



WILLIAM & MARY

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QUANTUM MECHANICS I NOTES

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CHAPTER 2

MATRIX MECHANICS AND OPERATORS



Vectors

$$\vec{V} = V_x \hat{x} + V_y \hat{y} + V_z \hat{z}$$

$$\vec{V} = (V_x, V_y, V_z)$$

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Meaning that

$$\begin{aligned}\vec{V} &= V_x(1, 0, 0) + V_y(0, 1, 0) \\ &\quad + V_z(0, 0, 1)\end{aligned}$$

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The Unitary Vectors of the basis are

$$\hat{x} = (1, 0, 0), \hat{y} = (0, 1, 0), \hat{z} = (0, 0, 1)$$

→ Row vectors (matrices of 1×3 in this example)

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There also exist the "Column Vector"

$$\vec{V} = \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix}; \text{ meaning}$$

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$$\vec{V} = \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix}; \text{ meaning}$$

$$\vec{V} = V_x \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + V_y \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + V_z \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Column vector:
matrices of 3×1
in this example

basic operations:

if "C" is a constant and

\vec{A} a row vector, then $a\vec{A}$

$$\vec{A} = (a_1, a_2, \dots, a_n)$$

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$$\begin{aligned} C\vec{A} &= C(a_1, a_2, \dots, a_n) \\ &= (Ca_1, Ca_2, \dots, Ca_n) \end{aligned}$$

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$$c\vec{A} = c(a_1, a_2, \dots, a_n)$$

$$= (ca_1, ca_2, \dots, ca_n)$$

the constant multiplies all the elements on the vector

→ same for a column vector

the same if A is a matrix of $m \times n$

$$cA = \begin{pmatrix} ca_{11} & ca_{12} & \dots & ca_{1n} \\ ca_{21} & ca_{22} & \dots & ca_{2n} \\ \vdots & & & \\ ca_{m1} & ca_{m2} & \dots & ca_{mn} \end{pmatrix}$$

and the product between two matrices ; in general
if $A = m \times n$ matrix
and $B = n \times p$

Next
⇒

$A = M \times n$ matrix, $B = n \times p$ matrix, then

$$AB = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & & & \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} & \dots & b_{1p} \\ b_{21} & b_{22} & \dots & b_{2p} \\ \vdots & & & \\ b_{n1} & b_{n2} & \dots & b_{np} \end{pmatrix}$$

$A = M \times n$ matrix, $B = n \times p$ matrix, then

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dot product

$$\begin{array}{cccc} b_{12} & \dots & b_{1p} \\ b_{22} & \dots & b_{2p} \\ \vdots & & \\ b_{n2} & \dots & b_{np} \end{array}$$

$$a_{11}b_{11} + a_{12}b_{21} + \dots + a_{1n}b_{n1}$$

$A = M \times n$ matrix, $B = n \times p$ matrix, then

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$$\begin{matrix} a_{11}b_{11} + a_{12}b_{21} + \dots + a_{1n}b_{n1} & a_{11}b_{12} + a_{12}b_{22} + \dots + a_{1n}b_{n2} \\ \vdots & \vdots \\ a_{m1}b_{11} + a_{m2}b_{21} + \dots + a_{mn}b_{n1} & a_{m1}b_{12} + a_{m2}b_{22} + \dots + a_{mn}b_{n2} \end{matrix}$$

all other elements



... etc

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all the other elements



... = 0

$$\begin{aligned} a_{11}b_{11} + a_{12}b_{21} + \dots + a_{1n}b_{n1} &= a_{11}b_{12} + a_{12}b_{22} + \dots + a_{1n}b_{n2} \\ a_{21}b_{11} + a_{22}b_{21} + \dots + a_{2n}b_{n1} & \end{aligned}$$

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$$\begin{array}{ll} a_{11}b_{11} + a_{12}b_{21} + \dots + a_{1n}b_{n1} & a_{11}b_{12} + a_{12}b_{22} + \dots + a_{1n}b_{n2} \\ a_{21}b_{11} + a_{22}b_{21} + \dots + a_{2n}b_{n1} & \end{array}$$

In that way we know how to
fill all the elements

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all the other elements



  the elements of the new matrix are given by

$$C_{ij} = \sum_{k=1}^n a_{ik} b_{kj}$$

for $i = 1, \dots, m$ and $j = 1, \dots, p$

Total time complexity $O(M \times N \times P)$

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Dot product is a multiplication of a row vector and column vector.

$$\vec{A} \cdot \vec{B} = (a_1, a_2, \dots, a_n) \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

$$\vec{A} \cdot \vec{B} = a_1b_1 + a_2b_2 + \dots + a_nb_n$$

this is just a scalar
Not a Vector

in general

$$(x_1, x_2, x_3, \dots, x_n)^T = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix}$$

↑
Transpose

in general

$$(x_1, x_2, x_3, \dots, x_n)^T = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix}$$

Transpose

and in the same way

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Transpose

and in the same way
 $x_1 \downarrow T$



The transpose of any row Vector is a Column Vector
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in general $[A^T]_{ij} = [A]_{ji}$

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in the same way:

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix}^+ = (x_1^*, x_2^*, x_3^*, \dots, x_n^*)$$

Back to Quantum Mechanics

Spin example $|\psi\rangle = c_+ |+\rangle + c_- |-\rangle$, we can think about the Quantum state, in a "ket" as a Column Vector in that sense:

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$$|+\hat{z}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |-\hat{z}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

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so that

$$|+\hat{z}\rangle = C_+ \begin{pmatrix} 1 \\ 0 \end{pmatrix} + C_- \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} C_+ \\ C_- \end{pmatrix}$$

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and for the bra representation:

$$\langle +\hat{z}| = (1, 0), \quad \langle -\hat{z}| = (0, 1) \quad \text{and}$$

$$\langle \psi | = C_+^* (1, 0) + C_-^* (0, 1) = (C_+^*, C_-^*)$$

• Orthonormality $\langle +z | -z \rangle = (1, 0) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0$

$$\langle +z | +z \rangle = (1, 0) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1$$

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• Amplitude of probability $\langle +z | \psi \rangle = (1, 0) \begin{pmatrix} c_+ \\ c_- \end{pmatrix} = c_+$

$$\langle -z | \psi \rangle = (0, 1) \begin{pmatrix} c_+ \\ c_- \end{pmatrix} = c_-$$

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is it possible to perform the product $|+z\rangle \times |-z\rangle$?

Operators

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

In general, the operator "transforms" the Quantum State; The state after the operator could be the initial state $\tilde{A}|\psi\rangle = a|\psi\rangle$

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In this case we said that $|\psi\rangle$ is an eigenstate of \tilde{A} and a is the eigenvalue

Rotation operator

$$\hat{R}(\varphi \hat{\vec{\alpha}}) = e^{-i \hat{J}_x \varphi / \hbar}$$

$$\hat{R}(\theta \hat{\vec{\beta}}) = e^{-i \hat{J}_y \theta / \hbar}$$

$$\hat{R}(\phi \hat{\vec{\gamma}}) = e^{-i \hat{J}_z \phi / \hbar}$$

Rotation operator

$$\left. \begin{aligned} \hat{R}(\varphi \hat{i}) &= e^{-i \hat{J}_x \varphi / \hbar} \\ \hat{R}(\theta \hat{j}) &= e^{-i \hat{J}_y \theta / \hbar} \\ \hat{R}(\phi \hat{k}) &= e^{-i \hat{J}_z \phi / \hbar} \end{aligned} \right\} \begin{array}{l} \varphi, \theta, \phi \quad \text{the angle of the} \\ \text{rotation, } \hat{i}, \hat{j}, \hat{k} \quad \text{the axis} \\ \text{of the rotation and} \\ \hat{J}_x, \hat{J}_y, \hat{J}_z \quad \text{the angular} \end{array}$$

Rotation operator

$$\hat{R}(\varphi \hat{i}) = e^{-i\hat{J}_x \varphi/\hbar}$$

$$\hat{R}(\theta \hat{j}) = e^{-i\hat{J}_y \theta/\hbar}$$

$$\hat{R}(\phi \hat{k}) = e^{-i\hat{J}_z \phi/\hbar}$$

momentum operator, with eigenvalues and eigenvectors

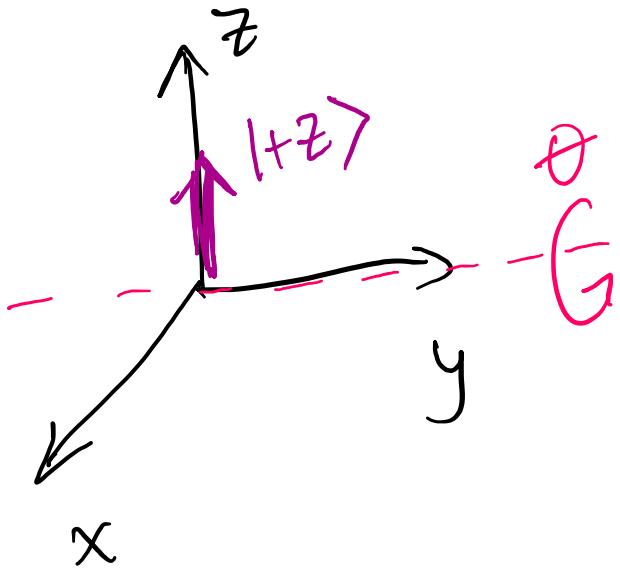
$$\hat{J}_x |\pm x\rangle = \left(\pm \frac{\hbar}{2}\right) |\pm x\rangle$$

$$\hat{J}_z |\pm z\rangle = \left(\pm \frac{\hbar}{2}\right) |\pm z\rangle$$

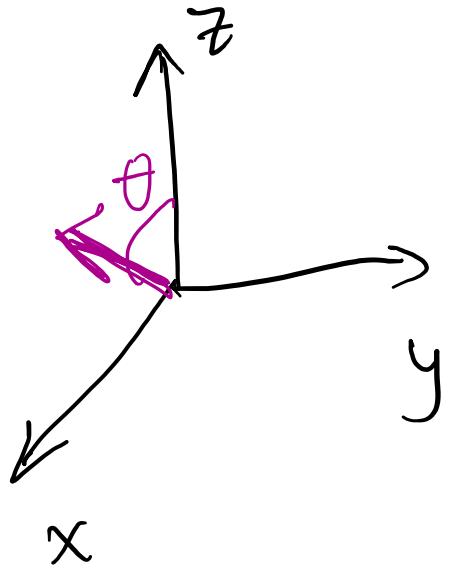
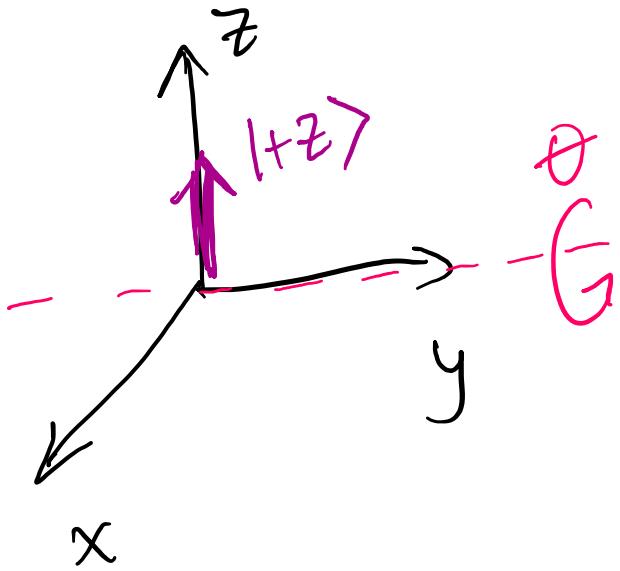
} φ, θ, ϕ the angle of the rotation, $\hat{i}, \hat{j}, \hat{k}$ the axis of the rotation and $\hat{J}_x, \hat{J}_y, \hat{J}_z$ the angular

$$\hat{J}_y |\pm y\rangle = \left(-\frac{\hbar}{2}\right) |\pm y\rangle$$

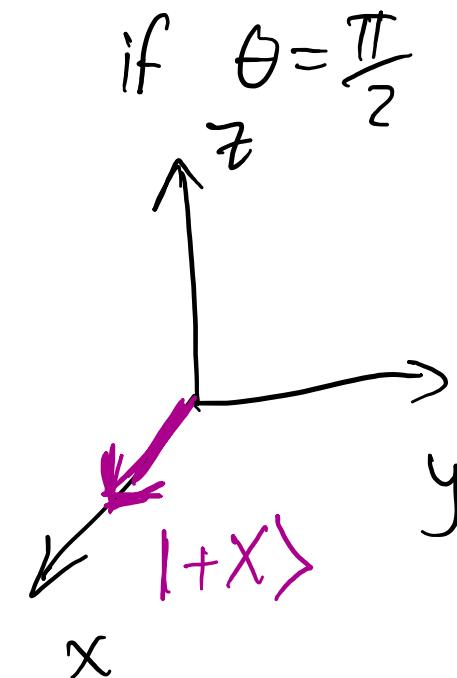
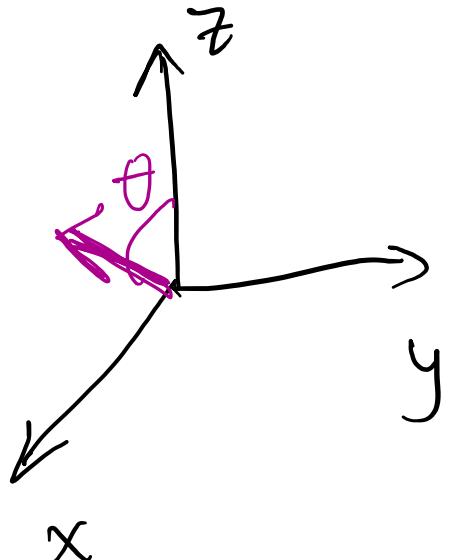
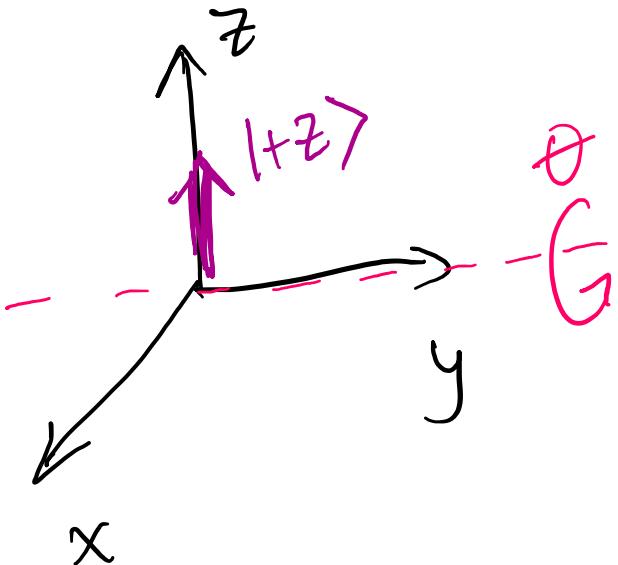
Example : Rotate the $|+z\rangle$ vector about the y axis



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$$\text{So } |+x\rangle = \hat{R}\left(\frac{\pi}{2}j\right) |+z\rangle$$

how to operate a general rotation

$$\hat{R}(\phi \hat{\vec{r}}) = e^{-i \frac{\hat{J}_z}{\hbar} \phi / \hbar} = \left[1 - \frac{i \phi \hat{J}_z}{\hbar} + \frac{1}{2!} \left(- \frac{i \phi \hat{J}_z}{\hbar} \right)^2 + \dots \right]$$

how to operate a general rotation

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$$e^X = \sum_{N=0}^{\infty} \frac{X^N}{N!}$$

how to operate a general rotation

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$$\hat{R}(\phi \hat{\vec{r}}) |\psi\rangle = \left[1 - \frac{i \phi \hat{J}_z}{\hbar} + \frac{1}{2!} \left(- \frac{i \phi \hat{J}_z}{\hbar} \right)^2 + \dots \right] |\psi\rangle$$

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it is convenient if $|\psi\rangle$ is in the \hat{J}_z basis, because $|+\hat{z}\rangle$ are eigenvectors of \hat{J}_z ; so that $\hat{J}_z |+\hat{z}\rangle = \left(\pm \frac{\hbar}{2} \right) |+\hat{z}\rangle$

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Something to Note: $[\hat{J}_z]^N |\psi\rangle = \underbrace{\hat{J}_z \cdot \hat{J}_z \cdots \hat{J}_z}_{N \text{ repetitions}} |\psi\rangle$

of the operator