## Introduction to Quantum Algorithms

K.C. Kong

Physics and Astronomy
University of Kansas


## YONSEI



## HW

- Install Qiskit / PennyLane / TensorFlow Quantum in your laptop or google colab.
- Create your IBM Quantum account (for IBMQ Lab and IBMQ Composer).
- Try simple Qiskit examples
- Example 1 with single gates on colab
- Example 2 with single qubit circuit on colab
- Example 3 with multiple qubits and measurements
- Check out NVIDIA CUDA Quantum for hybrid quantumclassical computing platform.
- Choose one QML example and run a sample code.


## ML SC ( <br> Google Summer of Code 2023

## Introduction

In 2023 ML 4 SCl is participating in the program as a GSoC umbrella organization. The ML4SCI organization has partnered with the Google Summer of Code in 2023 to broaden student participation in machine learning projects over a wide variety of scientific fields. ML4SCI participants will be mentored by scientists at top research universities and laboratories on research projects at the cutting edge of science. Projects span a wide range of scientific domains, including physics, astronomy, planetary science, quantum information science and others.

## For Students

In 2023 GSoC students work with their mentors for 175 hrs to produce open-source codes that apply machine learning solutions to solve science problems. Projects span three evaluation periods that allow for students and mentors to collaborate on their project and evaluate student progress. Detailed rules for the GSOC program can be found here. Interested students should look at the ideas page and contact the mentors. Candidates will be asked to complete an evaluation test for each project they apply to demonstrate the skills needed for the respective projects. In the next step, students will produce a

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## Very brief history of quantum computing

- 1924 The term "quantum mechanics" used by M. Born
- 1925 Formulation of matrix mechanics by Heisenberg, Born, Jordan
- 1925-1927: Copenhagen interpretation
- 1930 "The principles of quantum mechanics" by Dirac
- 1935 Einstein, Podolsky and Rosen
- 1935 "Quantum entanglement" and Schrödinger's cat by Schrodinger and Einstein
- 1947 "Spooky action at a distance" in a letter to M. Born by A. Einstein
- 1976 Attempt to create quantum information theory
- 1980 Quantum mechanical model of Turing machine by Benioff (ANL)
- 1981 "Simulating Physics with Computers" by Feynman
- 1985 Quantum Turing machine by Deutsch
- 1992 Deutsch-Jozsa algorithm
- 1993 First paper on quantum teleportation
- 1994 Shor's factoring algorithm (cf RSA encryption)
- 1996 Grover search algorithm (Bell)
- 2004 First five photon entanglement by China
- 2011 First commercially available quantum computer (D-Wave)
- 2017 First quantum teleportation of independent single-photon qubit ( 14 km ) by China
- 2018 US National Quantum Initiative Act
- 2019 Google quantum supremacy
- 2022 Nobel prize (Aspect, Clauser, Zeilinger) for violation of Bell's inequality
- 2022433 qubits by IBM
- 2023 Breakthrough Prize (Bennet, Brassard, Shor, Deutsch)


## Topics to discuss

- Introduction to QM and Single qubit
- System with two or more qubits
- Quantum algorithms
- Quantum Machine Learning
- https://kckong.ku.edu/Yonsei2023/
- https://ihepco.yonsei.ac.kr/event/247/


## Topics to discuss

1. Single qubit, Dirac notation, Bloch sphere and measurements
2. Quantum circuits, singlet qubit gate, two qubit gates, three qubit gates, no cloning, superdense coding, teleportation
3. Quantum algorithms, data embedding, Deutsch algorithm, DeutschJozsa, Bernstein-Vazirani algorithm, Simon's algorithm
4. Quantum Fourier Transformation and quantum phase estimation
5. Shor's algorithm and Grover's algorithm
6. Quantum machine learning, distance-based classifier
7. Quantum optimization, QUBO, Adiabatic theorem, variational quantum algorithms
8. QAOA, FALQON, ADAPT-QAOA
9. Single qubit-classifier using data re-uploading
10. Harrow-Hassidim-Lloyd Algorithm (Ax=b)
11. Quantum error correction, bit flip error correction, stabilizer formalism, phase flip error correction

## Machine Learning?

## Universal Approximation Theorem

- A feed-forward network with a single hidden layer containing a finite number of neurons can approximate continuous functions on compact subsets of R, 'under mild assumptions on the activation function.

Let $\varphi: \mathbb{R} \rightarrow \mathbb{R}$ be a nonconstant, bounded, and continuous function (called the activation function). Let $I_{m}$ denote the $m$-dimensional unit hypercube $[0,1]^{m}$. The space of real-valued continuous functions on $I_{m}$ is denoted by $C\left(I_{m}\right)$. Then, given any $\varepsilon>0$ and any function $f \in C\left(I_{m}\right)$, there exist an integer $N$, real constants $v_{i}, b_{i} \in \mathbb{R}$ and real vectors $w_{i} \in \mathbb{R}^{m}$ for $i=1, \ldots, N$, such that we may define:

$$
F(x)=\sum_{i=1}^{N} v_{i} \varphi\left(w_{i}^{T} x+b_{i}\right) \text { as an approximate realization of the function } f \text {; that is, }
$$

$$
|F(x)-f(x)|<\varepsilon \quad \text { for all } x \in I_{m} \text {. In other words, functions of the form } F(x) \text { are dense in } C\left(I_{m}\right) \text {. }
$$

- A. N. Kolmogorov, 1957
- G. Cybenko, 1989 with sigmoid activation

$$
S(x)=\frac{1}{1+e^{-x}}=\frac{e^{x}}{e^{x}+1}
$$

- K. Hornik, 1991, importance of the multilayer architecture
- Z. Lu et al, 2017, with deep neural network and ReLu activation


Let $p>0$ be a fixed number and $f(x)$ be a periodic function with period $2 p$, defined on $(-p, p)$. The Fourier series of $f(x)$ is a way of expanding the function $f(x)$ into an infinite series involving sines and cosines:

$$
\begin{equation*}
f(x)=\frac{a_{0}}{2}+\sum_{n=1}^{\infty} a_{n} \cos \left(\frac{n \pi x}{p}\right)+\sum_{n=1}^{\infty} b_{n} \sin \left(\frac{n \pi x}{p}\right) \tag{2.1}
\end{equation*}
$$

where $a_{0}, a_{n}$, and $b_{n}$ are called the Fourier coefficients of $f(x)$, and are given by the formulas

$$
\begin{align*}
a_{0}=\frac{1}{p} \int_{-p}^{p} f(x) d x, \quad a_{n} & =\frac{1}{p} \int_{-p}^{p} f(x) \cos \left(\frac{n \pi x}{p}\right) d x  \tag{2.2}\\
b_{n} & =\frac{1}{p} \int_{-p}^{p} f(x) \sin \left(\frac{n \pi x}{p}\right) d x
\end{align*}
$$








Neural network is a function-approximator.
Rectified Linear Unit
ReLU


$\operatorname{ReLu}=\max (0, x)$

$$
f(x)=x^{3}+x^{2}-x-1
$$



$$
\begin{aligned}
n_{1}(x) & =\operatorname{Relu}(-5 x-7.7) \\
n_{2}(x) & =\operatorname{Relu}(-1.2 x-1.3) \\
n_{3}(x) & =\operatorname{Relu}(1.2 x+1) \\
n_{4}(x) & =\operatorname{Relu}(1.2 x-.2) \\
n_{5}(x) & =\operatorname{Relu}(2 x-1.1) \\
n_{6}(x) & =\operatorname{Relu}(5 x-5) \\
F(x) & =-n_{1}(x)-n_{2}(x)-n_{3}(x) \\
& +n_{4}(x)+n_{5}(x)+n_{6}(x)
\end{aligned}
$$


(a)

(b) Input
layer
$1^{\text {st }}$ hidden layer
$2^{\text {nd }}$ hidden layer

Output layer


$$
y_{j}=f\left(\sum x_{i} \mathcal{w}_{i}\right) \quad y_{k}=f\left(\sum x_{j} \mathcal{w}_{j}\right) \quad y_{l}=f\left(\sum x_{k} \mathcal{w}_{k}\right)
$$

## Why Machine Learning?

## CHALLENGE: BIG DATA

Taken from J. Duarte's talk
, HL-LHC will reach 1 exabyte of data per year
1 PB = 1000 TB


Internet archive
~15 EB
1 EB = 1000 PB

SKA Phase 2 - mid-2020's
~1 EB science data
HL-LHC - 2026
~1 EB Physics data

# Dimensional Reduction in Collider Experiments and Phenomenological Studies 

## Dimensionality per event



Franceschini, Kim, Kong, Matchev, Park, Shyamsundar, 2206.13431
Review of Modern Physics

ML techniques applied at each stage



Theory

Phenomenology

The common goal is to find the optimal low-dimensional observables.

Data is obtained via InspireHEP
Che number of papers (in high energy physics) that has a keyword "Machine Learning", "Deep Learning", "Artificial Intelligence" or "Neural Networks" in their title.
he number of papers that has a keyword "Quantum Computer", "Quantum Computing", "Quantum Annealing" or "Quantum Machine Learning" in their title.


## Why Quantum Computing?

- Quantum simulation
- Cryptography
- Mathematics: factoring, hidden subgroup program, discrete logarithm problem
- Optimization
- Search algorithm
- Quantum Machine Learning
- Quantum Advantages?
- Learns better with small \# of data
- Faster convergence
- Less \# of parameters
- What are the interesting problems?


$$
|\psi\rangle=\cos \frac{\theta}{2}|0\rangle+e^{i \varphi} \sin \frac{\theta}{2}|1\rangle
$$

## QML: Variational Quantum Algorithms



## Single Qubit

- Notation: alternative representation
- Normalization conditions
- Quantum measurements
- Different bases
- Operators on qubits
- Simple quantum circuits


## Qubits and Pauli's matrices

$$
\begin{aligned}
& \sigma_{1}=\sigma^{x}=\left(\begin{array}{ll}
0 & 1 \\
1 & 0
\end{array}\right) \\
& \sigma_{2}=\sigma^{y}=\left(\begin{array}{cc}
0 & -i \\
i & 0
\end{array}\right) \\
& \sigma_{3}=\sigma^{z}=\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)
\end{aligned}
$$

- Qubit $(|\psi\rangle,|\psi\rangle) \equiv\langle\psi \mid \psi\rangle=1)$ :

$$
|\psi\rangle=\cos \frac{\theta}{2}|0\rangle+e^{i \phi} \sin \frac{\theta}{2}|1\rangle=\binom{\cos \frac{\theta}{2}}{e^{i \phi} \sin \frac{\theta}{2}}
$$

- Conjugate (dual vector or bra-vector):
$\langle\psi|=\cos \frac{\theta}{2}\langle 0|+e^{-i \phi} \sin \frac{\theta}{2}\langle 1|=\left(\begin{array}{ll}\cos \frac{\theta}{2} \quad e^{-i \phi} \sin \frac{\theta}{2}\end{array}\right)$
$\left[\sigma_{i}, \sigma_{j}\right] \equiv \sigma_{i} \sigma_{j}-\sigma_{j} \sigma_{i}=2 i \epsilon_{i j k} \sigma_{k} \cdot \mathrm{~A}$ set of all $|\psi\rangle$ (ket-vector) forms a vector space (Hilbert space)
$\left\{\sigma_{i}, \sigma_{j}\right\} \equiv \sigma_{i} \sigma_{j}+\sigma_{j} \sigma_{i}=2 \delta_{i j}$
- Pauli's matrices are generators of rotations in two
$\sigma_{i} \sigma_{j}=2 \delta_{i j}+i \epsilon_{i j k} \sigma_{k}$ dimensional complex plane.
$|0\rangle \equiv\binom{1}{0},|1\rangle \equiv\binom{0}{1}$

Computational basis

$$
R(\vec{\theta})=\exp \left(-i \frac{\vec{\theta} \cdot \vec{\sigma}}{2}\right)
$$

Hadamard basis

## Dirac Bracket Notation

- Consider a quantum system with two orthonormal states, $|0\rangle$ and $|1\rangle$ :

$$
\langle 0 \mid 0\rangle=\langle 1 \mid 1\rangle=1 \quad\langle 0 \mid 1\rangle=\langle 1 \mid 0\rangle=1 \quad\langle i \mid j\rangle=\delta_{i j}
$$

- In general, a qubit can be in an arbitrary superposition state $\psi=\alpha_{0}|0\rangle+\alpha_{1}|1\rangle$ with complex coefficients, $\alpha_{0}$ and $\alpha_{1}$, which are related to the probabilities to measure the state $|0\rangle$ and $|1\rangle$, correspondingly.

$$
\begin{aligned}
& P(0)=|\langle 0 \mid \psi\rangle|^{2}=\left|\alpha_{0}\right|^{2} \\
& P(1)=|\langle 1 \mid \psi\rangle|^{2}=\left|\alpha_{1}\right|^{2}
\end{aligned}
$$

- The total probability is equal to 1 , therefore $P(0)+P(1)=\left|\alpha_{0}\right|^{2}+\left|\alpha_{1}\right|^{2}=1$
- The two complex parameters $\alpha_{0}$ and $\alpha_{1}$ can be represented by the two real parameters (angles) $\theta$ and $\phi$ (considering the normalization condition, ignoring the overall phase)

$$
0 \leq \theta<\pi, 0 \leq \phi<2 \pi \quad|\psi\rangle=\cos \frac{\theta}{2}|0\rangle+e^{i \phi} \sin \frac{\theta}{2}|1\rangle=\binom{\cos \frac{\theta}{2}}{e^{i \phi} \sin \frac{\theta}{2}}
$$

## Bloch Sphere

- Each (normalized) state of the qubit can be uniquely associated with a point on the unit sphere.
$|\psi\rangle \longleftrightarrow(\theta, \phi) \longleftrightarrow \hat{r}=\left(\begin{array}{c}\sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta\end{array}\right)$
$|0\rangle: \theta=0, \phi=$ arbitrary $\longrightarrow \hat{r}=\left(\begin{array}{c}0 \\ 0 \\ 1\end{array}\right)$
$|1\rangle: \theta=\pi, \phi=$ arbitrary $\longrightarrow \hat{r}=\left(\begin{array}{c}0 \\ 0 \\ -1\end{array}\right)$


$|+i\rangle: \theta=\pi / 2, \phi=\pi / 2 \longrightarrow \hat{r}=\left(\begin{array}{l}0 \\ 1 \\ 0\end{array}\right)$




## Bloch Sphere

- $\{|0\rangle,|1\rangle\},\{|+\rangle,|-\rangle\},\{|+i\rangle,|-i\rangle\}$ are antipodal points on the Bloch sphere.
- Antipodal points are orthonormal, i.e., they represent two orthonormal qubit states (in Hilbert space)
- The antipodal point is obtained by

$$
\theta \rightarrow \pi-\theta, \quad \phi \rightarrow \pi+\phi
$$



$$
\begin{aligned}
|\tilde{\psi}\rangle= & \cos \frac{\pi-\theta}{2}|0\rangle+e^{i(\phi+\pi)} \sin \frac{\pi-\theta}{2}|1\rangle \\
= & \sin \frac{\theta}{2}|0\rangle-e^{i \phi} \cos \frac{\theta}{2}|1\rangle \\
\langle\tilde{\psi}|= & \sin \frac{\theta}{2}\langle 0|-e^{-i \phi} \cos \frac{\theta}{2}\langle 1| \\
\langle\tilde{\psi} \mid \psi\rangle= & \left(\sin \frac{\theta}{2}\langle 0|-e^{-i \phi} \cos \frac{\theta}{2}\langle 1|\right) \\
& \quad\left(\cos \frac{\theta}{2}|0\rangle+e^{i \phi} \sin \frac{\theta}{2}|1\rangle\right) \\
= & \sin \frac{\theta}{2} \cos \frac{\theta}{2}\langle 0 \mid 0\rangle-\cos \frac{\theta}{2} \sin \frac{\theta}{2}\langle 1 \mid 1\rangle=0
\end{aligned}
$$

## Standard Model

(Periodic Table for Elementary Particles)


## Standard Model

## (Periodic Table for Elementary Particles)




## Dirac and Vector Notation

- ket: $|a\rangle=\binom{a_{0}}{a_{1}}$, 2-dimensional complex vector
- bra: $\langle b|=(|b\rangle)^{\dagger}=\binom{b_{0}}{b_{1}}^{\dagger}=\left(b_{0}^{*} b_{1}^{*}\right)$
- Inner product: $\langle b \mid a\rangle=\left(b_{0}^{*} b_{1}^{*}\right)\binom{a_{0}}{a_{1}}=b_{0}^{*} a_{0}+b_{1}^{*} a_{1}$
- If $a \neq b,\langle b \mid a\rangle$ is in general a complex number.
- Outer product: $|a\rangle\langle b|=\binom{a_{0}}{a_{1}}\left(b_{0}^{*} b_{1}^{*}\right)=\binom{a_{0} b_{0}^{*} a_{0} b_{1}^{*}}{a_{1} b_{0}^{*} a_{1} b_{1}^{*}}$
- Standard basis: $|0\rangle=\binom{1}{0}$ and $|1\rangle=\binom{0}{1}$

$$
\langle 0 \mid 0\rangle=\langle 1 \mid 1\rangle=1 \quad\langle 0 \mid 1\rangle=\langle 1 \mid 0\rangle=1 \quad\langle i \mid j\rangle=\delta_{i j}
$$

## Quantum Measurements

- When we perform a measurement onto an orthogonal basis, the qubit collapses to one of the basis states with probability given by the corresponding amplitude. For example, if we perform a projection onto z-axis (the states $|0\rangle$ and $|1\rangle$ ), we get $P(0)=|\langle 0 \mid \psi\rangle|^{2}=\cos ^{2} \frac{\theta}{2}$ and $P(1)=|\langle 1 \mid \psi\rangle|^{2}=\sin ^{2} \frac{\theta}{2}$.
- Born rule: the probability that a state $|\psi\rangle$ collapses during a projective measurement onto a basis $\left\{|x\rangle,\left|x^{\perp}\right\rangle\right\}$ is given by $P(x)=|\langle x \mid \psi\rangle|^{2}$ and $P\left(x^{\perp}\right)=\left|\left\langle x^{\perp} \mid \psi\right\rangle\right|^{2}$.

$$
|\psi\rangle=\cos \frac{\theta}{2}|0\rangle+e^{i \phi} \sin \frac{\theta}{2}|1\rangle=\binom{\cos \frac{\theta}{2}}{e^{i \phi} \sin \frac{\theta}{2}}
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- Points in the "Northern hemisphere" of the Bloch sphere are more likely to collapse to the North pole (the state $|0\rangle$ ).
- Points in the "Southern hemisphere" of the Bloch sphere are more likely to collapse to the South pole (the state |17).
- Points on the "equator" of the Bloch sphere $\theta=\frac{\pi}{2}$ are equally likely to go on the North Pole or South pole.


## Measurement in a different basis

- What if we want to measure our state $|\psi\rangle=\cos \frac{\theta}{2}|0\rangle+e^{i \phi} \sin \frac{\theta}{2}|1\rangle$ in a different basis? For example,

$$
\begin{aligned}
& \theta=\frac{\pi}{2}, \phi=0 \longrightarrow|+\rangle=\cos \frac{\theta}{4}|0\rangle+\sin \frac{\theta}{4}|0\rangle=\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle) \\
& \theta=\frac{\pi}{2}, \phi=\pi \longrightarrow|-\rangle=\cos \frac{\theta}{4}|0\rangle+e^{-i \pi} \sin \frac{\theta}{4}|0\rangle=\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)
\end{aligned}
$$

- Born rule: the probability that a state $|\psi\rangle$ collapses during a projective measurement onto a basis $\left\{|x\rangle,\left|x^{\perp}\right\rangle\right\}$ is given by

$$
P(x)=|\langle x \mid \psi\rangle|^{2} \quad P\left(x^{\perp}\right)=\left|\left\langle x^{\perp} \mid \psi\right\rangle\right|^{2}
$$

## Measurement in a different basis

Rewrite the state $|\psi\rangle$ in the new basis $|+\rangle$ and $|-\rangle$

$$
\begin{gathered}
|0\rangle=\frac{1}{\sqrt{2}}(|+\rangle+|-\rangle) \quad|1\rangle=\frac{1}{\sqrt{2}}(|+\rangle-|-\rangle) \\
|\psi\rangle=\cos \frac{\theta}{2}|0\rangle+\sin \frac{\theta}{2} e^{i \phi}|1\rangle=\frac{1}{\sqrt{2}} \cos \frac{\theta}{2}(|+\rangle+|-\rangle)+\frac{1}{\sqrt{2}} \sin \frac{\theta}{2} e^{i \phi}(|+\rangle-|-\rangle) \\
=\frac{1}{\sqrt{2}}\left(\cos \frac{\theta}{2}+\sin \frac{\theta}{2} e^{i \phi}\right)|+\rangle+\frac{1}{\sqrt{2}}\left(\cos \frac{\theta}{2}-\sin \frac{\theta}{2} e^{i \phi}\right)|-\rangle \\
P(+)=\left|\frac{1}{\sqrt{2}}\left(\cos \frac{\theta}{2}+\sin \frac{\theta}{2} e^{i \phi}\right)\right|^{2} \quad P(-)=\left|\frac{1}{\sqrt{2}}\left(\cos \frac{\theta}{2}-\sin \frac{\theta}{2} e^{i \phi}\right)\right|^{2}
\end{gathered}
$$

## Quantum Measurements

- Sequential selective measurement:

- what is the probability of obtaining $|c\rangle$ ?
- Probabilities are multiplicative, we get $|\langle c \mid b\rangle|^{2}|\langle b \mid a\rangle|^{2}$
- Now let us sum over $b$ to consider the total probability for going through all possible $b$ routes.


$$
\begin{aligned}
\text { sum of probabilities } & =\sum_{b}|\langle c \mid b\rangle|^{2}|\langle b \mid a\rangle|^{2} \\
& =\sum_{b}\langle c \mid b\rangle\langle b \mid a\rangle\langle a \mid b\rangle\langle b \mid c\rangle
\end{aligned}
$$

## Quantum Measurements

- Now let us sum over $b$ to consider the total probability for going through all possible $b$ routes.

$$
|a\rangle \underset{\substack{ \\\longrightarrow \\\left|b^{\prime \prime}\right\rangle}}{\longrightarrow}|b\rangle \longrightarrow|c\rangle
$$

$$
\begin{aligned}
\text { sum of probabilities } & =\sum_{b}|\langle c \mid b\rangle|^{2}|\langle b \mid a\rangle|^{2} \\
& =\sum_{b}\langle c \mid b\rangle\langle b \mid a\rangle\langle a \mid b\rangle\langle b \mid c\rangle
\end{aligned}
$$

- If B -filter is absent, probability is $|\langle c \mid a\rangle|^{2}$


$$
|\langle c \mid a\rangle|^{2}=\left|\sum_{b}\langle c \mid b\rangle\langle b \mid a\rangle\right|^{2}=\sum_{b, b^{\prime}}\langle c \mid b\rangle\langle b \mid a\rangle\left\langle a \mid b^{\prime}\right\rangle\left\langle b^{\prime} \mid c\right\rangle
$$

## Quantum Circuits

- Quantum gates are repressed by unitary transformations (matrices), $U^{\dagger} U=U U^{\dagger}=I$ or $U^{-1}=U^{\dagger}$.

- A single qubit has 2 basis states, $|+\rangle=\binom{1}{0}$ and $|-\rangle=\binom{0}{1}$

$$
U=U_{00}|0\rangle\langle 0|+U_{01}|0\rangle\langle 1|+U_{10}|1\rangle\langle 0|+U_{11}|1\rangle\langle 1|=\left(\begin{array}{cc}
U_{00} & U_{01} \\
U_{10} & U_{11}
\end{array}\right)
$$

- Single qubit gates: X, Y, Z, Hadamard, phase shift etc
- Two qubit gates: Controlled, SWAP gate, Controlled Phase shift, etc
- Three quiet gates: Toffoli gates etc


## Single Qubit Gates

- X gate $=$ Not operator $=\sigma_{X}=$ bit flip $=$ NOT gate

$$
\begin{gathered}
\square \begin{array}{c}
\mathrm{x}
\end{array} \\
\sigma_{X}=X=\left(\begin{array}{ll}
0 & 1 \\
1 & 0
\end{array}\right)=|0\rangle\langle 1|+|1\rangle\langle 0| \\
\left.\sigma_{x}|0\rangle=|1\rangle \quad \sigma_{x}|j\rangle=|j \oplus=| 0\right\rangle
\end{gathered}
$$

- Interpretation on the Bloch sphere
- rotation around x-axis by $\pi$
- maps $|0\rangle \longrightarrow|1\rangle$ and $|1\rangle \longrightarrow|0\rangle$
- maps $|+i\rangle \longrightarrow|-i\rangle$ and $|-i\rangle \longrightarrow|+i\rangle$

$$
| \pm i\rangle=\frac{1}{\sqrt{2}}(|0\rangle \pm i|1\rangle)
$$

## Single Qubit Gates: Z-gate

- Z gate $=\sigma_{Z}=$ phase flip


$$
\begin{aligned}
& \sigma_{Z}|0\rangle=+|0\rangle \quad \sigma_{Z}|1\rangle=-|1\rangle \quad \sigma_{Z}|j\rangle=(-1)^{j}|j\rangle \\
& \sigma_{Z}|+\rangle=\left(\begin{array}{cc}
1 & 0 \\
0 & 01
\end{array}\right) \frac{1}{\sqrt{2}}\binom{1}{1}=\frac{1}{\sqrt{2}}\binom{1}{-1}=|-\rangle \\
& \sigma_{Z}|-\rangle=\left(\begin{array}{cc}
1 & 0 \\
0 & 01
\end{array}\right) \frac{1}{\sqrt{2}}\binom{1}{-1}=\frac{1}{\sqrt{2}}\binom{1}{1}=|+\rangle
\end{aligned}
$$

- Phase flip = rotation around z -axis by $\pi$

$$
\begin{aligned}
\sigma_{Z}|+i\rangle & =|-i\rangle \\
\sigma_{Z}|-i\rangle & =|+i\rangle
\end{aligned}
$$

## Single Qubit Gates: Y and phase shift

- Y gate $=\sigma_{Y}=$ bit and phase flip $=$ rotation around y -axis by $\pi$

$$
\begin{array}{ll}
\sigma_{Y}=Y=\left(\begin{array}{cc}
0 & -i \\
i & 0
\end{array}\right)=i \sigma_{X} \sigma_{Z} \\
\sigma_{Y}|+i\rangle=+|+i\rangle & \sigma_{Y}|+\rangle=-i|-\rangle
\end{array} \begin{array}{ll} 
\\
\sigma_{Y}|0\rangle=+i|1\rangle \\
\sigma_{Y}|-i\rangle=-|-i\rangle & \sigma_{Y}|-\rangle=+i|+\rangle
\end{array} \begin{gathered}
\sigma_{Y}|1\rangle=-i|0\rangle
\end{gathered}
$$

- Phase shift operator: $R_{\phi}=\left(\begin{array}{cc}1 & 0 \\ 0 & e^{i \phi}\end{array}\right)=P_{\phi}$

For $\phi=\pi, \quad R_{\pi}=Z=\left(\begin{array}{cc}1 & 0 \\ 0 & -1\end{array}\right) \quad$ For $\phi=\pi / 4$,
For $\phi=\pi / 2, \quad R_{\pi / 2}=S=\left(\begin{array}{cc}1 & 0 \\ 0 & i\end{array}\right)=\sqrt{Z} \quad R_{\pi}=T=\left(\begin{array}{cc}1 & 0 \\ 0 & e^{i \pi / 4}\end{array}\right)=\sqrt[4]{Z}$

## Single Qubit Gates

- X gate $=$ Not operator $=\sigma_{X}=$ bit flip $=$ NOT gate


$$
\begin{aligned}
\sigma_{X}|0\rangle & =|1\rangle \\
\sigma_{X}|1\rangle & =|0\rangle
\end{aligned}
$$

$$
\sigma_{X}=X=\left(\begin{array}{ll}
0 & 1 \\
1 & 0
\end{array}\right)=|0\rangle\langle 1|+|1\rangle\langle 0|
$$

$$
\sigma_{X}|j\rangle=|j \oplus 1\rangle
$$

- Z gate $=\sigma_{Z}=$ phase flip

$$
\sigma_{Z}=Z=\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)=|0\rangle\langle 0|-|1\rangle\langle 1|
$$



$$
\sigma_{Z}|0\rangle=+|0\rangle \quad \sigma_{Z}|1\rangle=-|1\rangle \quad \sigma_{Z}|j\rangle=(-1)^{j}|j\rangle
$$

- Y gate $=\sigma_{Y}=$ bit and phase flip

$$
\sigma_{Y}=Y=\left(\begin{array}{cc}
0 & -i \\
i & 0
\end{array}\right)=i \sigma_{X} \sigma_{Z} \quad \sigma_{Y}|j\rangle=i(-1)^{j}|j \oplus 1\rangle
$$

## Single Qubit Gates

- Hadamard operator: to switch between $Z$ and $X$ basis.

$$
\begin{aligned}
& -H=\frac{1}{\sqrt{2}}\left(\begin{array}{cc}
1 & 1 \\
1 & -1
\end{array}\right)=\frac{1}{\sqrt{2}}(|0\rangle\langle 0|+|0\rangle\langle 1|+|1\rangle\langle 0|-|1\rangle\langle 1|) \\
& H|0\rangle=\frac{1}{\sqrt{2}}\left(\begin{array}{cc}
1 & 1 \\
1 & -1
\end{array}\right)\binom{1}{0}=\frac{1}{\sqrt{2}}\binom{1}{1}=|+\rangle \quad H|+\rangle=|0\rangle \quad H|x\rangle=\frac{1}{\sqrt{2}}\left(|0\rangle+(-1)^{x}|1\rangle\right) \\
& H|1\rangle=\frac{1}{\sqrt{2}}\left(\begin{array}{cc}
1 & 1 \\
1 & -1
\end{array}\right)\binom{0}{1}=\frac{1}{\sqrt{2}}\binom{1}{-1}=|-\rangle \quad H|-\rangle=|1\rangle
\end{aligned}
$$

- The operator SH changes between the $Z$ and $Y$ basis.
- Most general 2 by 2 unitary matrix:

$$
\begin{aligned}
& U^{\dagger} U=1 \longrightarrow 4 \text { conditions } \\
& 2 \times 4=8 \text { parameters }
\end{aligned} \quad U=\left(\begin{array}{cc}
\cos \frac{\theta}{2} & e^{-i \lambda} \sin \frac{\theta}{2} \\
e^{i \phi} \sin \frac{\theta}{2} & e^{i(\phi+\lambda)} \cos \frac{\theta}{2}
\end{array}\right)
$$

## System with two or more qubits

- $H_{i}$ : Hilbert space spanned by $\{|0\rangle,|1\rangle\}$
- $H \equiv H_{1} \otimes H_{2}$ is called the Hilbert space of the combined system (tensor product space of $H_{1}$ and $H_{2}$.

|  | $H_{1}$ | $H_{2}$ | $H_{1} \otimes H_{2}$ |
| :--- | :---: | :--- | :--- |
| $\operatorname{dim}\left(H_{1}\right)=2=\operatorname{dim}\left(H_{2}\right)$ | $\|0\rangle$ | $\|0\rangle$ | $\|0\rangle=\|0\rangle \otimes\|0\rangle=\|00\rangle$ |
| $\operatorname{dim}\left(H_{1} \otimes H_{2}\right)=4$ | $\|1\rangle$ | $\|1\rangle$ | $\|1\rangle=\|0\rangle \otimes\|1\rangle=\|01\rangle$ |
|  |  |  | $\|2\rangle=\|1\rangle \otimes\|0\rangle=\|10\rangle$ |
|  |  | $\|3\rangle=\|1\rangle \otimes\|1\rangle=\|11\rangle$ |  |

- A system of two spin-1/2 particles (qubits): $2 \otimes 2=3 \oplus 1$
- n -qubit system:
computational basis or standard basis

$$
\begin{aligned}
|\psi\rangle= & \alpha_{0}|0 \cdots 00\rangle+\alpha_{1}|0 \cdots 01\rangle+\alpha_{2}|0 \cdots 10\rangle+\cdots+\alpha_{2^{n}-1}|1 \cdots 11\rangle \\
& \sum_{i=0}^{2^{n}-1}\left|\alpha_{i}\right|^{2}=1
\end{aligned}
$$

## Separable vs Entangled states

- Separable states: if a quantum state $|\psi\rangle$ is given by tensor product of two states, i.e., if $|\psi\rangle=|\alpha\rangle \otimes|\beta\rangle,|\psi\rangle$ is separable.

$$
|00\rangle=|0\rangle \otimes|0\rangle,|01\rangle=|0\rangle \otimes|1\rangle
$$

- Entangled states: if a quantum state is not separable, $|\psi\rangle$ is an entangled state.

$$
\begin{aligned}
|\psi\rangle & =\frac{1}{\sqrt{2}}(|00\rangle+|11\rangle) \\
|\phi\rangle=\frac{1}{\sqrt{2}}(|00\rangle+|01\rangle) & =\frac{1}{\sqrt{2}}(|0\rangle \otimes|0\rangle+|0\rangle \otimes|1\rangle)=\frac{1}{\sqrt{2}}|0\rangle \otimes(|0\rangle+|1\rangle)
\end{aligned}
$$

$\longrightarrow$ if Bob measures $|0\rangle$, Alice still has $50 \%$ probability for $|0\rangle$ and $|1\rangle$.

- Entangled states are crucial resources for QC, as there is no classical analog.
- Top quark pair production leads to a system of two qubits.
- Density matrix: more later


## Tensor Products of Operators

- Linearity: $\left(a_{1} A_{1}+a_{2} A_{2}\right) \otimes=a_{1} A_{1} \otimes B+a_{2} A_{2} \otimes B$
- Each term in a tensor product acts on its own component:

$$
(A \otimes B)|m n\rangle=(A \otimes B)(|m\rangle \otimes|n\rangle)=A|m\rangle \otimes B|n\rangle
$$

- Multiplication:

$$
(A \otimes B)(C \otimes D)=(A C \otimes B D)
$$

Reducible representation

- Matrix representation:

$$
\begin{aligned}
& |a\rangle=a_{0}|0\rangle+a_{1}|1\rangle=\binom{a_{0}}{a_{1}} \\
& |b\rangle=b_{0}|0\rangle+b_{1}|1\rangle=\binom{b_{0}}{b_{1}}
\end{aligned}
$$

$$
|a\rangle \otimes|b\rangle=\binom{a_{0}}{a_{1}} \otimes\binom{b_{0}}{b_{1}}=\binom{a_{0}\binom{b_{0}}{b_{1}}}{a_{1}\binom{b_{0}}{b_{1}}}=\left(\begin{array}{l}
a_{0} b_{0} \\
a_{0} b_{1} \\
a_{1} b_{0} \\
a_{1} b_{1}
\end{array}\right)
$$

- Cartesian product: $A=A_{1} \times A_{2} \times \cdots \times A_{n}=\left\{\left(a_{1}, a_{2}, \cdots, a_{n}\right) \mid a_{i} \in A_{i}\right\}$

$$
\begin{array}{ll}
\vec{a}=\left(a_{1}, a_{2}, \cdots, a_{n}\right) \in A \quad 2 \vec{a}=\left(2 a_{1}, 2 a_{2}, \cdots, 2 a_{n}\right) & \\
\operatorname{dim}\left(A_{1} \times A_{2}\right)=\operatorname{dim}\left(A_{1}\right)+\operatorname{dim}\left(A_{2}\right) & \mathbb{R}^{2}=\mathbb{R} \times \mathbb{R}
\end{array}
$$

- Tensor product:

$$
\begin{aligned}
& A=A_{1} \otimes A_{2},\left|a_{1}\right\rangle \in A_{1},\left|a_{2}\right\rangle \in A_{2} \\
& 2\left(\left|a_{1}\right\rangle \otimes\left|a_{2}\right\rangle\right)=\left(2\left|a_{1}\right\rangle\right) \otimes\left|a_{2}\right\rangle=\left|a_{1}\right\rangle \otimes\left(2\left|a_{2}\right\rangle\right) \\
& \operatorname{dim}\left(A_{1} \otimes A_{2}\right)=\operatorname{dim}\left(A_{1}\right) \cdot \operatorname{dim}\left(A_{2}\right)
\end{aligned}
$$

## Tensor Products of Operators

- Tensor product:

$$
\begin{aligned}
& A=A_{1} \otimes A_{2},\left|a_{1}\right\rangle \in A_{1},\left|a_{2}\right\rangle \in A_{2} \\
& 2\left(\left|a_{1}\right\rangle \otimes\left|a_{2}\right\rangle\right)=\left(2\left|a_{1}\right\rangle\right) \otimes\left|a_{2}\right\rangle=\left|a_{1}\right\rangle \otimes\left(2\left|a_{2}\right\rangle\right) \\
& \operatorname{dim}\left(A_{1} \otimes A_{2}\right)=\operatorname{dim}\left(A_{1}\right) \cdot \operatorname{dim}\left(A_{2}\right)
\end{aligned}
$$

For $A$ with $\left\{\alpha_{1}, \alpha_{2}, \cdots, \alpha_{n}\right\}$ basis and $B$ with $\left\{\beta_{1}, \beta_{2}, \cdots, \beta_{m}\right\}$ basis, $\operatorname{dim}(A)=n$ and $\operatorname{dim}(B)=m$ $A \otimes B$ with basis $\left\{\alpha_{i} \beta_{j}\right\}, \operatorname{dim}(A \otimes B)=n \cdot m$

- Direct product:

For $A$ with operation • and $B$ with operation $\circ$, one can consider $A \times B$ with operation $\star$.

$$
\begin{array}{lll}
a \in A & (a, b) \in A \times B & (a, b) \star\left(a^{\prime}, b^{\prime}\right)=\left(a \bullet a^{\prime}, b \circ b^{\prime}\right) \in A \times B \\
b \in B &
\end{array}
$$

- For operators $\quad A=\left(\begin{array}{ll}a_{00} & a_{01} \\ a_{10} & a_{11}\end{array}\right), B=\left(\begin{array}{ll}b_{00} & b_{01} \\ b_{10} & b_{11}\end{array}\right)$



## Tensor Products of Operators

- Commuting operators: $I=\sigma_{0}, X=\sigma_{1}, Y=\sigma_{2}, Z=\sigma_{3}$

$$
\sigma_{i} \sigma_{j}=\delta_{i j}+i \epsilon_{i j k} \sigma_{k} \quad M=\sum_{i=0}^{3} a_{i} \sigma_{i}, a_{i} \in \mathbb{C} \quad H=H^{\dagger}=\sum_{i=0}^{3} a_{i} \sigma_{i}, a_{i} \in \mathbb{R}
$$

$$
\begin{array}{ll}
|a\rangle=a_{0}|0\rangle+a_{1}|1\rangle \in H_{1} & |b\rangle=b_{0}|0\rangle+b_{1}|1\rangle \in H_{2} \\
I_{1} \otimes I_{2}=I_{1} & I_{1} \otimes I_{2}=I_{2} \\
X_{1} \otimes I_{2}=X_{1} & I_{1} \otimes X_{2}=X_{2} \\
Y_{1} \otimes I_{2}=Y_{1} & I_{1} \otimes Y_{2}=Y_{2} \\
Z_{1} \otimes I_{2}=Z_{1} & I_{1} \otimes Z_{2}=Z_{2}
\end{array} \longrightarrow Z_{1} Z_{2}=Z_{2} Z_{1}
$$

act on 1st state
act on 2nd state

- Example:

$$
Z_{1}|0\rangle=+1|0\rangle
$$

$$
\begin{aligned}
|\psi\rangle & =\left|b_{1} b_{2} b_{3}\right\rangle \quad b_{i} \in\{0,1\} \\
\left\langle Z_{1}\right\rangle & =\langle\psi| Z_{1}|\psi\rangle=\left\langle b_{1} b_{2} b_{3}\right| Z_{1} \otimes I_{2} \otimes I_{3}\left|b_{1} b_{2} b_{3}\right\rangle=\left\langle b_{1}\right| Z_{1}\left|b_{1}\right\rangle\left\langle b_{2}\right| I_{2}\left|b_{2}\right\rangle\left\langle b_{3}\right| I_{3}\left|b_{3}\right\rangle \\
& =(-1)^{b_{1}} \quad Z_{1}|j\rangle=(-1)^{j}|j\rangle
\end{aligned}
$$

## Tensor Products of Operators

- Bell basis for a two-qubit system

$$
\begin{aligned}
& \left|\Phi^{+}\right\rangle=\frac{1}{\sqrt{2}}(|00\rangle+|11\rangle) \\
& \left|\Phi^{-}\right\rangle=\frac{1}{\sqrt{2}}(|00\rangle-|11\rangle) \\
& \left|\Psi^{+}\right\rangle=\frac{1}{\sqrt{2}}(|01\rangle+|10\rangle) \\
& \left|\Psi^{-}\right\rangle=\frac{1}{\sqrt{2}}(|01\rangle-|10\rangle)
\end{aligned}
$$

- Overall phase is not important.

$$
\begin{aligned}
& |v\rangle \otimes\left(e^{i \phi}|w\rangle\right)=\left(e^{i \phi}|v\rangle\right) \otimes|w\rangle=e^{i \phi}(|v\rangle \otimes|w\rangle) \\
& \frac{1}{\sqrt{2}}\left(e^{i \phi}|00\rangle+e^{i \phi}|11\rangle\right)=\frac{1}{\sqrt{2}} e^{i \phi}(|00\rangle+|11\rangle) \sim \frac{1}{\sqrt{2}}(|00\rangle+|11\rangle)
\end{aligned}
$$

- Relative phase is important and observable. The interference term is crucial in QM.

$$
\frac{1}{\sqrt{2}}\left(e^{i \phi}|00\rangle+|11\rangle\right) \neq \frac{1}{\sqrt{2}}\left(|00\rangle+e^{i \phi}|11\rangle\right) \neq \frac{1}{\sqrt{2}}(|00\rangle+|11\rangle)
$$

## Partial Trace

- Partial trace

$$
\begin{aligned}
& A \otimes B=\left(\begin{array}{ll}
a_{00} & a_{01} \\
a_{10} & a_{11}
\end{array}\right) \otimes\left(\begin{array}{ll}
b_{00} & b_{01} \\
b_{10} & b_{11}
\end{array}\right)=\left(\begin{array}{lll}
a_{00}\left(\begin{array}{ll}
b_{00} & b_{01} \\
b_{10} & b_{11}
\end{array}\right) & a_{01}\left(\begin{array}{ll}
b_{00} & b_{01} \\
b_{10} & b_{11}
\end{array}\right) \\
a_{10}\left(\begin{array}{lll}
b_{00} & b_{01} \\
b_{10} & b_{11}
\end{array}\right) & a_{11}\left(\begin{array}{ll}
b_{00} & b_{01} \\
b_{10} & b_{11}
\end{array}\right)
\end{array}\right) \\
& =\left(\begin{array}{llll}
a_{00} b_{00} & a_{00} b_{01} & a_{01} b_{00} & a_{01} b_{01} \\
a_{00} b_{10} & a_{00} b_{11} & a_{01} b_{10} & a_{01} b_{11} \\
a_{10} b_{00} & a_{10} b_{01} & a_{11} b_{00} & a_{11} b_{01} \\
a_{10} b_{10} & a_{10} b_{11} & a_{11} b_{10} & a_{11} b_{11}
\end{array}\right) \xrightarrow[\text { tracing out }]{\operatorname{tr}_{2}}\left(\begin{array}{ccc}
a_{00} \operatorname{tr}(B) & a_{01} \operatorname{tr}(B) \\
a_{10} \operatorname{tr}(B) & a_{11} & \operatorname{tr}(B)
\end{array}\right)=\operatorname{tr}(B)\left(\begin{array}{ll}
a_{00} & a_{01} \\
a_{10} & a_{11}
\end{array}\right) \\
& \operatorname{tr}_{1} \downarrow \begin{array}{l}
\text { tracing out } \\
\text { 1st system }
\end{array}
\end{aligned}
$$

$$
\left(\begin{array}{ll}
b_{00} \operatorname{tr}(A) & b_{01} \operatorname{tr}(A) \\
b_{10} \operatorname{tr}(A) & b_{11} \operatorname{tr}(A)
\end{array}\right)=\operatorname{tr}(A)\left(\begin{array}{ll}
b_{00} & b_{01} \\
b_{10} & b_{11}
\end{array}\right)
$$

## Direct Sum of Vector Space

- If $V$ with bases $\left\{\left|\alpha_{1}\right\rangle, \cdots,\left|\alpha_{n}\right\rangle\right\}$ and $W$ with $\left\{\left|\beta_{1}\right\rangle, \cdots,\left|\beta_{m}\right\rangle\right\}$ are vector spaces, $V \oplus W$ is also a vector space with bases $\left\{\left|\alpha_{1}\right\rangle, \cdots,\left|\alpha_{n}\right\rangle,\left|\beta_{1}\right\rangle, \cdots,\left|\beta_{m}\right\rangle\right\}$ and $\operatorname{dim}(V \oplus W)=\operatorname{dim}(V)+\operatorname{dim}(W)$

$$
\begin{array}{ll}
|v\rangle=\binom{x_{1}}{x_{2}} & |w\rangle=\binom{y_{1}}{y_{2}} \\
O_{1}|v\rangle=O_{1}\binom{x_{1}}{x_{2}} & O_{2}|w\rangle=O_{2}\binom{y_{1}}{y_{2}}
\end{array}
$$

$$
|v\rangle \oplus|W\rangle=\left(\begin{array}{l}
x_{1} \\
x_{2} \\
y_{1} \\
y_{2}
\end{array}\right)
$$

$$
\left(O_{1}+O_{2}\right)(|v\rangle \oplus|W\rangle)=\left(\begin{array}{ll}
O_{1} & 0 \\
0 & O_{2}
\end{array}\right)\left(\begin{array}{l}
x_{1} \\
x_{2} \\
y_{1} \\
y_{2}
\end{array}\right)
$$

