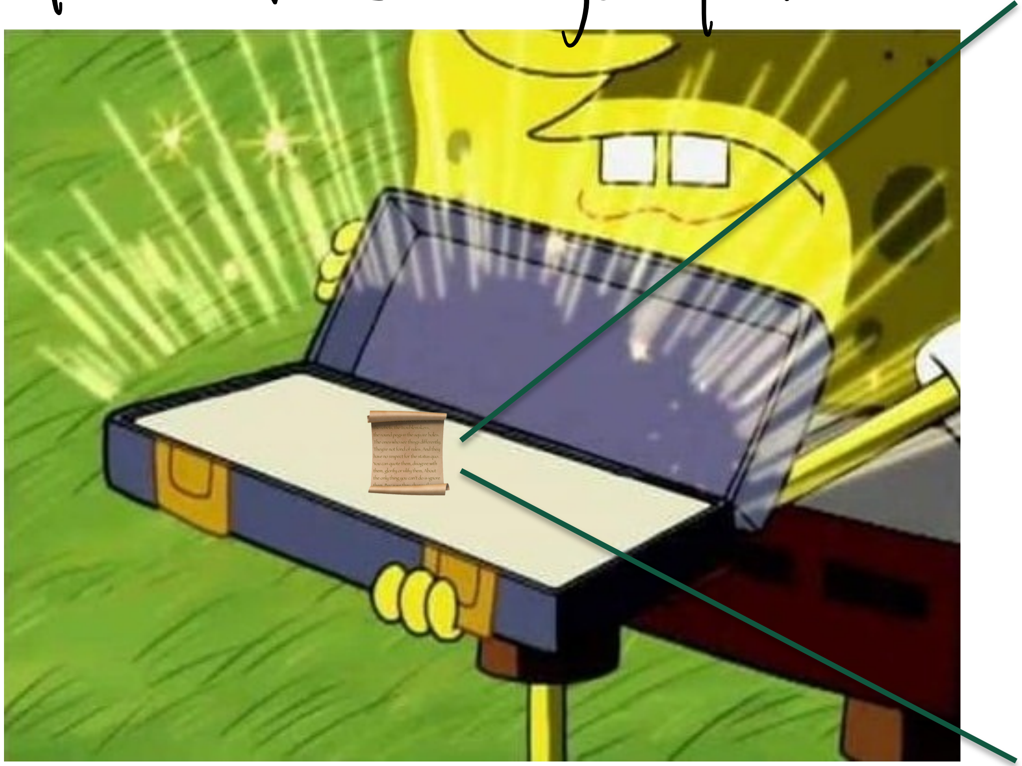


for example

In majority of the examples ($\hat{J}_z|+x\rangle$), we had to write $|+x\rangle$ in terms of the $|\pm z\rangle$ basis so the calculation becomes way easier (and clear)....

is it possible to change $\hat{J}_z$ instead??

to Solve the Schrödinger equation:



1.- Choose a basis

2.- Write the Hamiltonian in that basis

3.- "Diagonalize" the Hamiltonian to obtain the eigenvalues and eigenvectors

4.- Write the initial quantum state as a Superposition of the eigenvectors

5.- Add the time evolution by multiplyin by $e^{-i\omega_n t}$ $(\omega_n = \frac{E_n}{\hbar})$ Corresponding to every term.

to Solve the schrödinger equation:

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