

Introduction to Density matrices

Introduction to quantum computing using QSim

Jothishwaran C A

Indian Institute of Technology Roorkee

email: jc_a@ece.iitr.ac.in

The Identity Matrix

- Every single qubit state $|\psi\rangle$ can be represented in the computational basis as follows:

$$|\psi\rangle = \underbrace{\langle 0|\psi\rangle|0\rangle}_{\text{coordinates}} + \underbrace{\langle 1|\psi\rangle|1\rangle}_{\text{coordinates}}$$

moving the symbols around a bit it is possible to write:

$$\begin{aligned} |\psi\rangle &= |0\rangle\langle 0|\psi\rangle + |1\rangle\langle 1|\psi\rangle \\ &= (\underbrace{|0\rangle\langle 0| + |1\rangle\langle 1|}_{\text{no gate}})|\psi\rangle \end{aligned}$$

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

"no gate" gate

- The outer product sum given in parentheses is doing nothing to change $|\psi\rangle$.
- Therefore the object $|0\rangle\langle 0| + |1\rangle\langle 1|$ performs the same role as the Identity matrix.

The Identity Matrix: general results

- Everything done in the previous slide is true for any orthonormal single qubit basis: $\{|a\rangle, |b\rangle\}$

$$\Rightarrow |a\rangle\langle a| + |b\rangle\langle b| = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \text{ for all orthonormal basis.}$$

- This result can be generalized to multi-qubit states as well.
- These discussions will only deal with single qubit states and operators
- Outer products can be used to define transformations that can be applied to qubits.
- More generally outer products between complex vectors can be used to define all kinds of matrices.

Outer product matrices: the Hamiltonian

- It is possible to define matrices of the form:

$$\hat{H}(t) = r_0|0\rangle\langle 0| + z(t)|0\rangle\langle 1| + \bar{z}(t)|1\rangle\langle 0| + r_1|1\rangle\langle 1| ; \quad r_0, r_1 \in \mathbb{R}$$

$$\hat{H}(t) = \begin{bmatrix} r_0 & z(t) \\ \bar{z}(t) & r_1 \end{bmatrix} \quad z(t) \in \mathbb{C}$$

t - time

- This matrix is a Hermitian matrix and has the property:

physical $\hat{H}^\dagger(t) = \hat{H}(t)$

- Such matrices ultimately contain all the information about a qubit/quantum system.

From Hermitian to Unitary matrices

$\hat{H}(t)$, the Hamiltonian
also defines the gate operation

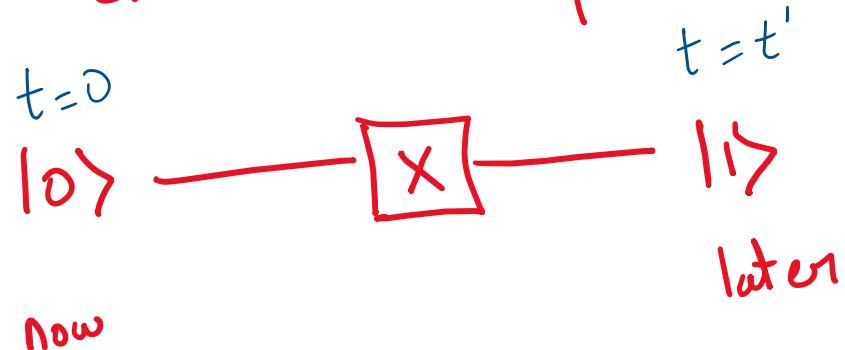
- The time evolution of any state $|\psi\rangle$ is given by:

single-qubit

$$i\hbar \frac{d}{dt} |\psi\rangle = \hat{H}(t) |\psi\rangle \quad - \text{differential equation}$$

this is one form of the Schrödinger equation

In Quantum computation : The state of the qubit
changes over time



Solving the Schrödinger Eqn will give the following relation

$$|\psi(t=t')\rangle = U(0,t') |\psi(t=0)\rangle$$

on
$$\boxed{U(0,t') |\psi(t=0)\rangle = |\psi(t=t')\rangle} \rightarrow \text{form of all gate transformation}$$

$$\underline{X|0\rangle} = \underline{|+\rangle}$$

now later

$$\underline{H|0\rangle} = \underline{|-\rangle}$$

If $\hat{H}(t)$ is Hermitian

then, $U(0,t')$ is unitary

$$U^+(0,t') = U(t',0) \rightarrow \begin{array}{l} \text{Unitary} \\ \text{time evolution} \\ \text{operator} \end{array}$$
$$U^+U = UU^+ = I$$

A Brief comment on Gate Sets

Gate set: $R_x, R_y, \sqrt{x}, S, T, CX \rightarrow$ for each there is
a different $\hat{H}(t)$
 $\Rightarrow Z(t)$ is a different

Summary:

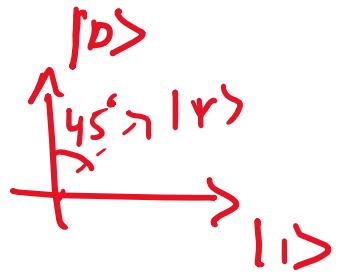
qubit is defined by it's Hamiltonian

\downarrow
 U {time evolution operator}

$U^\dagger U = U U^\dagger = I$; U - we consider this to be
the gate

A Question

Photon polarization - $|45^\circ\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$



If a photon in $|45^\circ\rangle$ is incident on a Polarizer oriented along $|0\rangle$, then 50% of the photons are transmitted

The same polarizer, but now a light source that randomly chooses to emit a photon in $|0\rangle$ or $|1\rangle$ with 50% probability. What fraction of the photons are transmitted?

$$|\Psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$$

Vertical Polarizer

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

Transmission Prob. = 50%.

what is the difference ??
Ans: different Transmission prob.

Transmission probability = 50%

If different, how to distinguish ??



Trans. Prob. = 100%.

$$\text{Trans. Prob.} = 0.5 \times 0.5 + 0.5 \times 0.5$$

$$= 0.5$$

Polarizer at angle θ

$$\text{Trans. Prob.} = |\cos(45^\circ - \theta)|^2$$

$$\begin{aligned}\text{Trans. Prob.} &= 0.5 \times |\cos \theta|^2 + 0.5 \times |\sin \theta|^2 \\ &= 0.5\end{aligned}$$

$$|\Psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$$

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

- Superposition
- A physically state from both $|0\rangle$ & $|1\rangle$
- Every photon has same polarization
- Transmission Prob. varies with Polarizer angle

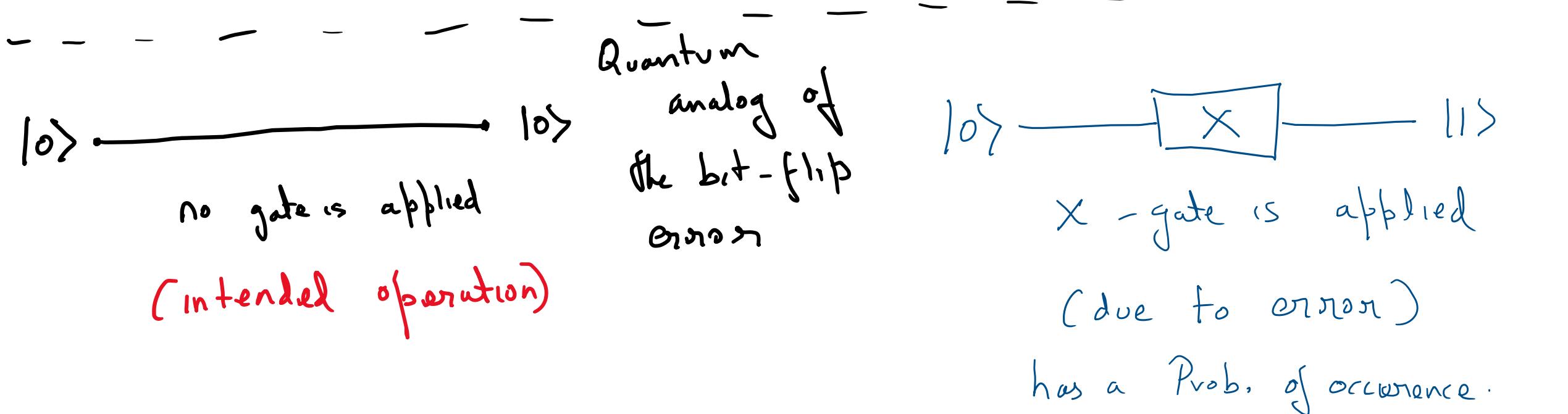
- No superposition
- A mixture, each photon is either in $|0\rangle$ or $|1\rangle$
- Mixture of photons with different polarization
- Transmission probability is const. (for this particular case)

Red is represented by $|y\rangle$ - a vector in \mathbb{C}^2

What mathematical object represents a mixture? \rightarrow Density matrix
[Should describe both red & blue cases]

Density Matrices were originally introduced

Jon von Neumann



Probability of error = 30% = 0.3

\Rightarrow 70% of the time the final state of the qubit is $|0\rangle$

& 30% of the time the final state of the qubit is $|1\rangle$

$$\rho = p_0 |0\rangle\langle 0| + p_1 |1\rangle\langle 1| \rightarrow p_0 - \text{prob. of finding } |0\rangle$$

$$= 0.7 \log_{10} + 0.3 \log_{10}$$

$$= 0.7 \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + 0.3 \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \Rightarrow P = \begin{bmatrix} 0.7 & 0 \\ 0 & 0.3 \end{bmatrix} - \text{density matrix of a mixed state}$$

In the limit error prob. $\rightarrow 0$

p_0 becomes closer 1 \Rightarrow the qubit is purely $|0\rangle$
 p_1 " " 0

$\therefore \rho = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = |0\rangle\langle 0|$ \rightarrow density matrix for a pure state.

The argument developed here is not only valid for $|0\rangle + |1\rangle$, it is valid for any number of states in a statistical mixture.

General form of Density operator

(can also be multi-qubit)

If a system is in a mixture of

States: $\{|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle \dots |\psi_n\rangle\}$

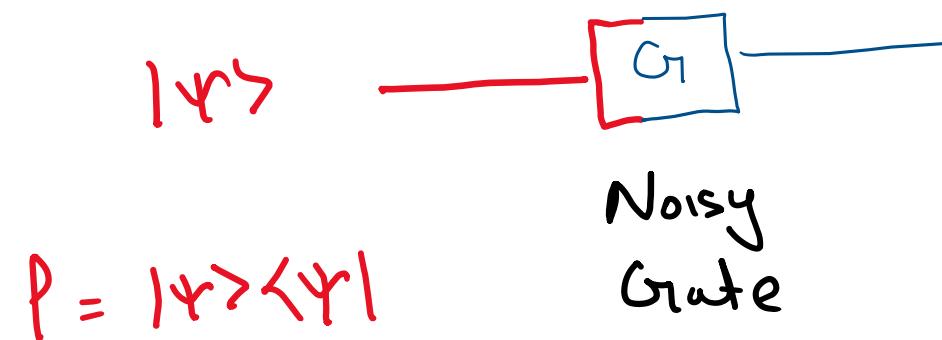
Probabilities $\{p_1, p_2, p_3 \dots p_n\}$

$$\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i| \quad ; \quad \rho^+ = \rho \quad ; \quad \text{Tr}(\rho) = 1$$

(qubit state)

[sum of diagonal elements]

Pure State



$$\sum_i p_i | \psi_i \rangle \langle \psi_i | \rightarrow$$

mixed state

$2^n \times 2^n$ matrix
with complex
elements

Noiseless gates : Unitary Transformations (U - a single operator)
- reversible

Noisy gates : Super operators - Krauss Operators

[primary aim
of QSim]

Collection of
operators

Not reversible

Lindblad operators