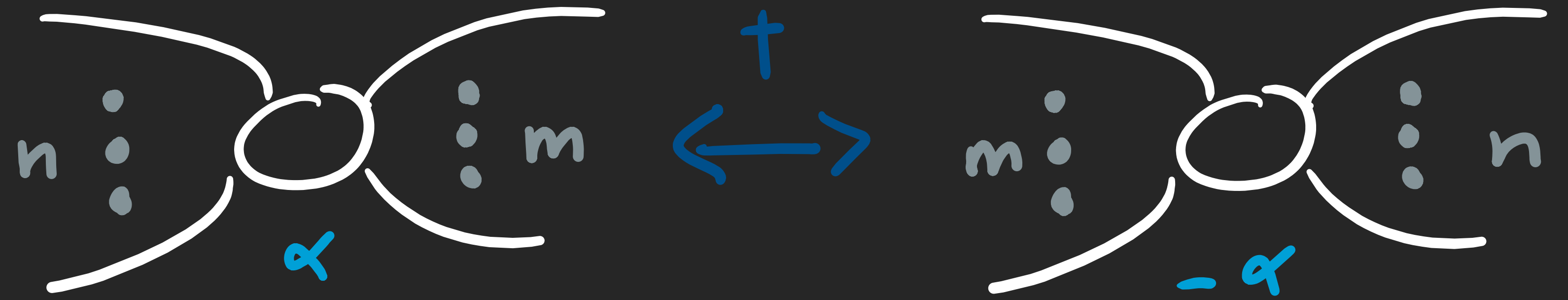
Measurement

The Dagger

i.e. the matrix adjoint
(conjugate transpose)



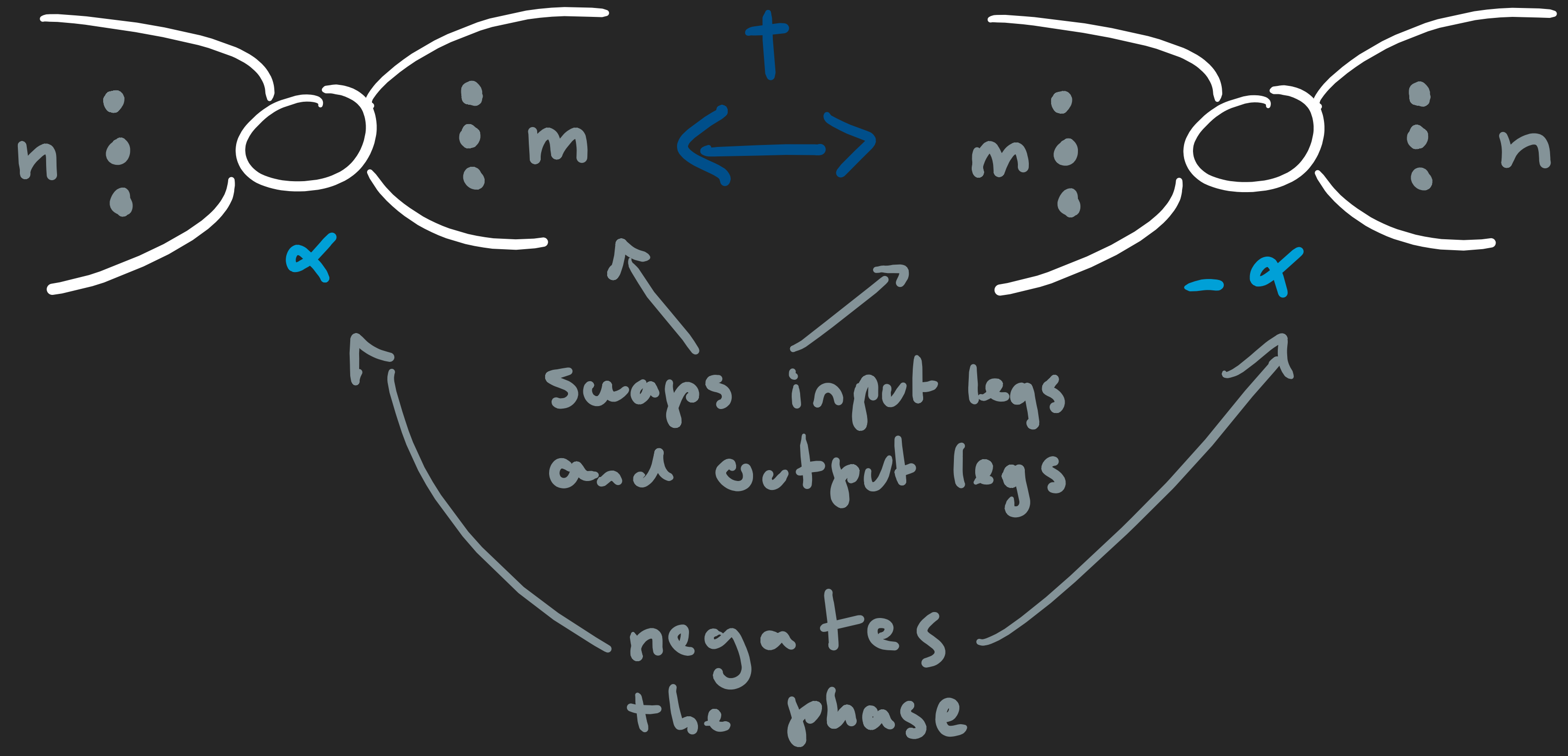
conjugate

$$\Big(\underbrace{|0\cdots0\rangle}_{m}\underbrace{\langle 0\cdots0|}_{n}+e^{i\alpha}\underbrace{|1\cdots1\rangle}_{m}\underbrace{\langle 1\cdots1|}_{n}\Big)^{\dagger}=\underbrace{|0\cdots0\rangle}_{n}\underbrace{\langle 0\cdots0|}_{m}+e^{-i\alpha}\underbrace{|1\cdots1\rangle}_{n}\underbrace{\langle 1\cdots1|}_{m}$$

transpose

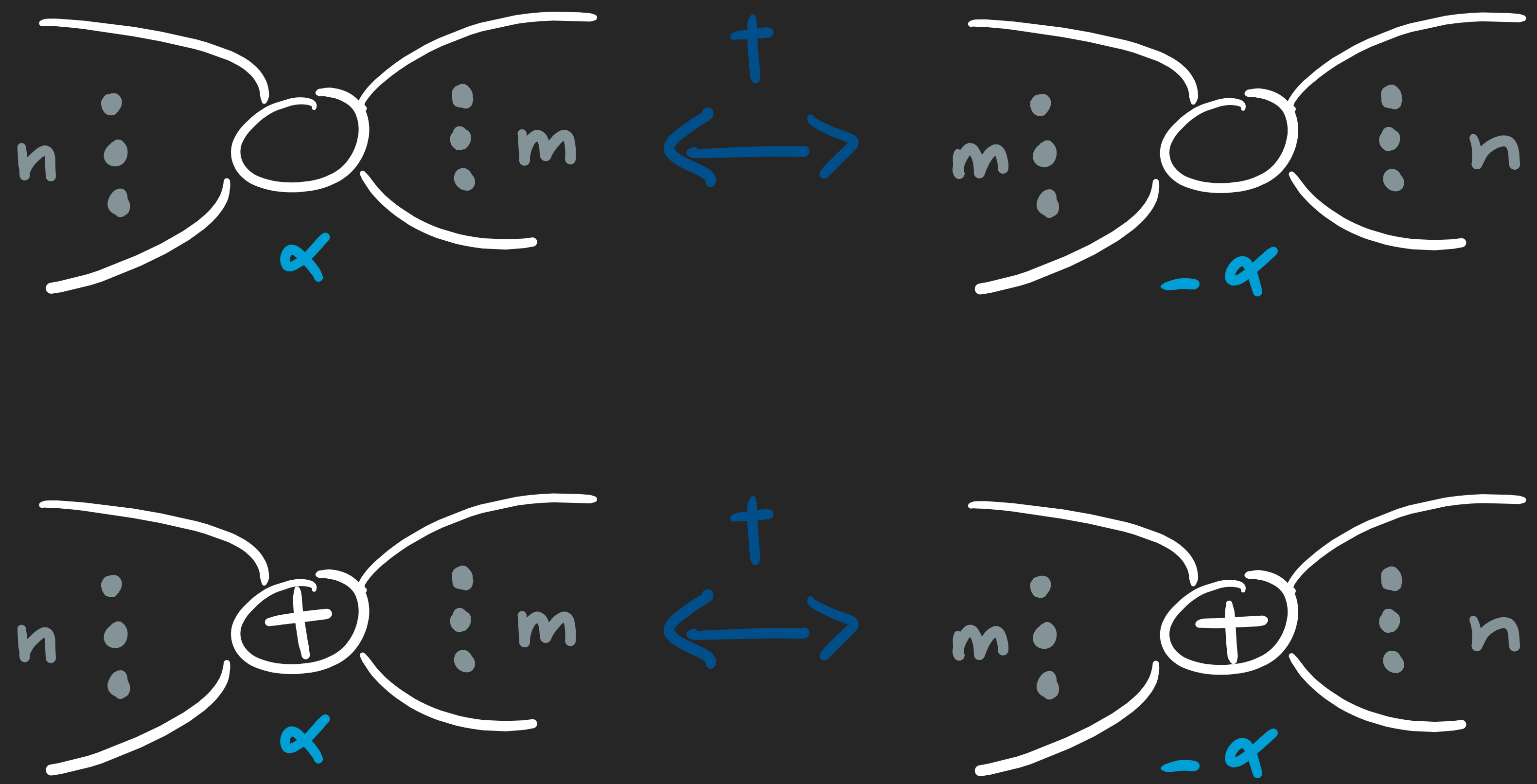
transpose

The Dagger

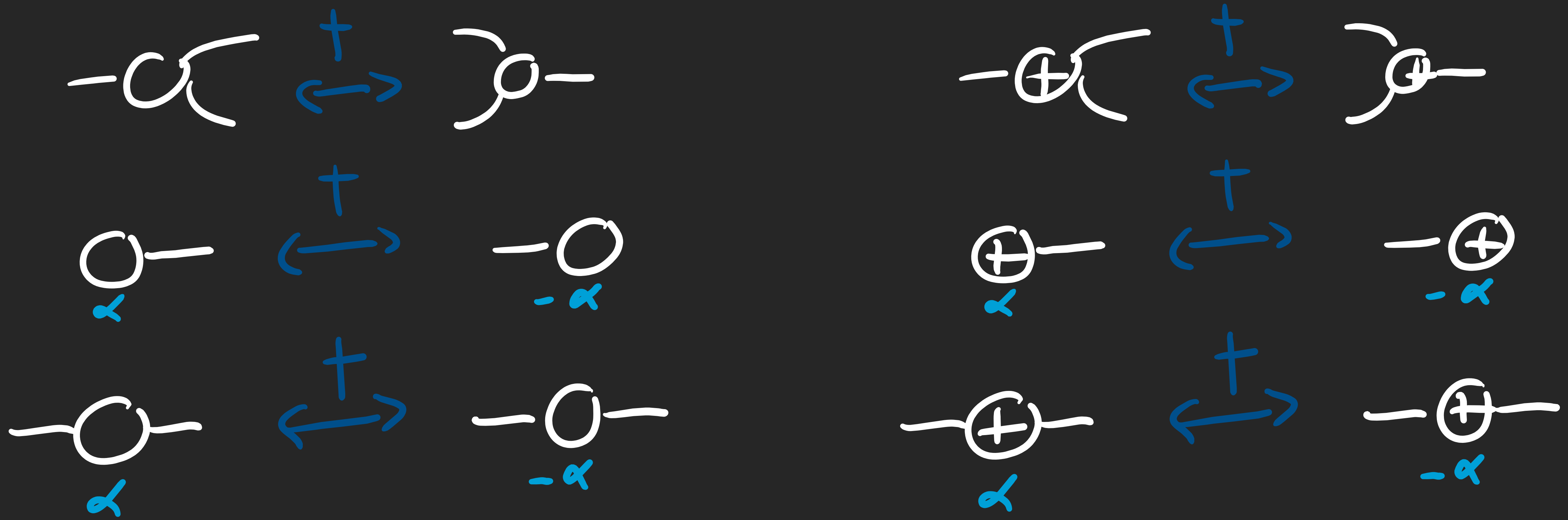


The Dagger

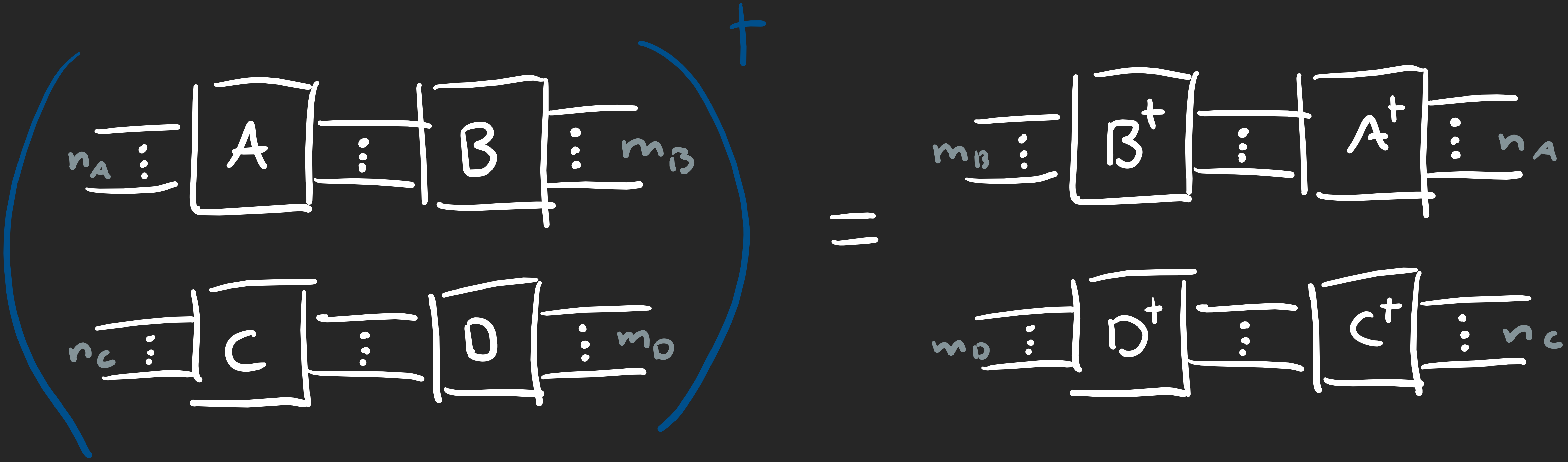
a.k.a.



The Dagger



The Dagger



Dagger of composite diagram = Invert sequential order & dagger of pieces

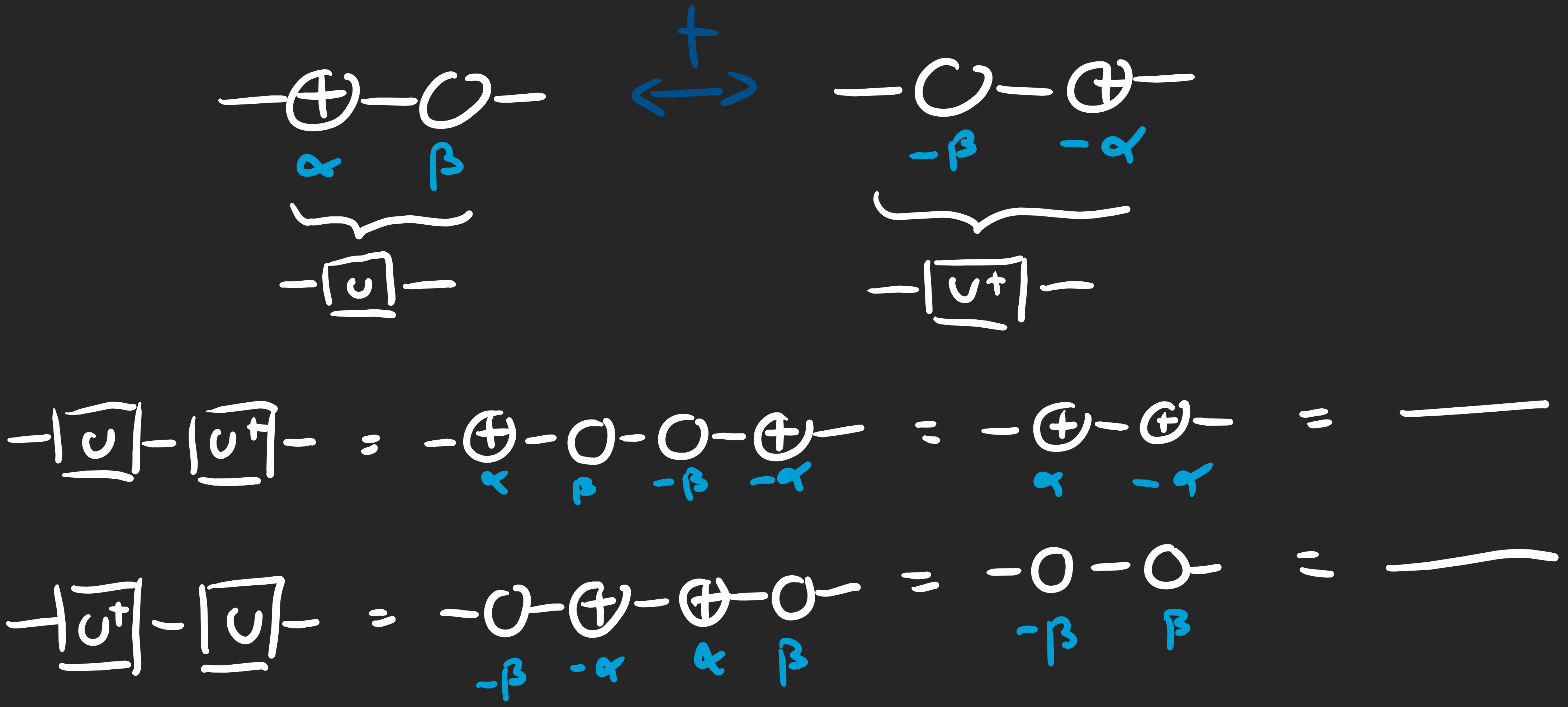
The Dagger

The dagger has no effect on numbers:

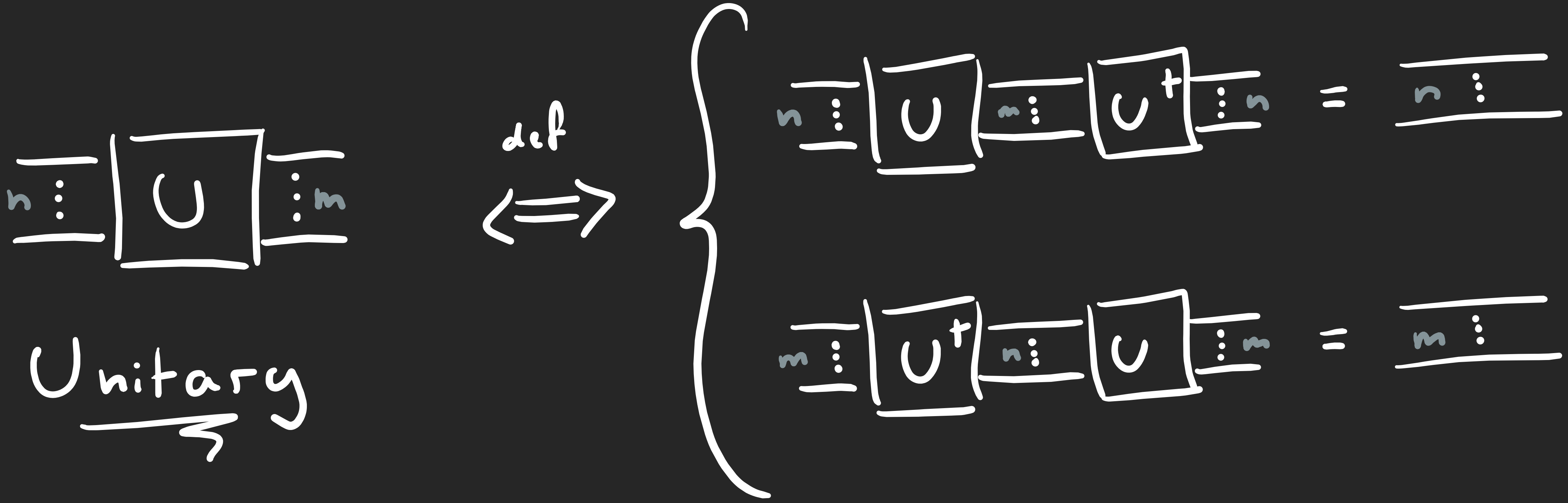
$$(r)^\dagger = r$$

for real numbers $r^* = r$

Unitaries and Isometries



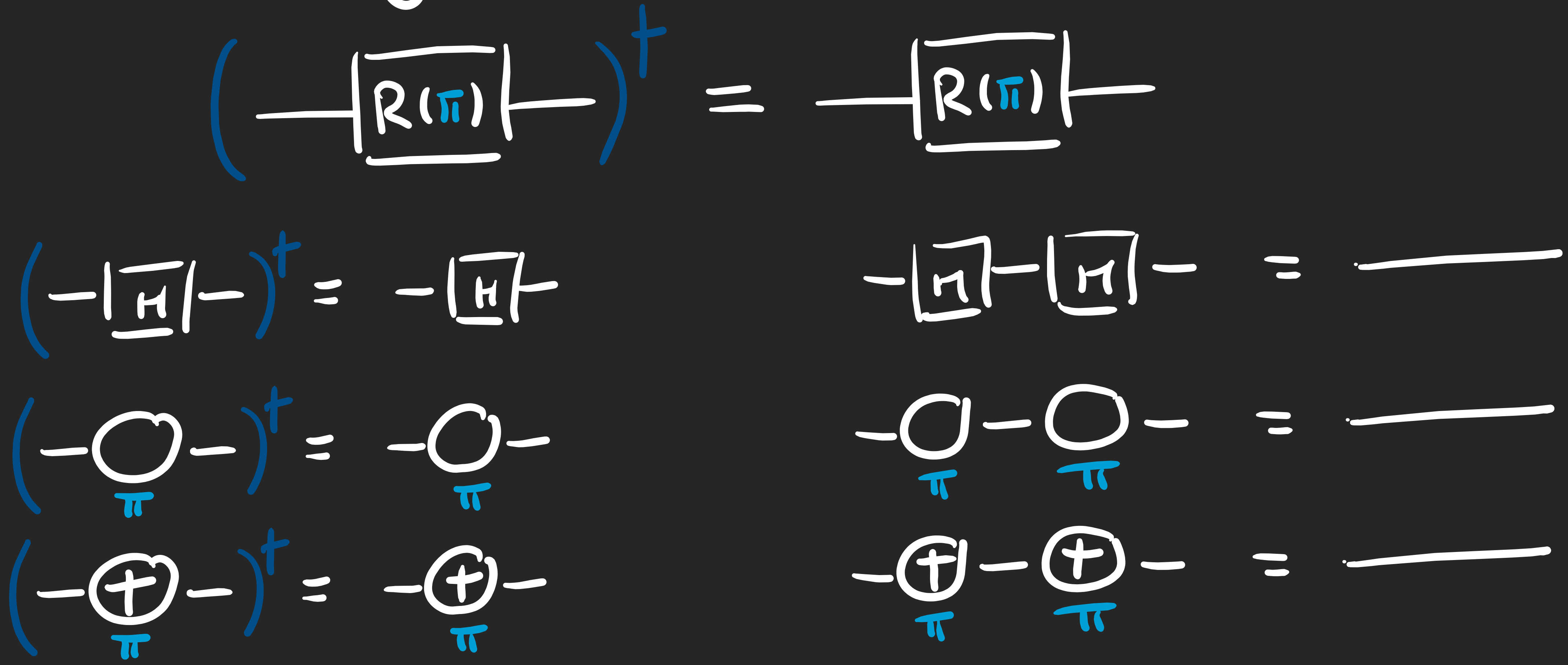
Unitaries and Isometries



Unitaries and Isometries

Rotations by π are "self-adjoint":

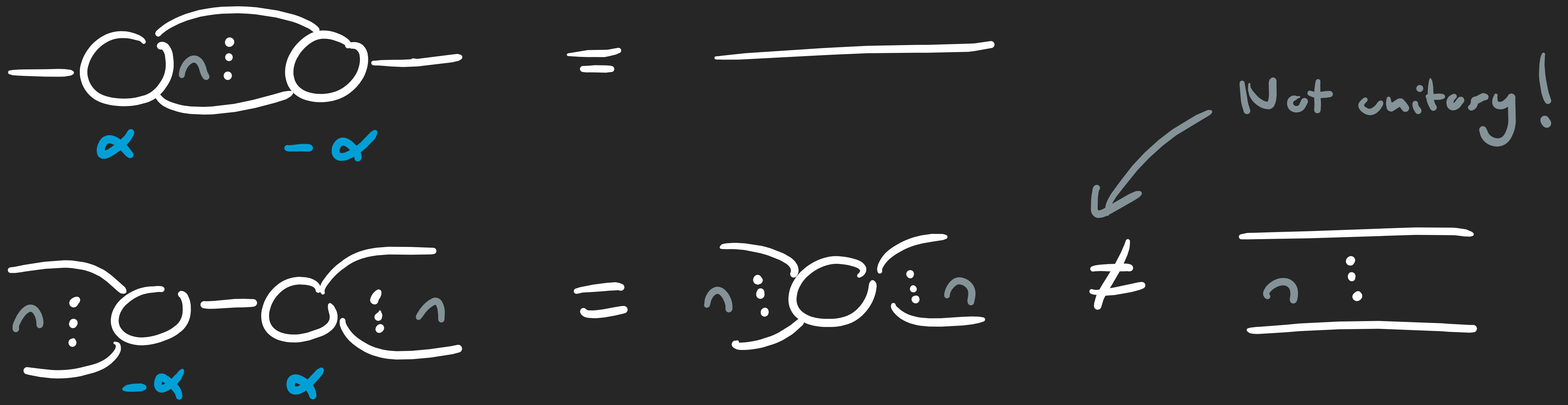
eg.



Unitaries and Isometries

Isometry

e.g.



The Fidelity

geodesic distance = distance along the unique great circle through 2 points

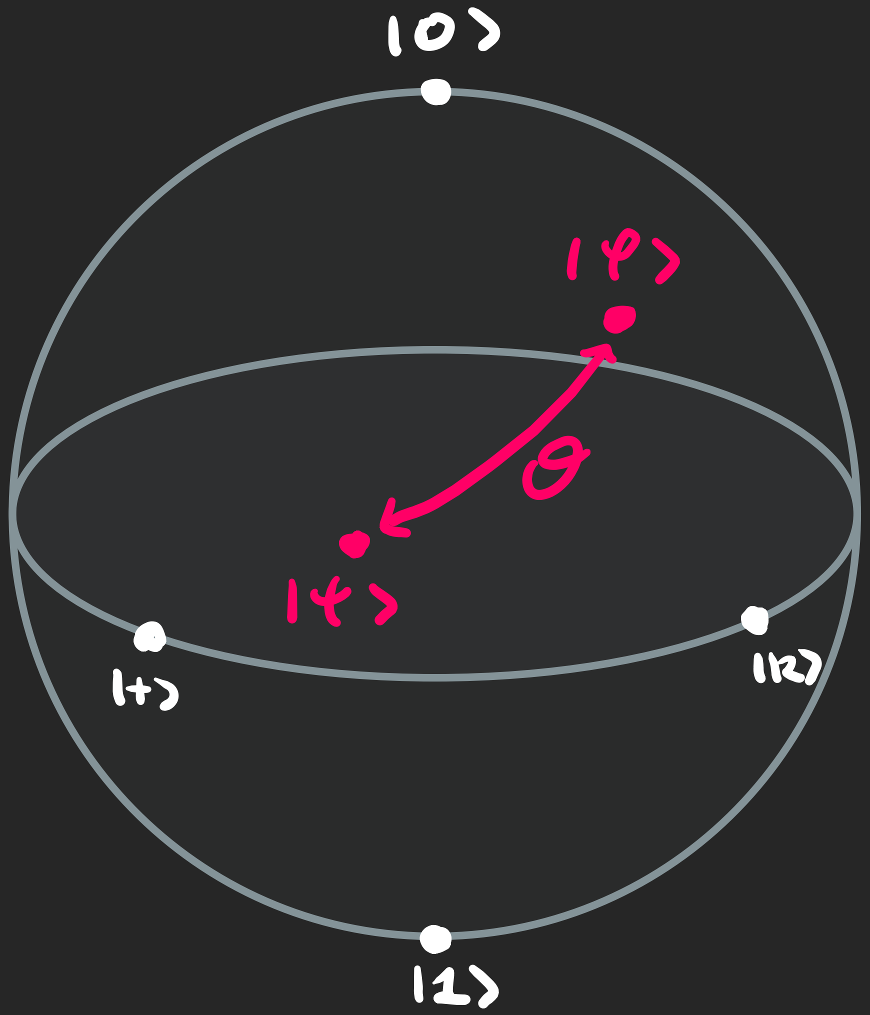
$$F(|\psi\rangle, |\varphi\rangle) := |\langle\psi|\varphi\rangle|^2$$

For 1-qubit states, the "Fidelity" is directly related to the $\boxed{\text{geodesic}}$ distance θ on the Bloch sphere:

$[0, \pi]$

$$|\langle\psi|\varphi\rangle|^2 = \cos^2\frac{\theta}{2} = \frac{\cos\theta + 1}{2}$$

$$\theta = \cos^{-1}\left(2\,|\langle\psi|\varphi\rangle|^2 - 1\right)$$



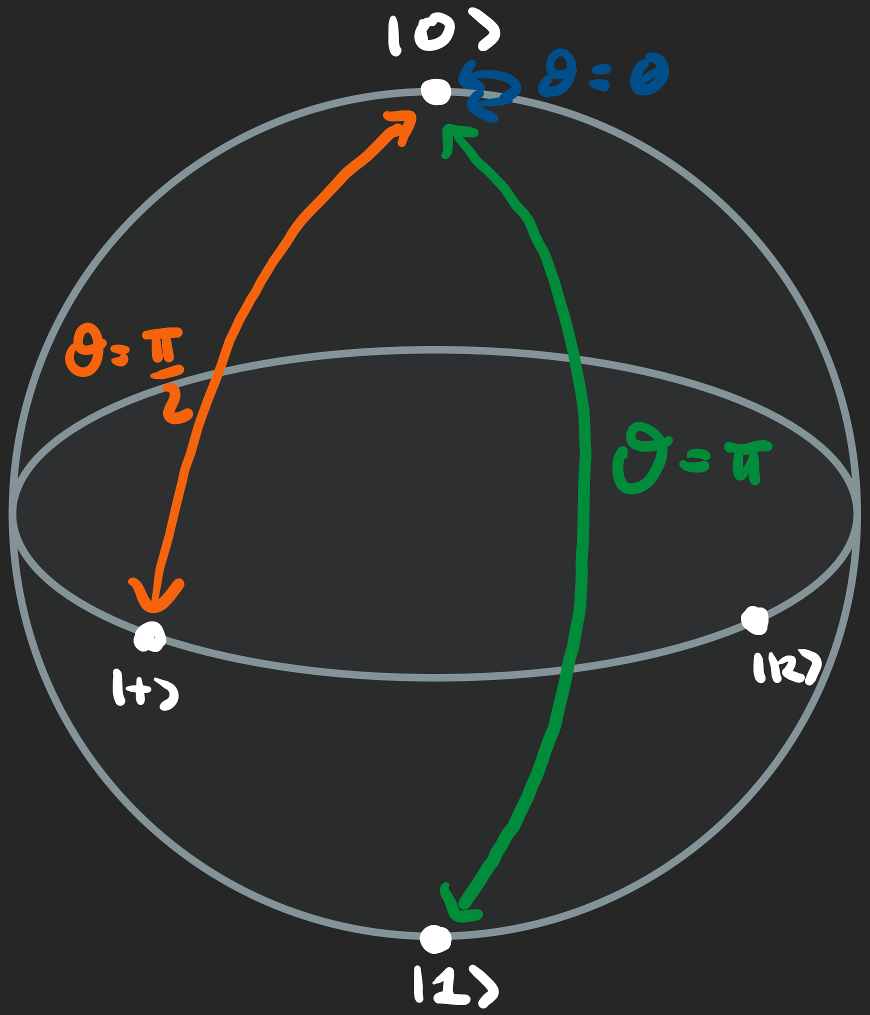
The Fidelity

Distance:	0	$\frac{\pi}{6}$	$\frac{\pi}{3}$	$\frac{\pi}{2}$	$\frac{2\pi}{3}$	$\frac{5\pi}{6}$	π
Fidelity:	1	$\frac{2+\sqrt{3}}{4}$	$\frac{3}{4}$	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{2-\sqrt{3}}{4}$	0

$$|\langle 0|0\rangle|^2 = \frac{\cos 0 + 1}{2} = 1$$

$$|\langle +|0\rangle|^2 = \frac{\cos \frac{\pi}{2} + 1}{2} = \frac{1}{2}$$

$$|\langle 0|1\rangle|^2 = \frac{\cos \pi + 1}{2} = 0$$



The Fidelity

$|\varphi\rangle = |\psi\rangle$

$|\psi\rangle$ on equator for $|\varphi\rangle$ (and vice versa)

$|\varphi\rangle$ and $|\psi\rangle$ antipodal

Distance:	0	$\frac{\pi}{6}$	$\frac{\pi}{3}$	$\frac{\pi}{2}$	$\frac{2\pi}{3}$	$\frac{5\pi}{6}$	π
Fidelity:	1	$\frac{2+\sqrt{3}}{4}$	$\frac{3}{4}$	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{2-\sqrt{3}}{4}$	0

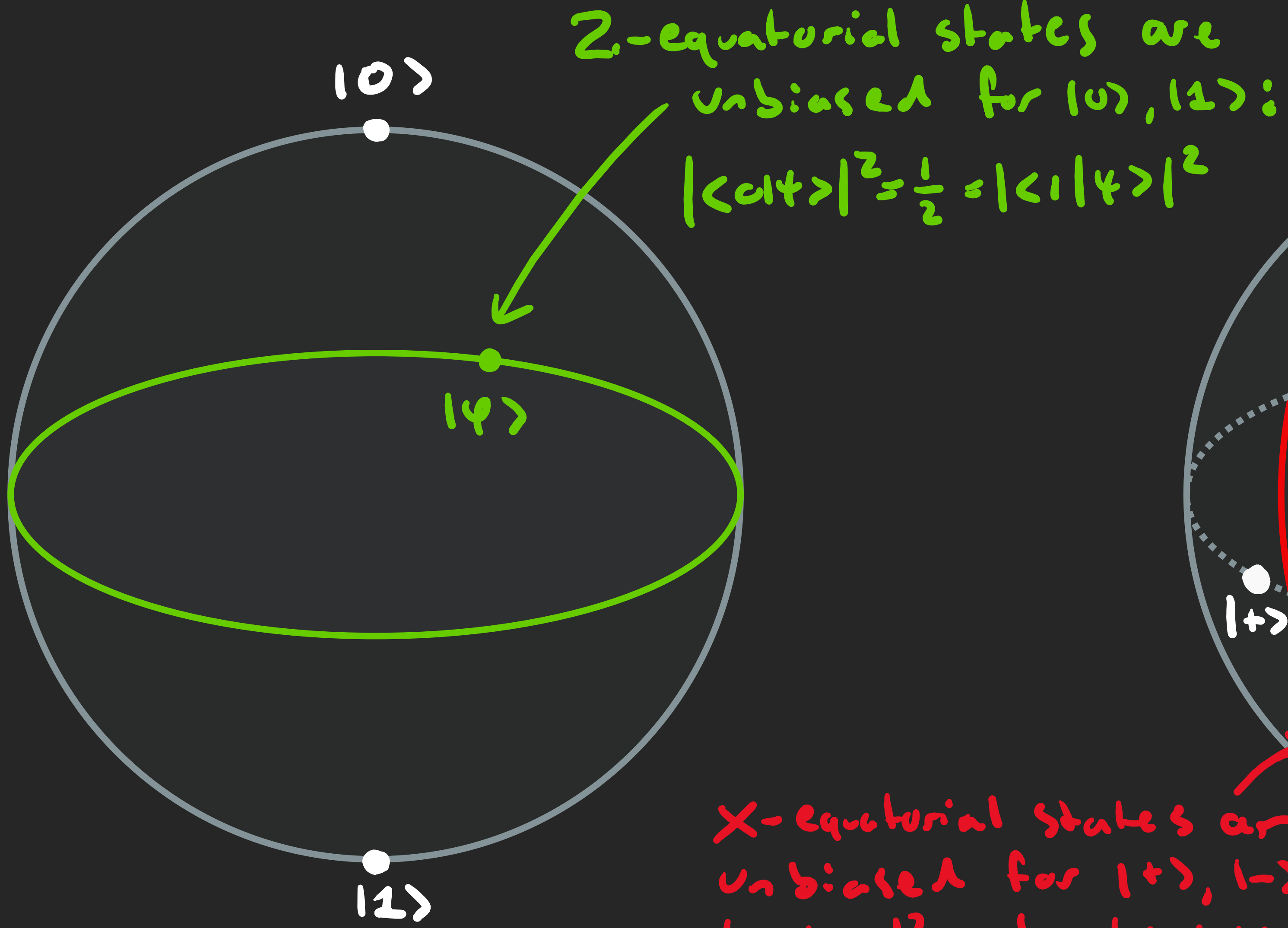
$|\varphi\rangle$ and $|\psi\rangle$ "unbiased"

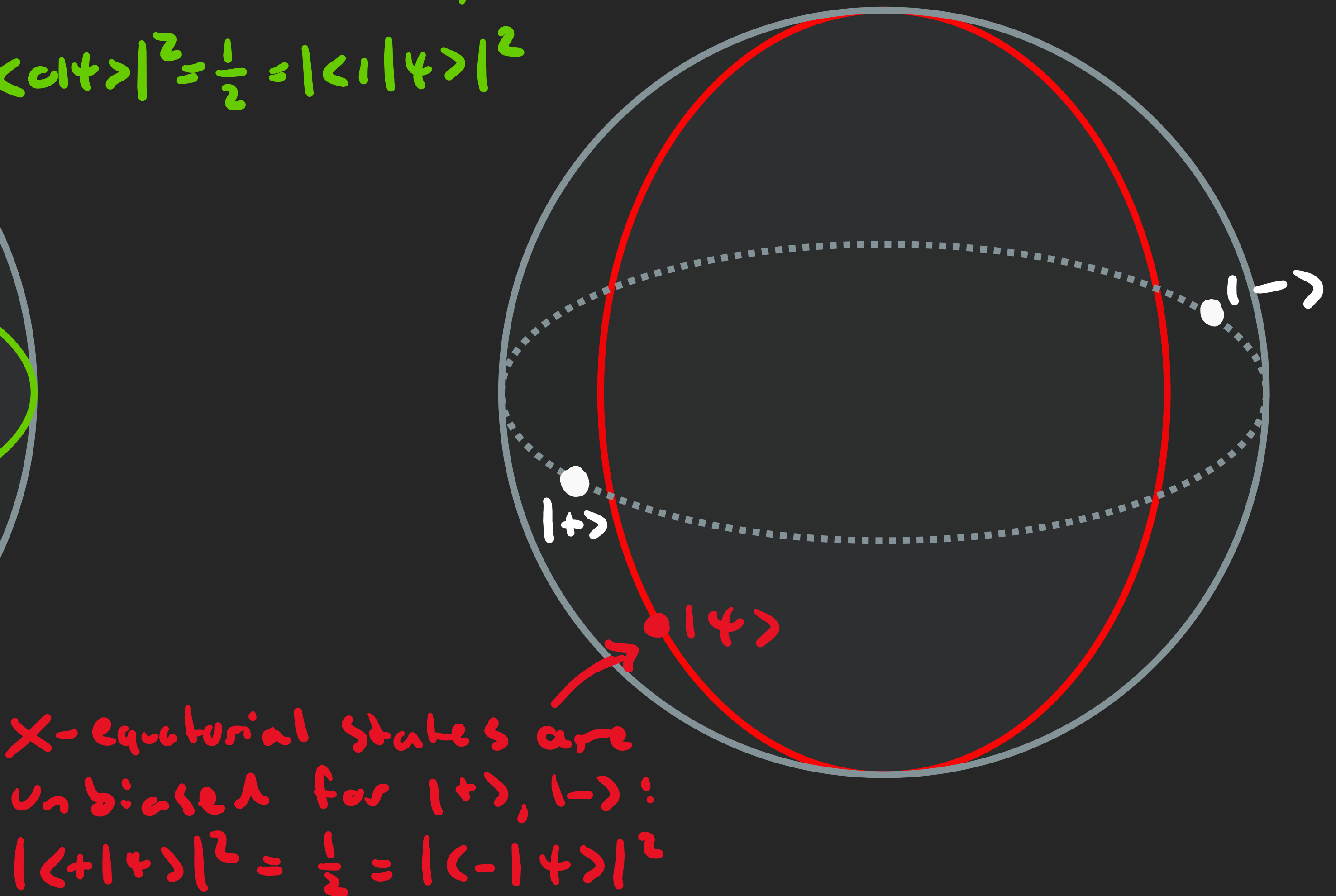
$|\varphi\rangle$ and $|\psi\rangle$ "orthogonal"

For n-qubit states, "unbiased" means

$$F(|\varphi\rangle, |\psi\rangle) = \frac{1}{2^n}$$

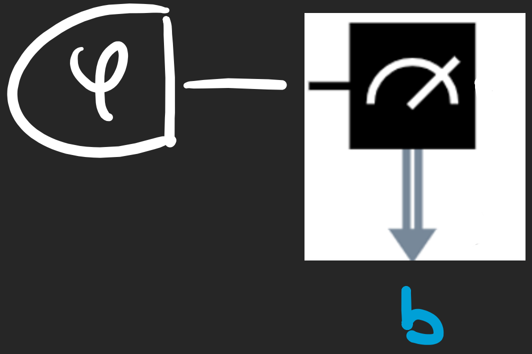
The Fidelity



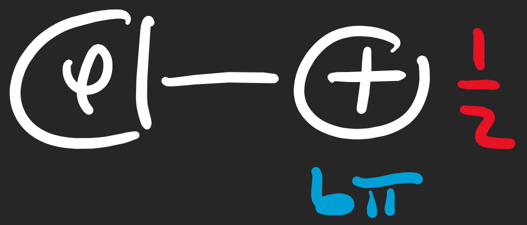


The Born Rule

The probability of outcome $b \in \{0, 1\}$ for a Z-basis measurement on a 1-qubit state $|\psi\rangle$ is given by its fidelity to $|b\rangle$



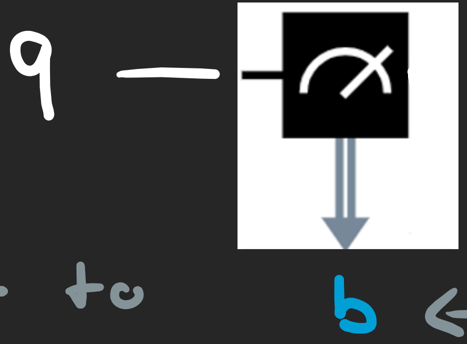
$$\mathbb{P}(b) = |\langle b|\psi\rangle|^2$$

$=$ 

Measurement

qubit discarded after measurement

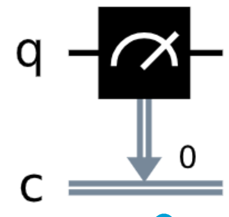
Demolition Measurement:



qubit to be measured

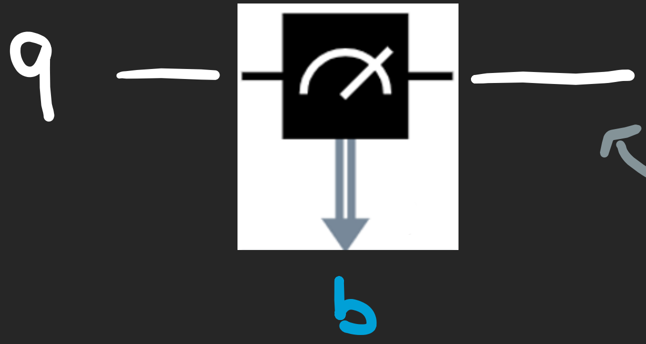
measurement outcome $b \in \{0,1\}$

```python
circ = QuantumCircuit(1, 1)
circ.measure(0, 0)
circ.draw("mpl")
```



outcome bit stored into "classical register"

Non-demolition Measurement:



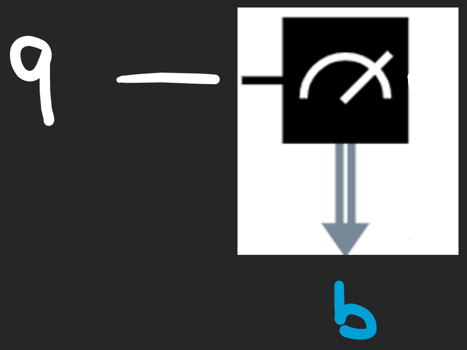
qubit still available after measurement (collapsed in state $|b\rangle$)

This is a Z-basis measurement

Measurement

$b \in \{0,1\}$ is the measurement outcome

Demolition Measurement:



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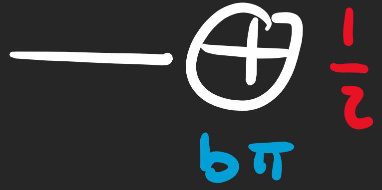
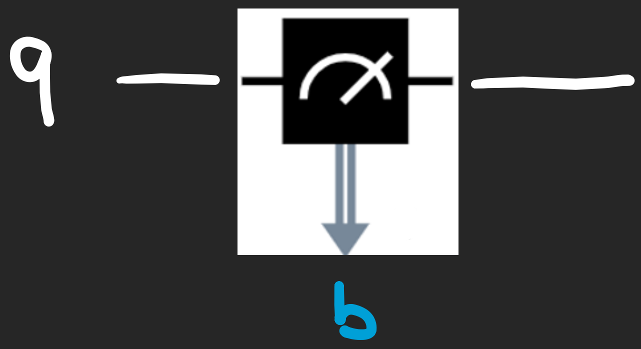


Z-basis

Non-demolition Measurement:



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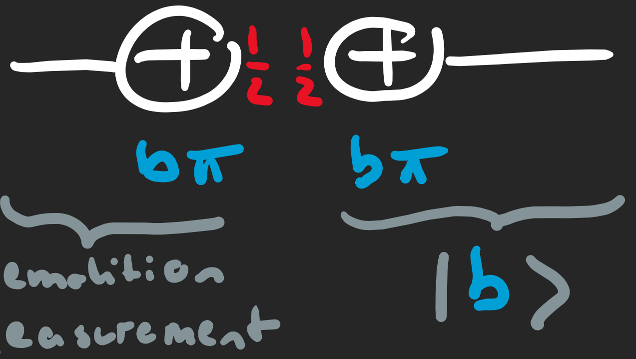


Measurement

Z-basis

X-basis

Demolition Measurement

$$\begin{cases} \langle 0| & \text{if } b=0 \\ \langle 1| & \text{if } b=1 \end{cases}$$

$$\begin{cases} \langle +| & \text{if } b=0 \\ \langle -| & \text{if } b=1 \end{cases}$$

$* \quad \cos(\theta) = 2\cos^2\left(\frac{\theta}{2}\right) - 1$

Spider Scalars

$$\longleftrightarrow \left| \underbrace{|0\ldots0\rangle}_{m}\underbrace{\langle 0\ldots0|}_{n} + e^{i\theta}\underbrace{|1\ldots1\rangle}_{m}\underbrace{\langle 1\ldots1|}_{n} \right|^2$$

$\underbrace{\qquad\qquad}_{n=0}$ input legs

$\underbrace{\qquad\qquad}_{m=0}$ output legs

$$= \left|1 + e^{i\theta}\right|^2$$

$$= (1+e^{i\theta})(1+e^{-i\theta})$$

$$= 2 + e^{i\theta} + e^{-i\theta} = 2(1+\cos\theta)$$

$$\overset{*}{=} 4\cos^2\left(\frac{\theta}{2}\right)$$

Spider Scalars

 $= |1+e^{i\theta}|^2 = 4\cos^2\left(\frac{\theta}{2}\right)$

 $= |1+e^{i\theta}|^2 = 4\cos^2\left(\frac{\theta}{2}\right)$

Special cases:

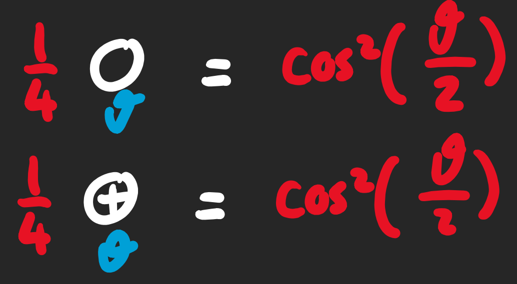
 $= 4$

 $= 0$

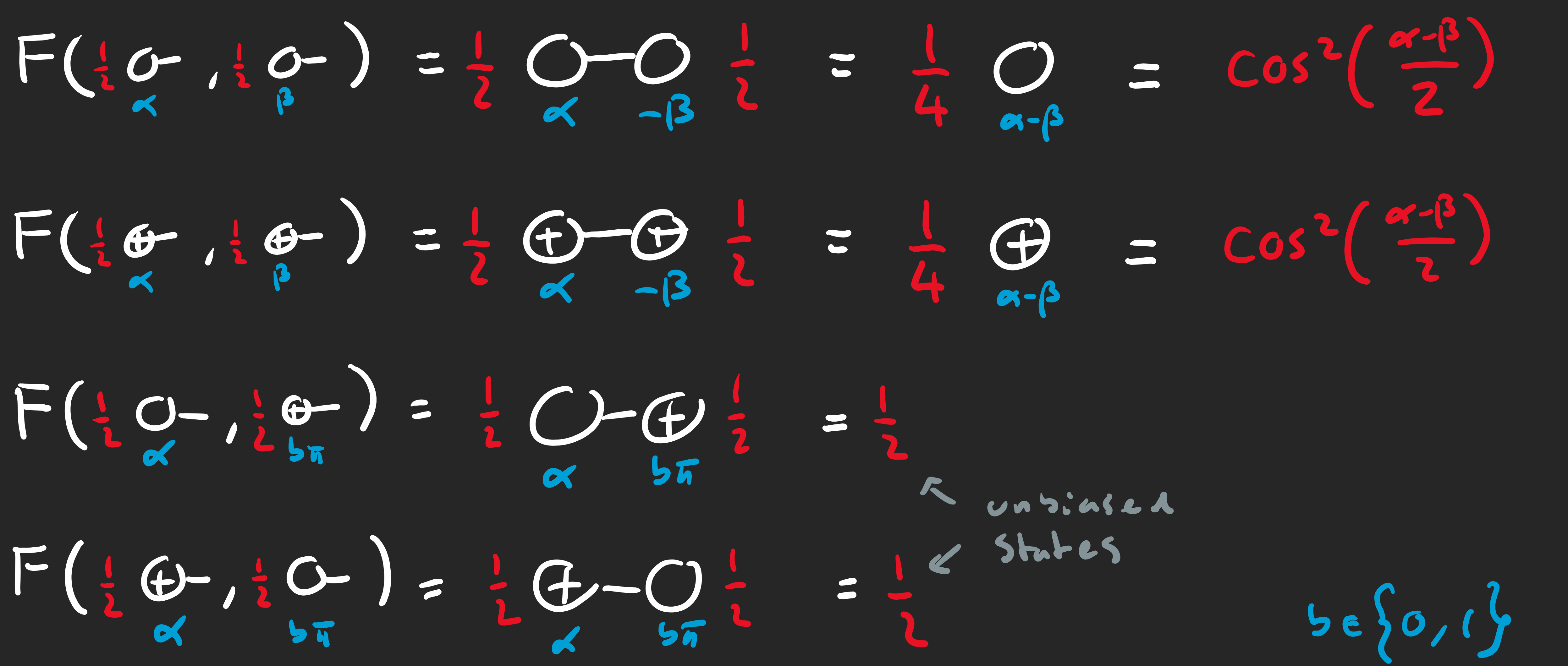
 $= 4$

 $= 0$

Fidelities

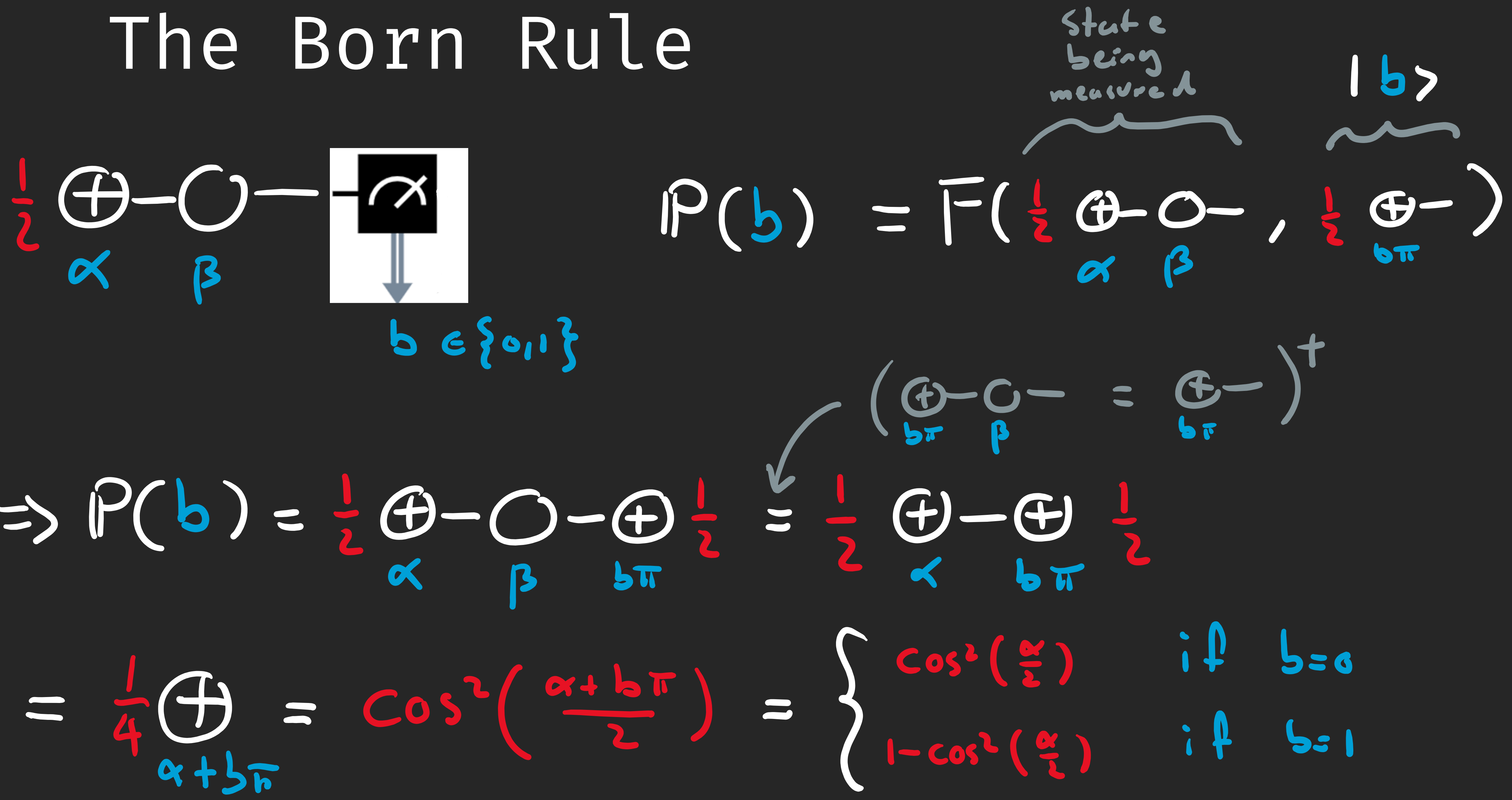


1/4 = cos²(θ/2)
1/4 = cos²(θ/2)

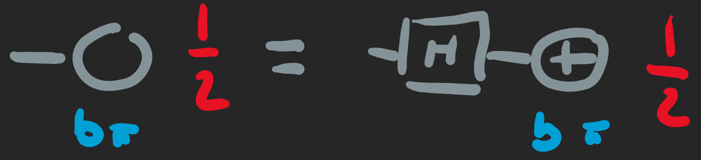


F(,) = 1/2 1/2 = 1/4 = cos²((α-β)/2)
F(,) = 1/2 1/2 = 1/4 = cos²((α-β)/2)
F(,) = 1/2 1/2 = 1/2
F(,) = 1/2 1/2 = 1/2
unbiased states
b ∈ {0,1}

The Born Rule



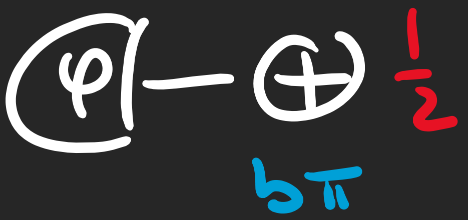
Measurement

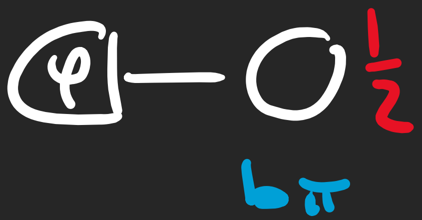


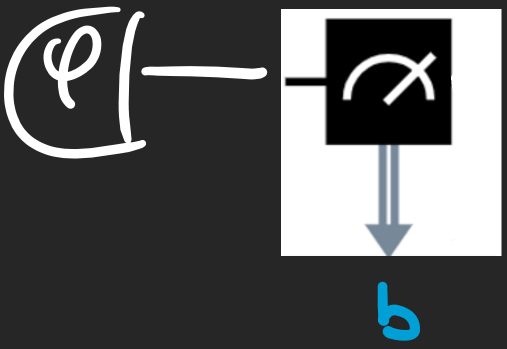
Z basis measurement

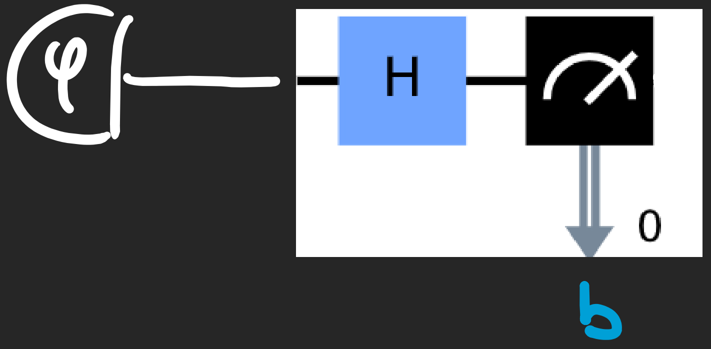
X basis measurement

$$\mathbb{P}(b|\psi) =$$

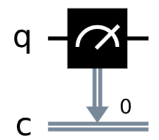






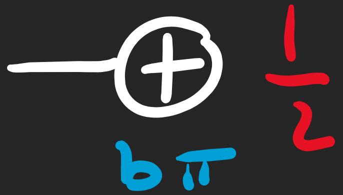


```python
circ = QuantumCircuit(1, 1)
circ.measure(0, 0)
circ.draw("mpl")
```



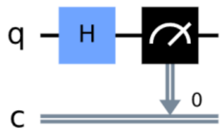
Z-basis

$\langle 0|, \langle 1|$



$$\underbrace{\langle \varphi |}_{\text{bra}} = \left(\underbrace{|\varphi\rangle}_{\text{ket}} \right)^{\dagger}$$

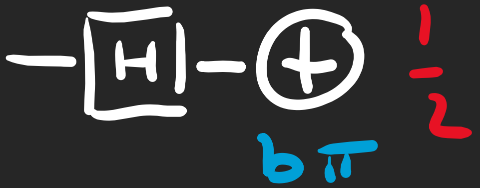
```python
circ = QuantumCircuit(1, 1)
circ.h(0)
circ.measure(0, 0)
circ.draw("mpl")
```



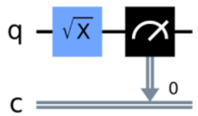
X-basis

$\langle +|, \langle -|$

=

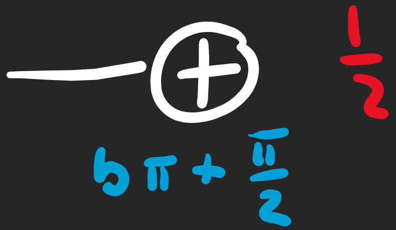



```python
circ = QuantumCircuit(1, 1)
circ.sx(0)
circ.measure(0, 0)
circ.draw("mpl")
```



Y-basis

$\langle R|, \langle L|$



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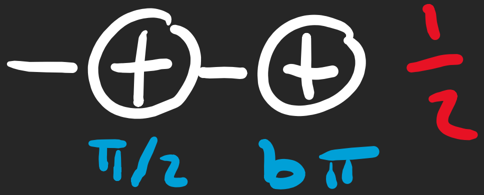


Measurement

backend = simulator (noiseless)

```python
from qiskit import QuantumCircuit, BasicAer, execute
from qiskit.visualization import plot_histogram
backend = BasicAer.get_backend('qasm_simulator')
```

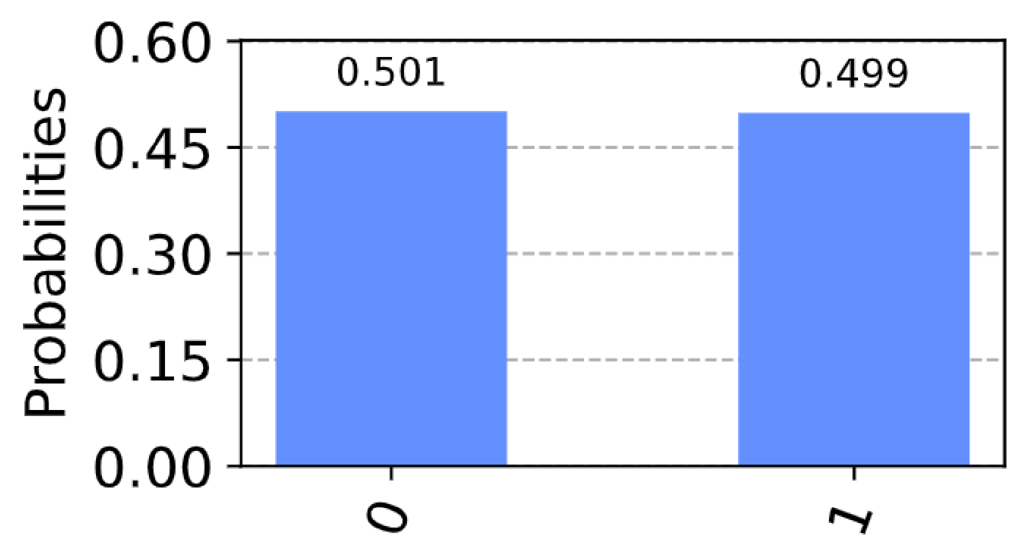
1-qubit + 1-bit circuit

measure q_0 into pos 0 of classical register

```python
circ = QuantumCircuit(1, 1)
# qubit starts in |0>
circ.h(0) # qubit now in |+>
circ.measure(0, 0)
job = execute(circ, backend, shots=10000)
counts = job.result().get_counts()
plot_histogram(counts, figsize=(3.5,2))
```

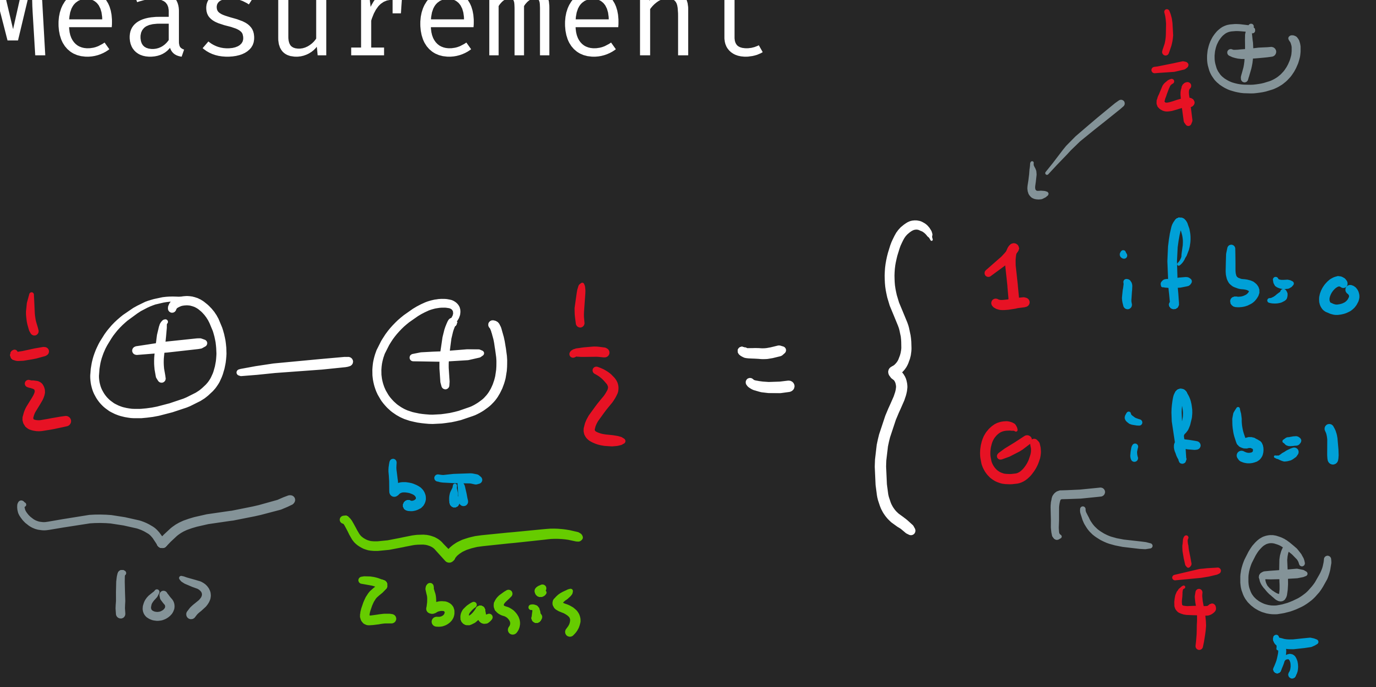
1. simulate 10k times
2. collect meas. outcomes
   return a dict of counts
3. plot probabilities

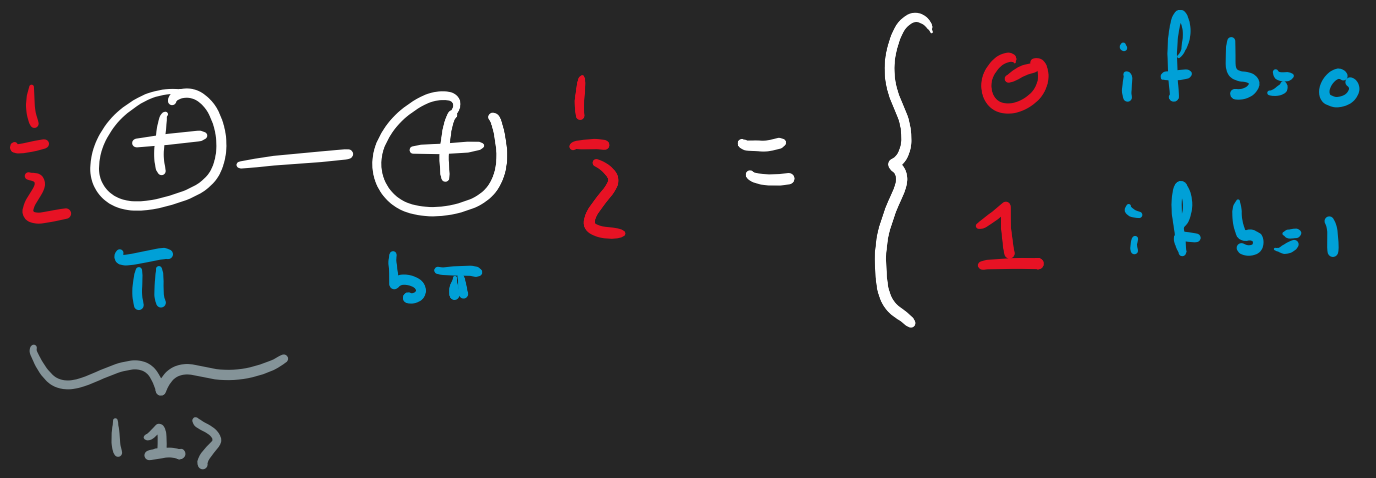
$$\mathbb{P}(b) = \frac{\text{count}(b)}{10000}$$



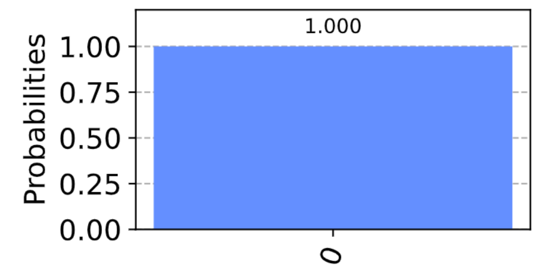
Z basis measurement

Measurement

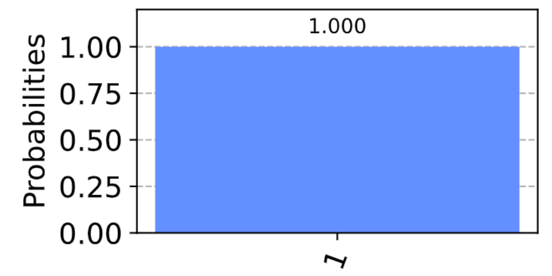





```
circ = QuantumCircuit(1, 1)
# qubit starts in |0>
circ.measure(0, 0)
job = execute(circ, backend, shots=10000)
counts = job.result().get_counts()
plot_histogram(counts, figsize=(3.5,2))
```



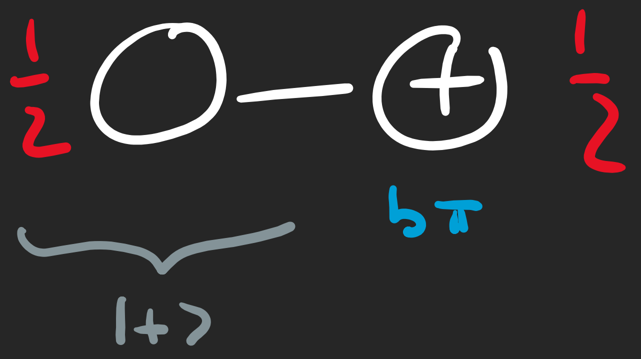

```
circ = QuantumCircuit(1, 1)
# qubit starts in |0>
circ.x(0) # qubit now in |1>
circ.measure(0, 0)
job = execute(circ, backend, shots=10000)
counts = job.result().get_counts()
plot_histogram(counts, figsize=(3.5,2))
```



Z basis measurement

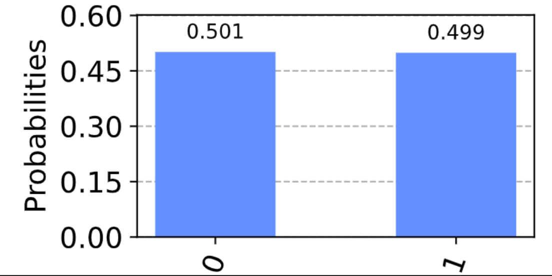
Measurement

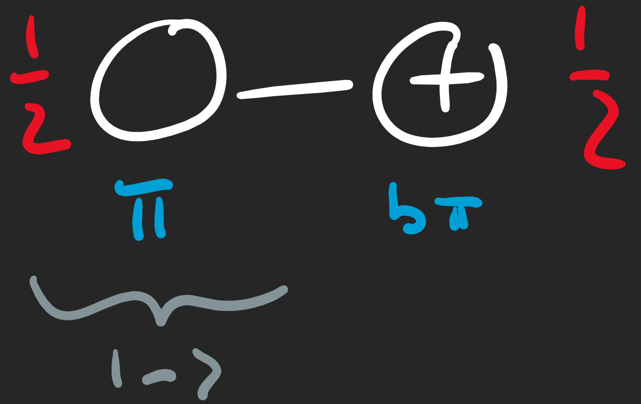
|+⟩ unbiased/equatorial in Z



$$= \begin{cases} \frac{1}{2} & \text{if } b=0 \\ \frac{1}{2} & \text{if } b=1 \end{cases}$$

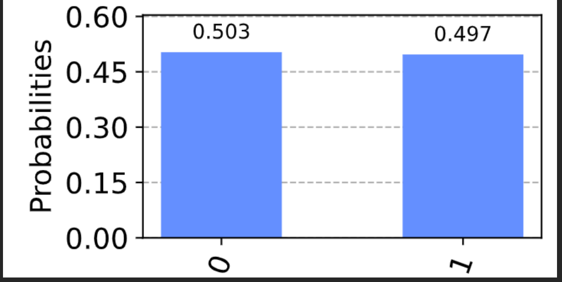
```
circ = QuantumCircuit(1, 1)
# qubit starts in |0>
circ.h(0) # qubit now in |+>
circ.measure(0, 0)
job = execute(circ, backend, shots=10000)
counts = job.result().get_counts()
plot_histogram(counts, figsize=(3.5,2))
```





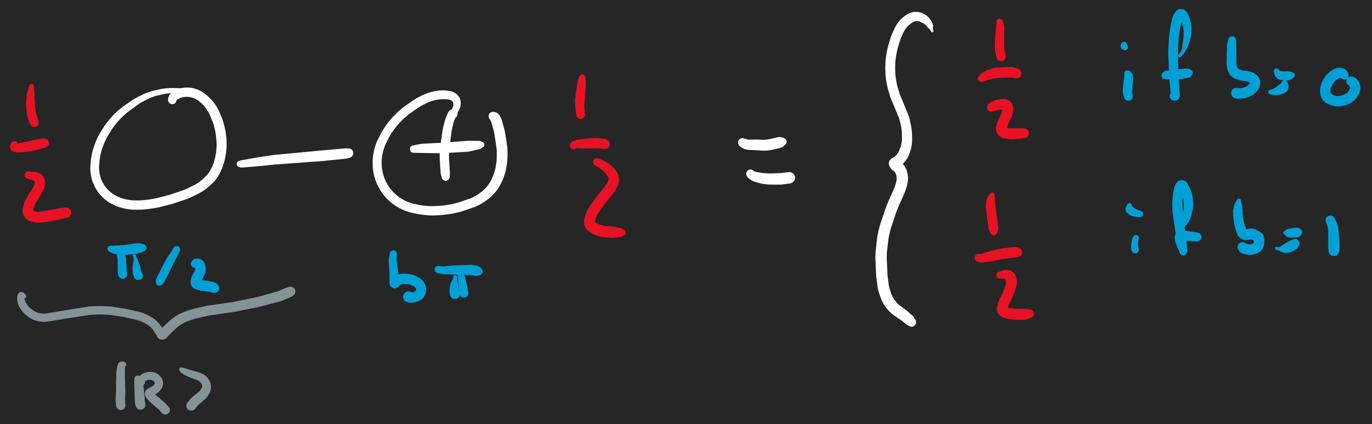
$$= \begin{cases} \frac{1}{2} & \text{if } b=0 \\ \frac{1}{2} & \text{if } b=1 \end{cases}$$

```
circ = QuantumCircuit(1, 1)
# qubit starts in |0>
circ.h(0); circ.z(0) # qubit now in |->
circ.measure(0, 0)
job = execute(circ, backend, shots=10000)
counts = job.result().get_counts()
plot_histogram(counts, figsize=(3.5,2))
```

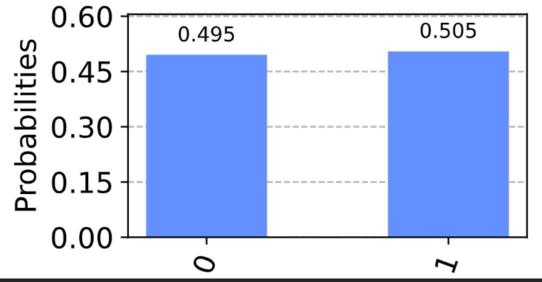


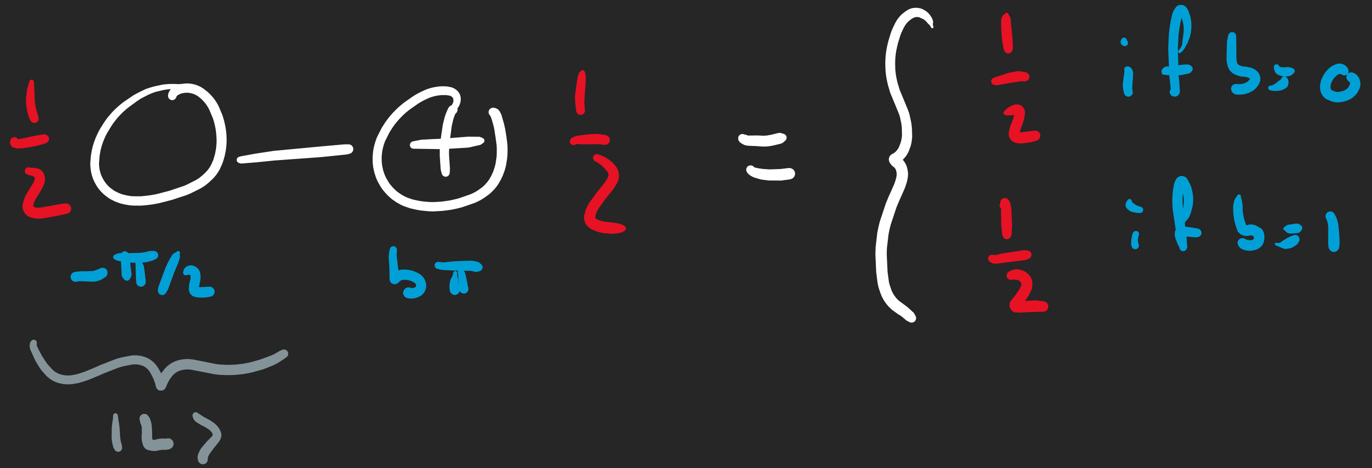
Z basis measurement

Measurement

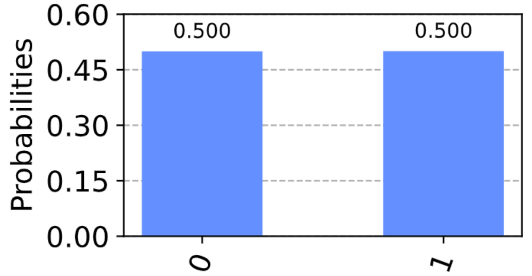



```
circ = QuantumCircuit(1, 1)
# qubit starts in |0>
circ.h(0); circ.s(0) # qubit now in |R>
circ.measure(0, 0)
job = execute(circ, backend, shots=10000)
counts = job.result().get_counts()
plot_histogram(counts, figsize=(3.5,2))
```



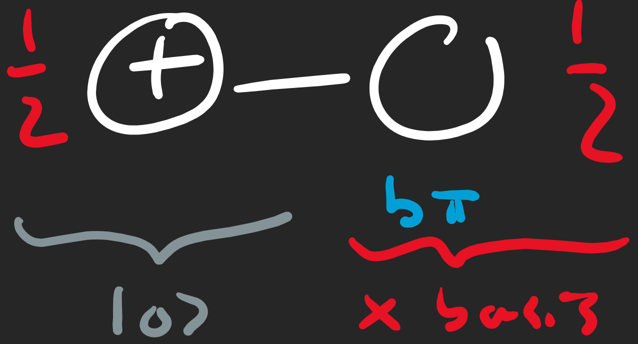



```
circ = QuantumCircuit(1, 1)
# qubit starts in |0>
circ.h(0); circ.sdg(0) # qubit now in |L>
circ.measure(0, 0)
job = execute(circ, backend, shots=10000)
counts = job.result().get_counts()
plot_histogram(counts, figsize=(3.5,2))
```



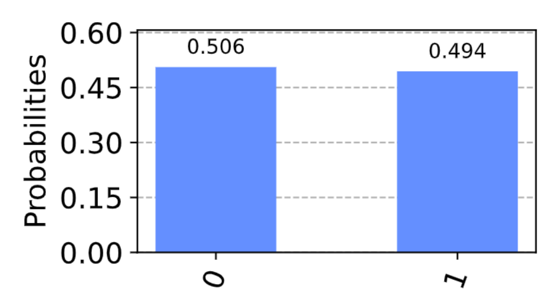
X basis measurement

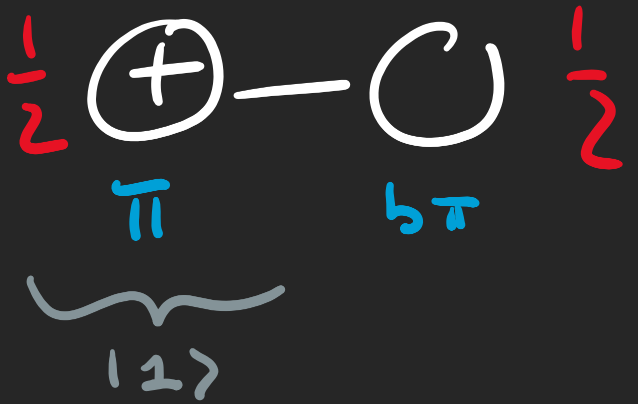
Measurement



$$= \begin{cases} \frac{1}{2} & \text{if } b=0 \\ \frac{1}{2} & \text{if } b=1 \end{cases}$$

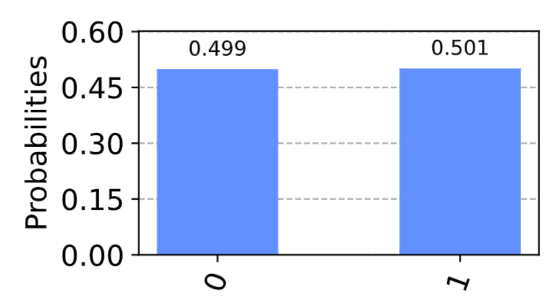
```python
circ = QuantumCircuit(1, 1)
# qubit starts in |0>
circ.h(0); circ.measure(0, 0) # X meas.
job = execute(circ, backend, shots=10000)
counts = job.result().get_counts()
plot_histogram(counts, figsize=(3.5,2))
```





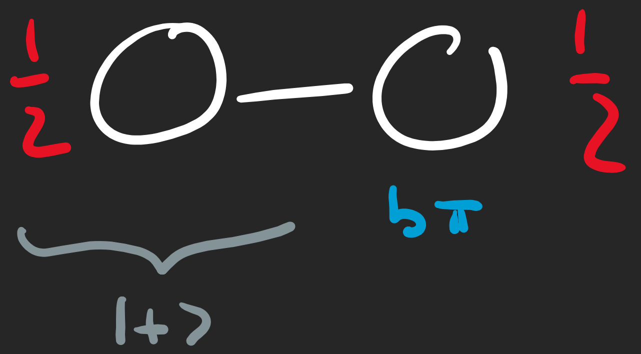
$$= \begin{cases} \frac{1}{2} & \text{if } b=0 \\ \frac{1}{2} & \text{if } b=1 \end{cases}$$

```python
circ = QuantumCircuit(1, 1)
# qubit starts in |0>
circ.x(0) # qubit now in |1>
circ.h(0); circ.measure(0, 0) # X meas.
job = execute(circ, backend, shots=10000)
counts = job.result().get_counts()
plot_histogram(counts, figsize=(3.5,2))
```



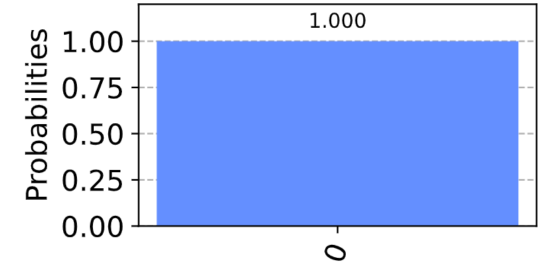
X basis measurement

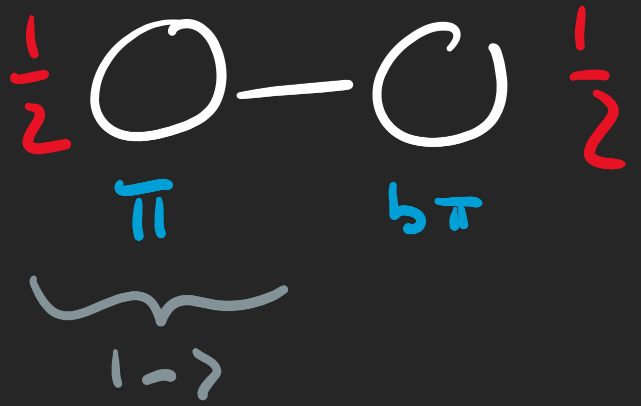
Measurement



$$= \begin{cases} 1 & \text{if } b=0 \\ 0 & \text{if } b=1 \end{cases}$$

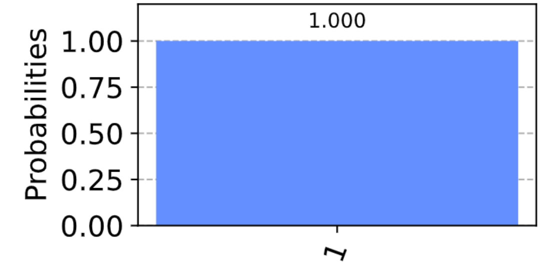
```
circ = QuantumCircuit(1, 1)
# qubit starts in |0>
circ.h(0) # qubit now in |+>
circ.h(0); circ.measure(0, 0) # X meas.
job = execute(circ, backend, shots=10000)
counts = job.result().get_counts()
plot_histogram(counts, figsize=(3.5,2))
```





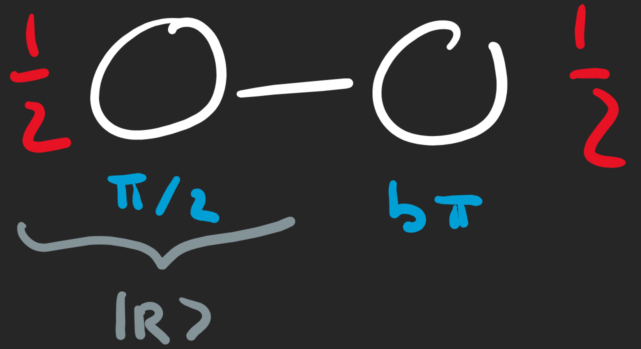
$$= \begin{cases} 0 & \text{if } b=0 \\ 1 & \text{if } b=1 \end{cases}$$

```
circ = QuantumCircuit(1, 1)
# qubit starts in |0>
circ.h(0); circ.z(0) # qubit now in |->
circ.h(0); circ.measure(0, 0) # X meas.
job = execute(circ, backend, shots=10000)
counts = job.result().get_counts()
plot_histogram(counts, figsize=(3.5,2))
```



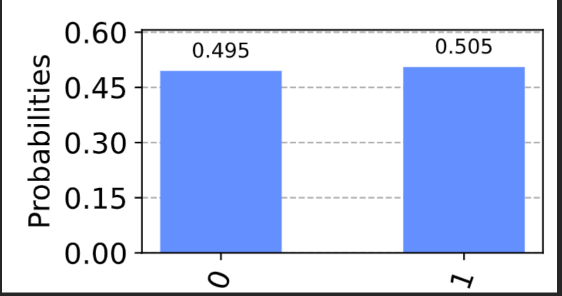
X basis measurement

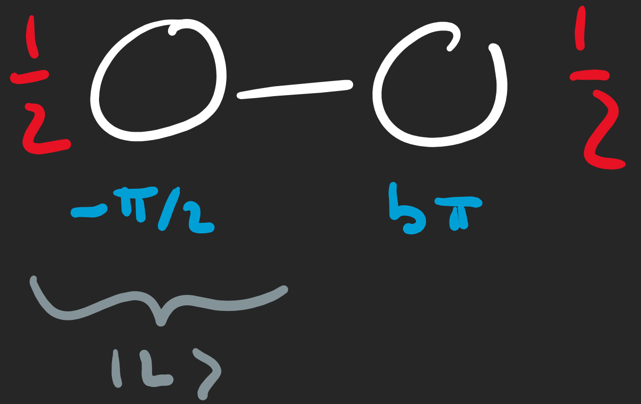
Measurement



$$= \begin{cases} \frac{1}{2} & \text{if } b=0 \\ \frac{1}{2} & \text{if } b=1 \end{cases}$$

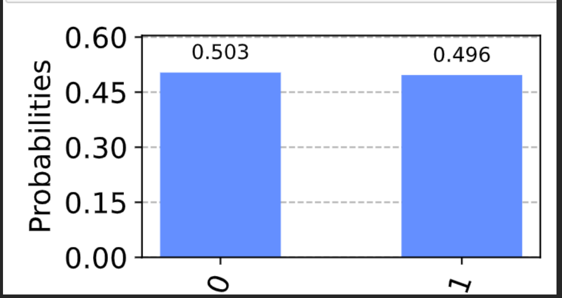
```
circ = QuantumCircuit(1, 1)
# qubit starts in |0>
circ.h(0); circ.s(0) # qubit now in |R>
circ.h(0); circ.measure(0, 0) # X meas.
job = execute(circ, backend, shots=10000)
counts = job.result().get_counts()
plot_histogram(counts, figsize=(3.5,2))
```





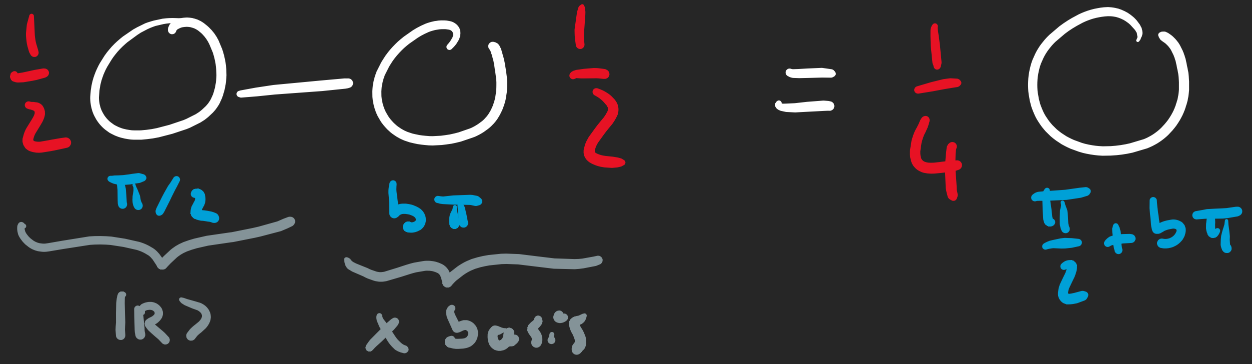
$$= \begin{cases} \frac{1}{2} & \text{if } b=0 \\ \frac{1}{2} & \text{if } b=1 \end{cases}$$

```
circ = QuantumCircuit(1, 1)
# qubit starts in |0>
circ.h(0); circ.sdg(0) # qubit now in |L>
circ.h(0); circ.measure(0, 0) # X meas.
job = execute(circ, backend, shots=10000)
counts = job.result().get_counts()
plot_histogram(counts, figsize=(3.5,2))
```



Measurement

e.g.

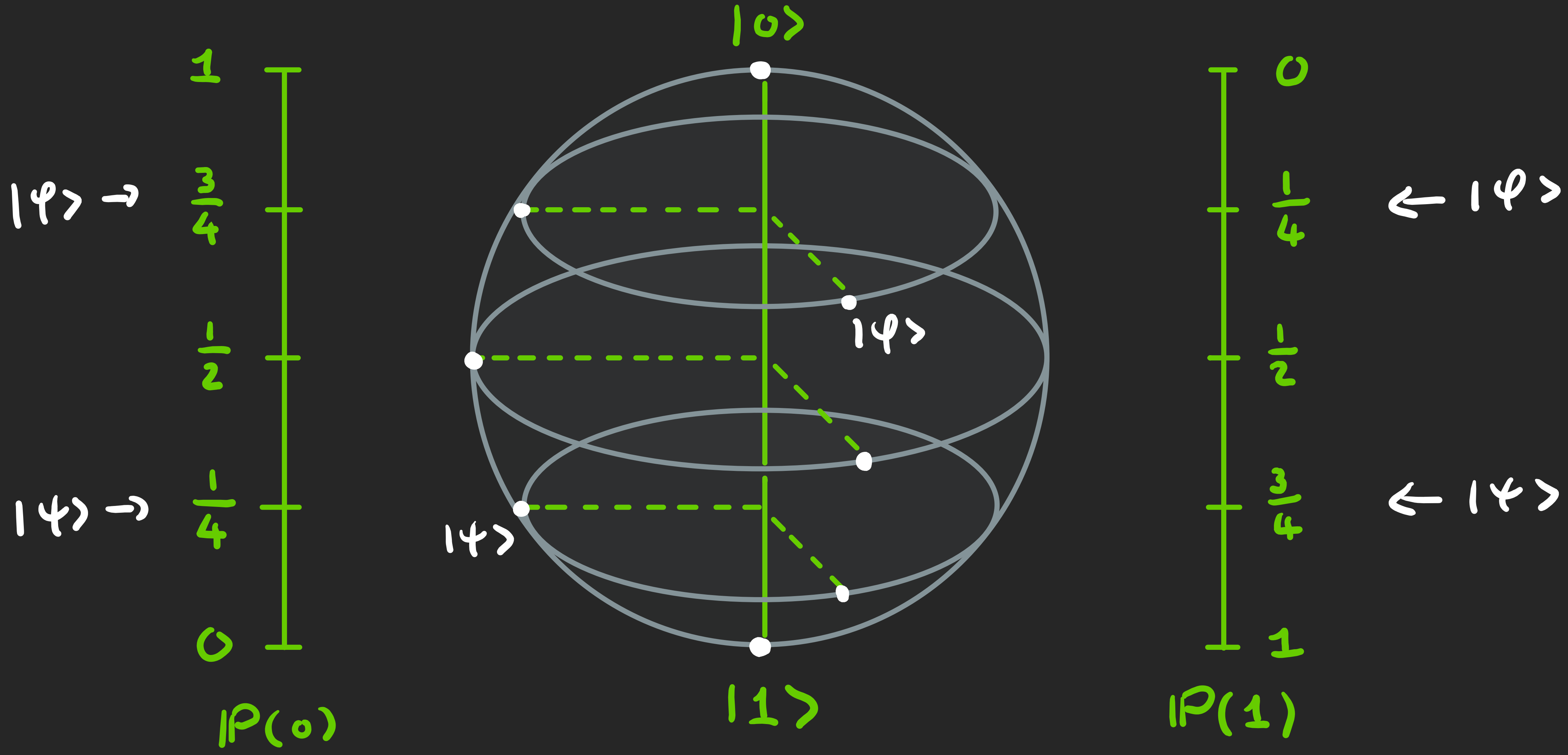


$$\cos^2\left(\frac{\pi/2 + b\pi}{2}\right) = \cos^2\left(\frac{\pm \pi/2}{2}\right) = \cos^2\left(\pm \pi/4\right) = \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}$$

$$= \cancel{\frac{1}{4}} \cdot \cancel{4} \cos^2\left(\frac{\pi/2 + b\pi}{2}\right) = \begin{cases} \frac{1}{2} & \text{if } b=0 \\ \frac{1}{2} & \text{if } b=1 \end{cases}$$

Measurement

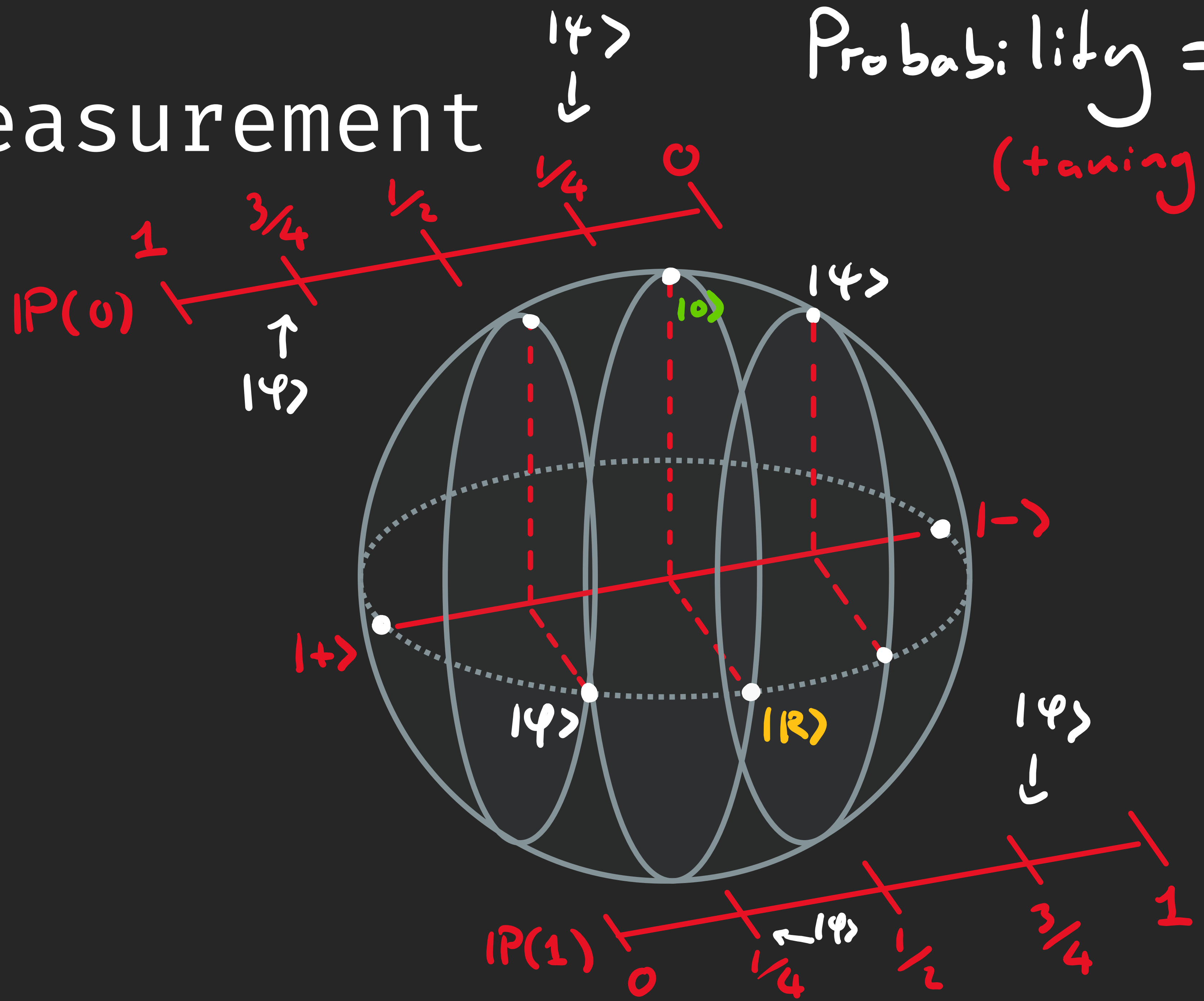
Probability = Latitude



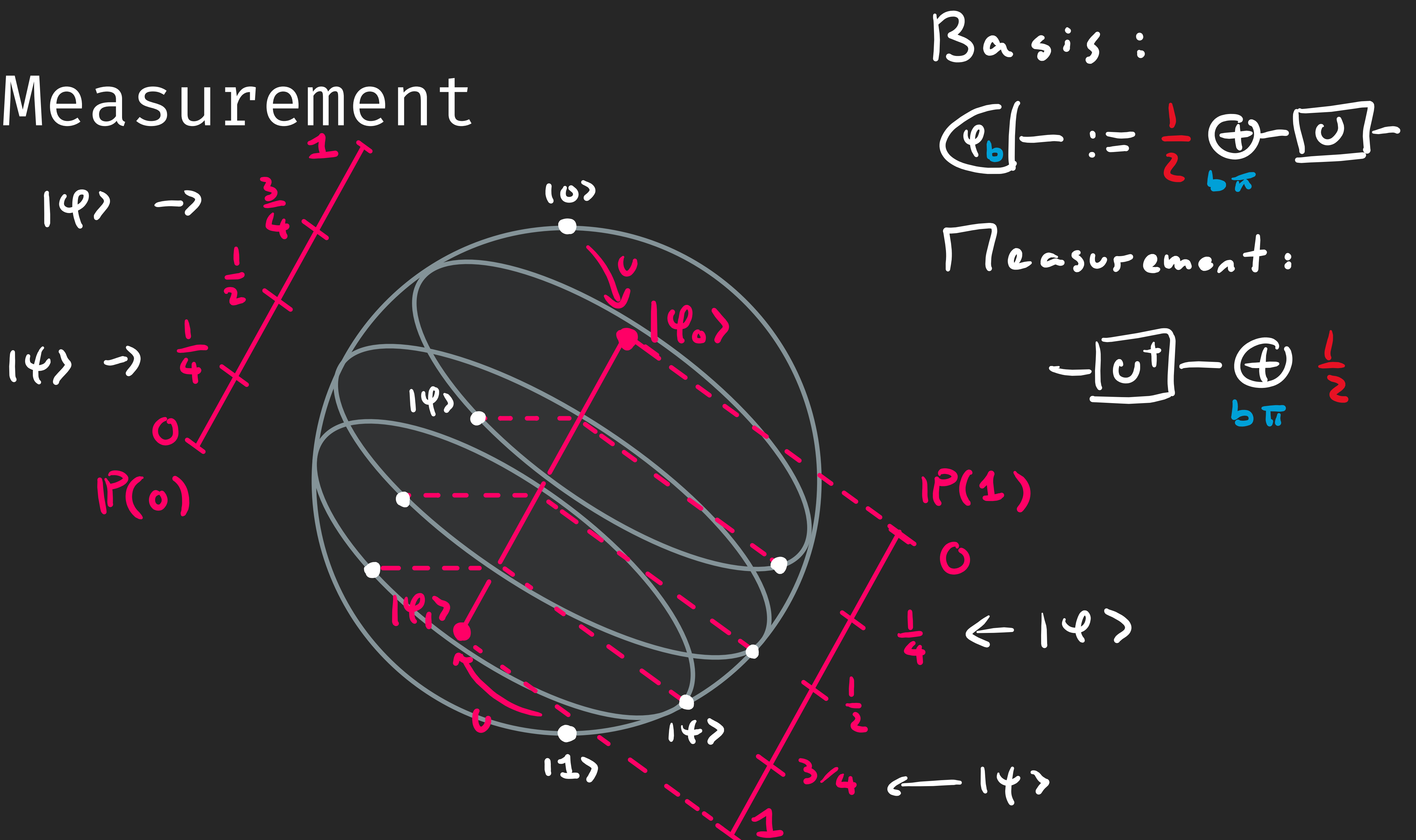
Measurement

Probability = Latitude

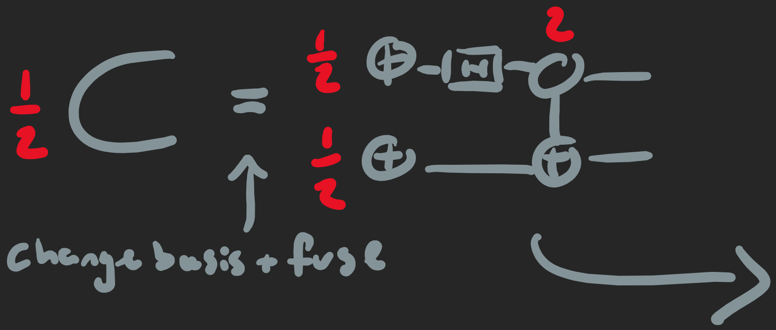
(taking poles along X)



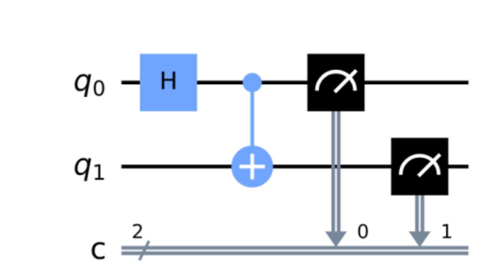
Measurement



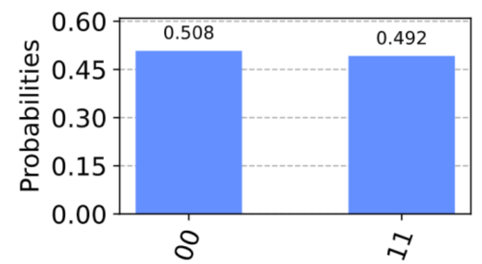
Measurement




```python
circ = QuantumCircuit(2, 2) # |00>
circ.h(0); circ.cx(0,1) # |bell>
circ.measure([0,1], [0,1])
circ.draw("mpl")
```




```python
job = execute(circ, backend, shots=10000)
counts = job.result().get_counts()
plot_histogram(counts, figsize=(3.5,2))
```

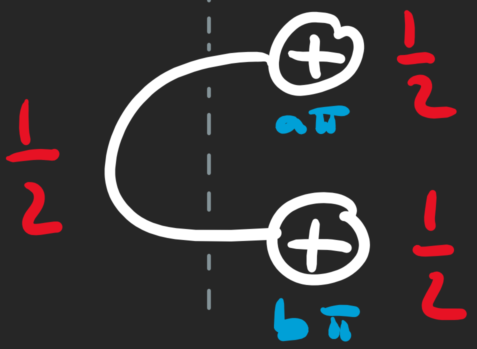


Entanglement ⇒ Correlation

2-qubit Bell state $|\Phi^+\rangle$

Z-basis measurements

$$\left\{\begin{array}{l} \oplus = 4 \\ \oplus_\pi = 0 \end{array}\right.$$

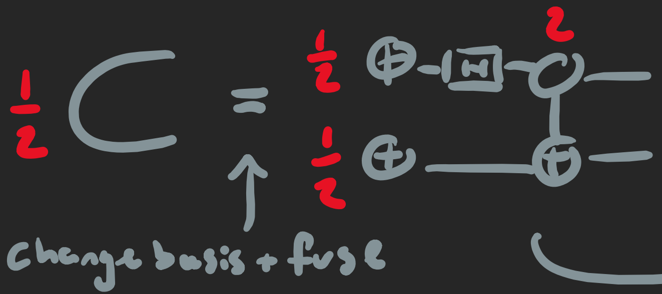


$$= \frac{1}{8} \oplus_{(a+b)\pi} = \begin{cases} \frac{1}{2} & \text{if } a \oplus b = 0 \\ 0 & \text{if } a \oplus b = 1 \end{cases}$$

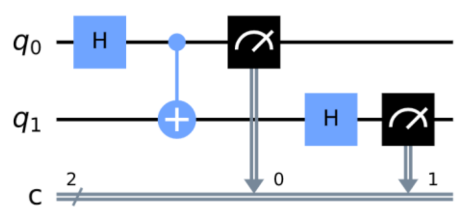
i.e. $a = b$

i.e. $a \neq b$

Measurement

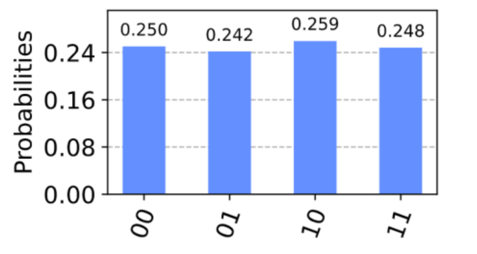



```python
circ = QuantumCircuit(2, 2) # |00>
circ.h(0); circ.cx(0, 1) # |bell>
circ.measure(0, 0) # Z meas. on q0
circ.h(1); circ.measure(1, 1) # X meas. on q1
circ.draw("mpl")
```

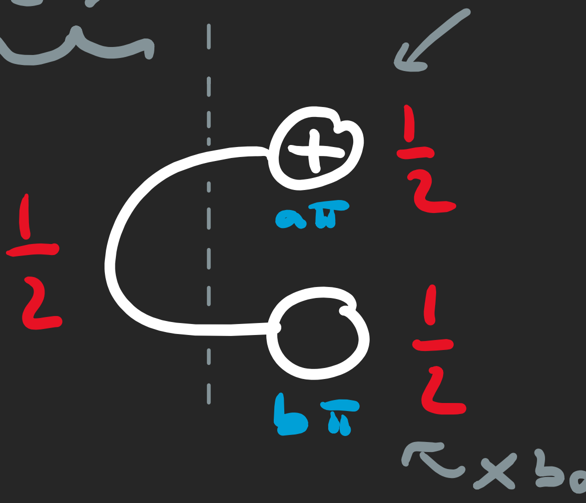


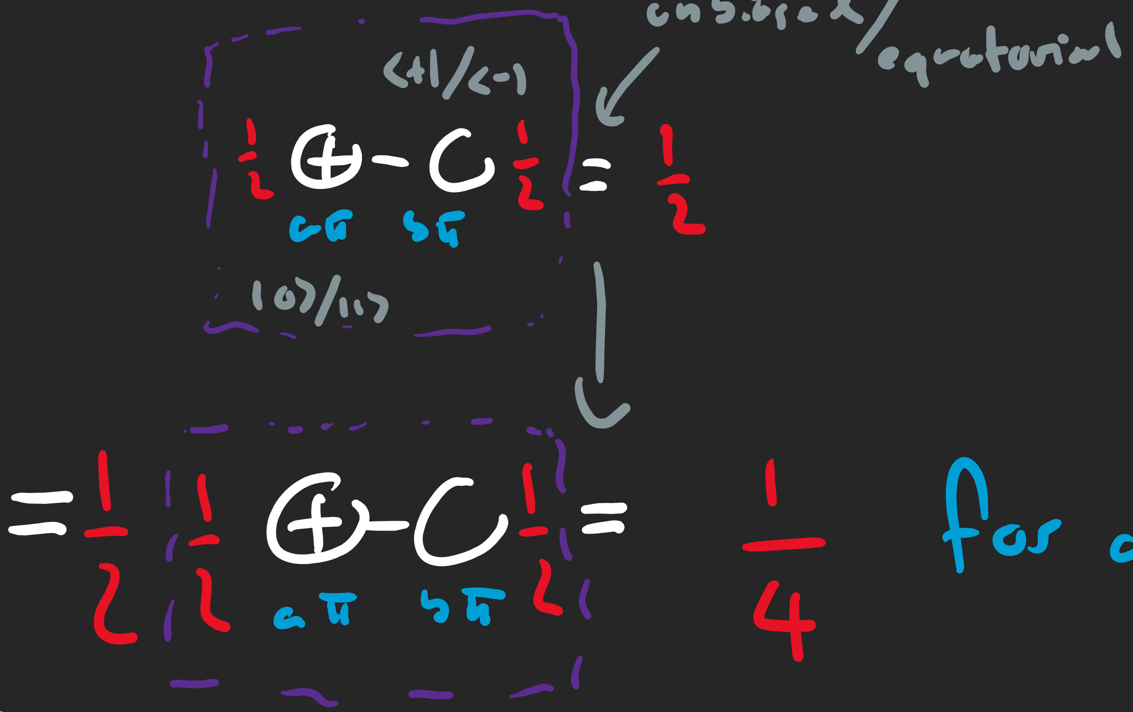
Entanglement ⇒ Correlation

```python
job = execute(circ, backend, shots = 10000)
counts = job.result().get_counts()
plot_histogram(counts, figsize=(3.5, 2))
```



2-qubit Bell state $|\Phi^+\rangle$



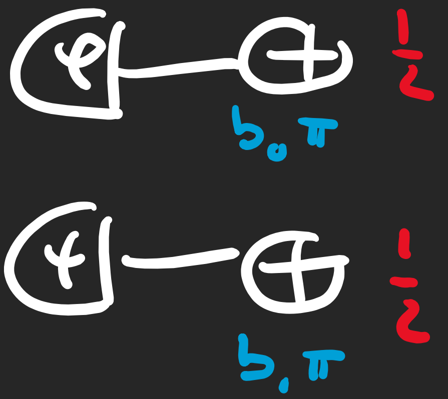


for all $a, b \in \{0, 1\}$

Measurement

Product states $\Rightarrow$ Probability distribution factors

$\mathbb{P}(\underline{b} \mid \varphi \times \psi) =$



$=$

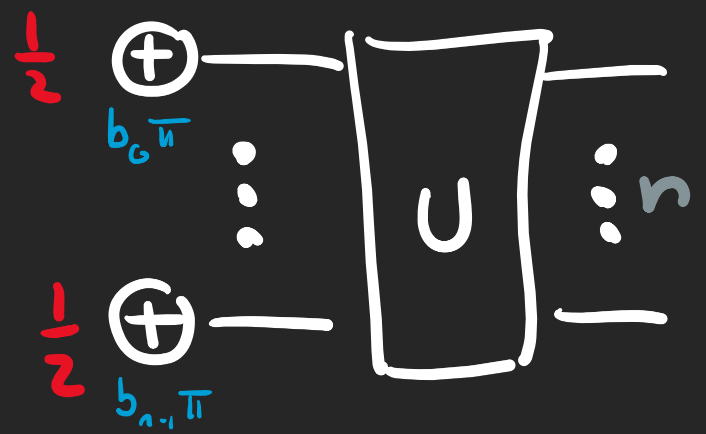
$$= \mathbb{P}(b_0 \mid \varphi) \cdot \mathbb{P}(b_1 \mid \psi)$$

Measurement

$|\underline{b}\rangle$ n-qubit Computational basis

Basis

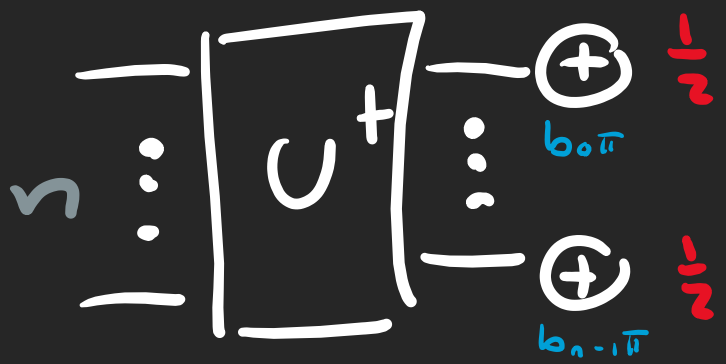
$|\varphi_{\underline{b}}\rangle :=$



State label: $\underline{b} \in \{0,1\}^n$

(n-bit string)

Measurement

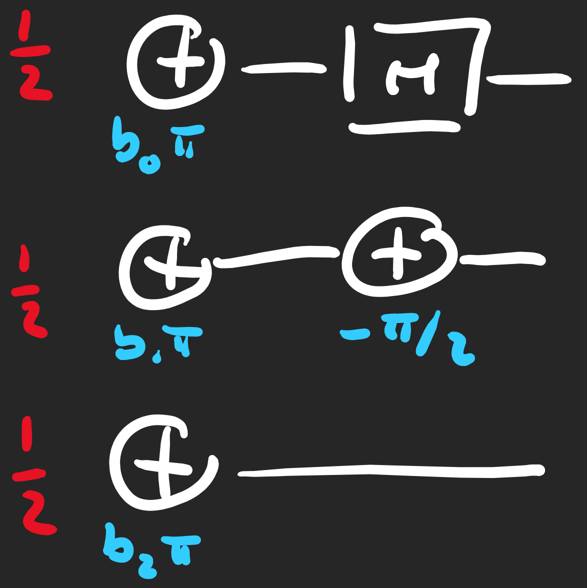


measurement outcome: $\underline{b} \in \{0,1\}^n$

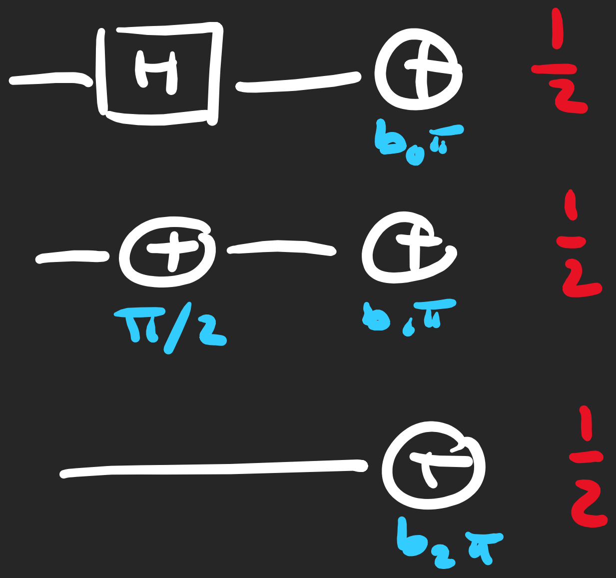
(n-bit string)

Measurement

3-qubit XYZ basis



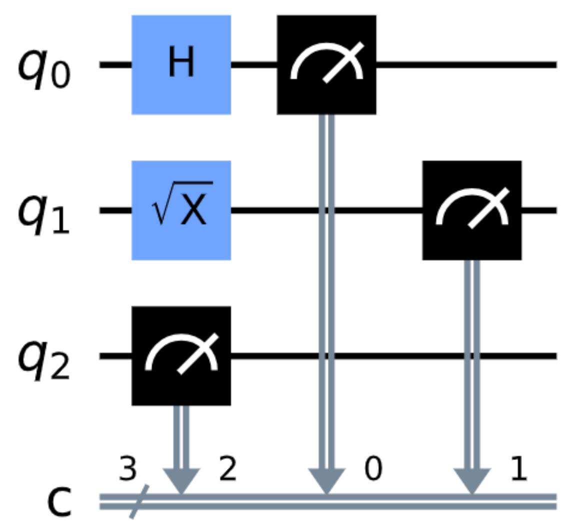
3-qubit XYZ measurement



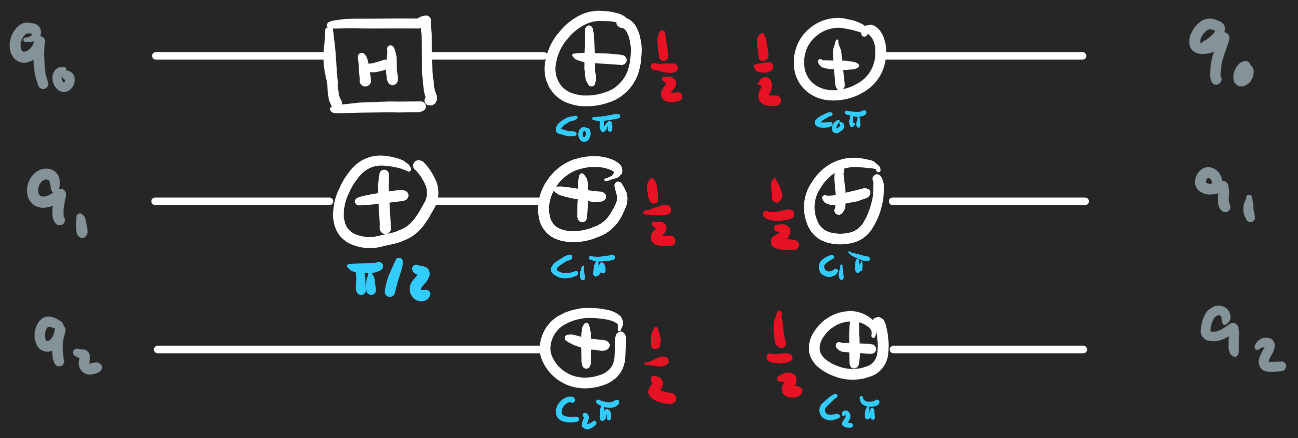
$$\underline{b} = b_2 b_1 b_0 \in \{0,1\}^3$$

Measurement

```
circ = QuantumCircuit(3, 3)
circ.h(0); circ.sx(1)
circ.measure([0, 1, 2], [0, 1, 2])
circ.draw("mpl")
```



3-qubit XYZ measurement



$c = [c_0, c_1, c_2]$

Mixed State Quantum Mechanics

Because of measurements, we need to introduce uncertainty into the theory:

Statevectors $\mapsto$ Density Matrices

$$|\psi\rangle \in \mathbb{C}^d \quad \mapsto \quad |\psi\rangle\langle\psi| \in \mathbb{C}^{d\times d}$$

$$\begin{pmatrix} \psi_{0\dots0} \\ \vdots \\ \psi_{1\dots1} \end{pmatrix} \qquad \begin{pmatrix} \psi_{0\dots0}\psi_{0\dots0} & \cdots & \psi_{0\dots0}\psi_{1\dots1} \\ \vdots & & \vdots \\ \psi_{1\dots1}\psi_{0\dots0} & \cdots & \psi_{1\dots1}\psi_{1\dots1} \end{pmatrix}$$

Mixed State Quantum Mechanics

$$A = \begin{pmatrix} A_{0\cdots 0,0\cdots 0} & \cdots & A_{0\cdots 0,1\cdots 1} \\ \vdots & & \vdots \\ A_{1\cdots 1,0\cdots 0} & \cdots & A_{1\cdots 1,1\cdots 1} \end{pmatrix} \in \mathbb{C}^{2^n \times 2^n}$$

row

$$A_{\underline{b},\underline{b}'} = \langle \underline{b} | A | \underline{b}' \rangle$$

column

$$\mathrm{Tr}(A) = \sum_{\underline{b} \in \{0,1\}^n} A_{\underline{b},\underline{b}} = \sum_{\underline{b} \in \{0,1\}^n} \langle \underline{b} | A | \underline{b} \rangle$$

Mixed State Quantum Mechanics

$|\psi\rangle$ n-qubit state in $\mathbb{C}^{2^n}$

$$\mathbb{P}(\underline{b} \mid \psi) = |\langle \underline{b} | \psi \rangle|^2 = \langle \underline{b} | \psi \rangle \langle \psi | \underline{b} \rangle$$

$$= \sum_{\underline{b}' \in \{0,1\}^n} \langle \underline{b}' | \underline{b} \rangle \langle \underline{b} | \psi \rangle \langle \psi | \underline{b}' \rangle$$

$$= \mathrm{Tr}\left(|\underline{b}\rangle\langle \underline{b} | \psi \rangle\langle \psi | \right)$$

Mixed State Quantum Mechanics

ρ density matrix in $\mathbb{C}^{2^n \times 2^n}$

$$\mathbb{P}(\underline{b} \mid \rho) = \cancel{|\langle \underline{b} | \psi \rangle|^2} = \langle \underline{b} | \rho | \underline{b} \rangle$$

$$= \sum_{\underline{b}' \in \{0,1\}^n} \langle \underline{b}' | \underline{b} \rangle \langle \underline{b} | \rho | \underline{b}' \rangle$$

$$= \mathrm{Tr}\left(|\underline{b}\rangle\langle\underline{b}| \rho \right)$$

Mixed State Quantum Mechanics

$$\mathbb{P}(\underline{b} \mid \rho) \in \mathbb{R} \iff \langle \underline{b} | \rho | \underline{b} \rangle = \left(\langle \underline{b} | \rho | \underline{b} \rangle \right)^*$$

$$= \langle \underline{b} | \rho^\dagger | \underline{b} \rangle$$

$$\mathbb{P}(\underline{b} \mid \rho) \geq 0 \iff \langle \underline{b} | \rho | \underline{b} \rangle \geq 0$$

$$\sum_{\underline{b} \in \{0,1\}^n} \mathbb{P}(\underline{b} \mid \rho) = 1 \iff \mathrm{Tr}(\rho) = \sum \langle \underline{b} | \rho | \underline{b} \rangle = 1$$

Mixed State Quantum Mechanics

Density matrices:

$$\rho \in \mathbb{C}^{2^n \times 2^n}$$

(i) self-adjoint: $\rho^\dagger = \rho$

(ii) positive: $\langle \varphi | \rho | \varphi \rangle \geq 0 \quad \forall |\varphi\rangle \in \mathbb{C}^{2^n}$

(iii) normalised: $\mathrm{Tr}(\rho) = 1$

Mixed State Quantum Mechanics

Density matrices from statevectors:

$$|\psi\rangle\langle\psi| \in \mathbb{C}^{2^n \times 2^n}$$

(i) self-adjoint: $(|\psi\rangle\langle\psi|)^\dagger = |\psi\rangle\langle\psi|$ ✓

(ii) positive: $\langle\varphi|\psi\rangle\langle\psi|\varphi\rangle = |\langle\varphi|\psi\rangle|^2 \geq 0$ ✓

(iii) normalised: $\mathrm{Tr}(|\psi\rangle\langle\psi|) = \langle\psi|\psi\rangle = 1$ ✓

Mixed State Quantum Mechanics

Unitary transformations extend to density matrices:

$$|\psi\rangle \in \mathbb{C}^{2^n} \longmapsto U|\psi\rangle \in \mathbb{C}^{2^n}$$

$$|\psi\rangle\langle\psi| \in \mathbb{C}^{2^n \times 2^n} \longmapsto U|\psi\rangle\langle\psi|U^\dagger \in \mathbb{C}^{2^n \times 2^n}$$

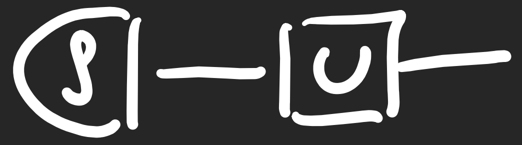
$$\rho \in \mathbb{C}^{2^n \times 2^n} \longmapsto U\rho U^\dagger \in \mathbb{C}^{2^n \times 2^n}$$

Graphical Formalism

$\rho \in \mathbb{C}^{2\times 2}$ $\longleftrightarrow$

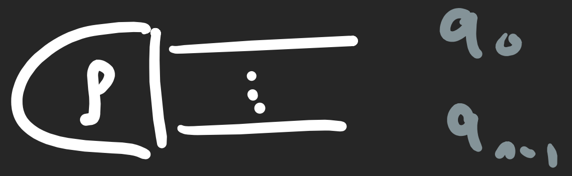
self-adjoint
positive

$U \rho U^\dagger$ $\longleftrightarrow$



Graphical Formalism

$\rho \in \mathbb{C}^{2^n \times 2^n}$ $\longleftrightarrow$



self-adjoint
positive

$U \rho U^\dagger$ $\longleftrightarrow$

Graphical Formalism

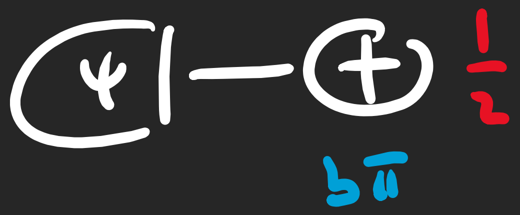
Nothing changed in the graphical formalism: secretly, we were already using density matrices!

$\cancel{|\psi\rangle} \rightarrow |\psi\rangle\langle\psi|$ $\longleftrightarrow$ 

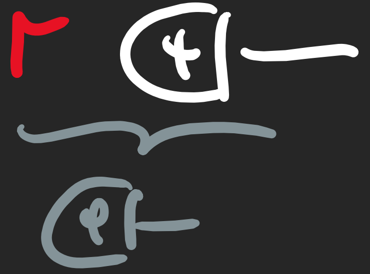
$\cancel{U|\psi\rangle} \rightarrow U|\psi\rangle\langle\psi|U^\dagger$ $\longleftrightarrow$ 

Graphical Formalism

To a trained eye, our convention for numbers would have immediately given the game away:



$\longleftrightarrow \quad |\langle b|\psi\rangle|^2 = \mathrm{Tr}(|b\rangle\langle b|\psi\rangle\langle\psi|)$



$\longleftrightarrow \quad r|\psi\rangle\langle\psi| = \underbrace{(\sqrt{r}|\psi\rangle)}_{|\varphi\rangle}(\langle\psi|\sqrt{r})$

Mixed State Quantum Mechanics

Uncertainty = Convex combination

States $(\rho_k)_{k\in K}$
Probabilities $(q_k)_{k\in K}$

$q_k \in [0,1]$

$\sum_k q_k = 1$

$\Rightarrow$ uncertain state:

$$\rho = \sum_{k\in K} q_k \rho_k$$

Mixed State Quantum Mechanics

50% $|0\rangle$, 50% $|1\rangle$

$$\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Note that this sum is <u>**NOT**</u> that of state vectors:

$$\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle = |+\rangle \qquad |+\rangle\langle +| = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \neq \rho$$

(non-zero off-diagonal coefficients)

Graphical Formalism

We introduce sums of diagrams to model uncertainty:

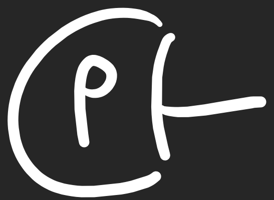
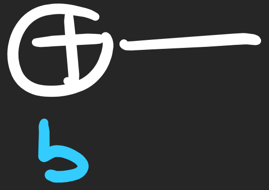
probabilities

diagrams corresponding to each case

$$\sum_{k} p_k$$

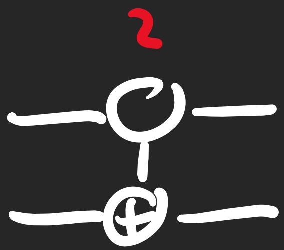
possible cases

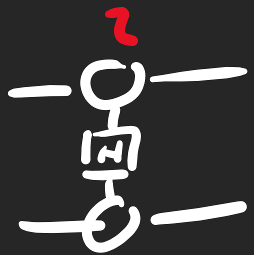
Graphical Formalism

 $:=$ $\sum_{b\in\{0,1\}} \frac{1}{2}$ 

Parametrised

$50\%\ |0\rangle\ ,\ 50\%\ |1\rangle$

$:=$ $\frac{3}{4}$ 

$+\ \frac{1}{4}$ 

Explicit

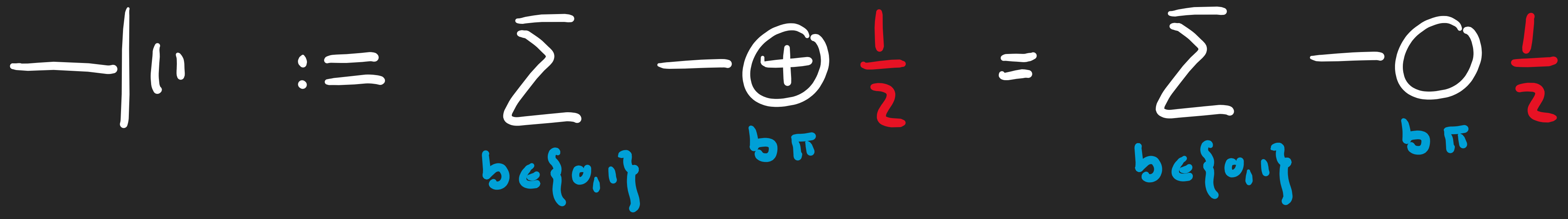
$75\%\ CX\ ,\ 25\%\ CZ$

Graphical Formalism

$$\sum_k \sqrt{p_k}\, |\psi_k\rangle \quad \longleftrightarrow \quad \sum_k p_k$$ 

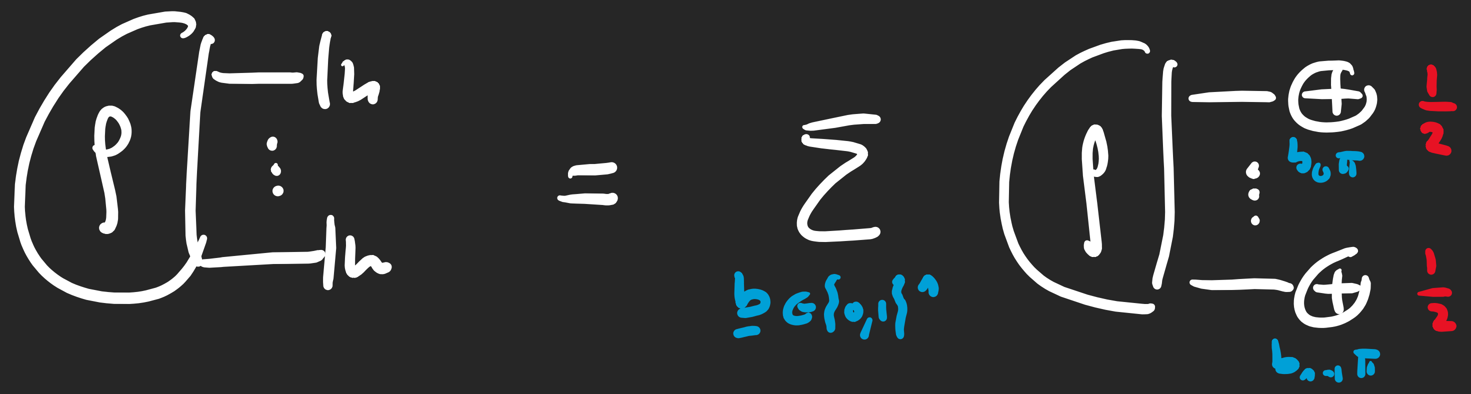
$$\sum_k p_k\, |\psi_k\rangle\langle\psi_k| \quad \longleftrightarrow \quad \sum_k p_k$$ 

The Discarding Map



the electrical ground symbol indicates the discarding map

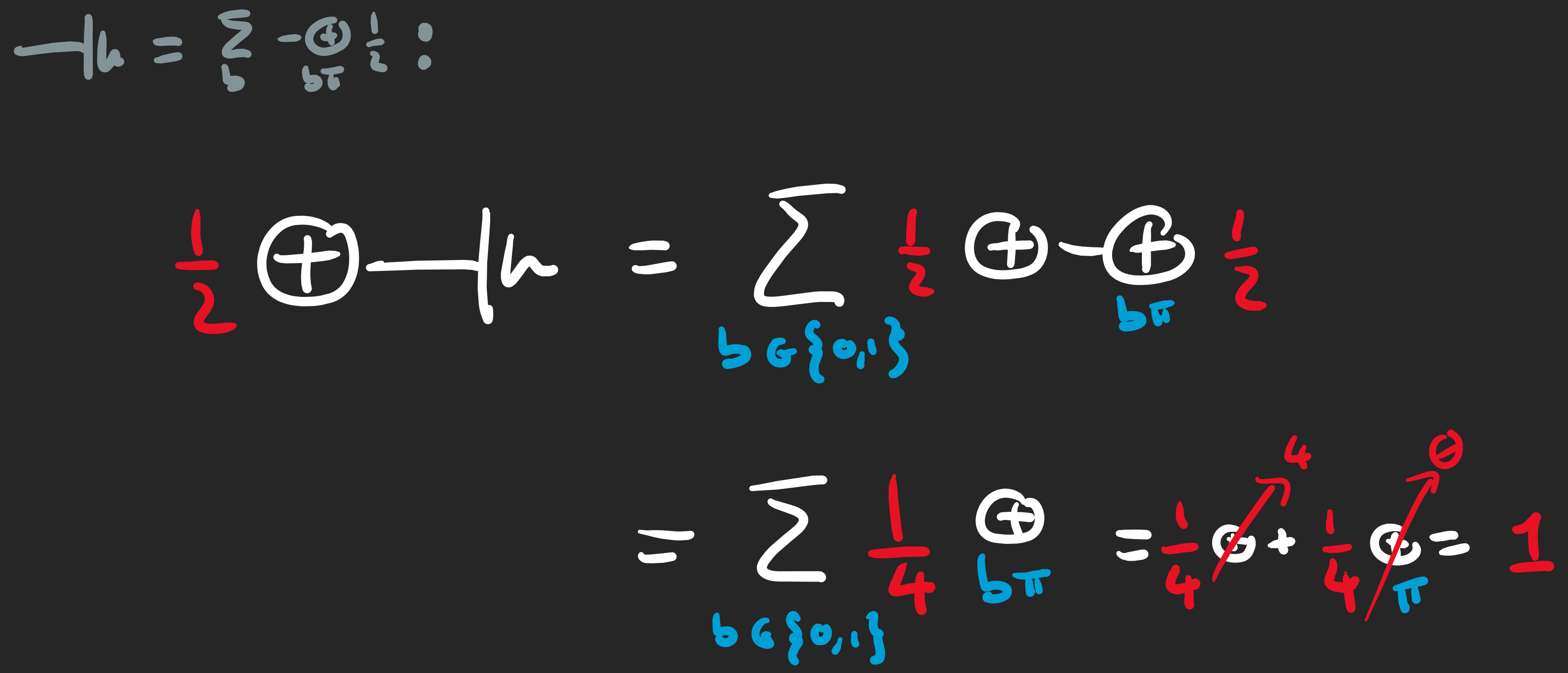
The Discarding Map



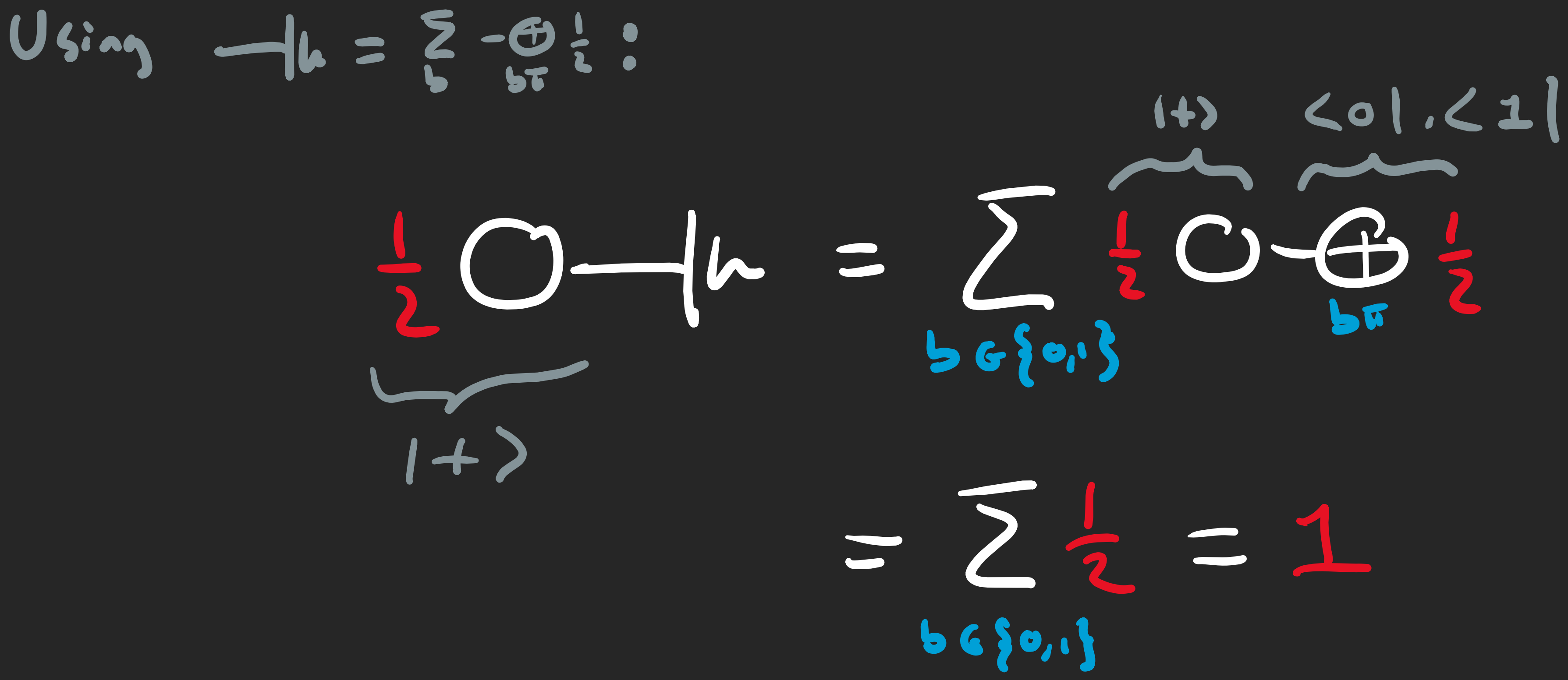
$$= \sum_{\underline{b} \in \{0,1\}^n} \langle \underline{b} | \rho | \underline{b} \rangle = \mathrm{Tr}(\rho)$$

The Discarding Map

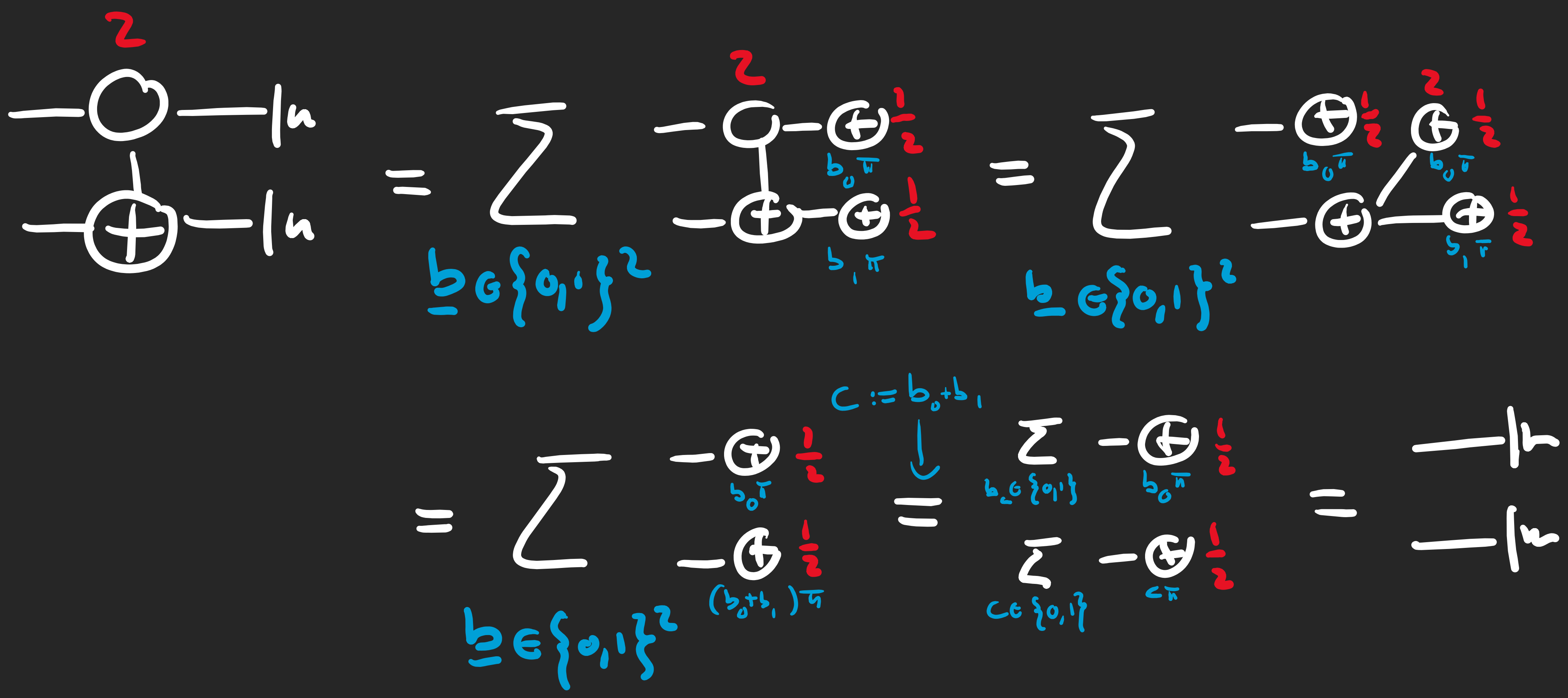
Using



The Discarding Map



The Discarding Map



The Discarding Map

* Trace is cyclic:

$$\mathrm{Tr}(ABC) = \mathrm{Tr}(CAB) = \mathrm{Tr}(BCA)$$

$$= \mathrm{Tr}(U\rho U^\dagger)$$

$$\overset{*}{=} \mathrm{Tr}(U^\dagger U \rho)$$

$$= \mathrm{Tr}(\rho) =$$

U unitary $\Rightarrow U^\dagger U = I$

The Discarding Map

$$= \mathrm{Tr}(U \boxtimes U^\dagger)$$

$$= \mathrm{Tr}(U^\dagger U \boxtimes)$$

$$= \mathrm{Tr}(\boxtimes) =$$

* more entanglement $\Leftrightarrow$ more uncertainty

The Maximally Mixed State

(Entanglement $\Rightarrow$ Correlation)

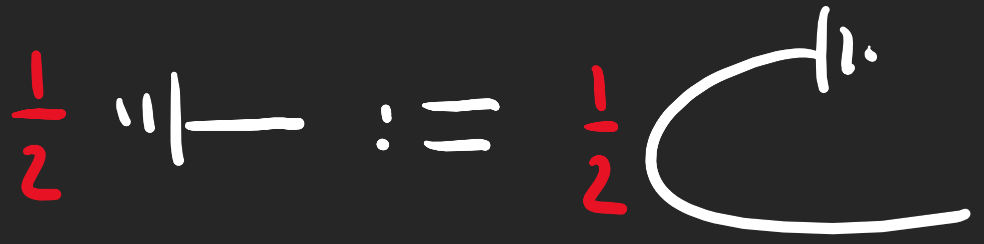
$\Rightarrow$ (Part of an entangled state not available $\Rightarrow$ Other parts of the state are uncertain*)

qubit q_0 not available

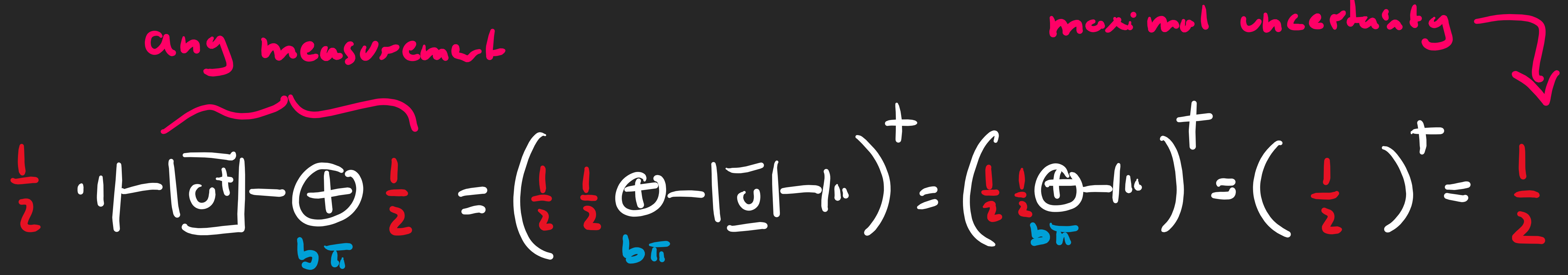
qubit q_1 is uncertain:

$\begin{cases} 50\% & |0\rangle \\ 50\% & |1\rangle \end{cases}$

The Maximally Mixed State

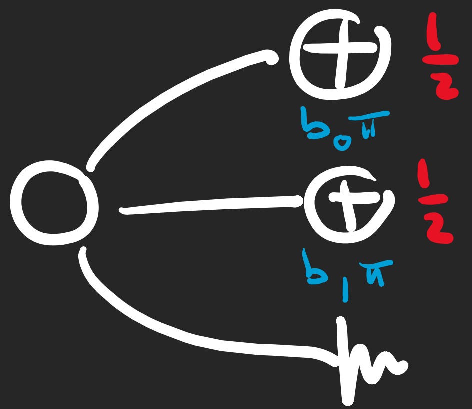


Maximally mixed state



Partial Measurements

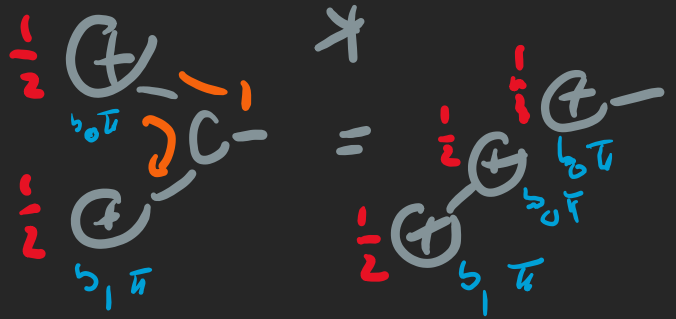
Not all qubits measured $\Rightarrow$ Discard unmeasured qubits to compute probabilities

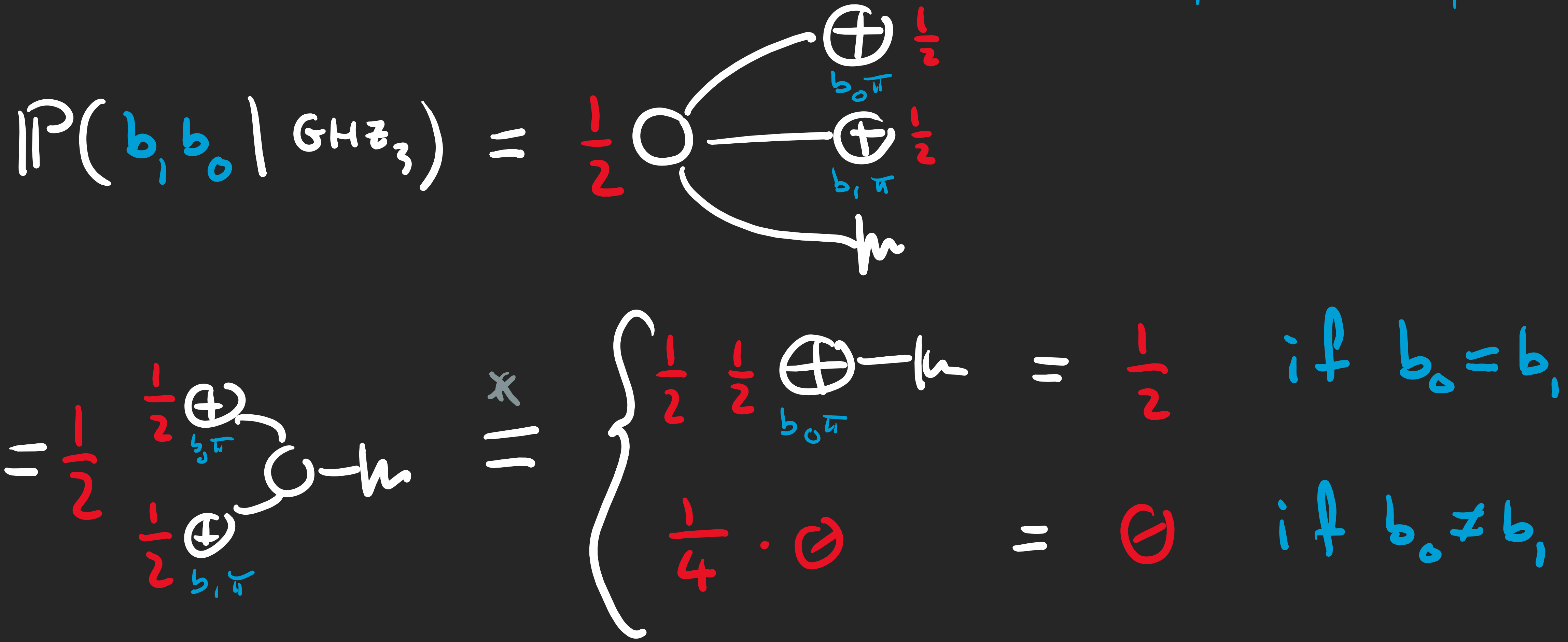
$\mathbb{P}(b_1 b_0 \mid GHZ_3) = \frac{1}{2}$ 

qubits 1 and 2 measured

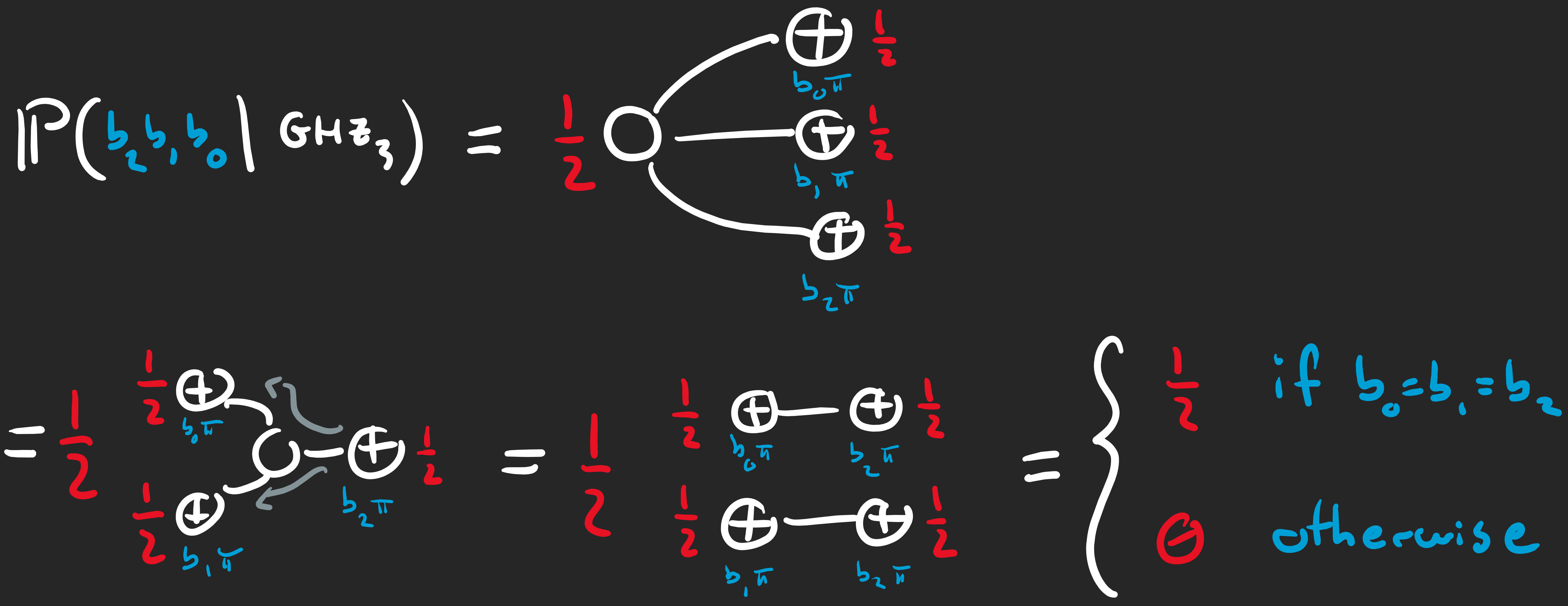
qubit 3 not measured

Partial Measurements



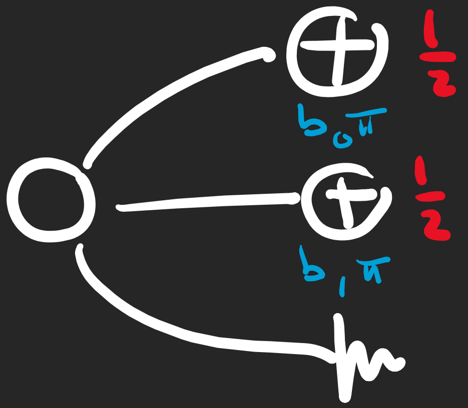


Partial Measurements



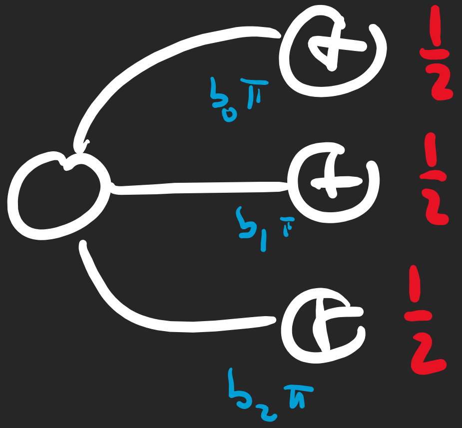
Partial Measurements

$$\mathbb{P}(b_1 b_0 \mid GHZ_3) = \frac{1}{2}$$



marginalisation of probability distribution!

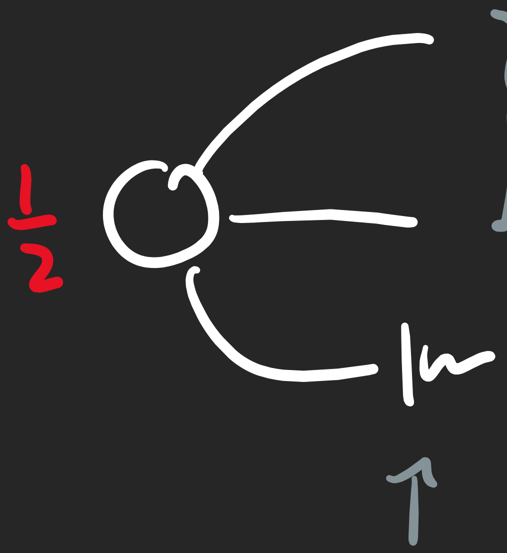
$$= \sum_{b_2 \in \{0,1\}} \frac{1}{2}$$



$$= \sum_{b_2 \in \{0,1\}} P(b_2 b_1 b_0 \mid GHZ_3)$$

Marginal/Conditional States

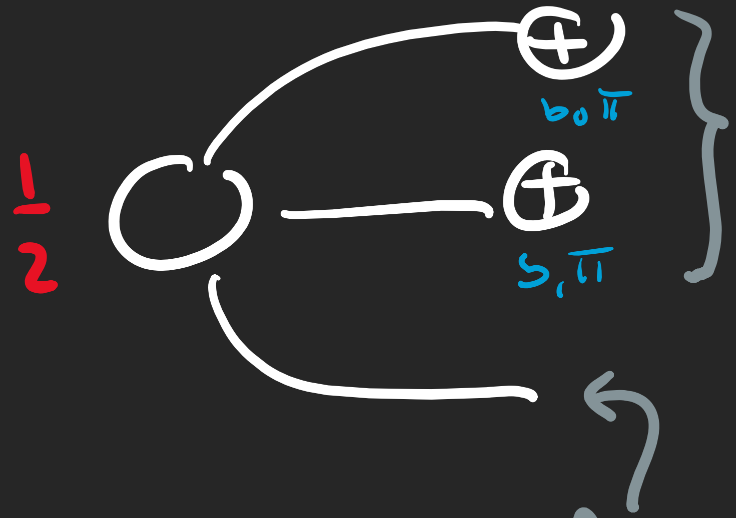
Marginal State



State of qubits q_0, q_1

qubit q_2 unavailable or disregarded

Conditional State



qubits q_0, q_1 measured with outcomes $b_1 b_0$

State of qubit 3

Marginal States

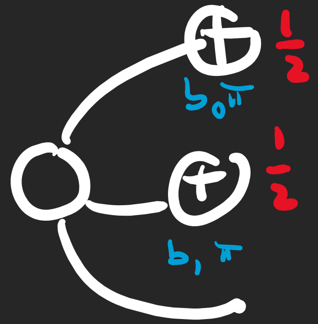
Marginal State = Uncertainty

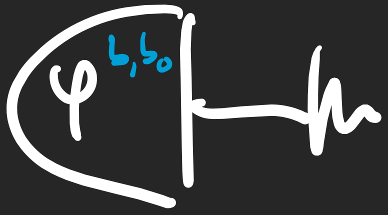
Always normalised:

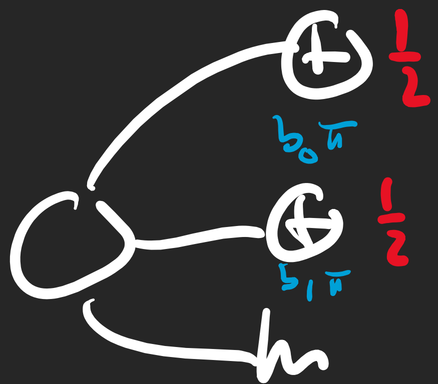
Conditional States

Conditional state = State when a given outcome is observed

Norm of conditional state = probability

$:= \frac{1}{2}$


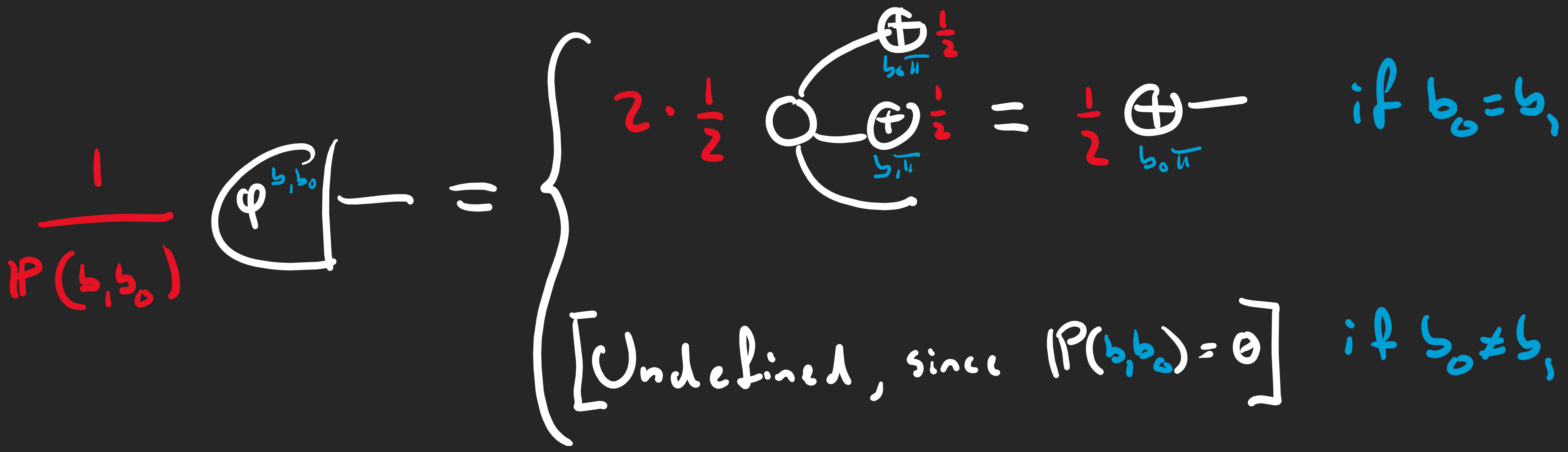
$\Rightarrow$


$= \frac{1}{2}$


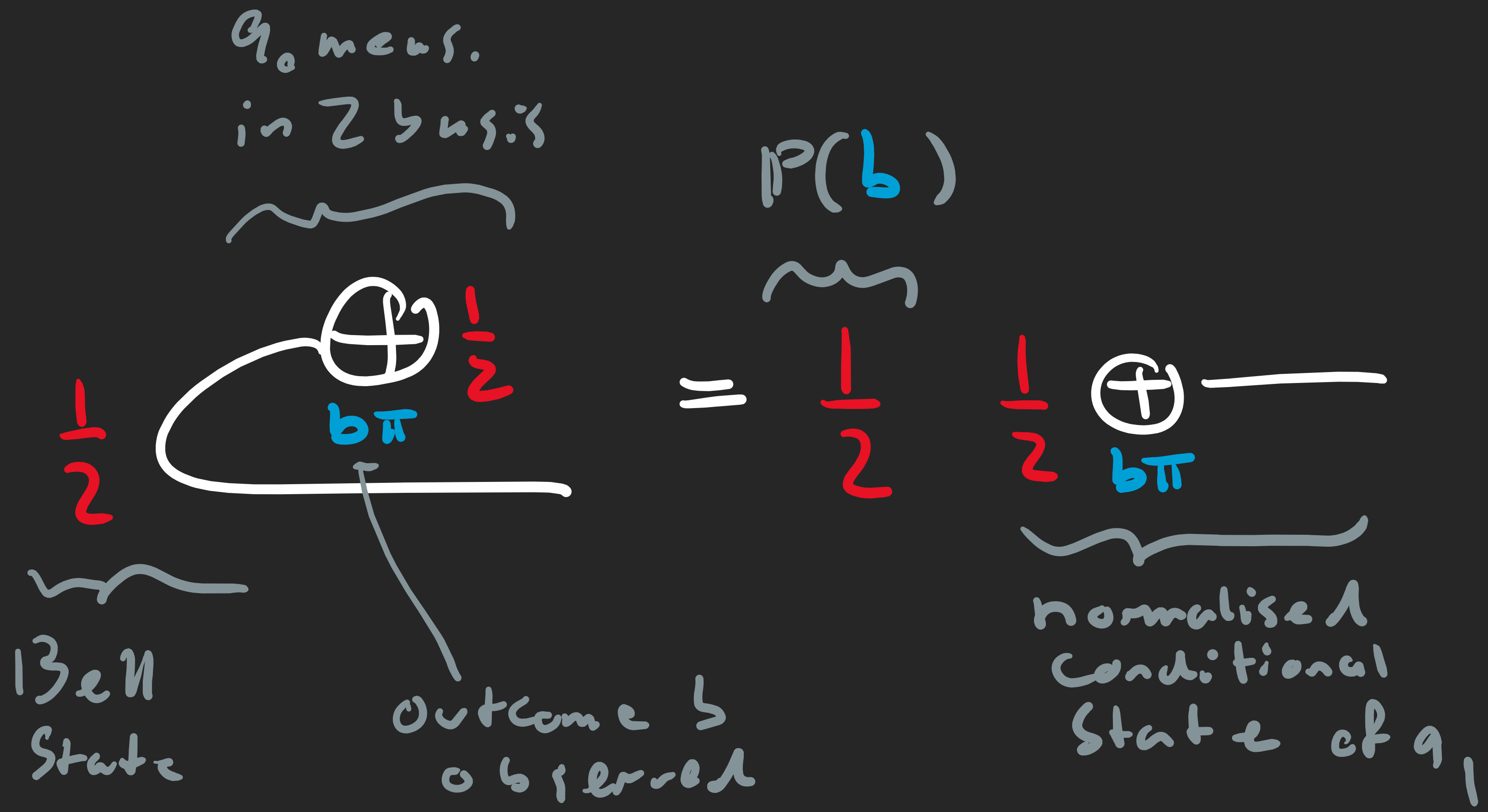
$= \mathbb{P}(b_1 b_0 \mid GHZ_3)$

Conditional States

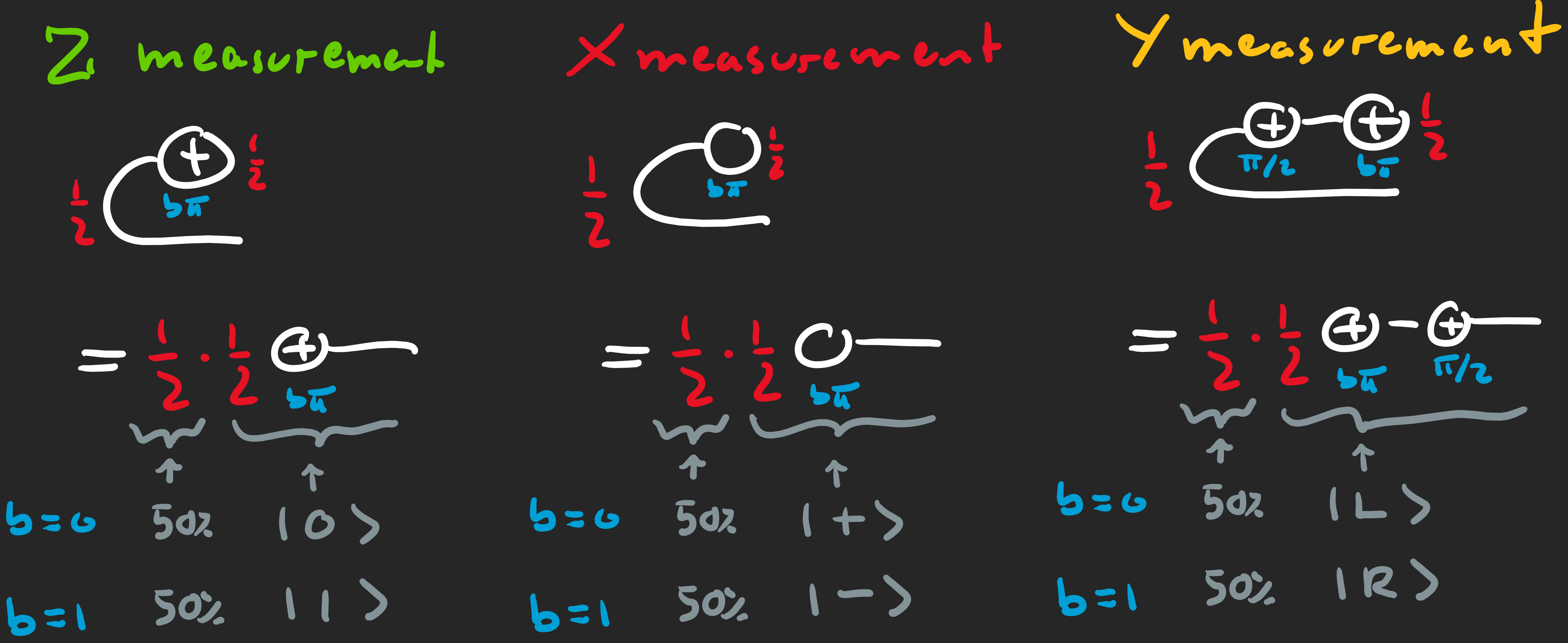
Must renormalise before further use:



Conditional States



Conditional States

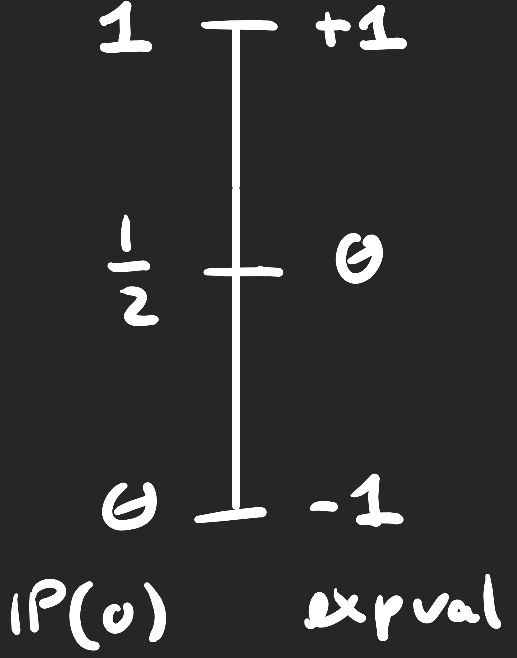


Tomography

(Because outcomes are binary, considering expectation values is lossless.)

Instead of measurement outcome probabilities, we now consider <u>Expectation Values</u>:

$$
\begin{aligned}
\text{expval} &:= \mathbb{P}(0) - \mathbb{P}(1) \\
&= 2\mathbb{P}(0) - 1 \\
&= 1 - 2\mathbb{P}(1)
\end{aligned}
$$



Tomography

$\Pi \in \{X, Y, Z\} \implies$ measure q in Π

$$\langle \Pi \rangle_\rho := \mathbb{P}(0 \mid \rho, \Pi) - \mathbb{P}(1 \mid \rho, \Pi)$$

where $\mathbb{P}(b \mid \rho, \Pi) =$ probability of outcome b measuring ρ in Π basis.

Tomography

$$\Pi \in \{X, Y, Z\} \implies \text{measure } q \text{ in } \Pi$$

if $\rho = |\psi\rangle\langle\psi|$

$$\langle \Pi \rangle_\rho = \mathrm{Tr}(\Pi \rho) = \langle \psi | \Pi | \psi \rangle$$

$$X := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad Y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad Z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Tomography

Inner product : $(A, B) := \frac{1}{2}\mathrm{Tr}(A, B) \in \mathbb{R}$

e.g. $\begin{cases} (X, X) = \frac{1}{2}\mathrm{Tr}(XX) = \frac{1}{2}\mathrm{Tr}(I) = 1 \\ (X, Y) = \frac{1}{2}\mathrm{Tr}(iZ) = 0 \end{cases}$

$\{I, X, Y, Z\}$ form an orthonormal basis for the $\mathbb{R}$-vector space of self-adjoint matrices $A \in \mathbb{C}^{2\times 2}$:

$$A = \sum_{\Pi \in \{I, X, Y, Z\}} \frac{1}{2}\mathrm{Tr}(\Pi A) \cdot \Pi$$

Tomography

$\rho \in \mathbb{C}^{2\times 2}$ density matrix

self-adjoint matrix in $\mathbb{C}^{2\times 2}$

$$\rho = \sum_{\sigma \in \{I, X, Y, Z\}} \frac{1}{2} \underbrace{\mathrm{Tr}(\sigma \rho)}_{\text{expectation value in } [-1,+1]} \cdot \sigma$$

Note: $\mathrm{Tr}(I\rho) = \mathrm{Tr}(\rho) = 1$

Tomography

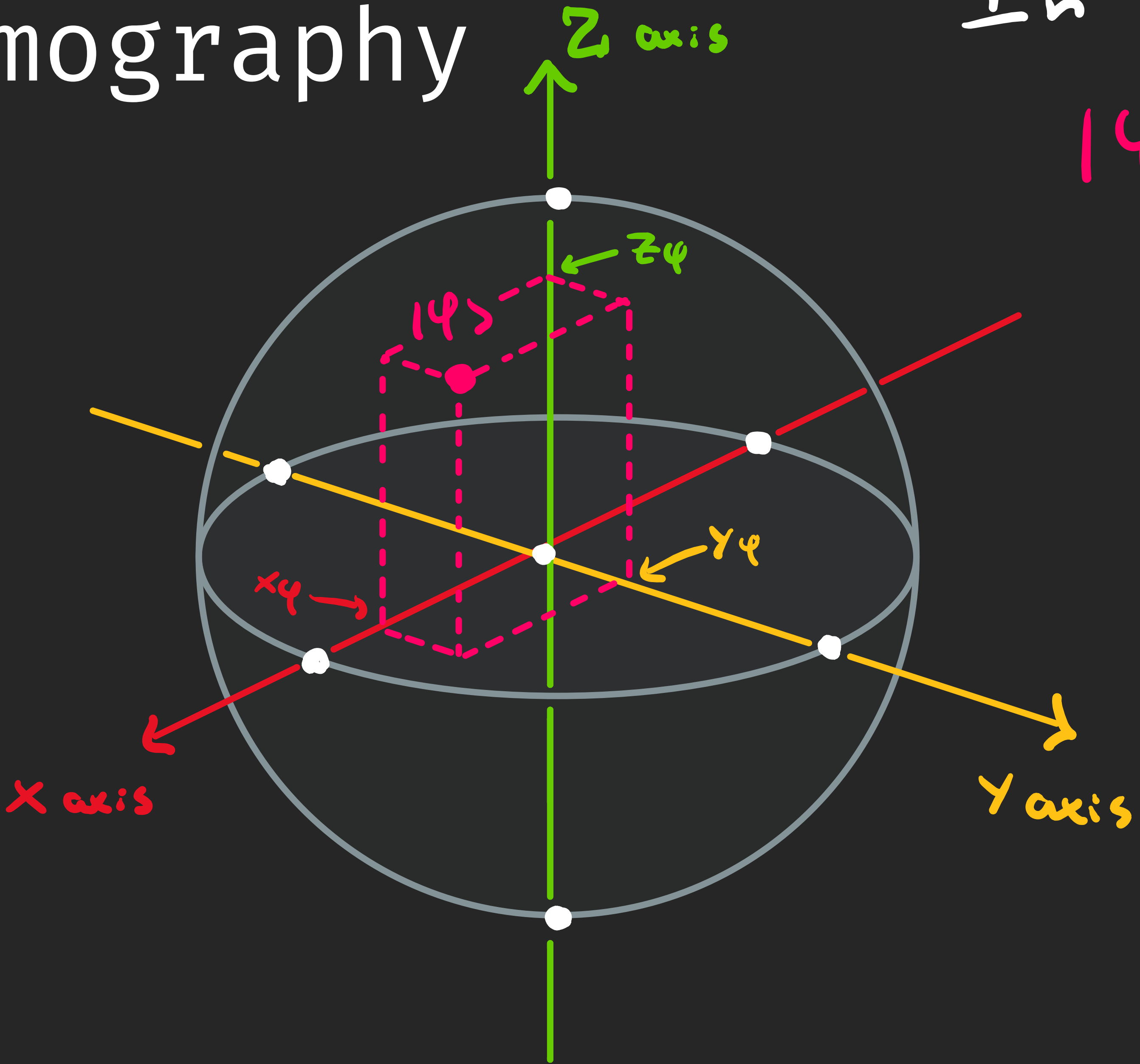
$\rho \in \mathbb{C}^{2\times 2}$ density matrix

self-adjoint matrix in $\mathbb{C}^{2\times 2}$

$$\rho = \sum_{M \in \{I, X, Y, Z\}} \frac{1}{2} \underbrace{\mathrm{Tr}(M\rho)}_{} \cdot M$$

expectation value in [-1, +1]

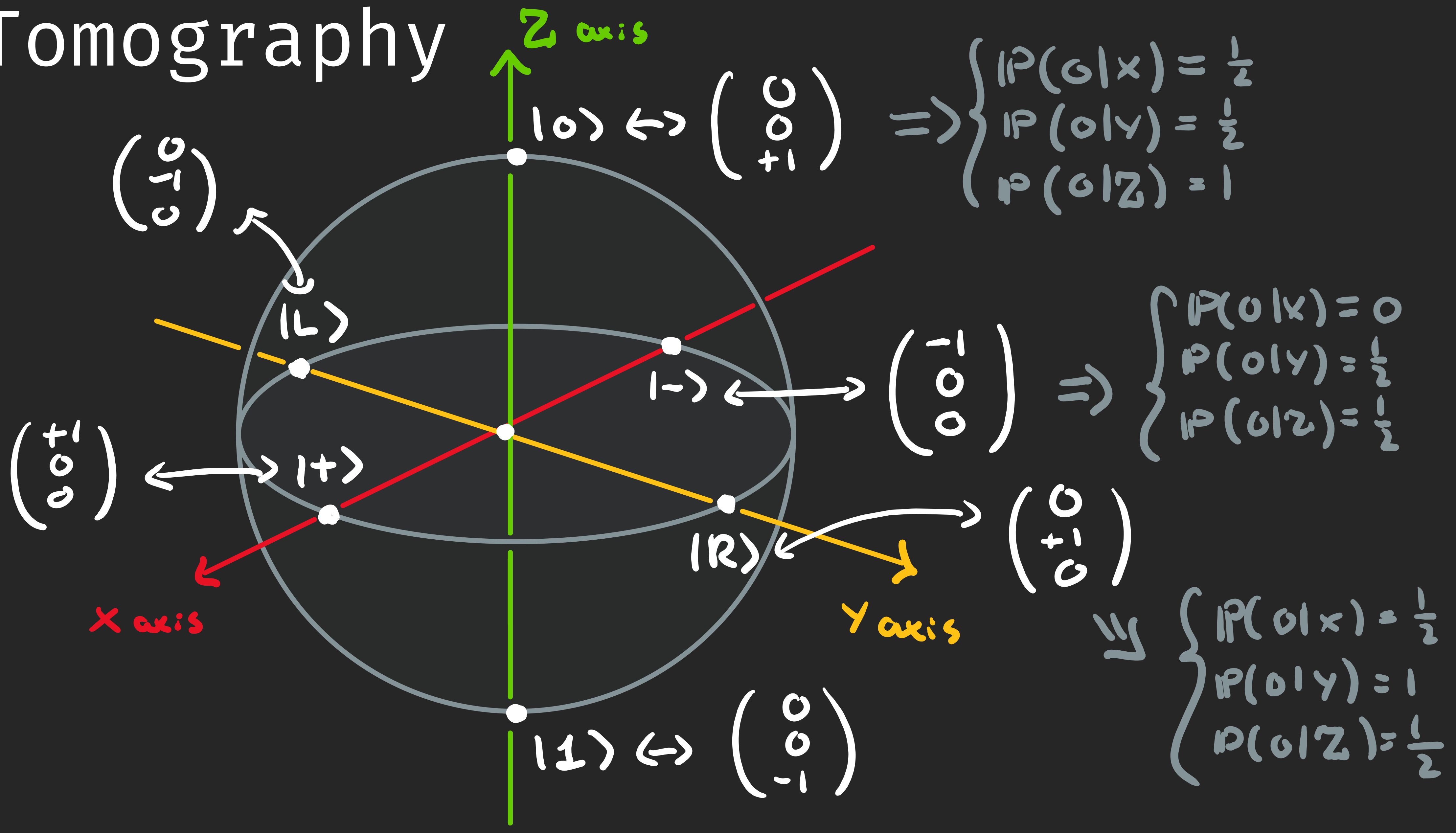
Tomography



In Cartesian coordinates:

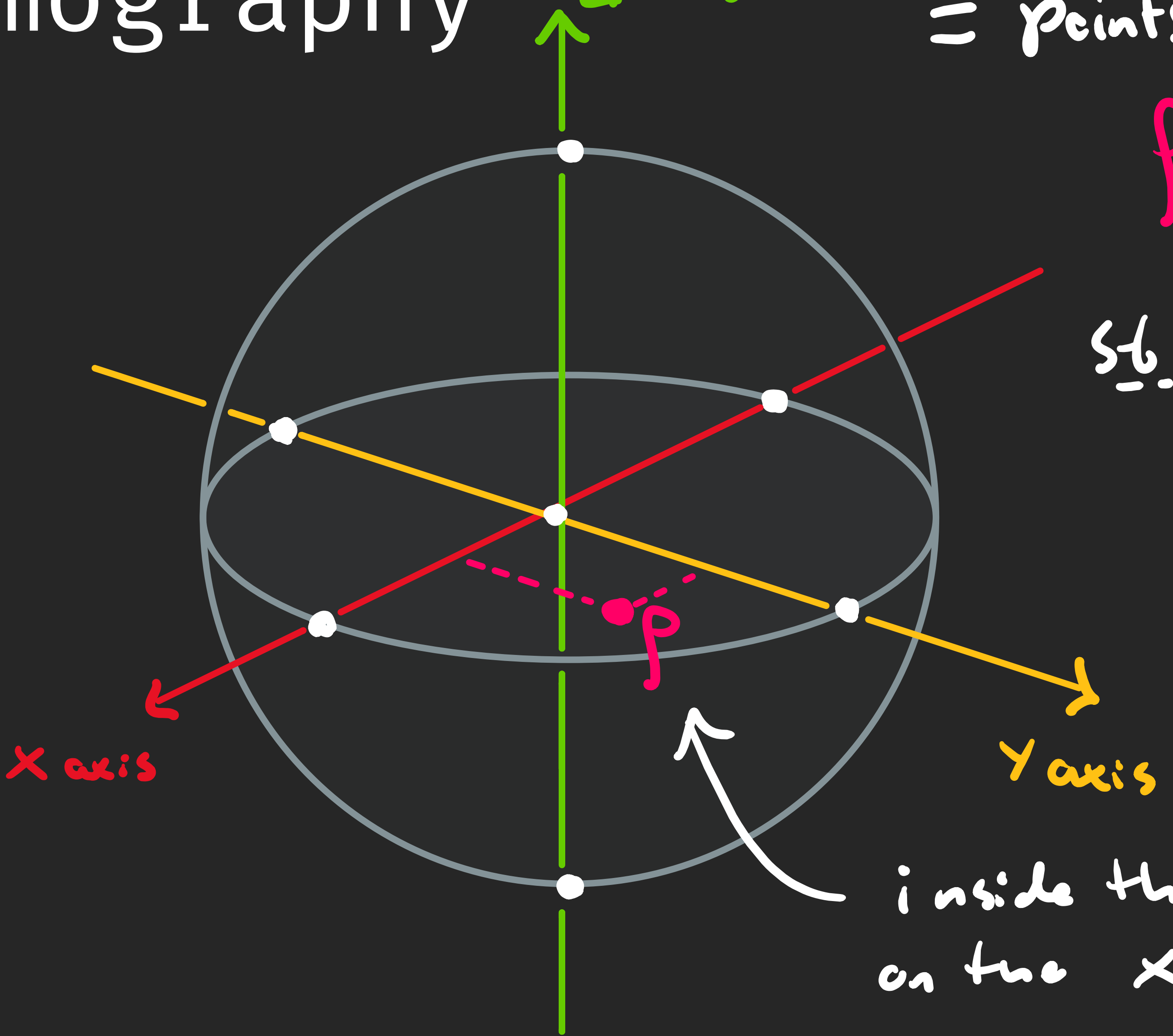
$$|\psi\rangle \longleftrightarrow \begin{pmatrix} x_\psi \\ y_\psi \\ z_\psi \end{pmatrix} = \begin{pmatrix} X \text{ expval on } |\psi\rangle \\ Y \text{ expval on } |\psi\rangle \\ Z \text{ expval on } |\psi\rangle \end{pmatrix}$$

Tomography



Z axis
X axis
Y axis
|0⟩ ↔ $\begin{pmatrix}0\\0\\+1\end{pmatrix}$
$\Rightarrow \begin{cases} \mathbb{P}(0|x) = \frac{1}{2} \\ \mathbb{P}(0|y) = \frac{1}{2} \\ \mathbb{P}(0|Z) = 1 \end{cases}$
$\begin{pmatrix}0\\-1\\0\end{pmatrix}$
|L⟩
|−⟩ ↔ $\begin{pmatrix}-1\\0\\0\end{pmatrix}$
$\Rightarrow \begin{cases} \mathbb{P}(0|x) = 0 \\ \mathbb{P}(0|y) = \frac{1}{2} \\ \mathbb{P}(0|Z) = \frac{1}{2} \end{cases}$
$\begin{pmatrix}+1\\0\\0\end{pmatrix}$ ↔ |+⟩
|R⟩ ↔ $\begin{pmatrix}0\\+1\\0\end{pmatrix}$
$\Rightarrow \begin{cases} \mathbb{P}(0|x) = \frac{1}{2} \\ \mathbb{P}(0|y) = 1 \\ \mathbb{P}(0|Z) = \frac{1}{2} \end{cases}$
|1⟩ ↔ $\begin{pmatrix}0\\0\\-1\end{pmatrix}$

Tomography



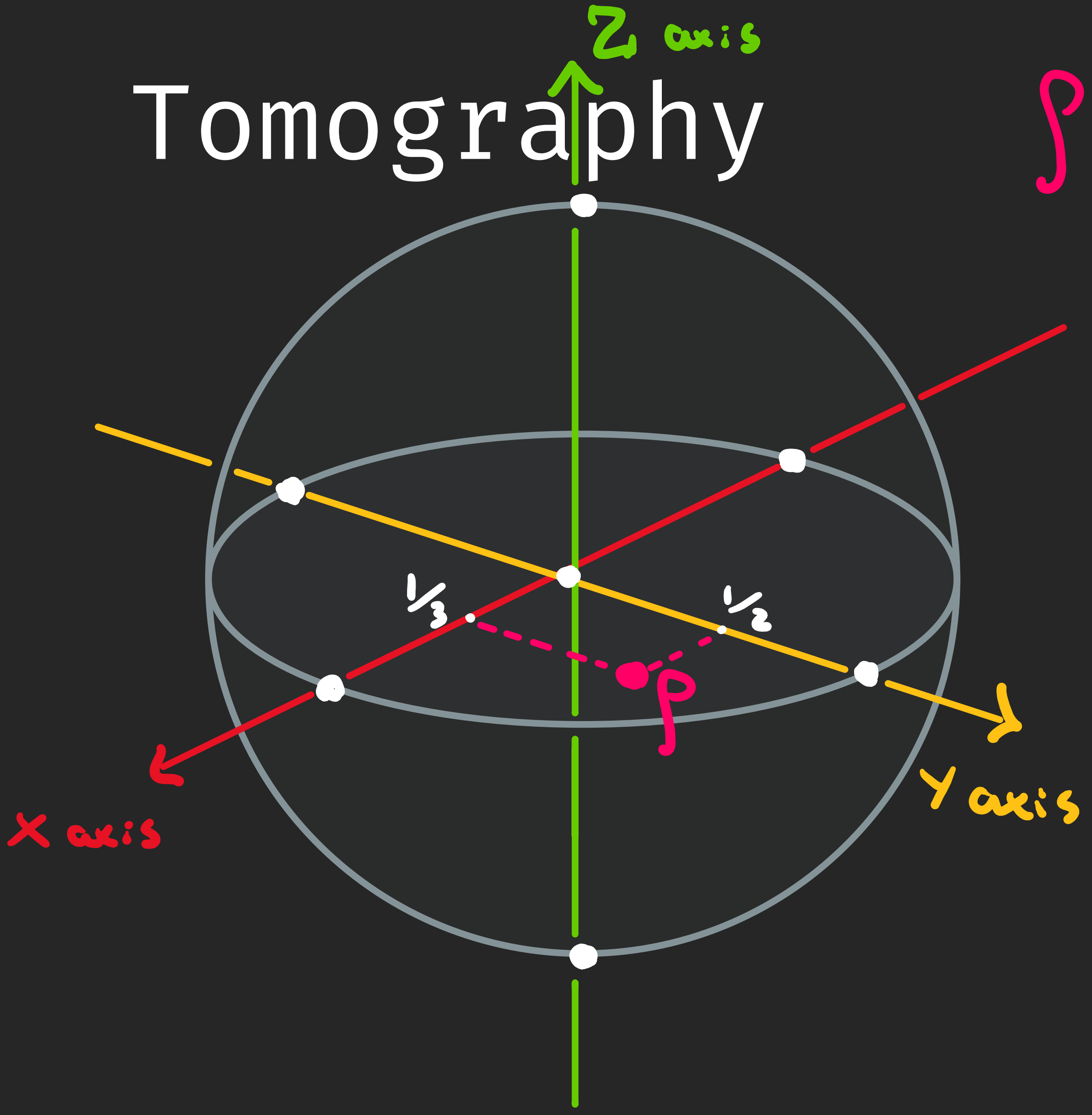
inside the ball, on the XY plane

Mixed states = points in the Bloch Ball

$$\rho \longleftrightarrow \begin{pmatrix} x_\rho \\ y_\rho \\ z_\rho \end{pmatrix}$$

s.t. $\underbrace{x_\rho^2 + y_\rho^2 + z_\rho^2 \leq 1}$

Tomography



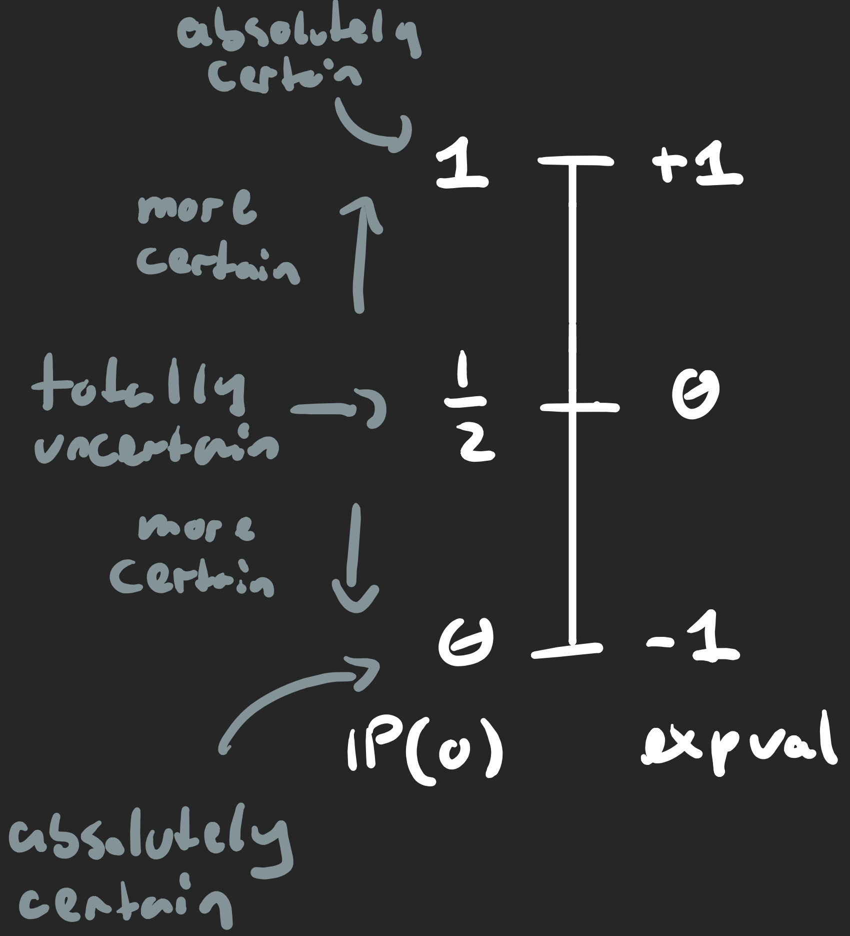
$$\rho = \frac{1}{2}\Big[\, \mathrm{Tr}(I\rho)\, I + \mathrm{Tr}(X\rho)\, X + \mathrm{Tr}(Y\rho)\, Y + \mathrm{Tr}(Z\rho)\, Z \,\Big]$$

$$= \frac{1}{2}\Big[\, \overset{1}{\cancel{\mathrm{Tr}(I\rho)}}\, I + \overset{1/3}{\cancel{\mathrm{Tr}(X\rho)}}\, X + \underset{1/2}{\cancel{\mathrm{Tr}(Y\rho)}}\, Y + \underset{0}{\cancel{\mathrm{Tr}(Z\rho)}}\, Z \,\Big]$$

$$= \frac{1}{2}\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{3}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + 0\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right]$$

$$= \begin{pmatrix} 1/2 & 1/6 - 1/4\, i \\ 1/6 + 1/4\, i & 1/2 \end{pmatrix}$$

Uncertainty Principle



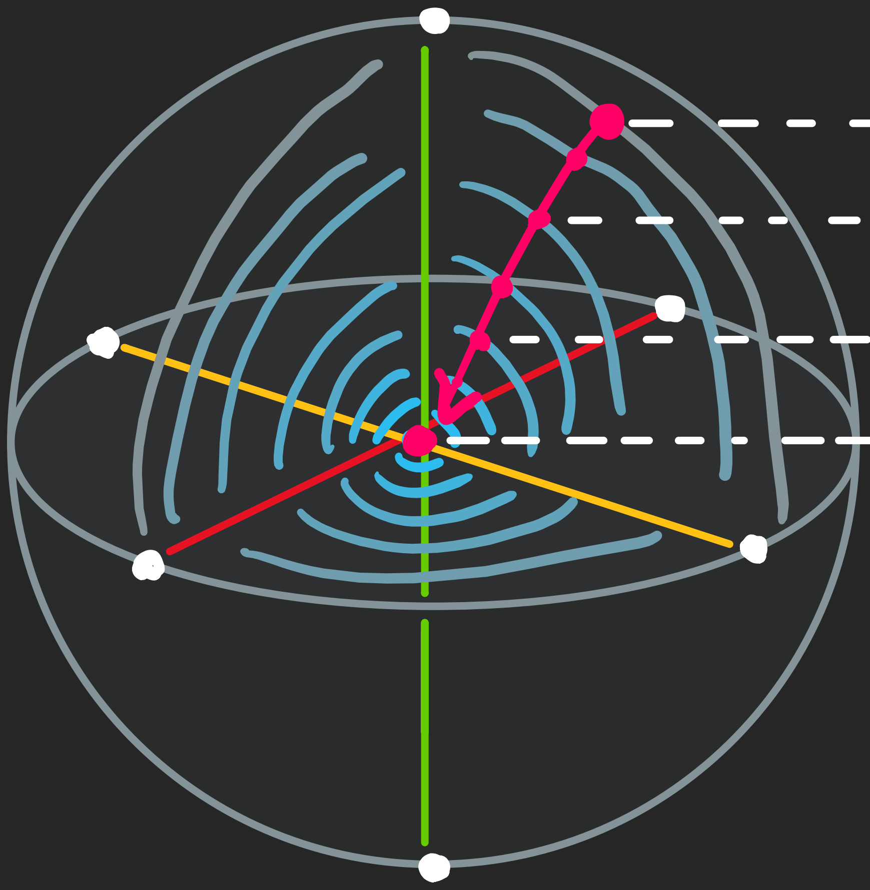
Larger |expval| $\Rightarrow$ more certainty

$$|X \text{ expval}|^2 + |Y \text{ expval}|^2 + |Z \text{ expval}|^2 \leq 1$$

More certainty in one measurement

$\Rightarrow$ less certainty in the others!

Tomography



surface = $\overbrace{\text{pure states}}^{\text{no uncertainty}}$

$\downarrow$ increasing uncertainty / mixedness

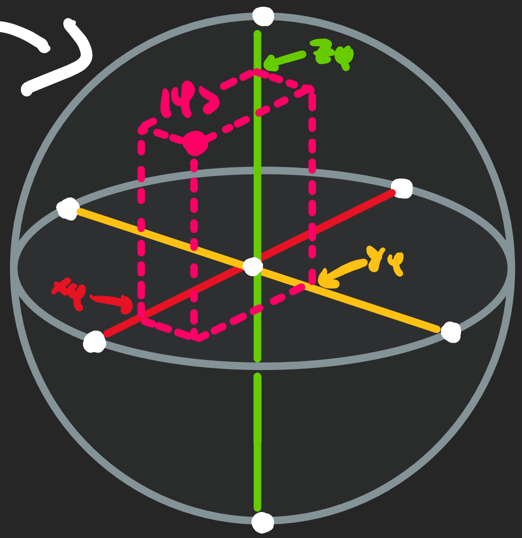
center = maximally mixed state

$$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{cases} \mathbb{P}(0|x) = \mathbb{P}(1|x) = \frac{1}{2} \\ \mathbb{P}(0|y) = \mathbb{P}(1|y) = \frac{1}{2} \\ \mathbb{P}(0|z) = \mathbb{P}(1|z) = \frac{1}{2} \end{cases}$$

Tomography

3 measurements are enough to identify a 1-qubit state:

$$\begin{array}{llll} X \text{ meas} & \longrightarrow & X \text{ exp val} & \longrightarrow \\ Y \text{ meas} & \longrightarrow & Y \text{ exp val} & \longrightarrow \\ Z \text{ meas} & \longrightarrow & Z \text{ exp val} & \longrightarrow \end{array} \begin{pmatrix} x_\psi \\ y_\psi \\ z_\psi \end{pmatrix}$$



Pauli Measurements

Indexed right-to-left: $P_{n-1} \cdots P_1 P_0$

"Pauli string" $\underline{P} \in \{I, X, Y, Z\}^n$

<u>Pauli measurement</u> $\longleftrightarrow$ "Pauli string"

$P_j \in \{X, Y, Z\} \Rightarrow$ measure q_j in P_j

$P_j = I \Rightarrow$ don't measure q_j

(outcome 0 100% by default)

Tomography

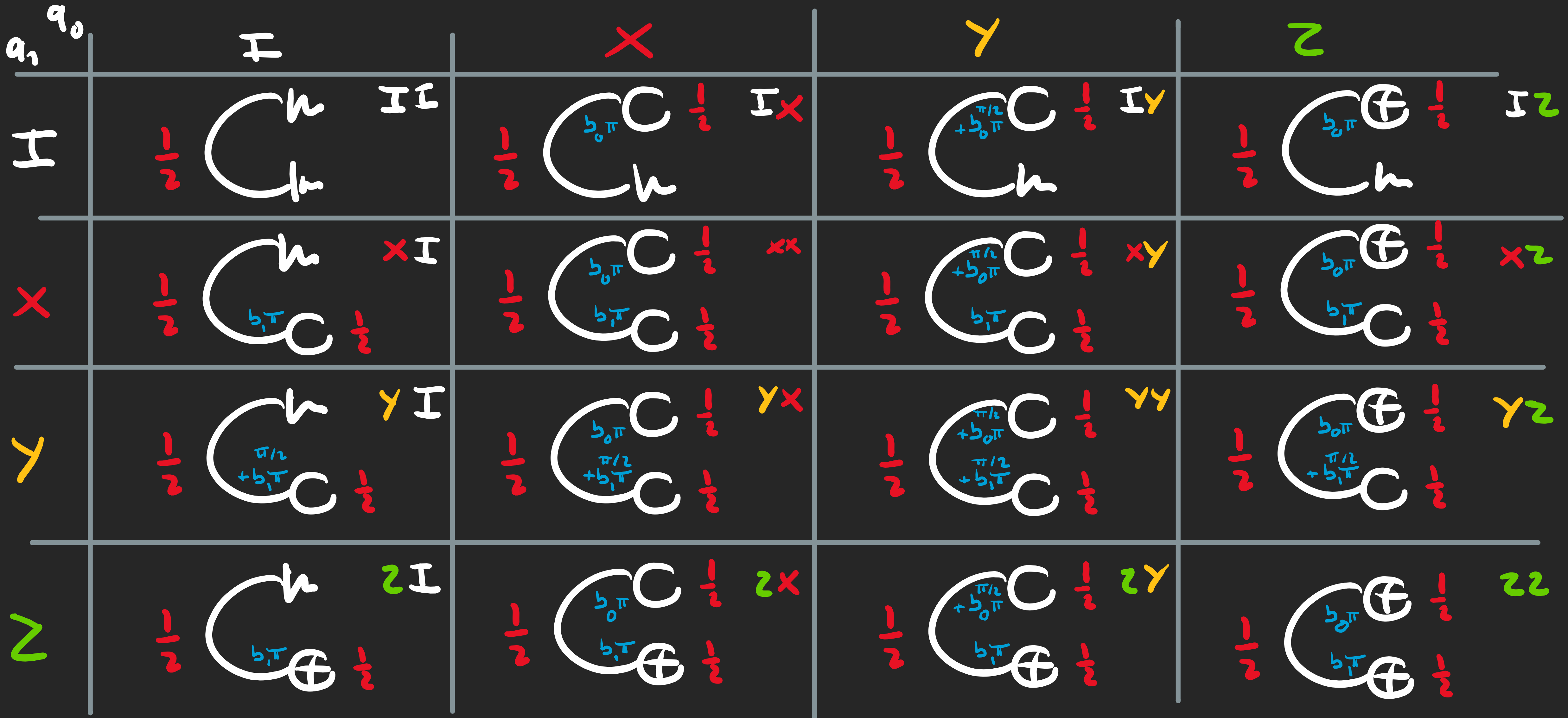
$$\rho \in \mathbb{C}^{2^n \times 2^n} \quad \text{density matrix}$$

$$\rho = \sum_{\underline{P} \in \{I, X, Y, Z\}^n} \frac{1}{2^n} \underbrace{\mathrm{Tr}\left[\bigotimes_{i=0}^{n-1} P_i \, \rho\right]}_{\text{expectation value in } [-1,+1]} \overbrace{\bigotimes_{i=0}^{n-1} P_i}^{\text{self-adjoint matrix in } \mathbb{C}^{2\times 2}}$$

$$\bigotimes_{i=0}^{n-1} P_i := P_{n-1} \otimes \dots \otimes P_0 \in \mathbb{C}^{2^n \times 2^n}$$

Pauli Measurements

Bell state $\frac{1}{2}$



b_j = outcome of Π_j on qubit q_j

Tomography

Define the expectation value for a Pauli measurement:

$$\text{expval}(\Pi) := \mathbb{P}(b_1 \oplus \ldots \oplus b_n = 0) - \mathbb{P}(b_1 \oplus \ldots \oplus b_n = 1)$$

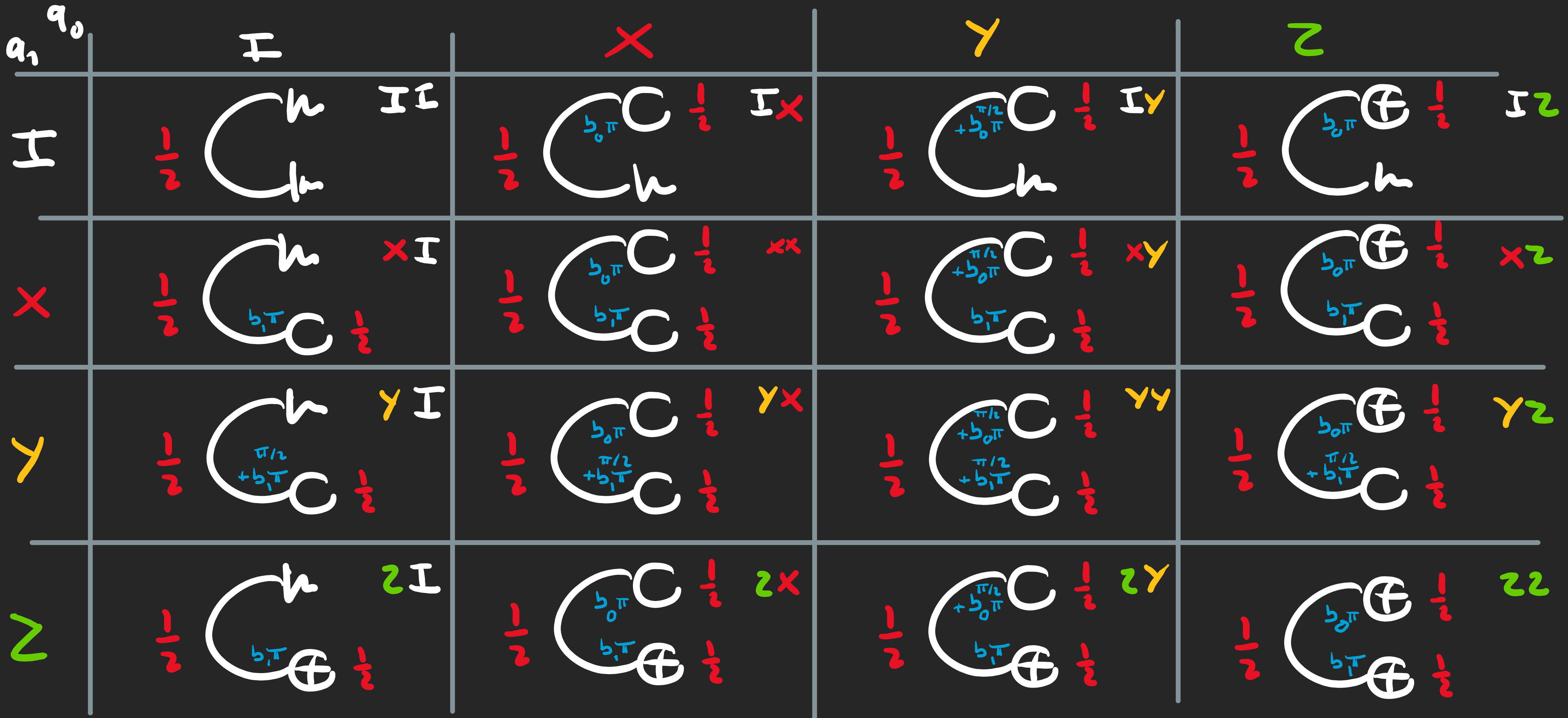
skip $I \ldots I$
($b_j = 0$ always)

To identify a generic n-qubit state:

1. perform the $4^n - 1$ non-trivial Pauli measurements
2. compute expectation values from outcom distribution

Pauli Measurements

Bell state $\frac{1}{2}$



Tomography

q_1 \ q_0	I	X	Y	Z
I	//	$\mathbb{P}(b_0) = \frac{1}{2}$	$\mathbb{P}(b_0) = \frac{1}{2}$	$\mathbb{P}(b_0) = \frac{1}{2}$
X	$\mathbb{P}(b_1) = \frac{1}{2}$	$\mathbb{P}(b_1 b_0) = \begin{cases} \frac{1}{2} & b_0 = b_1 \\ 0 & b_0 \neq b_1 \end{cases}$	$\mathbb{P}(b_1 b_0) = \frac{1}{4}$	$\mathbb{P}(b_1 b_0) = \frac{1}{4}$
Y	$\mathbb{P}(b_1) = \frac{1}{2}$	$\mathbb{P}(b_1 b_0) = \frac{1}{4}$	$\mathbb{P}(b_1 b_0) = \begin{cases} 0 & b_0 = b_1 \\ \frac{1}{2} & b_0 \neq b_1 \end{cases}$	$\mathbb{P}(b_1 b_0) = \frac{1}{4}$
Z	$\mathbb{P}(b_1) = \frac{1}{2}$	$\mathbb{P}(b_1 b_0) = \frac{1}{4}$	$\mathbb{P}(b_1 b_0) = \frac{1}{4}$	$\mathbb{P}(b_1 b_0) = \begin{cases} \frac{1}{2} & b_0 = b_1 \\ 0 & b_0 \neq b_1 \end{cases}$

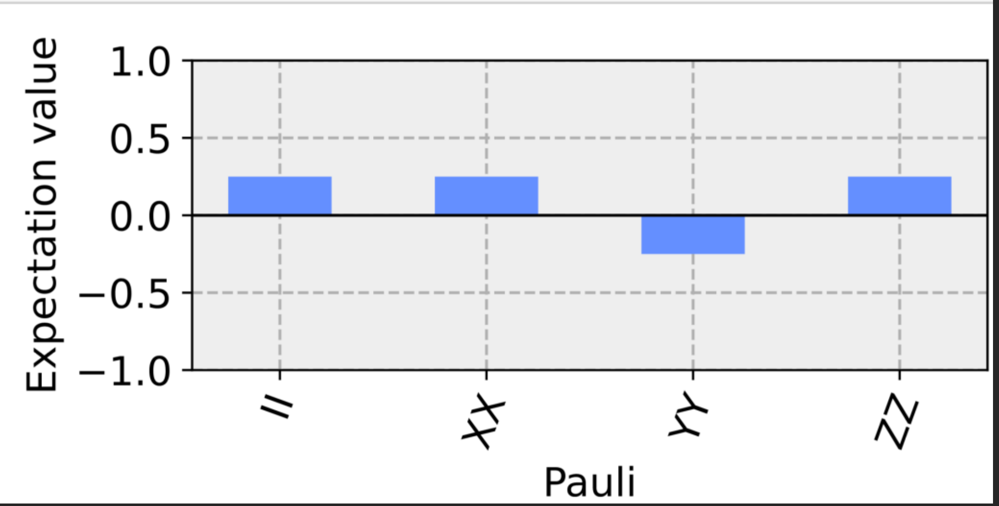
$$\text{expval}(IX) = P(0) - P(1) = 1/2 - 1/2 = 0$$

$$\text{expval}(YY) = P(00) + P(11) - P(10) - P(11) = 0 + 0 - \tfrac{1}{2} - \tfrac{1}{2} = -1$$

Tomography

q_1 \ q_0	I	X	Y	Z
I	(expval = +1)	expval = 0	expval = 0	expval = 0
X	expval = 0	expval = +1	expval = 0	expval = 0
Y	expval = 0	expval = 0	expval = −1	expval = 0
Z	expval = 0	expval = 0	expval = 0	expval = +1

```python
from qiskit.visualization import plot_state_paulivec
circc = QuantumCircuit(2) # q1q0 initial state |00>
circ.h(0); circ.cx(0, 1) # q1q0 in Bell state |Phi+>
plot_state_paulivec(circ, figsize=(5,2))
```



Tomography

Note: Qiskit's `plot_state_paulivec` says "expectation value", but in fact it displays the coefficient of the density matrix, which is $\frac{1}{2^n}$ times the exp. value.

We have thus characterised the Bell state as:

$$\frac{1}{2}\rho = \frac{1}{4}\left(I \otimes I + X \otimes X - Y \otimes Y + Z \otimes Z\right)$$

$\frac{1}{2^n}$, where $n=2$ here

Tomography

$\frac{1}{2}$  $= |\Phi^+\rangle\langle\Phi^+|$

$$= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0 & 0 & 1\end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix}1 & 0 & 0 & 1\\0 & 0 & 0 & 0\\0 & 0 & 0 & 0\\1 & 0 & 0 & 1\end{pmatrix} \in \mathbb{C}^{4\times 4}$$

Tomography

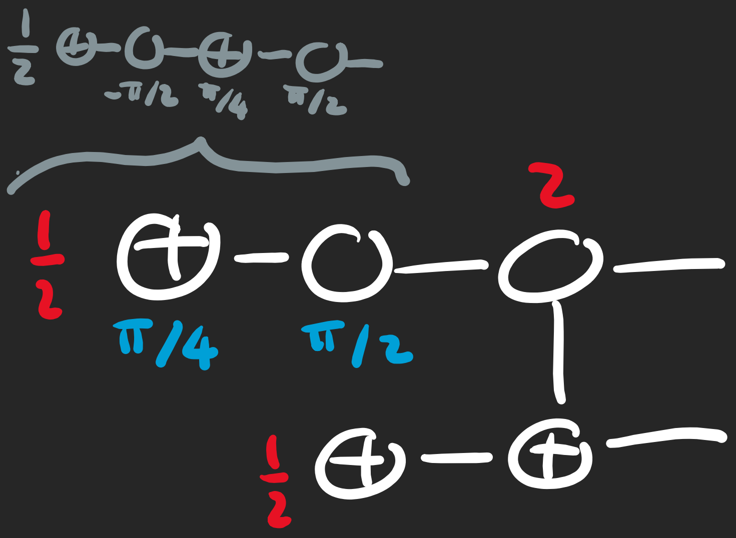
$$Y\otimes Y=\left(\begin{array}{c|c} 0Y & -iY \\ \hline iY & 0Y \end{array}\right) \qquad iY=\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$$\frac{1}{4}\left(I\otimes I+X\otimes X-Y\otimes Y+Z\otimes Z\right)$$

$$=\frac{1}{4}\left(\left(\begin{array}{cc|cc} 1&0&0&0\\ 0&1&0&0\\ \hline 0&0&1&0\\ 0&0&0&1 \end{array}\right)+\left(\begin{array}{cc|cc} 0&0&0&1\\ 0&0&1&0\\ \hline 0&1&0&0\\ 1&0&0&0 \end{array}\right)-\left(\begin{array}{cc|cc} 0&0&0&-1\\ 0&0&1&0\\ \hline 0&1&0&0\\ -1&0&0&0 \end{array}\right)+\left(\begin{array}{cc|cc} 1&0&0&0\\ 0&-1&0&0\\ \hline 0&0&-1&0\\ 0&0&0&1 \end{array}\right)\right)$$

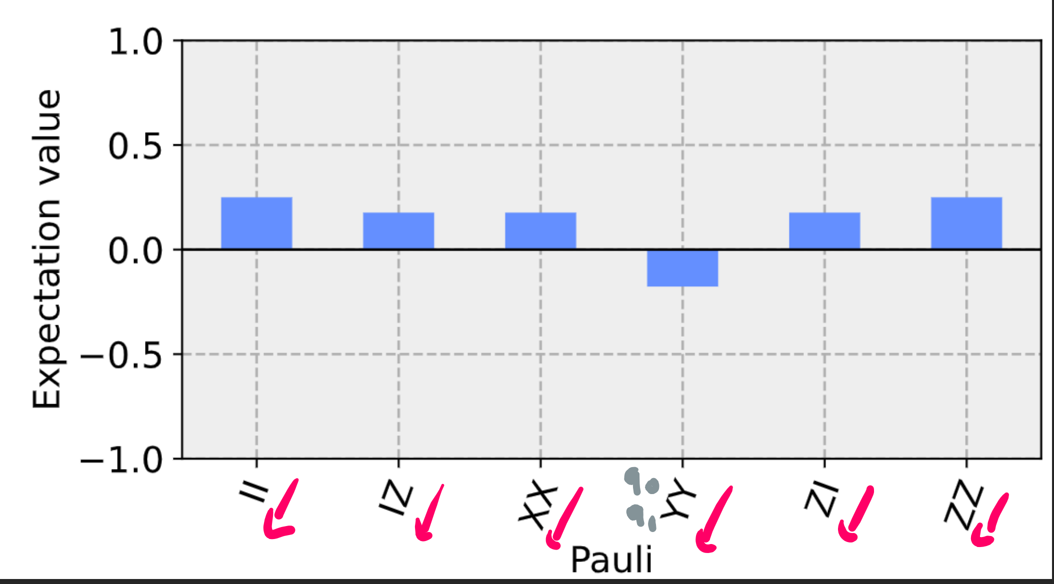
$$=\frac{1}{4}\left(\begin{array}{c|c} \begin{pmatrix}1&0\\0&1\end{pmatrix}+\begin{pmatrix}1&0\\0&-1\end{pmatrix} & \begin{pmatrix}0&1\\1&0\end{pmatrix}-\begin{pmatrix}0&-1\\1&0\end{pmatrix} \\ \hline \begin{pmatrix}0&1\\1&0\end{pmatrix}-\begin{pmatrix}0&1\\-1&0\end{pmatrix} & \begin{pmatrix}1&0\\0&1\end{pmatrix}+\begin{pmatrix}-1&0\\0&1\end{pmatrix} \end{array}\right)=\frac{1}{4}\begin{pmatrix} 2&0&0&2\\ 0&0&0&0\\ 0&0&0&0\\ 2&0&0&2 \end{pmatrix}=\frac{1}{2}\begin{pmatrix} 1&0&0&1\\ 0&0&0&0\\ 0&0&0&0\\ 1&0&0&1 \end{pmatrix}$$

Tomography



$$= \frac{1}{4}\left(I\otimes I + \frac{1}{\sqrt{2}} X\otimes X - \frac{1}{\sqrt{2}} Y\otimes Y + \frac{1}{\sqrt{2}} I\otimes Z + \frac{1}{\sqrt{2}} Z\otimes I + Z\otimes Z \right)$$

```python
from math import pi
circ = QuantumCircuit(2)
circ.ry(pi/4, 0); circ.cx(0,1)
plot_state_paulivec(circ, figsize=(6, 3))
```



(Paulistrings read right-to-left)

```python
from qiskit.visualization.utils import _paulivec_data
{s : e for s, e in zip(*_paulivec_data(circ))}
```

```
{'II': 1.0,
 'ZI': 0.7071067811865475,
 'XX': 0.7071067811865476,
 'YY': -0.7071067811865476,
 'IZ': 0.7071067811865475,
 'ZZ': 1.0}
```

$\leftarrow 1/\sqrt{2}$

$\leftarrow -1/$

actual expectation values

Tomography

We don't need $4^n - 1$ measurements:
the 3^n in $\{X, Y, Z\}^n$ are enough

e.g.
$$\begin{cases} \mathbb{P}(b_1 b_0 \mid I_2 Z_1 X_0) = \sum_{b_2 \in \{0,1\}} \mathbb{P}(b_2 b_1 b_0 \mid X_2 Z_1 X_0) \\ \\ \mathbb{P}(b_1 \mid I_2 Z_1 I_0) = \sum_{b_2, b_0 \in \{0,1\}} \mathbb{P}(b_2 b_1 b_0 \mid X_2 Z_1 X_0) \end{cases}$$

Tomography

We don't need $4^n - 1$ measurements:
the 3^n in $\{X, Y, Z\}^n$ are enough

$$
\begin{tikzcd}
 & I_2 Z_1 X_0 \arrow[r] \arrow[dr] & I_2 I_1 X_0 \\
X_2 Z_1 X_0 \arrow[ur] \arrow[r] \arrow[dr] & X_2 I_1 X_0 \arrow[ur] \arrow[dr] & I_2 Z_1 I_0 \\
 & X_2 Z_1 I_0 \arrow[ur] \arrow[r] & X_2 I_1 I_0
\end{tikzcd}
$$

Hamiltonians

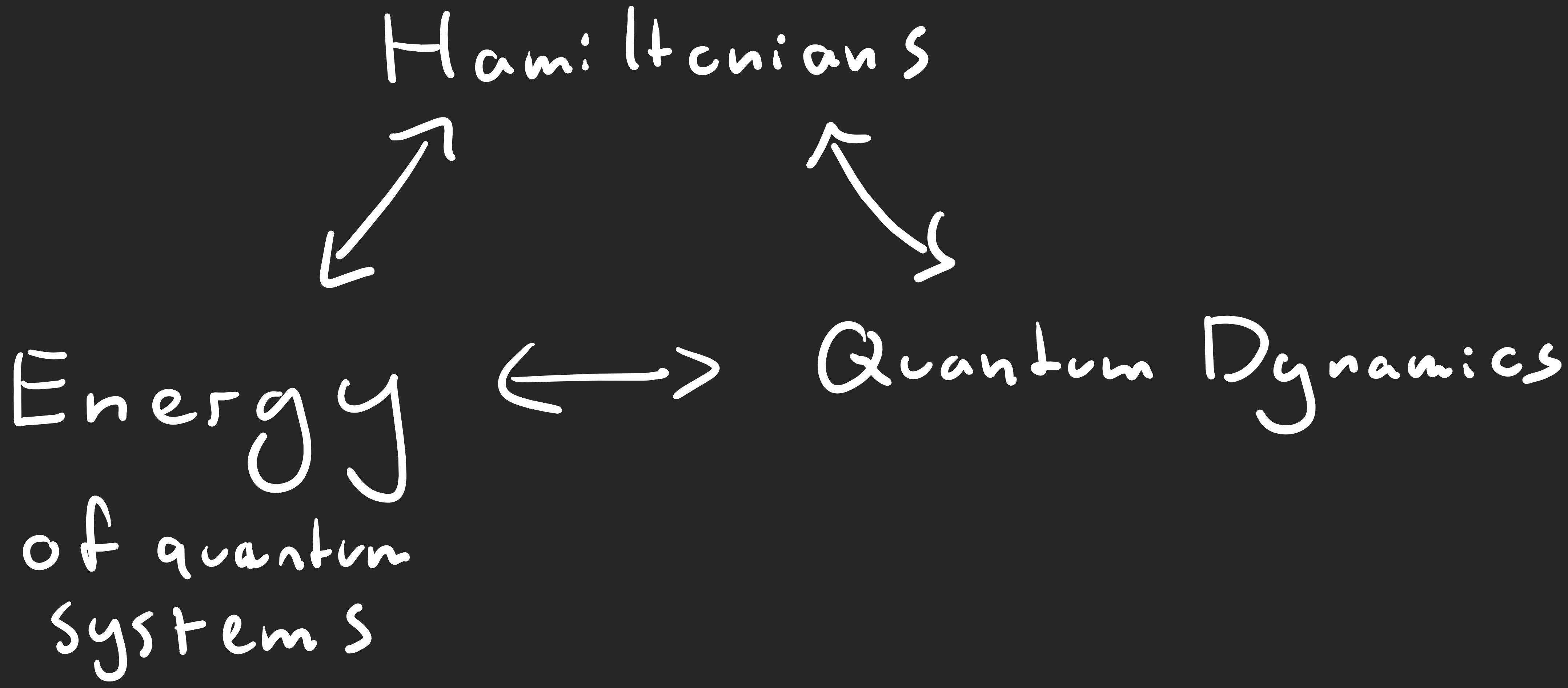
coefficients in $\mathbb{R}$

Hamiltonians = linear combinations of Pauli measurement expvals.

e.g. the molecular Hamiltonian for the Hydrogen molecule H_2 in the 4-qubit Hartree-Fock approximation (STO-3G minimal basis set):

$$H = -0.042IIII + 0.178ZIII + 0.178IZII - 0.243IIZI - 0.243IIIZ + 0.171ZZII + 0.123ZIZI + 0.168ZIIZ + 0.168IZZI + 0.123IZIZ + 0.176IIZZ + 0.045YXXY - 0.045YYXX - 0.045XXYY + 0.045XYYX$$

Hamiltonians



Hamiltonians

Hamiltonian

$$H = \sum_{\underline{P} \in \{I, X, Y, Z\}^n} H_{\underline{P}} \cdot \bigotimes_{i=0}^{n-1} P_i$$

Hydrogen molecule Hamiltonian

$$H_{H_2} = \begin{aligned} &0.011\ ZZ \\ +&0.398\ ZI \\ +&0.398\ IZ \\ +&0.181\ XX \end{aligned}$$

Shorthands for

$Z \otimes Z$, $Z \otimes I$, $I \otimes Z$, $X \otimes X$

Alternatively:

$Z_1 Z_0$, $Z_1 I_0$, $I_1 Z_0$, $X_1 X_0$

Hamiltonians

$$H = \sum_{\underline{\sigma} \in \{I, X, Y, Z\}^n} H_{\underline{\sigma}} \cdot \bigotimes_{i=0}^{n-1} \sigma_i$$

quantum state

$$\rho = \frac{1}{2^n} \sum_{\underline{\sigma} \in \{I, X, Y, Z\}^n} \rho_{\underline{\sigma}} \cdot \bigotimes_{i=0}^{n-1} \sigma_i$$

expvals from tomography

$$H_{H_2} = \begin{array}{l} 0.011\ ZZ \\ +0.398\ ZI \\ +0.398\ IZ \\ +0.181\ XX \end{array}$$

Bell state

$$\frac{1}{2} C = \begin{array}{l} 0.25\ II \\ +0.25\ XX \\ -0.25\ YY \\ +0.25\ ZZ \end{array}$$

Hamiltonians

$$H = \sum_{\underline{\Pi} \in \{I,X,Y,Z\}^n} H_{\underline{\Pi}} \cdot \bigotimes_{i=0}^{n-1} \Pi_i$$

$$H_{H_2} = \begin{aligned} &0.011\ ZZ \\ &+0.398\ ZI \\ &+0.398\ IZ \\ &+0.181\ XX \end{aligned}$$

$$\rho = \frac{1}{2^n} \sum_{\underline{\Pi} \in \{I,X,Y,Z\}^n} \rho_{\underline{\Pi}} \cdot \bigotimes_{i=0}^{n-1} \Pi_i$$

$$\frac{1}{2}C = \begin{aligned} &0.25\ II \\ &+0.25\ XX \\ &-0.25\ YY \\ &+0.25\ ZZ \end{aligned}$$

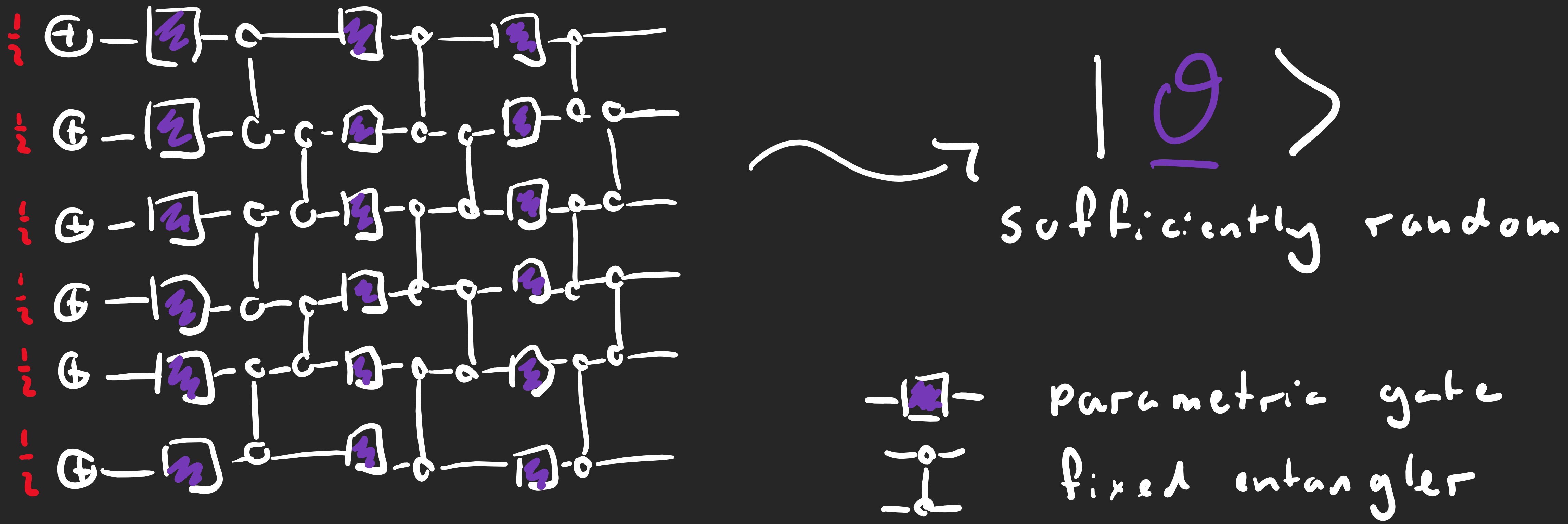
expected value
for Hamiltonian

$$\langle H \rangle_\rho := \sum_{\underline{\Pi} \in \{I,X,Y,Z\}^n} H_{\underline{\Pi}} \cdot \rho_{\underline{\Pi}}$$

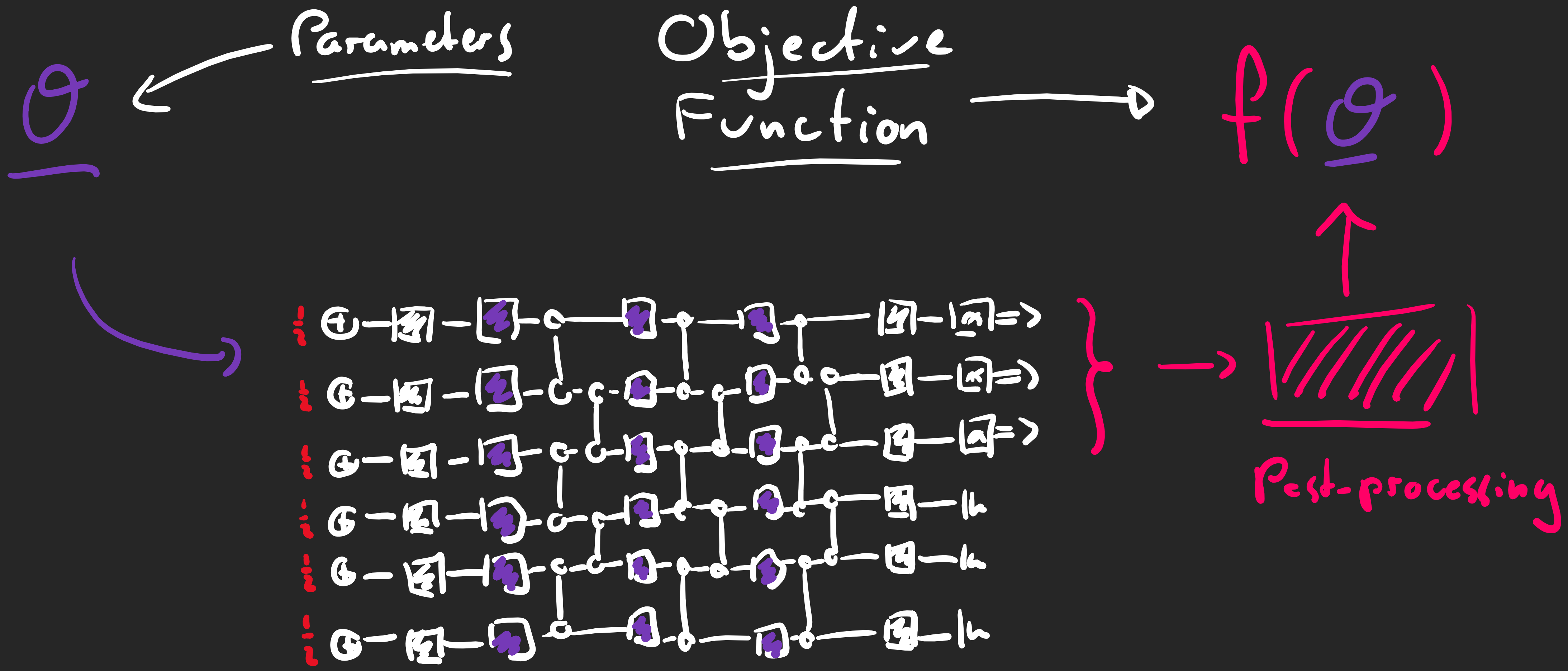
$$\langle H_{H_2} \rangle_{\frac{1}{2}C} = \underbrace{0.011}_{ZZ} + \underbrace{0.181}_{XX}$$

Variational Quantum Circuits

If a family of structured circuits is "sufficiently random", by tweaking their parameters we can explore a large region in the space of quantum states.



Parameter Optimisation



*: barren plateaus => init values close to θ (see appendix)

Parameter Optimisation

random $\underline{\theta}_0$

```python
from qiskit.algorithms.optimizers import COBYLA
rng = np.random.default_rng(seed=0)
optimizer = COBYLA(maxiter=100)
init_params = rng.uniform(-pi/16, pi/16, size=num_params)
opt_params, value, nfev = optimizer.optimize(num_params, obj_fun, initial_point=init_params)
```

$\underline{\theta}_N$ $f(\underline{\theta}_N)$ $f(\underline{\theta})$ $\underline{\theta}_0$

return

termination conditions are met

$$\underline{\theta}_0 \xrightarrow{QC} f(\underline{\theta}_0) \xrightarrow{opt} \underline{\theta}_1 \xrightarrow{QC} f(\underline{\theta}_1) \xrightarrow{opt} \underline{\theta}_2 \xrightarrow{QC} f(\underline{\theta}_2) \xrightarrow{opt} \cdots \xrightarrow{opt} \underline{\theta}_N \xrightarrow{QC} f(\underline{\theta}_N)$$

Parameter Optimisation

Gradient-free optimisers:

- COBYLA
- SPSA

Gradient-based optimisers:

- Gradient Descent
- ADAM
- Quantum Natural Gradient

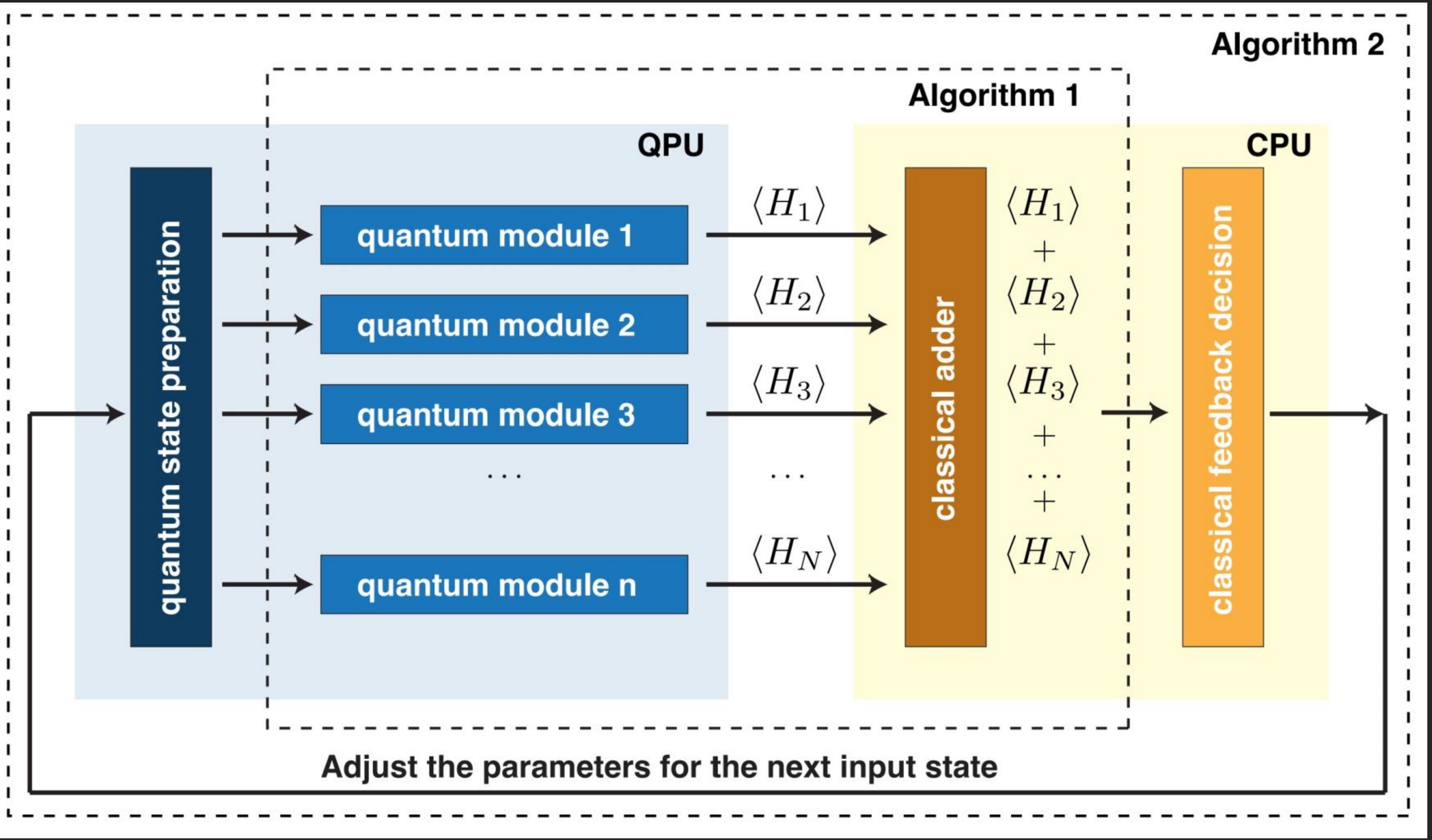
```
from qiskit.algorithms.optimizers import SPSA, COBYLA, GradientDescent, ADAM
```

See Qiskit optimizers documentation

```
Optimizer.optimize(num_vars, objective_function,
                   gradient_function=None,
                   variable_bounds=None,
                   initial_point=None)
```

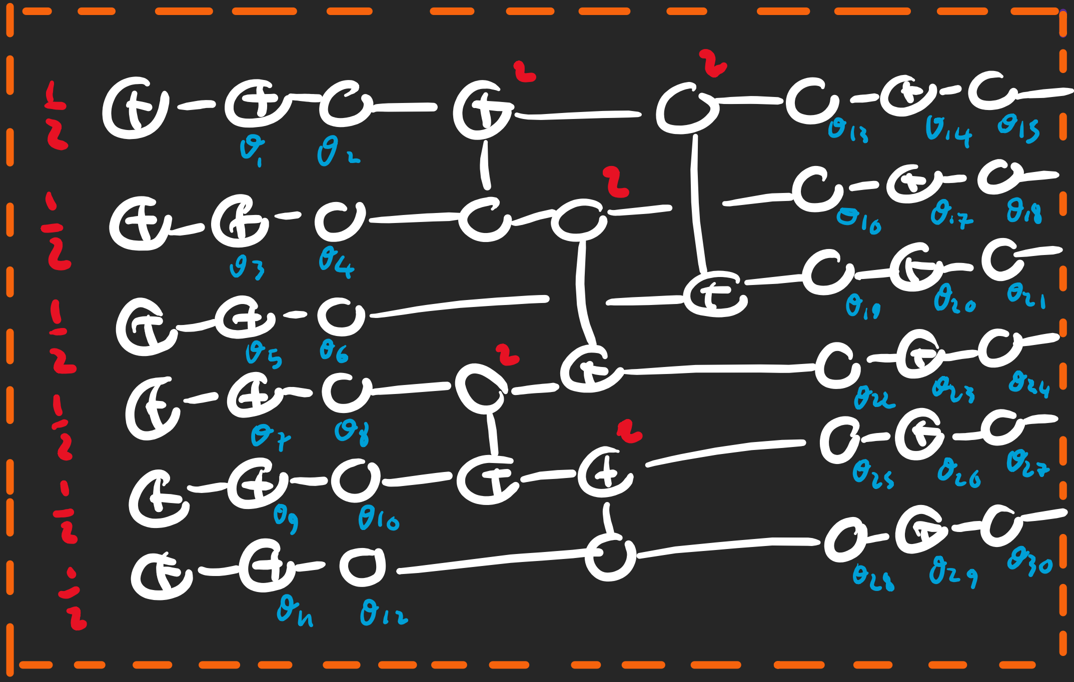
Variational Quantum Eigensolver (VQE)

A variational eigenvalue solver on a quantum processor [arXiv:1304.3061](https://arxiv.org/abs/1304.3061)



VQE

$$\mathcal{H} = \sum_{\underline{\Gamma}\in\{I,X,Y,Z\}} \mathcal{H}_{\underline{\Gamma}} \bigotimes_{i=0}^{n-1} \Gamma_i$$



State ansatz $|\underline{\theta}\rangle$

enough to measure the $\underline{\Gamma}$ for which $\mathcal{H}_{\underline{\Gamma}} \neq 0$

$\Rightarrow$ tomography

$\Downarrow$

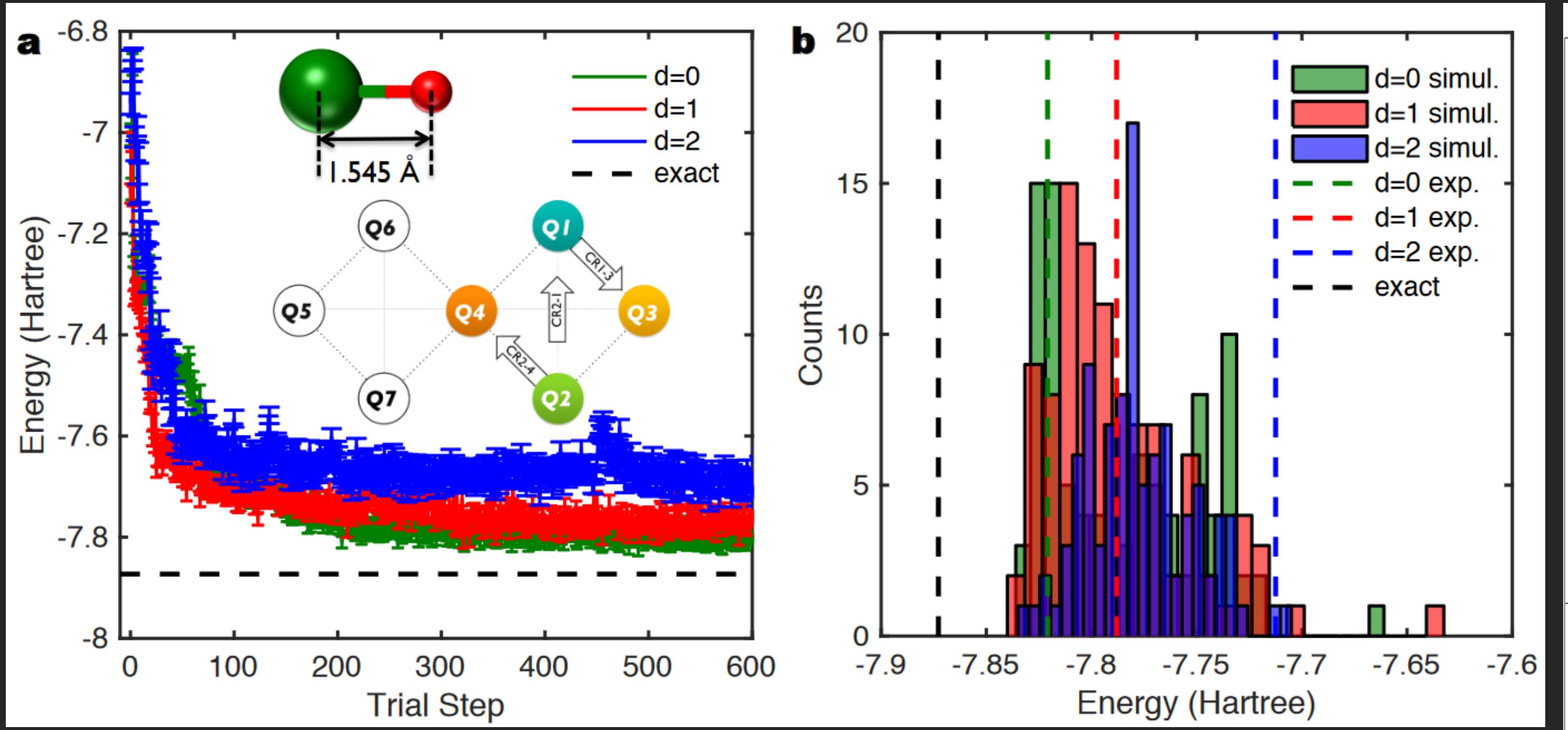
$$f(\underline{\theta}) = \langle \mathcal{H} \rangle_{|\underline{\theta}\rangle}$$

objective function

VQE

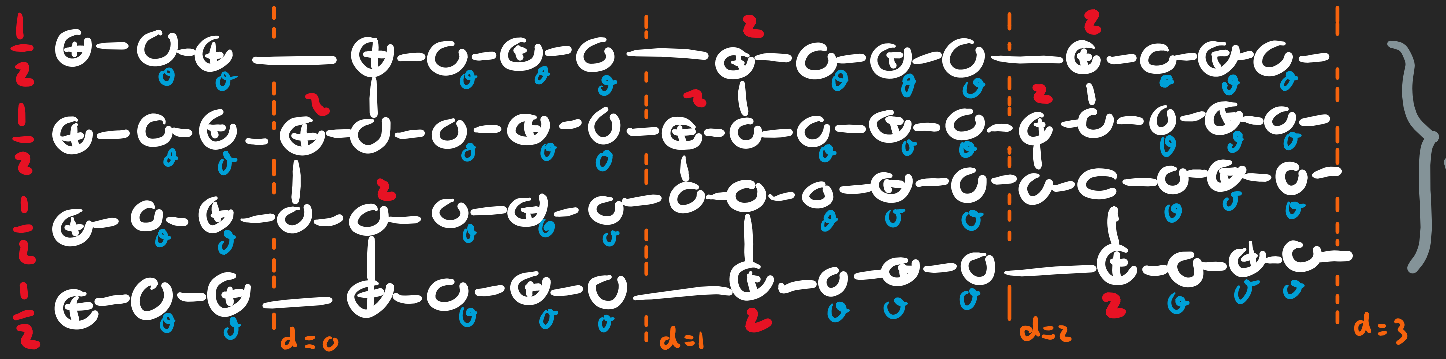
Each group of terms requires a single Pauli measurement.

(eg. ZZXX)



LiH at bond distance

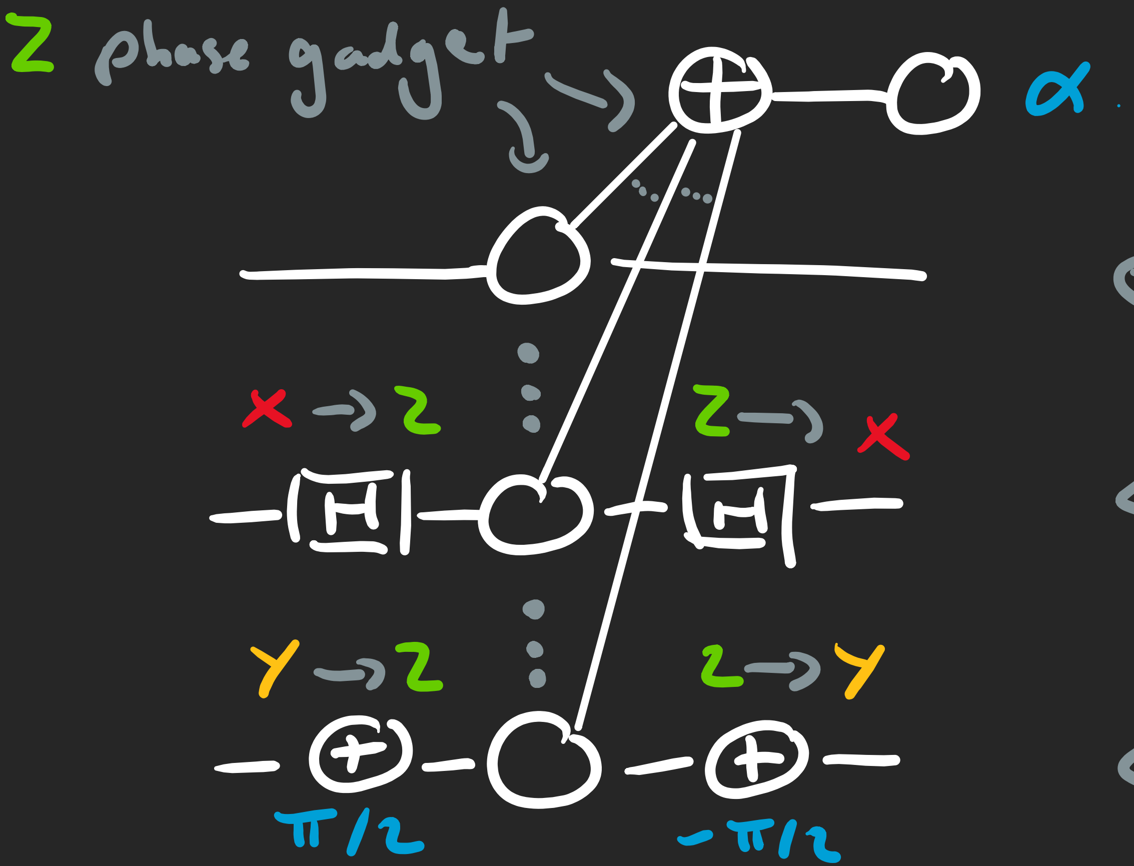
ZIII -0.096022 ZZII -0.206128 IZII 0.364746 IIZI 0.096022 IIZZ -0.206128 IIIZ -0.364746 ZIZI -0.145438 ZIZZ 0.056040 ZIIZ 0.110811 ZZZI -0.056040 ZZZZ 0.080334 ZZIZ 0.063673 IZZI 0.110811 IZZZ -0.063673 IZIZ -0.095216	XZII -0.012585 XIII 0.012585 IIXZ 0.012585 IIXI 0.012585 XZXZ -0.002667 XZXI -0.002667 XIXZ 0.002667 XIXI 0.002667 XZIZ 0.007265 XIIZ -0.007265 IZXZ 0.007265 IZXI 0.007265	XXII -0.029640 IXII 0.002792 IIXX -0.029640 IIIX 0.002792 XIXX -0.008195 XIIX -0.001271 XXXI -0.008195 XXXX 0.028926 XXIX 0.007499 IXXI -0.001271 IXXX 0.007499 IXIX 0.009327	YYII 0.029640 IIYY 0.029640 YYYY 0.028926	ZXII 0.002792 IIZX -0.002792 ZIZX -0.016781 ZIIX 0.016781 ZXZI -0.016781 IXZI -0.016781 ZXZX -0.009327 ZXIX 0.009327 IXZX -0.009327	ZIXZ -0.011962 ZIXI -0.011962 ZZXZ 0.000247 ZZXI 0.000247	ZIXX 0.039155 ZZXX -0.002895 ZZIX -0.009769 IZXX -0.024280 IZIX -0.008025	ZIYY -0.039155 ZZYY 0.002895 IZYY 0.024280	XZZI -0.011962 XIZI 0.011962 XZZZ -0.000247 XIZZ 0.000247
XZXX 0.008195 XZIX 0.001271	XZYY -0.008195 XIYY 0.008195	XZZX -0.001271 XIZX 0.001271 IZZX 0.008025	XXZI -0.039155 XXZZ -0.002895 XXIZ 0.024280 IXZZ -0.009769 IXIZ 0.008025	YYZI 0.039155 YYZZ 0.002895 YYIZ -0.024280	XXXZ -0.008195 IXXZ -0.001271	YYXZ 0.008195 YYXI 0.008195	XXYY -0.028926 IXYY -0.007499	YYXX -0.028926 YYIX -0.007499
XXZX -0.007499	YYZX 0.007499	ZZZX 0.009769	ZXXZ -0.001271 ZXXI -0.001271 ZXIZ 0.008025	ZXXX 0.007499	ZXYY -0.007499	ZXZZ -0.009769		



tomography (25 measurements)

Pauli Gadgets

Pauli Gadgets = Phase Gadgets + leg change of basis



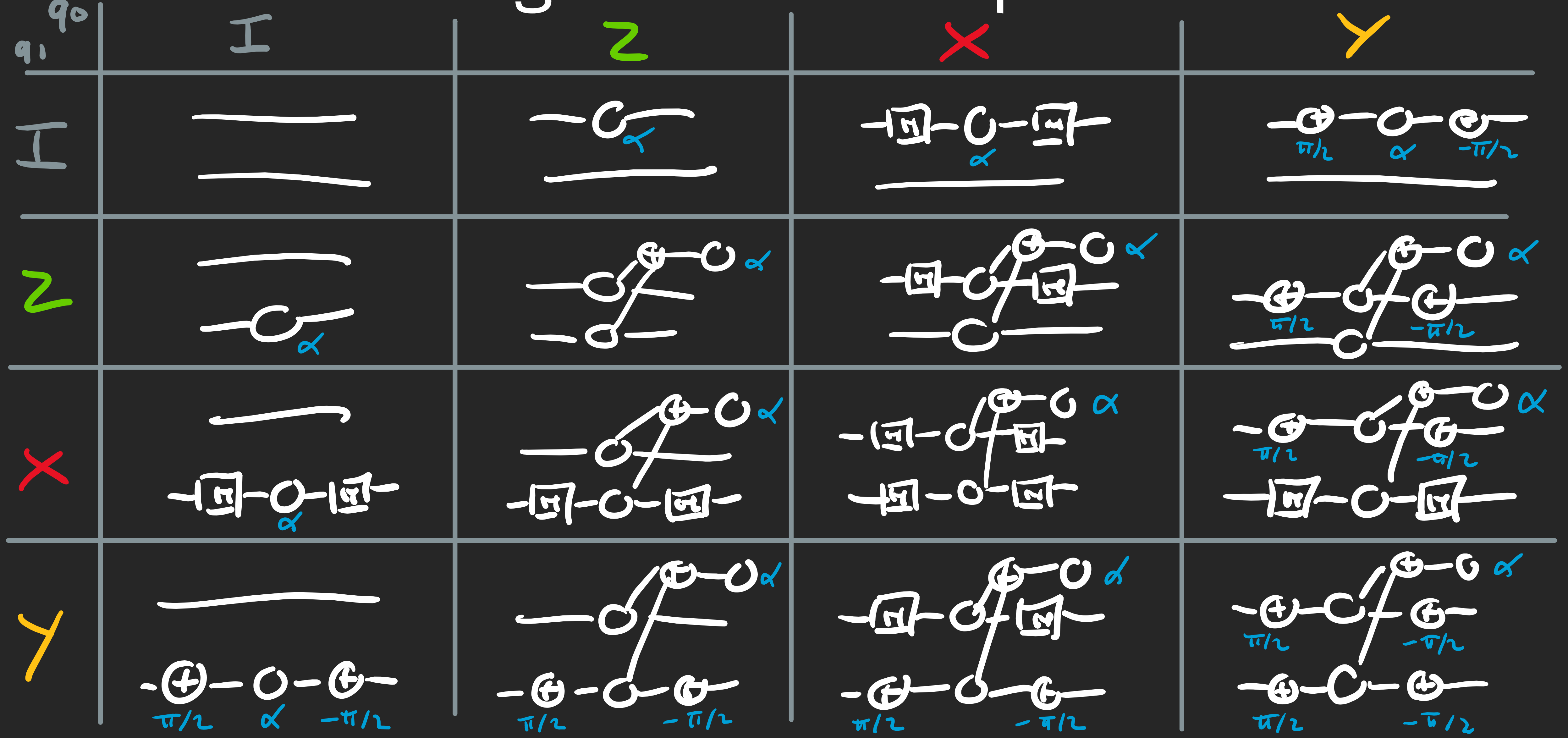
← a Z leg

← an X leg

← a Y leg

(15 non-trivial gadgets ⇒ 15-dimensional space of 2-qubit rotations)

Pauli Gadgets on 2 qubits



Pauli Gadgets

Pauli Gadgets are the coordinate directions in the space (Lie group) of n-qubit rotations.

# of Pauli Gadgets on n qubits (except id) = dimension of space of n-qubit rotations $SU(2^n)$

$$\underbrace{4^n - 1}_{\text{All strings of } n \text{ characters from } \{I, Z, X, Y\}, \text{ not all } I.}$$

Quantum Dynamics

A Diagrammatic Approach
to Quantum Dynamics
arXiv:1905.13111
Categorical Quantum Dynamics
arXiv:1709.09772

Hamiltonian $\longleftrightarrow$ Unitary Evolution

H
(on n qubits)

$n \vdots \boxed{\exp(-iHt)} \vdots n$

the quantum system is rotated as time progresses

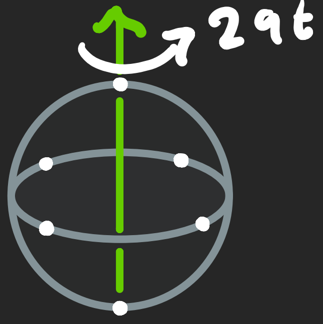
Quantum Dynamics

Some simple cases:

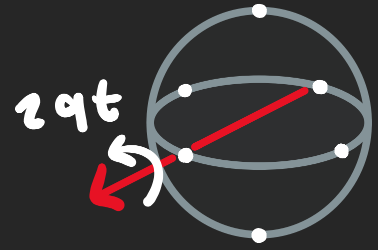
angular velocity 2q

time

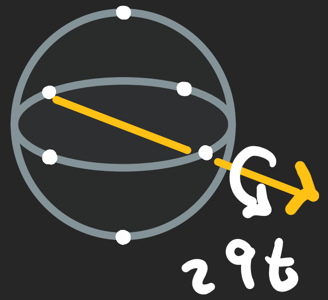
$$qZ \longrightarrow R_Z(2qt)$$



$$qX \longrightarrow R_X(2qt)$$



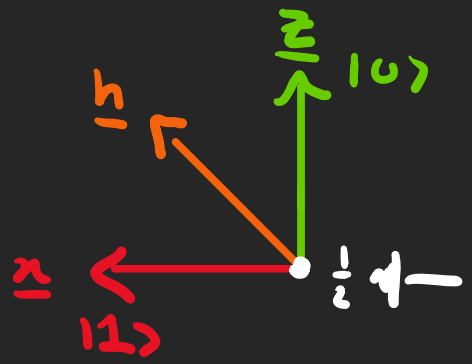
$$qY \longrightarrow R_Y(2qt)$$

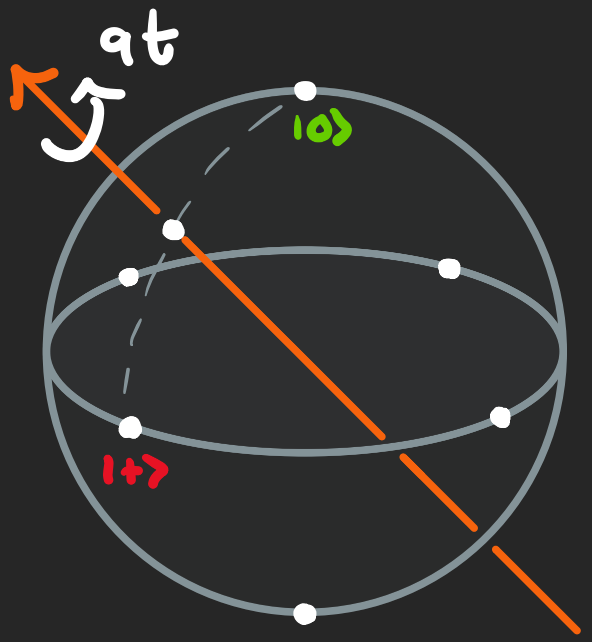


Quantum Dynamics

$$q \underbrace{\frac{1}{\sqrt{2}}(Z+X)}_{\text{mid-way through } Z \text{ and } X} \longrightarrow R_H(2qt)$$

$\Rightarrow$ Hadamard axis!





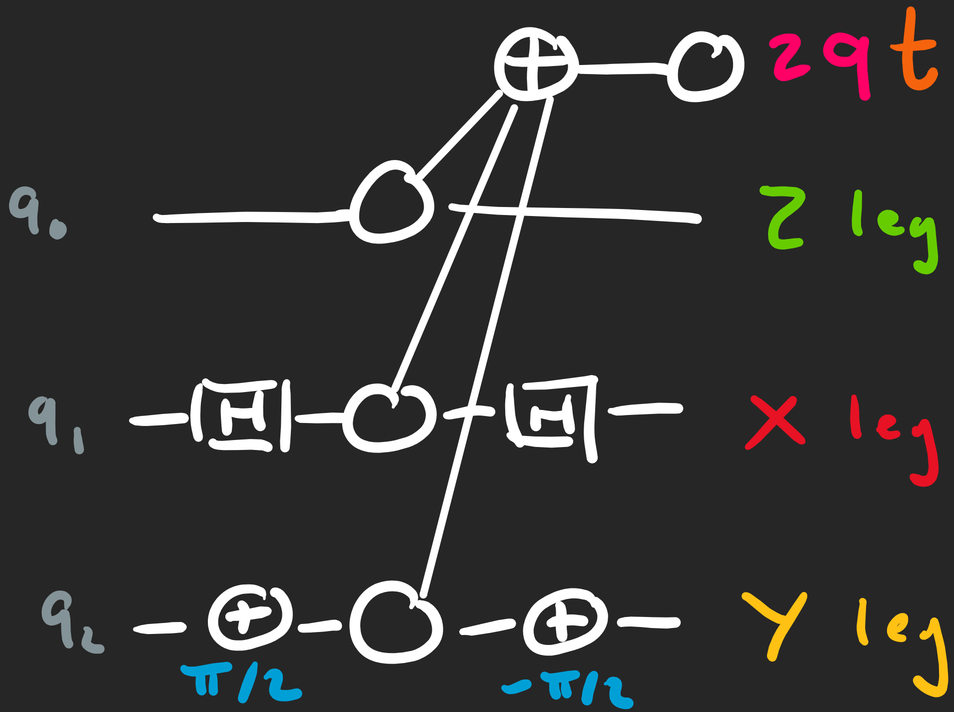
$$\underline{h} = \frac{1}{\sqrt{2}}(\underline{z}+\underline{x}) \quad \text{as 3D vectors}$$

Quantum Dynamics

Pauli terms $\longleftrightarrow$ Pauli gadgets

e.g. $q\, Y \otimes X \otimes Z \longrightarrow$

$(q\, Y_2 X_1 Z_0)$



https://en.wikipedia.org/wiki/Lie_product_formula

Trotterization

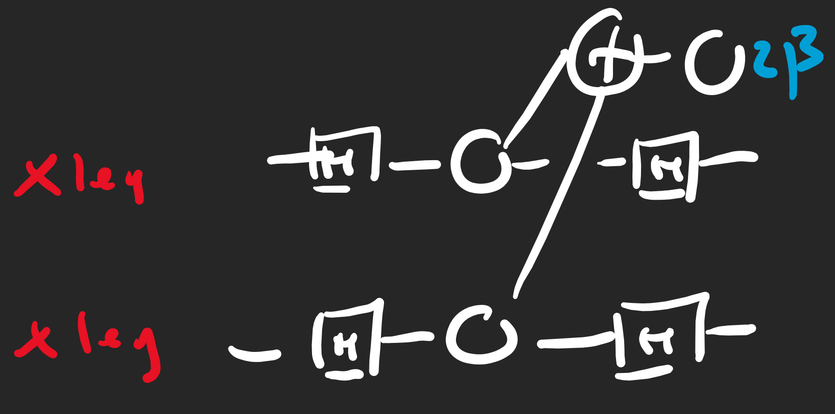
Generic n-qubit Hamiltonian $\Longrightarrow$ Circuit to simulate quantum dynamics is very complicated!

e.g. $\mathcal{H} = 0.011\, Z_0 Z_1 + 0.398\, Z_0 + 0.398\, Z_1 + 0.181\, X_0 X_1$

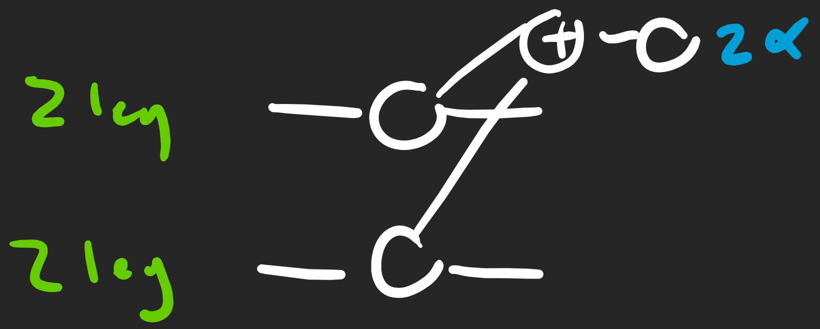
$$e^{-i\mathcal{H}t}$$

Trotterization

Problem:



$$e^{-i(\alpha Z\otimes Z + \beta X\otimes X)} \neq e^{-i\alpha Z\otimes Z} \; e^{-i\beta X\otimes X}$$



Trotterization

$$e^{-i\left(\overbrace{\sum_{\underline{\Pi}} H_{\underline{\Pi}} \bigotimes_{i=0}^{n-1} \Pi_i}^{\text{generic n-qubit Hamiltonian}}\right) t}$$

$\neq$ (in general) sequential composition over $\underline{\Pi}$

$$\left(e^{-i H_{\underline{\Pi}} t \bigotimes_{i=0}^{n-1} \Pi_i} \right)$$

n-qubit Pauli gadget!

Trotterization

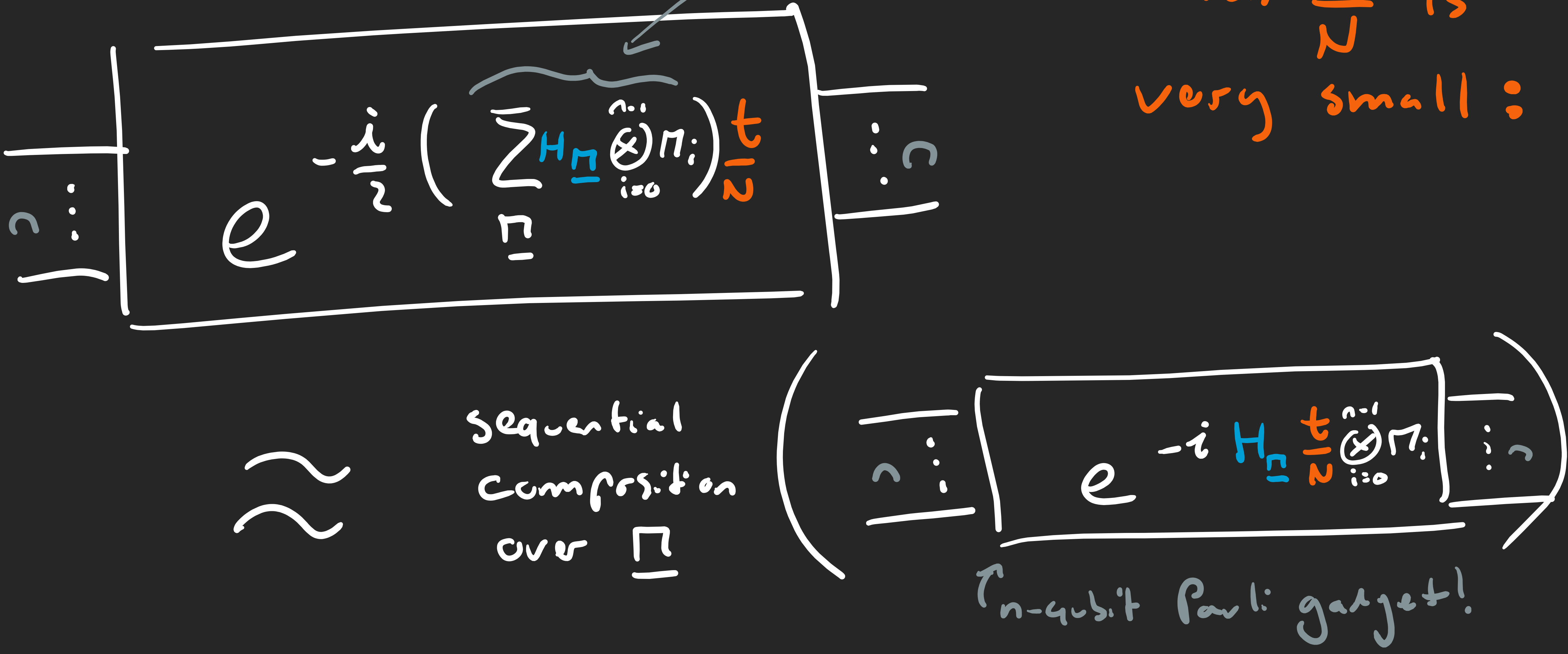
<u>Solution</u>: Chop rotation into tiny time intervals

$$\boxed{e^{-iHt}} = \underbrace{\boxed{e^{-iH\frac{t}{N}}} \cdots \boxed{e^{-iH\frac{t}{N}}}}_{\text{N very small rotations}}$$

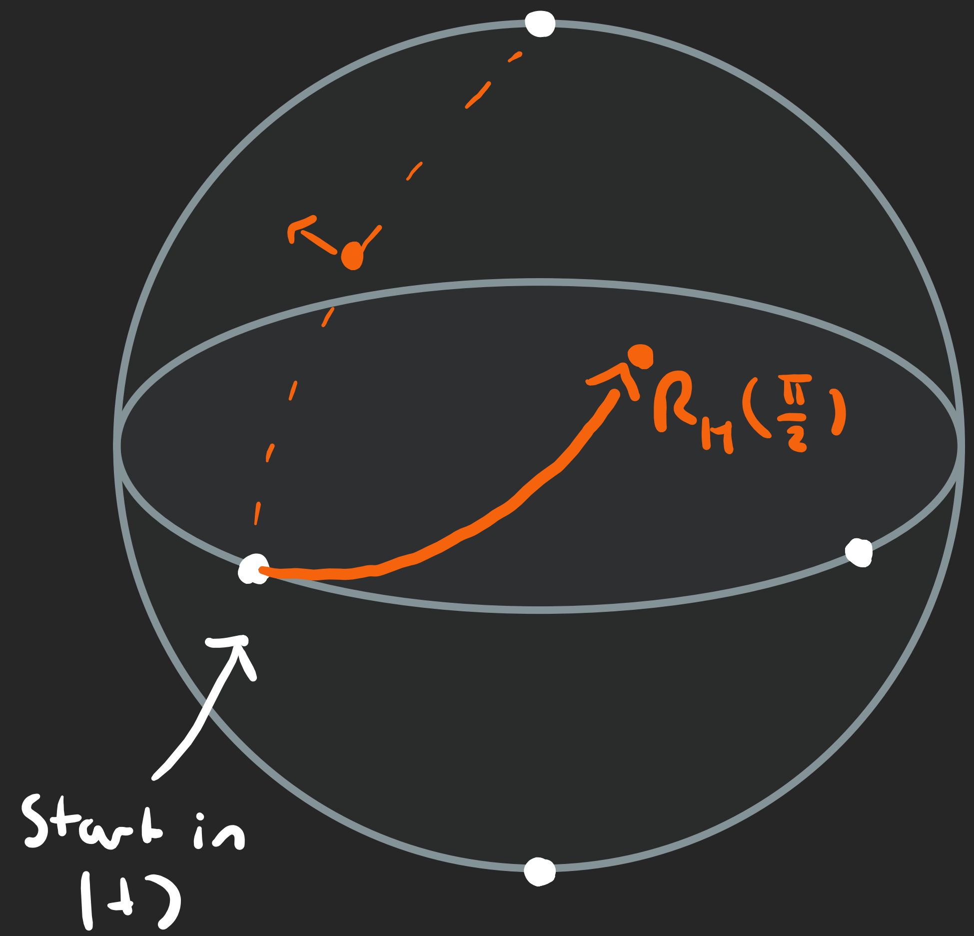
Trotterization

generic n-qubit Hamiltonian

When $\frac{t}{N}$ is very small:

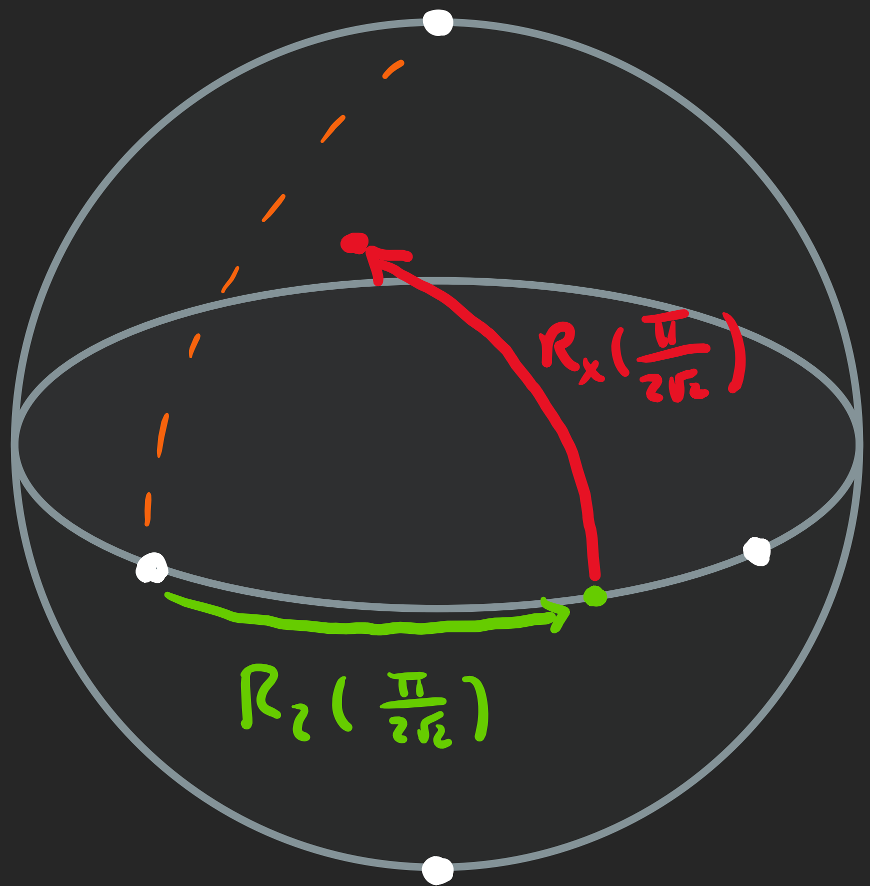


$$\frac{1}{\sqrt{2}}(Z+X) \to R_H(t) \quad \text{vs.} \quad \begin{array}{l} \frac{1}{\sqrt{2}} Z \to R_Z\left(\frac{2t}{\sqrt{2}}\right) \\ \frac{1}{\sqrt{2}} X \to R_X\left(\frac{2t}{\sqrt{2}}\right) \end{array}$$

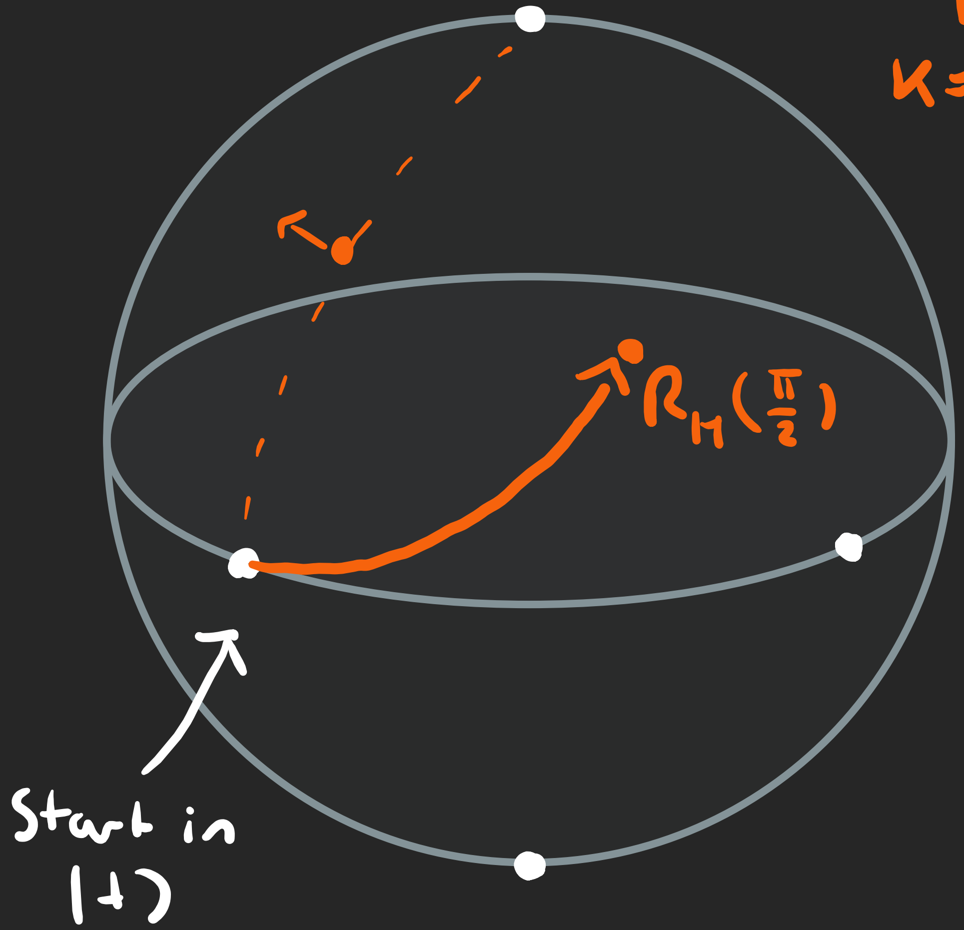


$t = \frac{\pi}{4}$

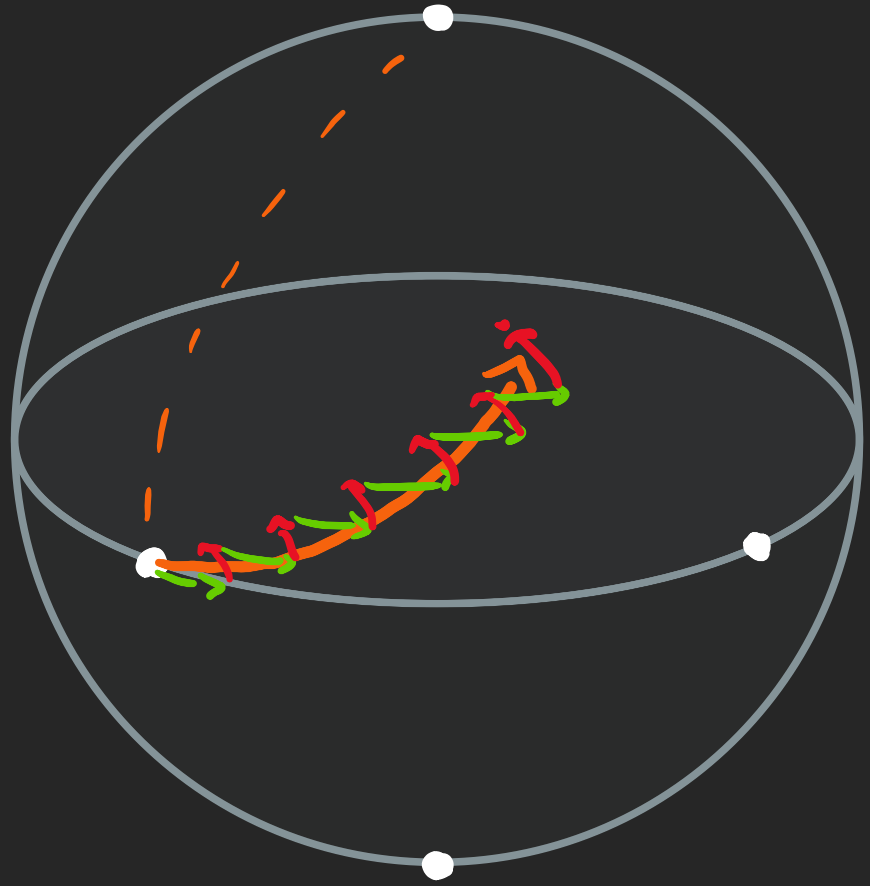
(not small)



$$\frac{1}{\sqrt{2}}(Z+X) \rightarrow R_H(t) \quad \text{vs.} \quad \begin{aligned} \frac{1}{\sqrt{2}}Z &\rightarrow R_Z\left(\frac{2t}{\sqrt{2}}\right) \\ \frac{1}{\sqrt{2}}X &\rightarrow R_X\left(\frac{2t}{\sqrt{2}}\right) \end{aligned}$$

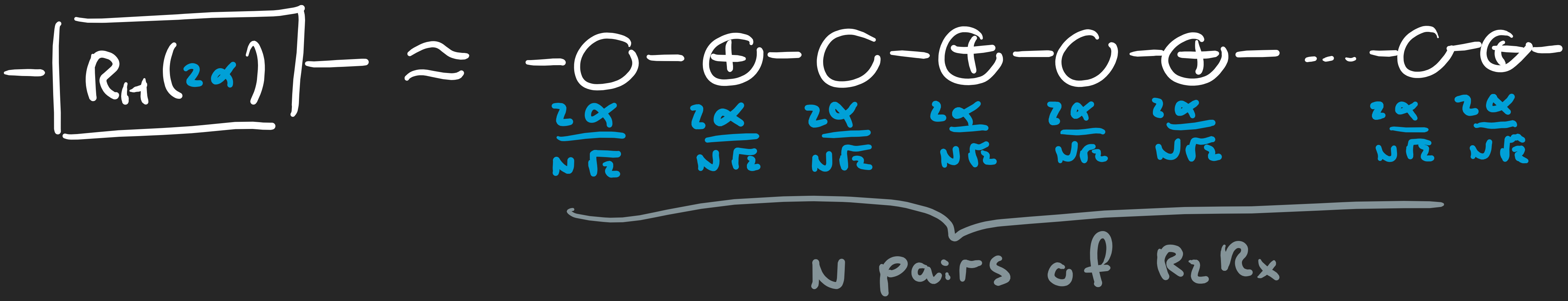


trotterised in $K=6$ small steps of $\Delta t = \frac{\pi}{24}$



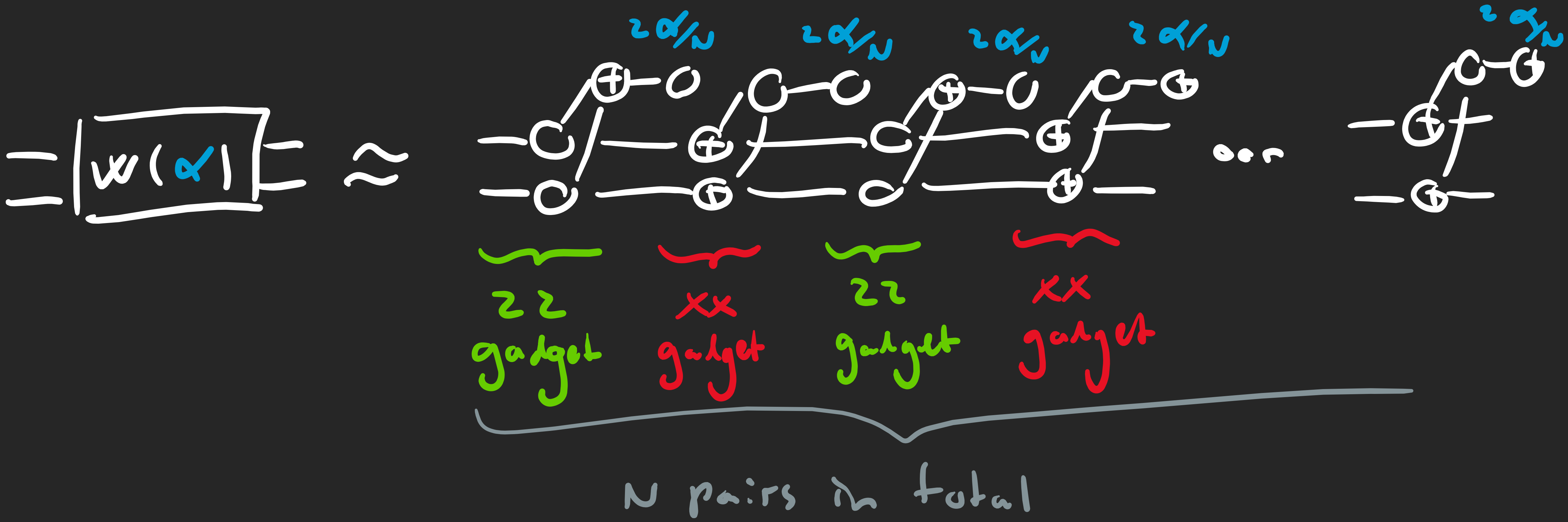
Trotterization

$$R_H(2\alpha) = e^{-i\alpha\frac{1}{\sqrt{2}}(Z+X)}$$



Trotterization

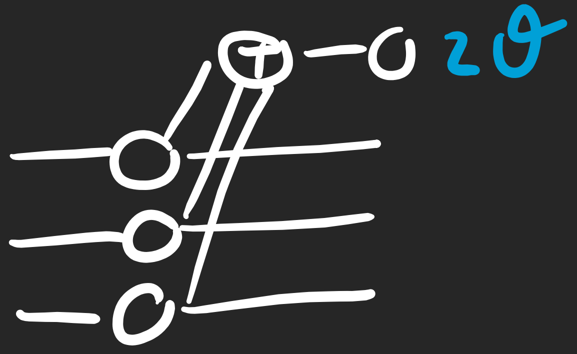
$$W(\alpha) := e^{-i\alpha(XX+ZZ)}$$



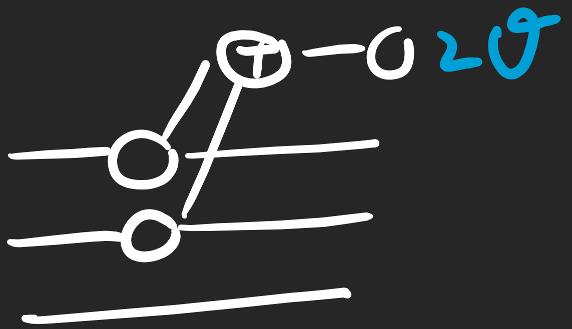
Trotterization

$$H = \frac{1}{2}\left(-3 Z_0 Z_1 Z_2 + Z_0 Z_1 - Z_1 Z_2 + 1\right)$$

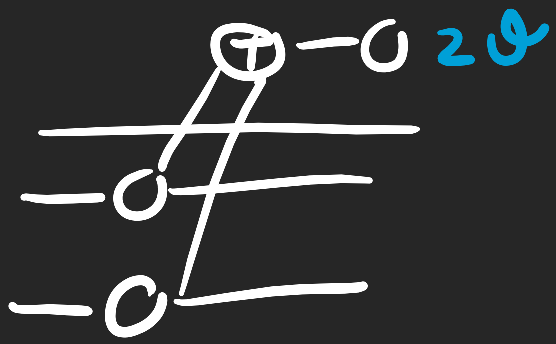
irrelevant!



$\theta\, Z_0 Z_1 Z_2$



$\theta\, Z_0 Z_1$

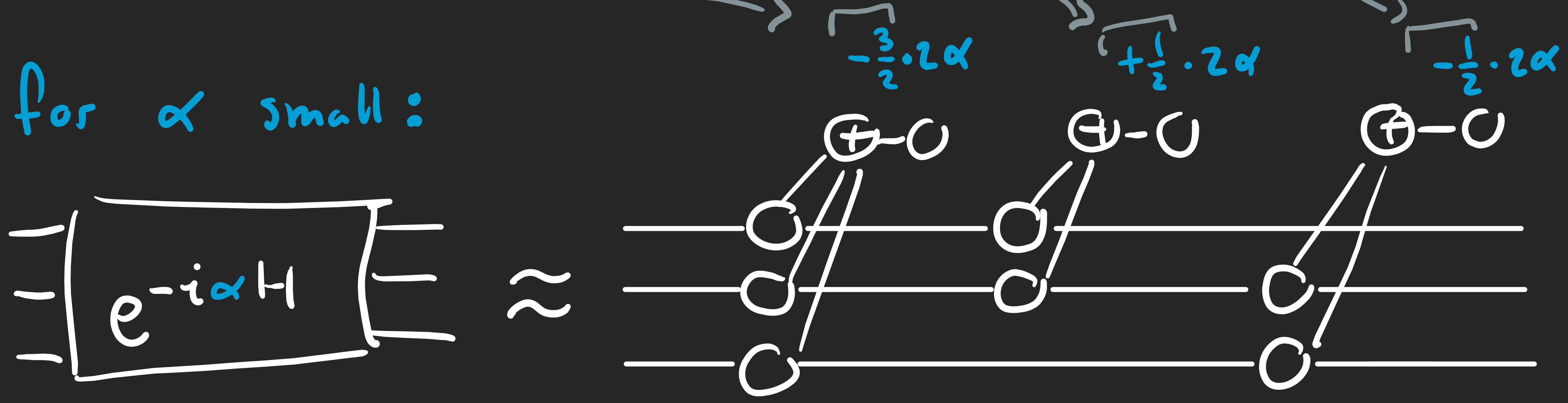


$\theta\, Z_1 Z_2$

Trotterization

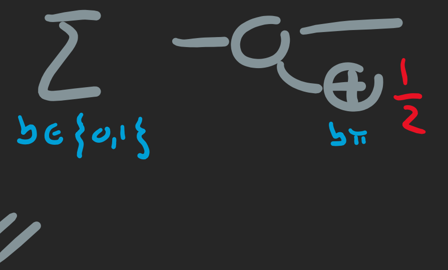
$$H = -\frac{3}{2} Z_0 Z_1 Z_1 + \frac{1}{2} Z_0 Z_1 - \frac{1}{2} Z_1 Z_2 + \frac{1}{2}$$

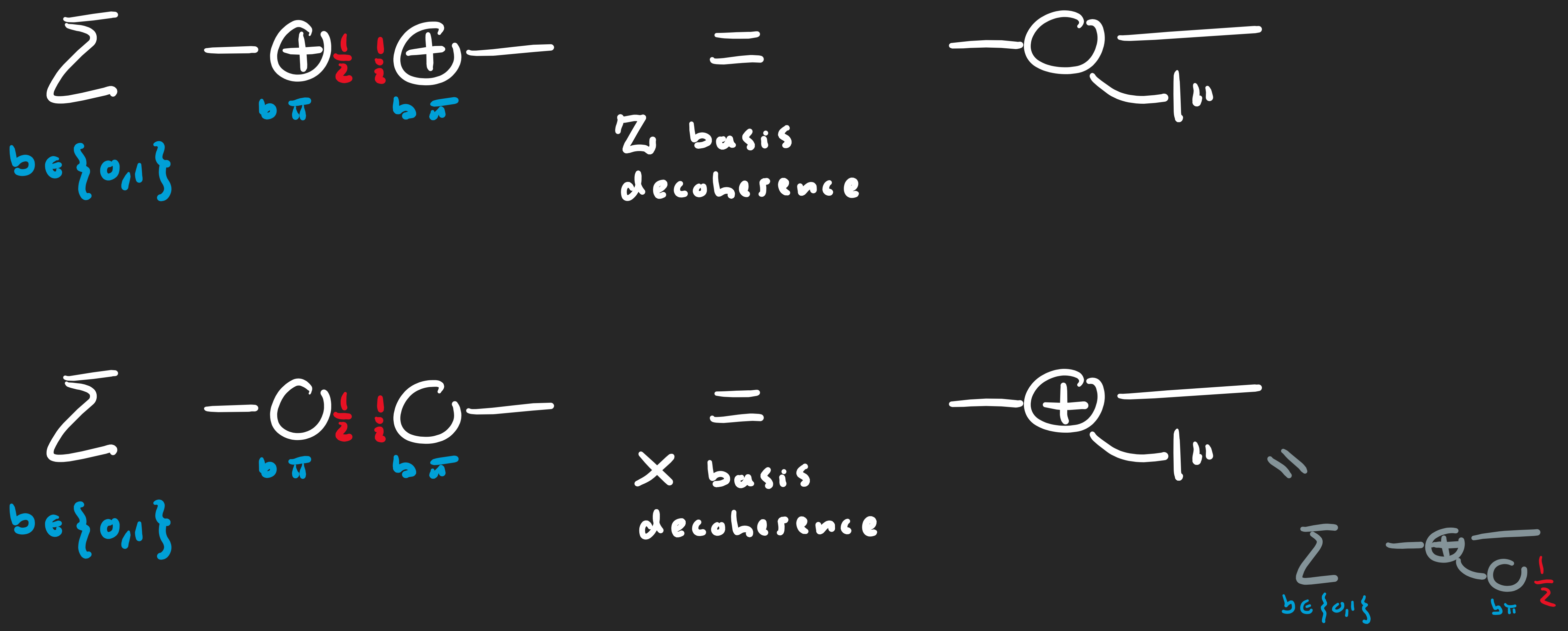
for α small:



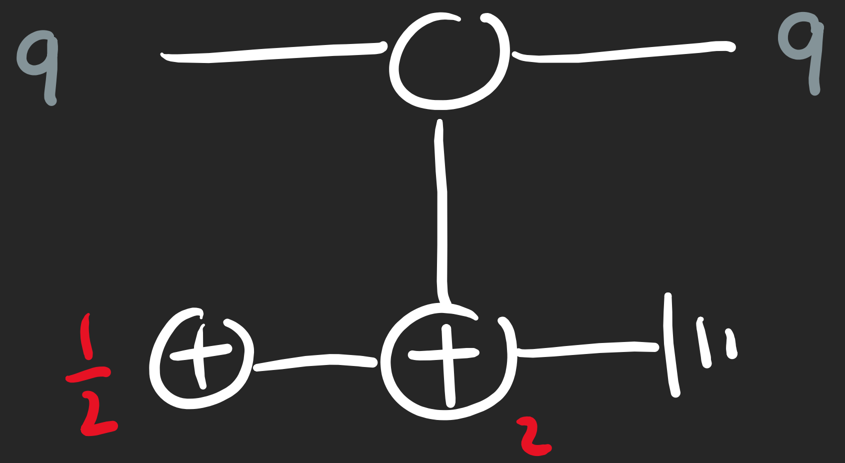
Appendix: Decoherence

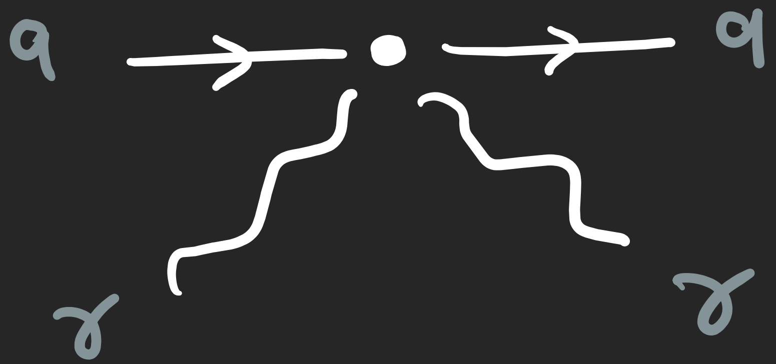
Decoherence Maps





Decoherence Maps





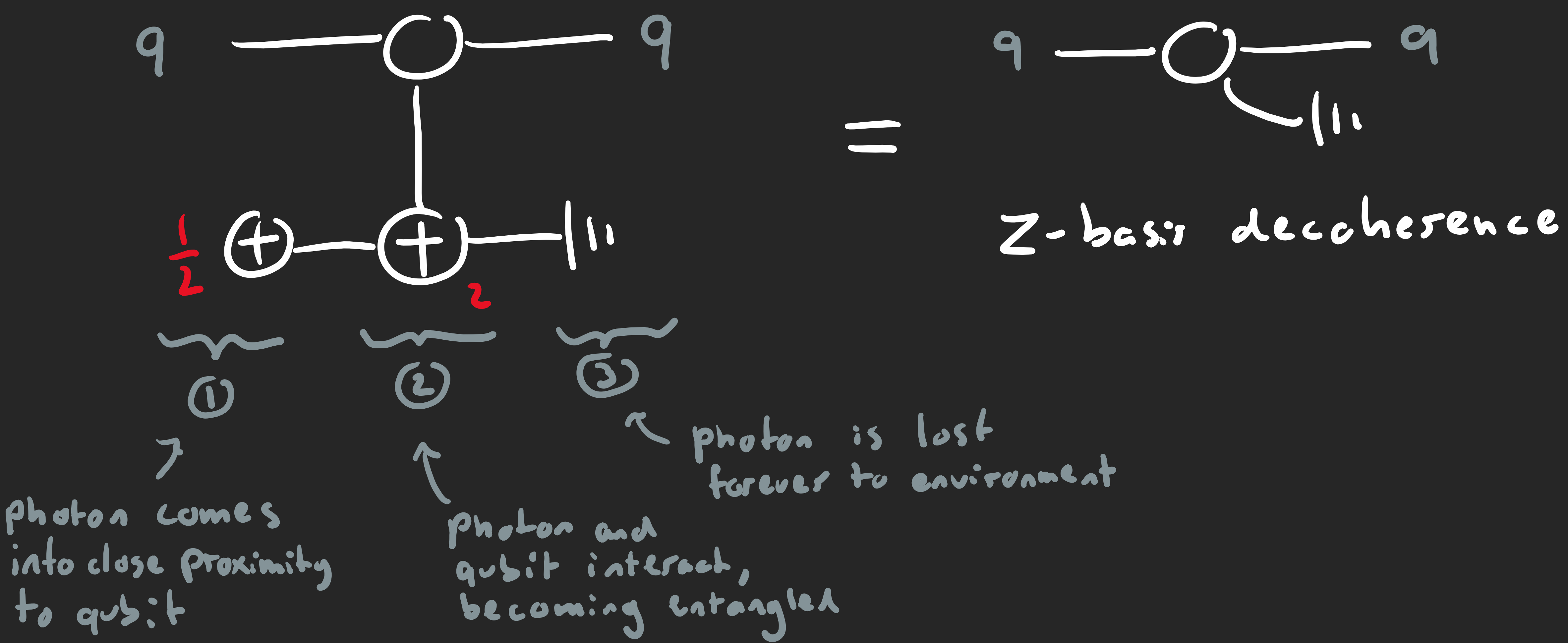
1 2 3

photon comes into close proximity to qubit

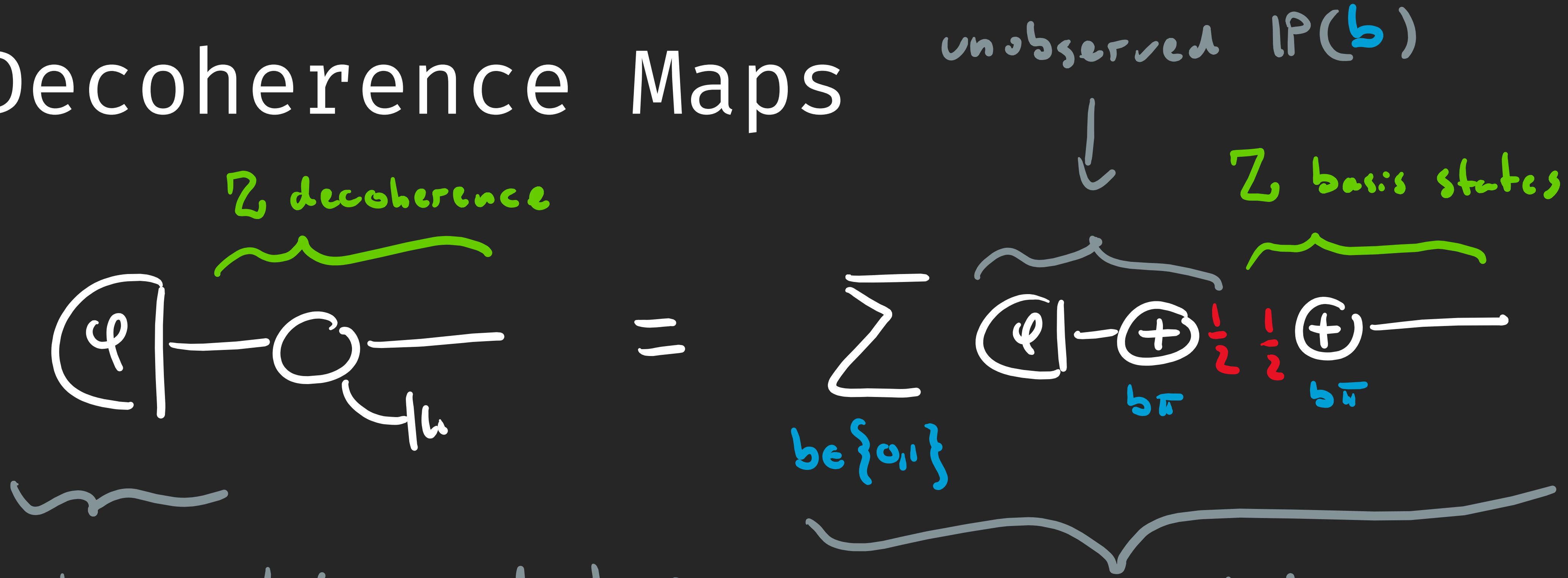
photon and qubit interact, becoming entangled

photon is lost forever to environment

Decoherence Maps



Decoherence Maps



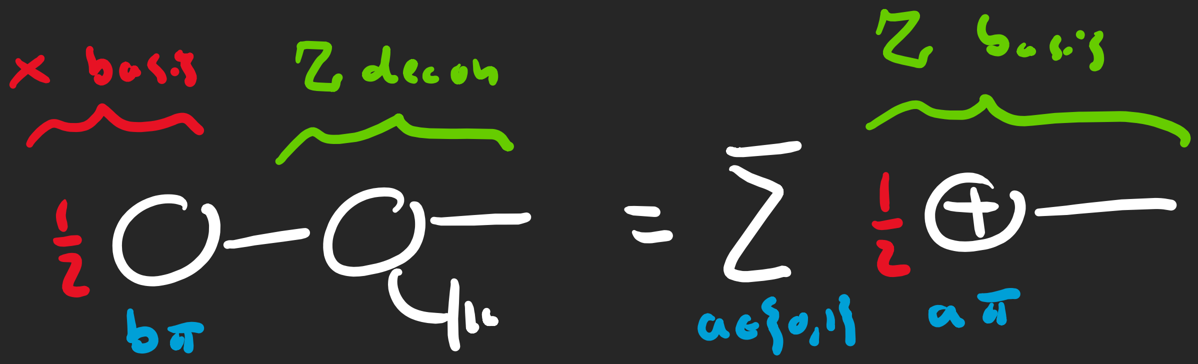
quantum state $|\varphi\rangle$ $\overset{\text{decohere}}{\longmapsto}$ classical state

$$\mathbb{P}(0|\varphi)\,|0\rangle\langle 0| + \mathbb{P}(1|\varphi)\,|1\rangle\langle 1|$$

Decoherence Maps

same basis states

= no change



other basis state

= total uncertainty

~~IBMQ~~ Superconducting QC Measurements