# Application of Quantum Computation to Quantum Field Theory

- Basics & Spin system -

## Masazumi Honda

(本多正純)





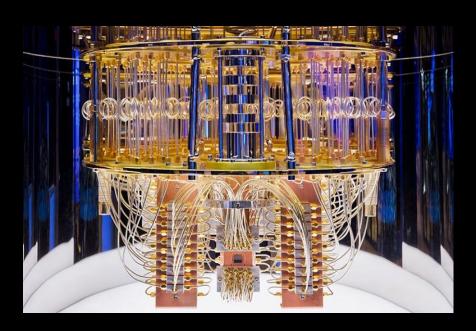


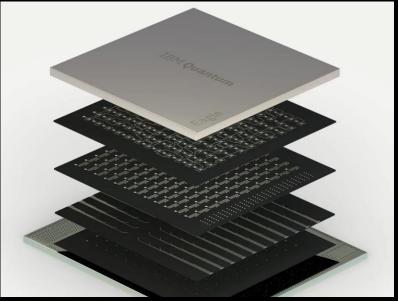






## Quantum computer sounds growing well...





#### **Article**

## Evidence for the utility of quantum computing before fault tolerance

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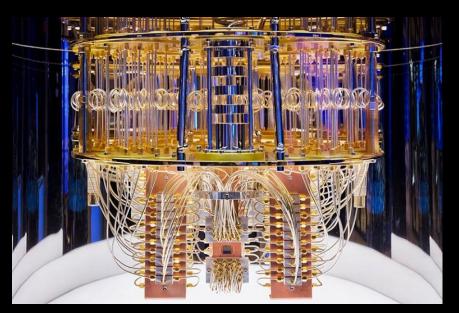
Accepted: 18 April 2023

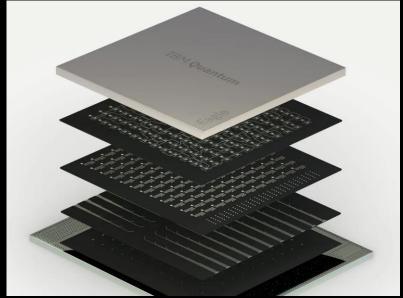
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Quantum computing promises to offer substantial speed-ups over its classical

## Quantum computer sounds growing well...



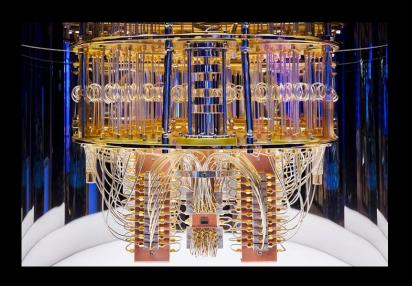


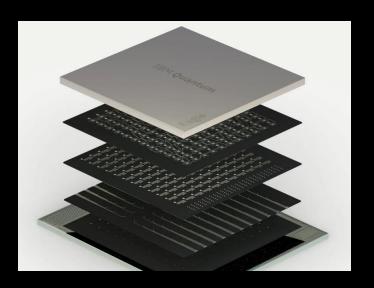
#### **Article**

## Evidence for the utility of quantum computing before fault tolerance

## How can we use it for us?

## Applications mentioned in media?





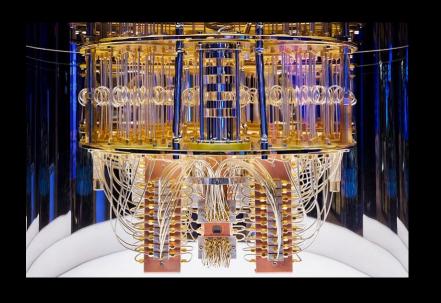


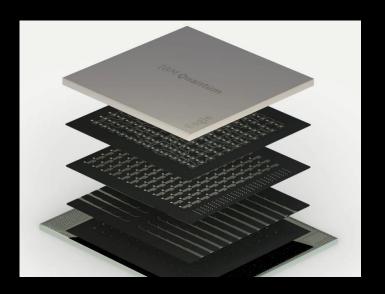






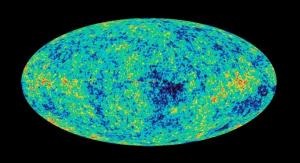
## In my mind...













#### This lecture is on

# Application of Quantum Computation to Quantum Field Theory (QFT)

• Generic motivation:

simply would like to use powerful computers?

Specific motivation:

#### This lecture is on

# Application of Quantum Computation to Quantum Field Theory (QFT)

#### • Generic motivation:

simply would like to use powerful computers?

#### Specific motivation:

Quantum computation is suitable for operator formalism

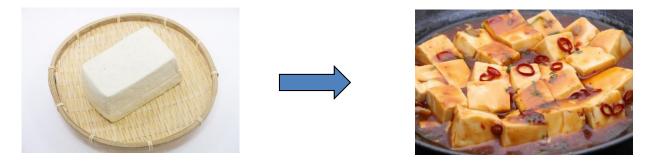
→ Liberation from infamous sign problem in Monte Carlo?

## Sign problem in Monte Carlo simulation

#### Conventional approach to simulate QFT: (this

(this point will be elaborated tomorrow)

1 Discretize Euclidean spacetime by lattice:



& make path integral finite dimensional:

$$\int D\phi \ \mathcal{O}(\phi)e^{-S[\phi]} \qquad \longrightarrow \qquad \int d\phi \ \mathcal{O}(\phi)e^{-S(\phi)}$$

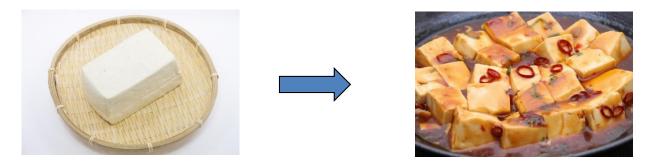


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② Numerically Evaluate it by (Markov Chain) Monte Carlo method regarding the Boltzmann factor as a probability:

$$\langle \mathcal{O}(\phi) \rangle \simeq \frac{1}{\sharp (\mathsf{samples})} \sum_{i \in \mathsf{samples}} \mathcal{O}(\phi_i)$$

### Sign problem in Monte Carlo simulation (Cont'd)

#### Markov Chain Monte Carlo:

$$\int d\phi \ \mathcal{O}(\phi) e^{-S(\phi)}$$
probability

problematic when Boltzmann factor isn't R≥0 & is highly oscillating

#### Examples w/ sign problem:

- -topological term complex action chemical potential indefinite sign of fermion determinant real time "  $e^{iS(\phi)}$  " much worse

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### In operator formalism,

sign problem is absent from the beginning

## Cost of operator formalism

We have to play with huge vector space

since QFT typically has ∞-dim. Hilbert space

regularization needed!

Technically, computers have to

memorize huge vector & multiply huge matrices

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Quantum computers do this job?

## Should we care now as "users"?

Quantum computers don't have sufficient powers yet.

Shouldn't we start to care after quantum supremacy comes?

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Quantum computers don't have sufficient powers yet.

Shouldn't we start to care after quantum supremacy comes?

#### I personally think:

<sup>3</sup> Many things to do even now in various contexts

(numerical/analytic/purely algorithmic/lat/th/ph/astro/cosmo)

For instance,

• we haven't established

how to put QCD efficiently on quantum computers

how to efficiently pick up various real time physics

(e.g. scattering/dynamical hadronization)

■ only few examples so far to take a serious continuum limit

## Plan of the lectures

(If 2nd lecture in each day ends early, then we start hands-on early)

### <u>Day 1</u>

- Lecture 1: introduction, basics of quantum computation
- Lecture 2: Spin system on quantum computer (QC)
- Hands-on 1: Basics on IBM's qiskit

## <u>Day 2</u>

- Lecture 3: Quantum field theory (QFT) on QC
- Lecture 4: QFT on QC, error correction & future prospects
- Hands-on 2: Time evolution of spin system

## Plan of lecture 1

- 0. Introduction
- 1. Qubits and gates
- 2. Some demonstrations in IBM Q Experience
- 3. Quantum simulation of Spin system
- 4. Summary

## Qubit = Quantum Bit

Qubit = Quantum system w/ 2 dim. Hilbert space

#### **Basis:**

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
 "computational basis"

#### Generic state:

$$\alpha |0\rangle + \beta |1\rangle$$
 w/  $|\alpha|^2 + |\beta|^2 = 1$ 

Ex.) Spin 1/2 system:

$$|0\rangle = |\uparrow\rangle, \qquad |1\rangle = |\downarrow\rangle$$

(We don't need to mind how it is realized as "users")

## Single qubit operations

• Acting unitary operator:  $|\psi\rangle \to U|\psi\rangle$  (multiplying 2x2 unitary matrix)

$$|\psi
angle \ 
ightarrow \ U|\psi
angle$$

In quantum circuit notation,

$$|\psi\rangle - U - U|\psi\rangle$$

$$= \alpha |0\rangle + \beta |1\rangle = \alpha U|0\rangle + \beta U|1\rangle$$

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#### • Measurement:

$$|\psi\rangle$$
 
$$= \alpha|0\rangle + \beta|1\rangle$$
 
$$C \quad \text{(classical number)}$$
 
$$\begin{cases} c = 0 \text{ w/ probability } |\alpha|^2 \\ c = 1 \text{ w/ probability } |\beta|^2 \end{cases}$$

X,Y,Z gates: (just Pauli matrices)

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

X is "NOT": 
$$X|0\rangle = |1\rangle$$
,  $X|1\rangle = |0\rangle$ 

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#### $R_X, R_Y, R_Z$ gates:

$$R_X(\theta) = e^{-\frac{i\theta}{2}X}, \quad R_Y(\theta) = e^{-\frac{i\theta}{2}Y}, \quad R_Z(\theta) = e^{-\frac{i\theta}{2}Z}$$

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#### Hadamard gate:

$$H = \frac{1}{\sqrt{2}}(X+Z) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1\\ 1 & -1 \end{pmatrix}$$
$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \equiv |+\rangle, \qquad H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \equiv |-\rangle$$

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T gate:

$$T = e^{\frac{\pi i}{8}} R_Z \left(\frac{\pi}{4}\right) = \begin{pmatrix} 1 & 0 \\ 0 & e^{\frac{i\pi}{4}} \end{pmatrix}$$

## Multiple qubits

#### 2 qubits – 4 dim. Hilbert space:

$$|\psi\rangle = \sum_{i,j=0,1} c_{ij} |ij\rangle, \qquad |ij\rangle \equiv |i\rangle \otimes |j\rangle$$

$$|00\rangle = \begin{pmatrix} 1\\0\\0\\0 \end{pmatrix}, \qquad |01\rangle = \begin{pmatrix} 0\\1\\0\\0 \end{pmatrix}, \qquad |10\rangle = \begin{pmatrix} 0\\0\\1\\0 \end{pmatrix}, \qquad |11\rangle = \begin{pmatrix} 0\\0\\0\\1 \end{pmatrix}$$

#### N qubits – 2<sup>N</sup> dim. Hilbert space:

$$|\psi\rangle = \sum_{i_1,\dots i_N=0,1} c_{i_1\dots i_N} |i_1\dots i_N\rangle,$$

$$|i_1 i_2 \cdots i_N\rangle \equiv |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_N\rangle$$

## Two qubit gates used here

#### Controlled *X* (NOT) gate:

$$\int CX|00\rangle = |00\rangle, \qquad CX|01\rangle = |01\rangle, 
CX|10\rangle = |11\rangle, \qquad CX|11\rangle = |10\rangle$$

#### or equivalently

$$CX|0\rangle \otimes |\psi\rangle = |0\rangle \otimes |\psi\rangle, \qquad CX|1\rangle \otimes |\psi\rangle = |1\rangle \otimes X|\psi\rangle$$

$$CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} =$$

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$$CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} =$$

#### **SWAP** gate:

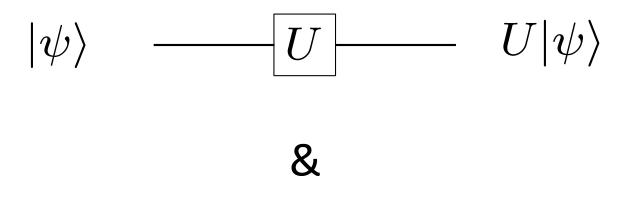
$$\mathsf{SWAP}|\psi\rangle\otimes|\phi\rangle=|\phi\rangle\otimes|\psi\rangle$$

$$SWAP = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{array}{c} & & & \\$$

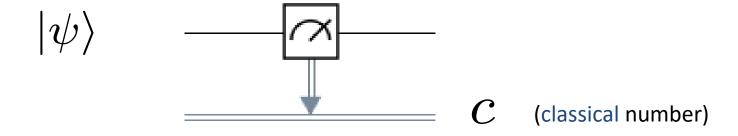
We'll see this is useful to compute Renyi entropy

## Rule of the game

Do something interesting by a combination of action of Unitary operators:

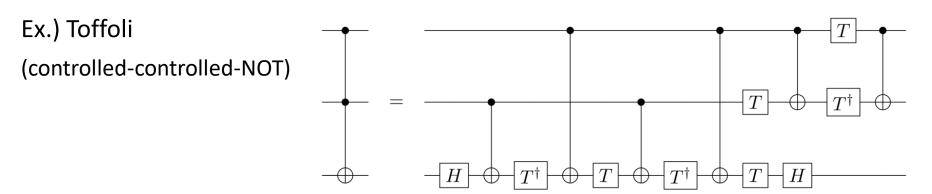


#### measurements:



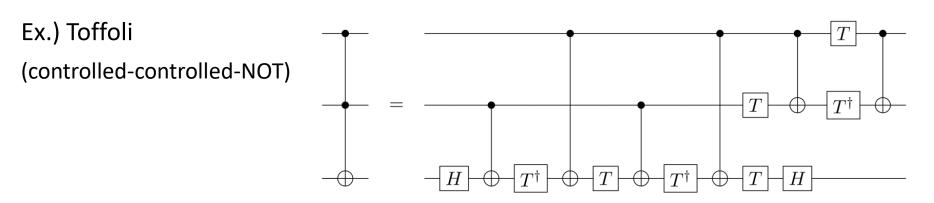
## **Universality**

•Any unitary gate is a combination of single qubit gates & CX ("Single qubit gates & CX are universal")



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•Any single qubit gate is approximated by a combination of H & T in arbitrary precision (next slide)

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad T = \begin{pmatrix} 1 & 0 \\ 0 & e^{\frac{i\pi}{4}} \end{pmatrix}$$

• *H*, *T* & *CX* are universal

## Approximation of single qubit gate by H & T

① Get a rotation with angle  $2\pi \times (irrational)$ :

$$THTH = e^{\frac{i\pi}{4}} R_{\vec{n}}(\theta)$$
 with  $R_{\vec{n}}(\theta) \equiv e^{-\frac{i}{2}\vec{n}\cdot\vec{\sigma}}$ 

where

re
$$\vec{n} = \frac{1}{\sqrt{1 + \cos^2(\pi/8)}} \begin{pmatrix} \cos(\pi/8) \\ \sin(\pi/8) \\ \cos(\pi/8) \end{pmatrix} \& \cos(\theta/2) \equiv \cos^2(\pi/8)$$

$$2\pi \times \text{(irrational)!}$$

2 Use Weyl's uniform distribution theorem:

$$\frac{\theta}{2\pi} \mathbf{Z}$$
 is uniformly distributed mod 1  $\Longrightarrow$  approximate  $R_{\vec{n}}(\alpha)$  for  $\forall \alpha$ 

3 Construct rotation around another axis:

$$HR_{\vec{n}}(\alpha)H = R_{\vec{m}}(\alpha)$$
 with  $\vec{m} = \frac{1}{\sqrt{1 + \cos^2(\pi/8)}} \begin{pmatrix} \cos(\pi/8) \\ -\sin(\pi/8) \\ \cos(\pi/8) \end{pmatrix}$ 

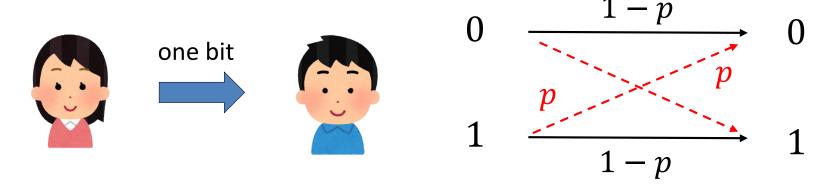
(4) Approximate  $\forall$  single qubit gate:  $R_{\vec{n}}(\alpha)R_{\vec{m}}(\beta)$   $R_{\vec{n}}(\gamma)$  (To achieve accuracy  $\epsilon$ , it requires  $\mathcal{O}(\log^c(1/\epsilon))$  gates w/  $c\sim 2$ ) [Solovay '95, Kitaev '97]

## Errors in classical computers

Computer interacts w/ environment error/noise

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Computer interacts w/ environment error/noise

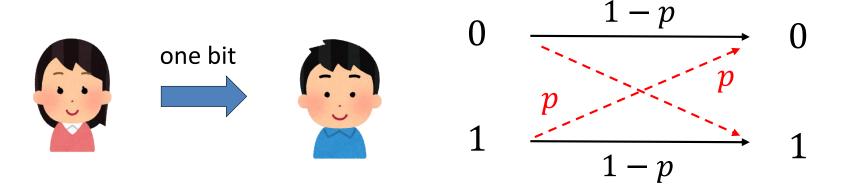


Suppose we send a bit but have "error" in probability p

A simple way to correct errors:

## Errors in classical computers

Computer interacts w/ environment error/noise



Suppose we send a bit but have "error" in probability p

#### A simple way to correct errors:

- ① Duplicate the bit (encoding):  $0 \rightarrow 000$ ,  $1 \rightarrow 111$
- 2 Error detection & correction by "majority voting":

$$001 \to 000$$
,  $011 \to 111$ , etc...

$$P_{\text{failed}} = 3p^2(1-p) + p^3$$
 (improved if  $p < 1/2$ )

## Errors in quantum computers

(we'll come back to this point tomorrow)

Computer interacts w/ environment error/noise



Unknown unitary operators are multiplied:

(in addition to decoherence & measurement errors)

$$|\psi\rangle$$
 error!  $U|\psi\rangle$  not only bit flip!

We need to include "quantum error corrections" but it seems to require a huge number of qubits

~ major obstruction of the development

## FTQC vs NISQ

### Fault Tolerant Quantum Computer (FTQC)

- large quantum computer w/ sufficient error correction
- our dream
- expected to show "quantum supremacy" if it is realized
- not sure if it is realized in future

## Noisy Intermediate-Scale Quantum computer (NISQ)

[cf. Preskill '18]

- intermediate quantum computer w/ non-negligible errors
- current/near future device
- not sure if ∃ problems to give "quantum supremacy"

## (Classical) simulator for Quantum computer

### Quantum computation ⊂ Linear algebra

The same algorithm can be implemented in classical computer but w/o speed-up (1 quantum step = many classical steps)

Simulator = Tool to simulate quantum computer by classical computer

- Doesn't have errors → ideal answers
   (More precisely, classical computer also has errors but its error correction is established)
- The same code can be run in quantum computer w/ speed-up

Useful to test algorithm & estimate computational resources

(~# of qubits, gates)

## **Short summary**

- Qubit = Quantum bit
- Important gates:

$$R_X(\theta) = e^{-\frac{i\theta}{2}X}, \quad R_Y(\theta) = e^{-\frac{i\theta}{2}Y}, \quad R_Z(\theta) = e^{-\frac{i\theta}{2}Z}$$

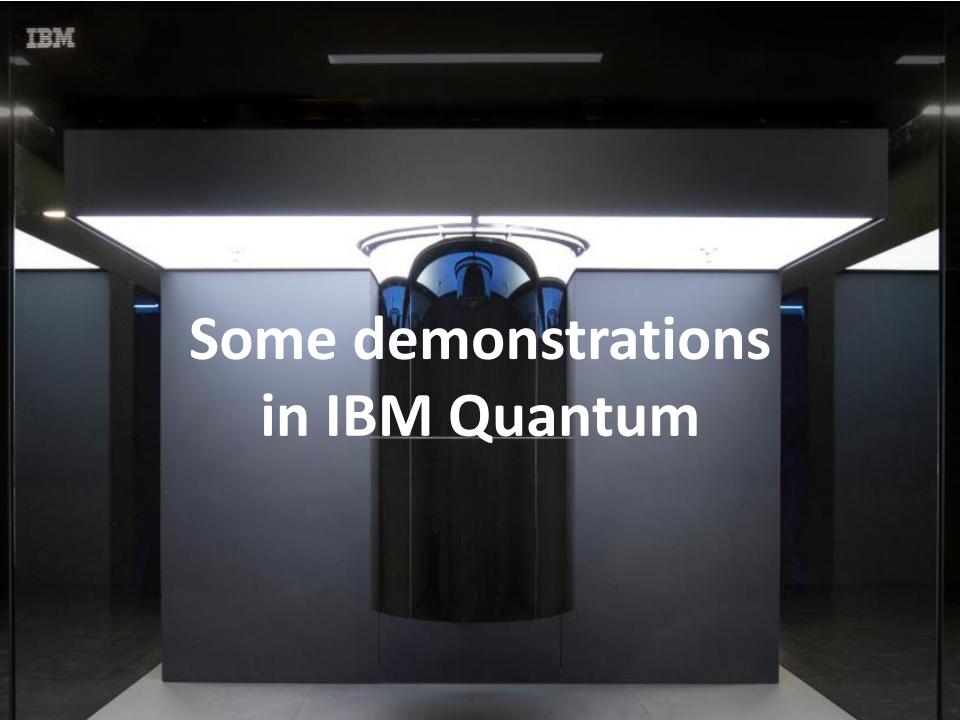
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$$CX|0\rangle \otimes |\psi\rangle = |0\rangle \otimes |\psi\rangle, \quad CX|1\rangle \otimes |\psi\rangle = |1\rangle \otimes X|\psi\rangle$$

- Do something interesting by a combination of acting unitary op. & measurement
- *H*, *T* & *CX* are universal

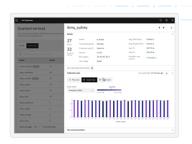
$$T = e^{\frac{\pi i}{8}} R_Z \left(\frac{\pi}{4}\right) = \begin{pmatrix} 1 & 0\\ 0 & e^{\frac{i\pi}{4}} \end{pmatrix}$$

- Real quantum computer has errors
- Simulator = Tool to simulate quantum computer by classical computer



#### Real quantum computers. Right at your fingertips.

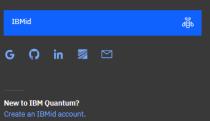
IBM offers cloud access to the most advanced quantum computers available. Learn, develop, and run programs with our quantum applications and systems.



#### View quantum system details

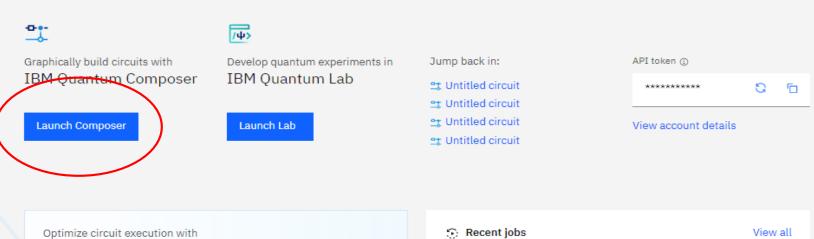
Check out the status, topology, calibration data, and access details of your IBM quantum systems.

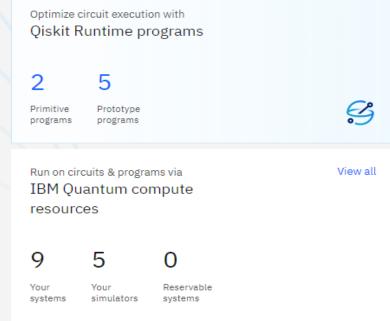
#### Sign in to IBM Quantum

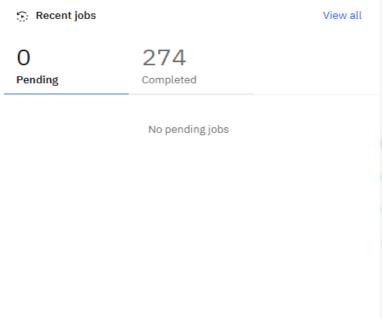


Having trouble signing in:

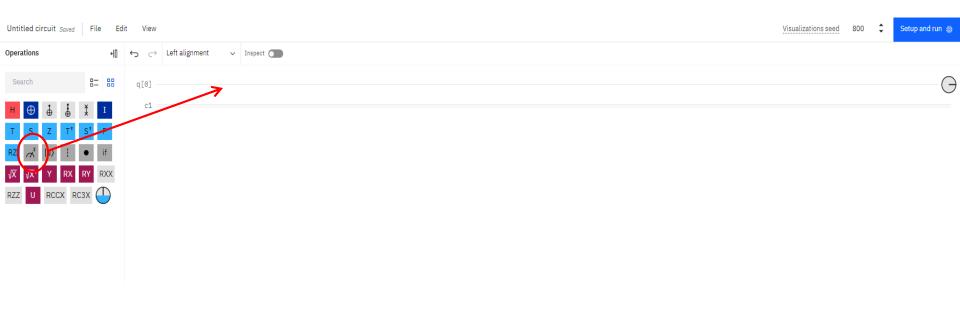
#### Welcome, Honda Masazumi



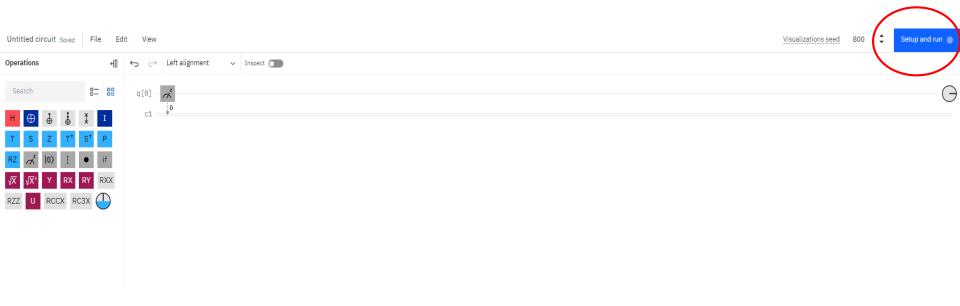




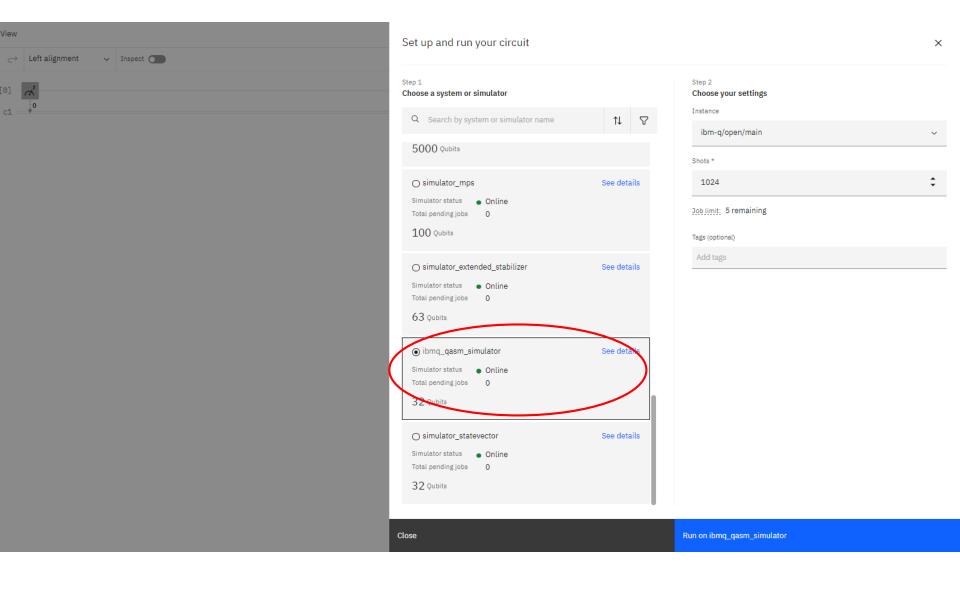
# A trivial problem: measure |0|



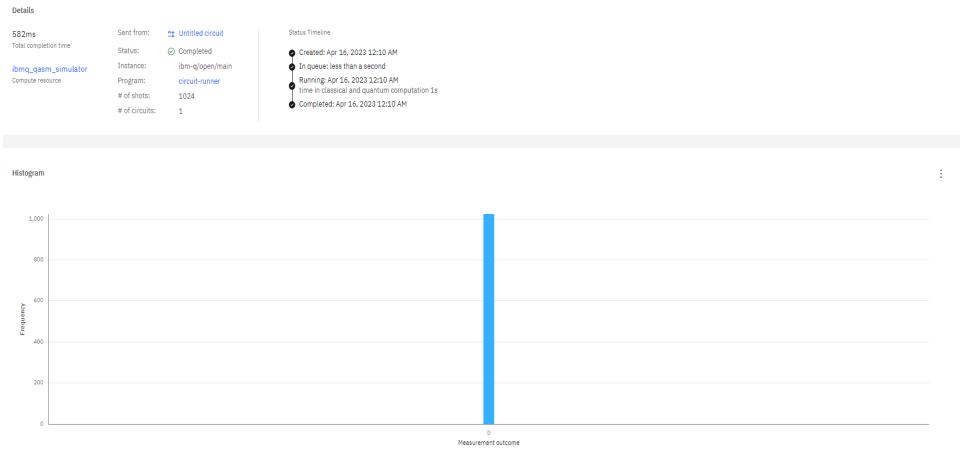
## A trivial problem: measure $|0\rangle$ (Cont'd)



## Measure 1024 times in simulator

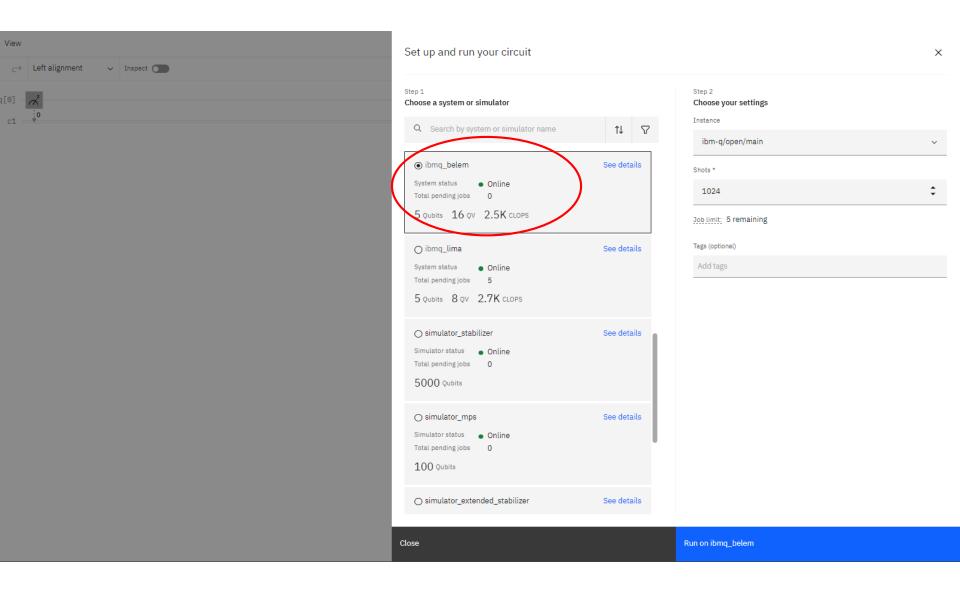


# Trivial result

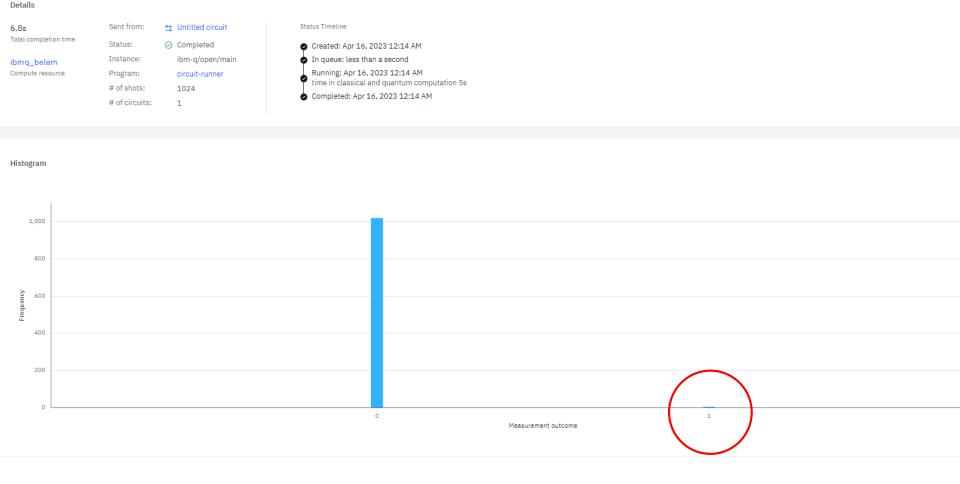


#### Of Course!

### Measure 1024 times in quantum computer

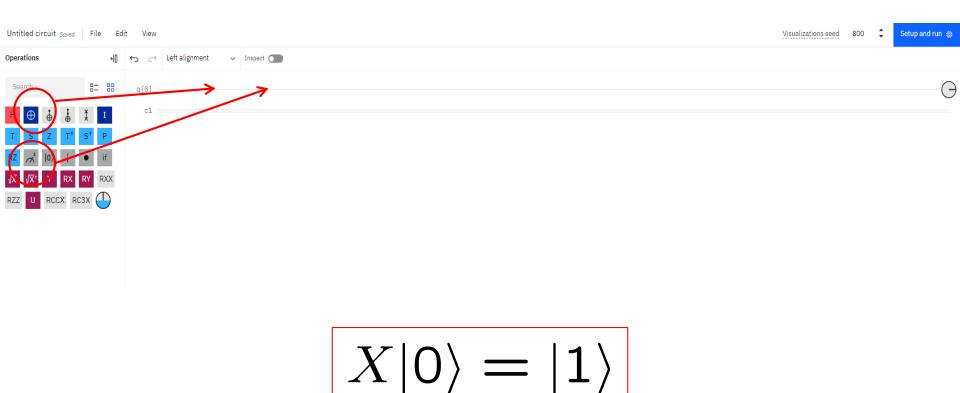


# Result of quantum computer?

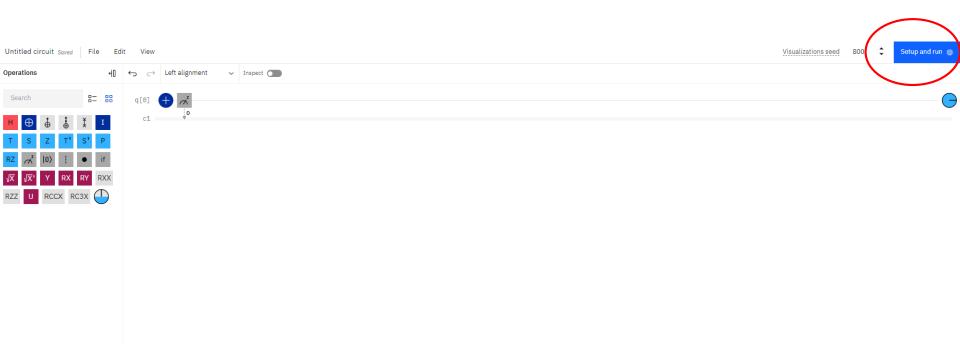


This is the error!

## Another trivial problem: measure |1>



## Another trivial problem: measure 1) (Cont'd)



## Result of simulator (1024 shots)

#### Details

730ms Total completion time

 Status:
 ⊘ Completed

 Instance:
 ibm-q/open/main

 Program:
 circuit-runner

 # of shots:
 1024

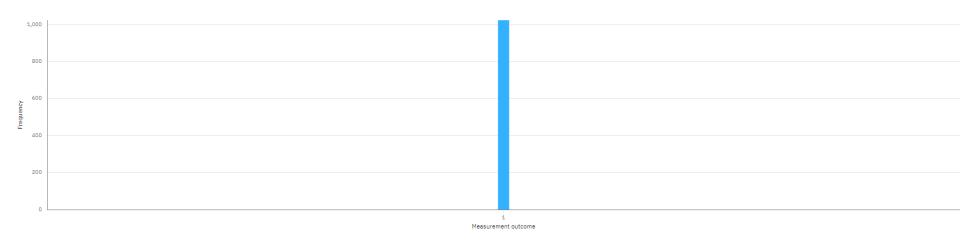
 # of circuits:
 1

■ Untitled circuit

Status Timeline

- Oreated: Apr 16, 2023 12:24 AM
- In queue: less than a second
- Running: Apr 16, 2023 12:24 AM
- time in classical and quantum computation 1s
- Completed: Apr 16, 2023 12:24 AM

#### Histogram



## Result of quantum computer (1024shots)

Details

3.5s Total completion time

ibmq\_belem

Compute resource

ntitled circuit

ibm-q/open/main

circuit-runner

○ Completed

Status:

Instance:

Program:

Status Timeline

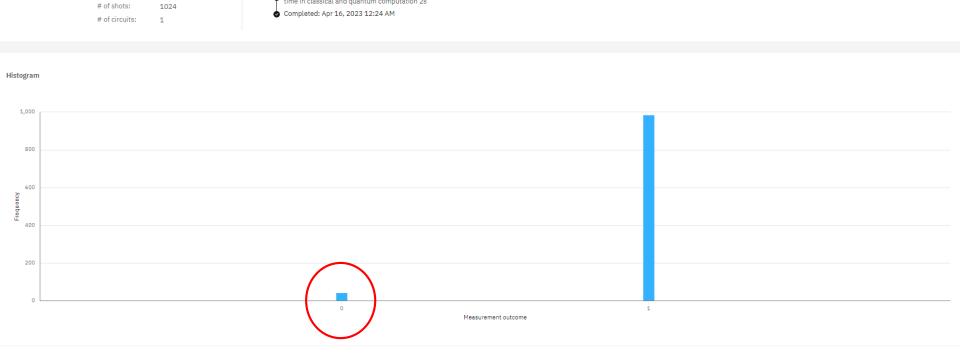
Oreated: Apr 16, 2023 12:24 AM

Running: Apr 16, 2023 12:24 AM

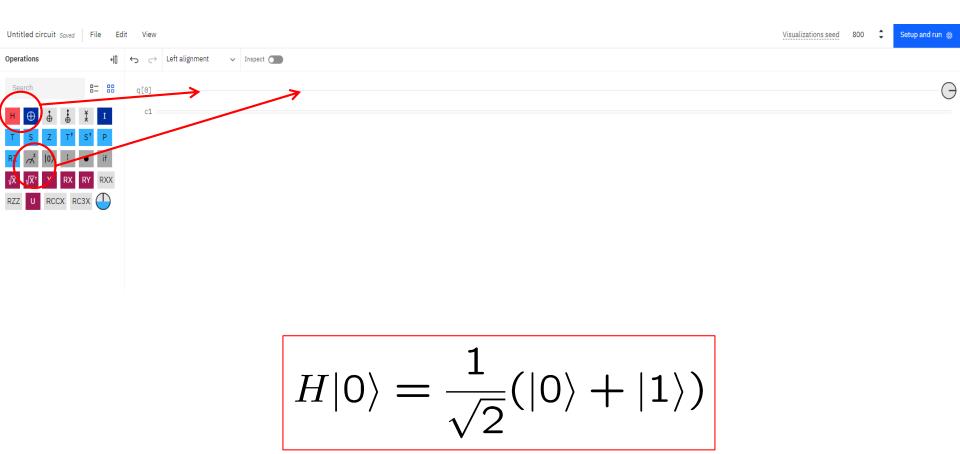
Error again

time in classical and quantum computation 2s

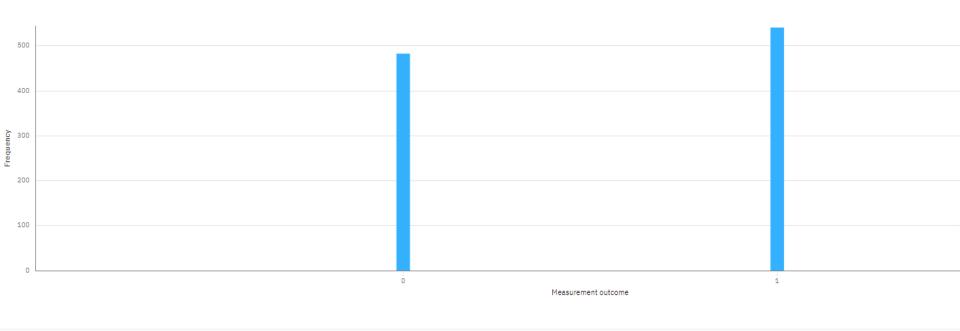
In queue: less than a second



#### The simplest nontrivial problem: Hadamard gate

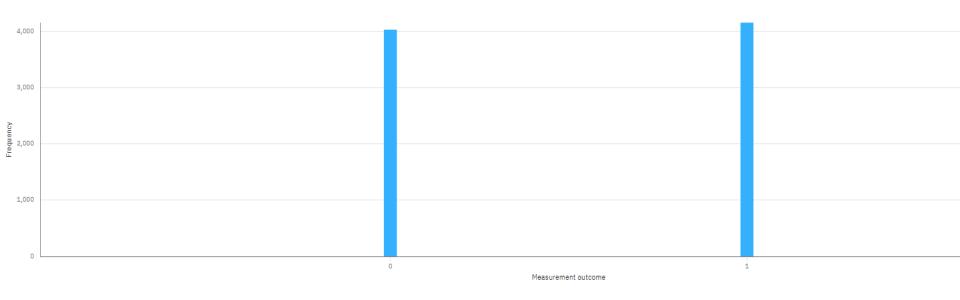


## Result of simulator (1024 shots)



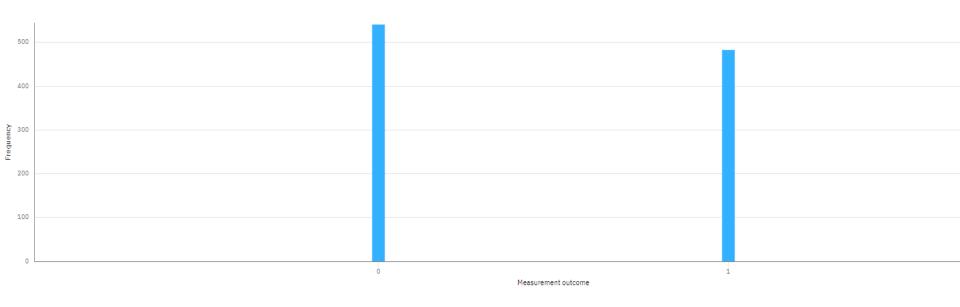
Not exactly 50:50 because of statistical errors

# Result of simulator (8192 shots)



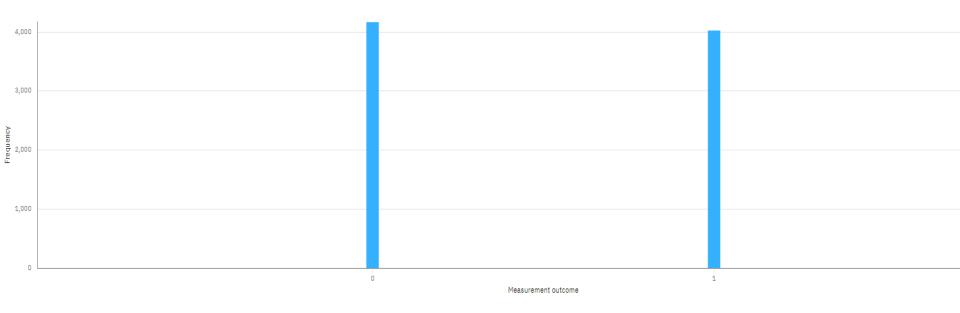
### Improved!

## Result of quantum computer (1024 shots)



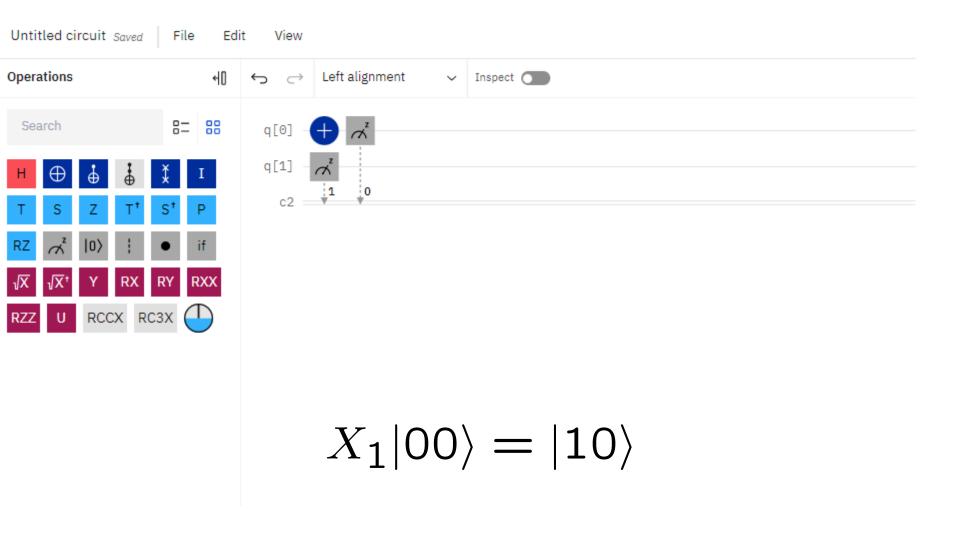
∃ Both errors & statistical errors

## Result of quantum computer (8192 shots)



Statistical errors are improved

# A trivial problem for 2 qubits



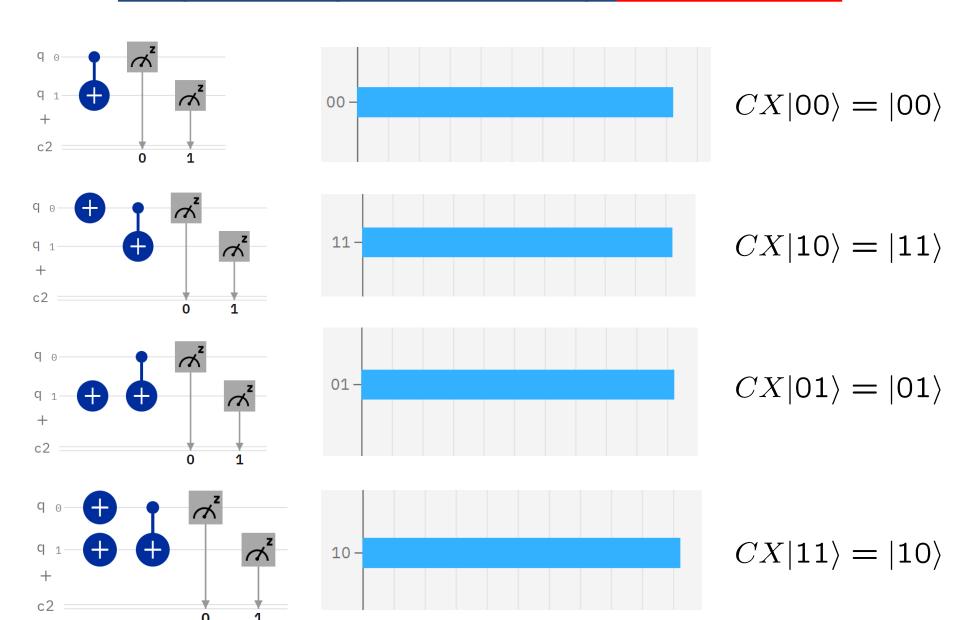
## Result of simulator (1024 shots)

$$X_1|00\rangle = |10\rangle$$

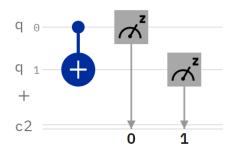


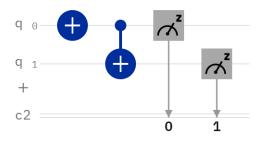
Note that notation is different from the ket notation

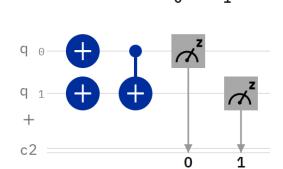
# 2 qubit operation by simulator



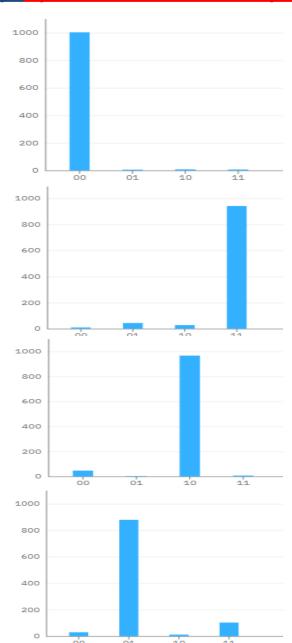
### 2 qubit operation by quantum computer (1024 shots)







c2



$$CX|00\rangle = |00\rangle$$

$$CX|10\rangle = |11\rangle$$

$$CX|01\rangle = |01\rangle$$

$$CX|11\rangle = |10\rangle$$

# Tutorial 0: Play with IBMQ

(until the end of this class)

## Plan of the lectures

(If 2nd lecture in each day ends early, then we start hands-on early)

#### <u>Day 1</u>

- Lecture 1: introduction, basics of quantum computation
- Lecture 2: Spin system on quantum computer (QC)
- Hands-on 1: Basics on IBM's qiskit

### <u>Day 2</u>

- Lecture 3: Quantum field theory (QFT) on QC
- Lecture 4: QFT on QC, error correction & future prospects
- Hands-on 2: Time evolution of spin system

Quantum simulation of Spin system

# The (1+1)d transverse Ising model

#### Hamiltonian (w/ open b.c.):

 $(X_n, Y_n, Z_n: \sigma_{1,2,3} \text{ at site } n)$ 

$$\widehat{H} = -J \sum_{n=1}^{N-1} Z_n Z_{n+1} - h \sum_{n=1}^{N} X_n - m \sum_{n=1}^{N} Z_n$$

For simplicity, take  $N=2\ \&\ m=0$  for a while:

$$\widehat{H} = -JZ_1Z_2 - h(X_1 + X_2)$$

Let's construct the time evolution op.  $e^{-i\hat{H}t}$ 

## Warm up: 2-site transverse Ising model

$$\hat{H} = -JZ_1Z_2 - h(X_1 + X_2)$$

We are going to

- construct time evolution operator
- obtain vacuum state
- compute vacuum expectation values
- compute Renyi entropy

# Time evolution operator

Time evolution of any state is studied by acting the operator

$$e^{-i\hat{H}t} = e^{-i(H_X + H_{ZZ})t}$$

where

$$H_X = -h(X_1 + X_2), \quad H_{ZZ} = -JZ_1Z_2$$

How do we express this in terms of elementary gates?

(such as  $X, Y, Z, R_{X,Y,Z}, CX$  etc...)

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How do we express this in terms of elementary gates?

(such as  $X, Y, Z, R_{X,Y,Z}, CX$  etc...)

#### Step 1: Suzuki-Trotter decomposition:

(<sup>3</sup> higher order improvements)

$$e^{-i\hat{H}t} = \left(e^{-i\hat{H}\frac{t}{M}}\right)^{M}$$
 (M: large positive integer) 
$$\simeq \left(e^{-iH_X\frac{t}{M}}e^{-iH_{ZZ}\frac{t}{M}}\right)^{M} + \mathcal{O}(1/M)$$

## Time evolution operator (Cont'd)

$$e^{-i\hat{H}t} \simeq \left(e^{-iH_X\frac{t}{M}}e^{-iH_{ZZ}\frac{t}{M}}\right)^M$$

acting on qubit 2 acting on qubit 1

The 1st one is trivial:

$$e^{-iH_X \frac{t}{M}} = e^{-i\frac{ht}{M}X_2} e^{-i\frac{ht}{M}X_1} = R_X^{(2)} \left(\frac{2ht}{M}\right) R_X^{(1)} \left(\frac{2ht}{M}\right)$$

## Time evolution operator (Cont'd)

$$e^{-i\hat{H}t} \simeq \left(e^{-iH_X\frac{t}{M}}e^{-iH_{ZZ}\frac{t}{M}}\right)^M$$

acting on qubit 2 acting on qubit 1

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The 2nd one is nontrivial:

$$e^{-iH_{ZZ}\frac{t}{M}} = e^{-i\frac{Jt}{M}Z_1Z_2} = \cos\frac{Jt}{M} - iZ_1Z_2\sin\frac{Jt}{M}$$

One can show (see next slide)

$$e^{-i\frac{Jt}{M}Z_1Z_2} = CXR_Z^{(2)}\left(\frac{2Jt}{M}\right)CX$$

## Time evolution operator (Cont'd)

$$e^{-icZ_1Z_2} = CXR_Z^{(2)}(2c)CX$$

#### **Proof:**

$$CXR_Z^{(2)}(2c)CX|0\rangle \otimes |\psi\rangle$$

$$= CXR_Z^{(2)}(2c)|0\rangle \otimes |\psi\rangle = CX|0\rangle \otimes R_Z(2c)|\psi\rangle$$

$$= |0\rangle \otimes R_Z(2c)|\psi\rangle = \cos c|0\rangle \otimes |\psi\rangle - i\sin c \, Z|0\rangle \otimes Z|\psi\rangle$$

$$CXR_Z^{(2)}(2c)CX|1\rangle \otimes |\psi\rangle$$

$$= CXR_Z^{(2)}(2c)|1\rangle \otimes X|\psi\rangle = CX|1\rangle \otimes R_Z(2c)X|\psi\rangle = |1\rangle \otimes XR_Z(2c)X|\psi\rangle$$

$$= \cos c|1\rangle \otimes XX|\psi\rangle - i\sin c \, |1\rangle \otimes XZX|\psi\rangle$$

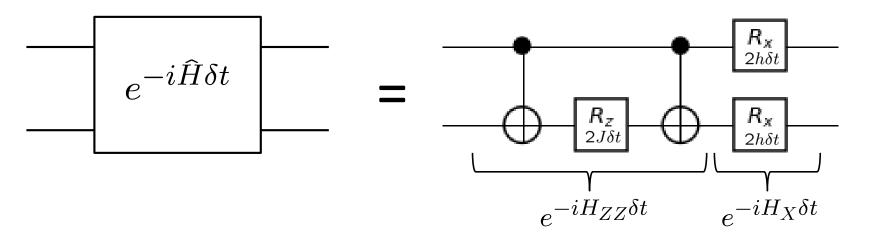
$$= \cos c|1\rangle \otimes |\psi\rangle - i\sin c \, Z|1\rangle \otimes Z|\psi\rangle$$

Thus,

$$CXR_Z^{(2)}(2c)CX|\varphi\rangle\otimes|\psi\rangle = \cos c|\varphi\rangle\otimes|\psi\rangle - i\sin c \, Z|\varphi\rangle\otimes Z|\psi\rangle$$
$$= e^{-icZ_1Z_2}|\varphi\rangle\otimes|\psi\rangle$$

## Quantum circuit for time evolution op.

$$H_X = -h(X_1 + X_2), \qquad H_{ZZ} = -JZ_1Z_2$$
 
$$\delta t = \frac{t}{M} \ll 1$$



$$+\mathcal{O}(\delta t)$$

# Survival probability of free vacuum

For I = 0, the ground state is

$$\hat{H}|_{J=0} = -h(X_1 + X_2)$$

$$|++\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle + |1\rangle}{\sqrt{2}} = H^{(2)}H^{(1)}|00\rangle$$

We can compute survival probability of the free vacuum:

$$P(t) = \left| \langle + + | e^{-i\hat{H}t} | + + \rangle \right|^{2}$$

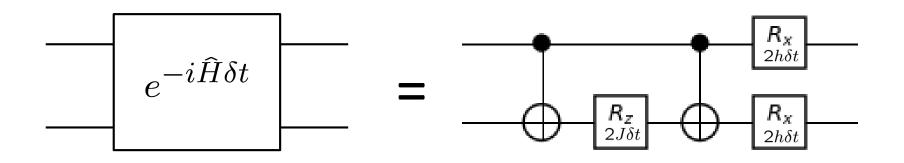
$$= \left| \langle 00 | H^{(2)}H^{(1)}e^{-i\hat{H}t}H^{(2)}H^{(1)} | 00 \rangle \right|^{2}$$

Measure the probability having  $|00\rangle$  inside the state

$$H^{(2)}H^{(1)}e^{-i\hat{H}t}H^{(2)}H^{(1)}|00\rangle$$

## Demonstration for the survival probability

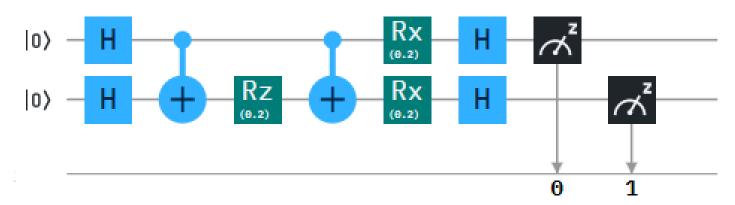
$$P(t) = \left| \langle + + | e^{-i\hat{H}t} | + + \rangle \right|^2 = \left| \langle 00 | H^{(2)} H^{(1)} e^{-i\hat{H}t} H^{(2)} H^{(1)} | 00 \rangle \right|^2$$



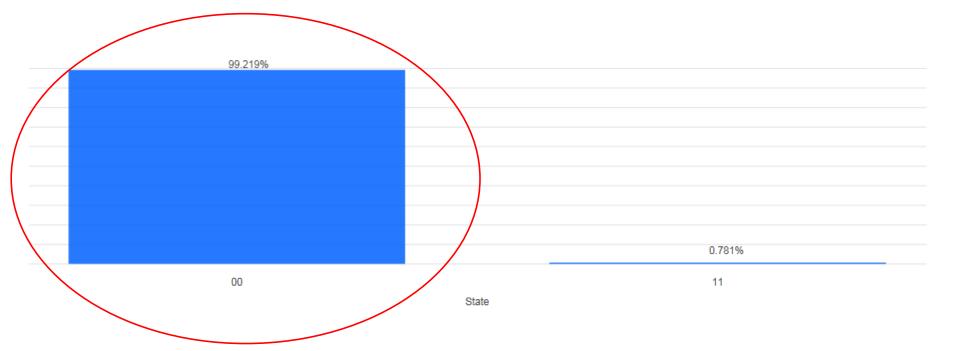
Let's compute it for J = 1, h = 1, t = 0.1, M = 1

$$\delta t = \frac{t}{M}$$

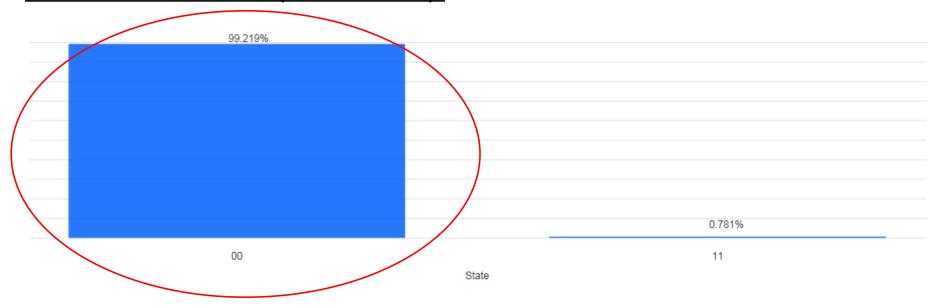
#### Demonstration for the survival probability (Cont'd)



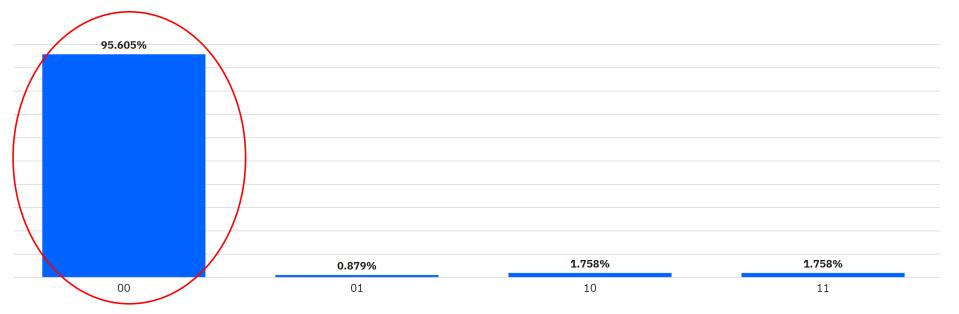
#### Result by simulator w/ 1024 shots:



#### Result of simulator (1024 shots):

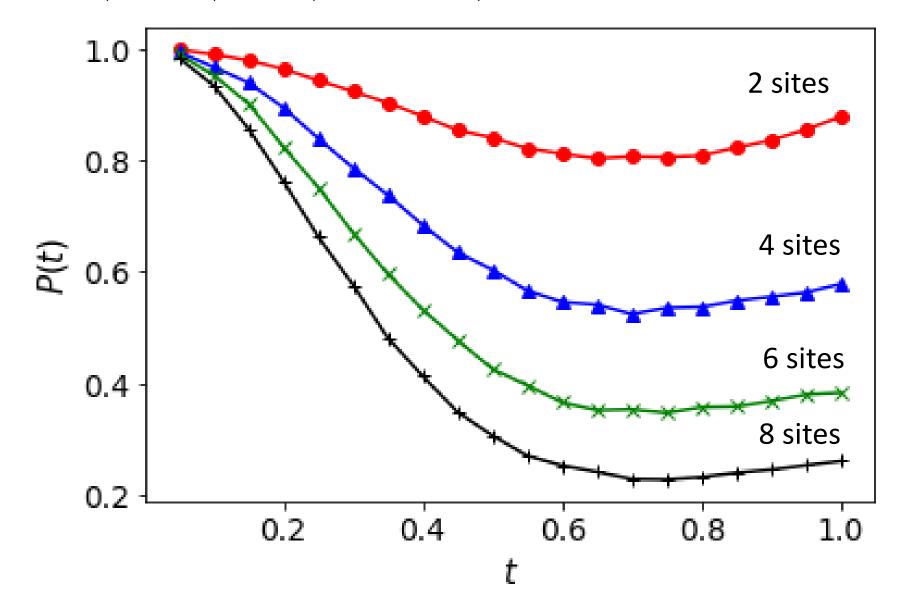


#### Result of quantum computer (1024 shots):



### More serious computation

J = 1, h = 1, t = 1, M = 100, 10000 shots



## Computational costs for large size system

$$P(t) = |\langle + \dots + | e^{-i\hat{H}t} | + \dots + \rangle|^{2}$$
$$e^{-i\hat{H}t} \simeq \left(e^{-iH_{X}\frac{t}{M}}e^{-iH_{ZZ}\frac{t}{M}}\right)^{M}$$

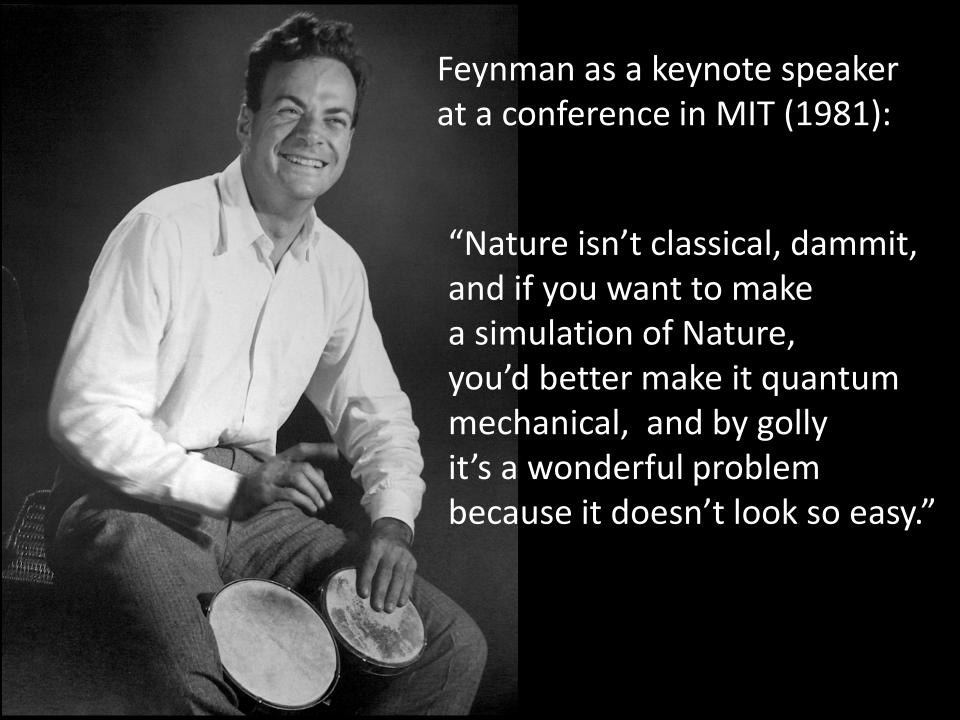
#### **Classical** computer

multiplications of matrices to vectors w/ sizes =  $2^N$ 

exponentially large steps

### **Quantum** computer

- •time evolution = O(NM) experimental operations
- \*taking the inner product is done by acting N gates & a measurement  $polynomial\ steps$



## Constructing vacuum (ground state)

<sup>∃</sup>various quantum algorithms to construct vacuum:

- adiabatic state preparation
- algorithms based on variational method
- imaginary time evolution etc..

Here, let's apply

adiabatic state preparation

## Adiabatic state preparation of vacuum

Step 1: Choose an initial Hamiltonian  $H_0$  of a simple system whose ground state  $|vac_0\rangle$  is known and unique

Step 2:

<u>Step 3</u>:

## Adiabatic state preparation of vacuum

Step 1: Choose an initial Hamiltonian  $H_0$  of a simple system whose ground state  $|vac_0\rangle$  is known and unique

Step 2: Introduce adiabatic Hamiltonian  $H_A(t)$  s.t.

$$\begin{cases} \bullet \ H_A(0) = H_0, \ H_A(T) = H_{\text{target}} \\ \bullet \ \left| \frac{dH_A}{dt} \right| \ll 1 \text{ for } T \gg 1 \end{cases}$$

<u>Step 3</u>:

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Step 3: Use the adiabatic theorem

If  $H_A(t)$  has a unique ground state w/ a finite gap for  $\forall t$ , then the ground state of  $H_{\text{target}}$  is obtained by

$$|\text{vac}\rangle = \lim_{T \to \infty} \mathcal{T} \exp\left(-i \int_0^T dt \, H_A(t)\right) |\text{vac}_0\rangle$$

## For transverse Ising model

$$\widehat{H} = -J \sum_{n=1}^{N-1} Z_n Z_{n+1} - h \sum_{n=1}^{N} X_n - m \sum_{n=1}^{N} Z_n$$

Choose

$$\begin{cases} H_0 = -h \sum_{n=1}^{N} X_n & | \operatorname{vac}_0 \rangle = | + \cdots + \rangle \\ H_A(t) = \left(1 - \frac{t}{T}\right) H_0 + \frac{t}{T} \hat{H} \end{cases}$$

Discretize the integral:

$$\mathcal{T} \exp \left(-i \int_0^T dt \ H_A(t)\right) |\mathsf{vac}_0> \simeq U(T) U(T-\delta t) \cdots U(2\delta t) U(\delta t) |\mathsf{vac}_0>$$

where

$$U(t) = e^{-iH_A(t)\delta t}, \ \delta t = \frac{T}{M} \ll 1$$

## **Magnetization**

Once we get the vacuum, we can compute VEV of operators:

$$\langle vac|\mathcal{O}|vac \rangle$$

It is easiest to compute magnetization:

$$\frac{1}{N}\langle \operatorname{vac}|\sum_{n=1}^{N} Z_{n}|\operatorname{vac}\rangle = \frac{1}{N}\sum_{n=1}^{N}\sum_{i_{1}\cdots i_{N}=0,1}\langle \operatorname{vac}|Z_{n}|i_{1}\cdots i_{N}\rangle\langle i_{1}\cdots i_{N}|\operatorname{vac}\rangle$$

$$= \frac{1}{N}\sum_{n=1}^{N}\sum_{i_{1}\cdots i_{N}=0,1}(-1)^{i_{n}}|\langle i_{1}\cdots i_{N}|\operatorname{vac}\rangle|^{2}$$

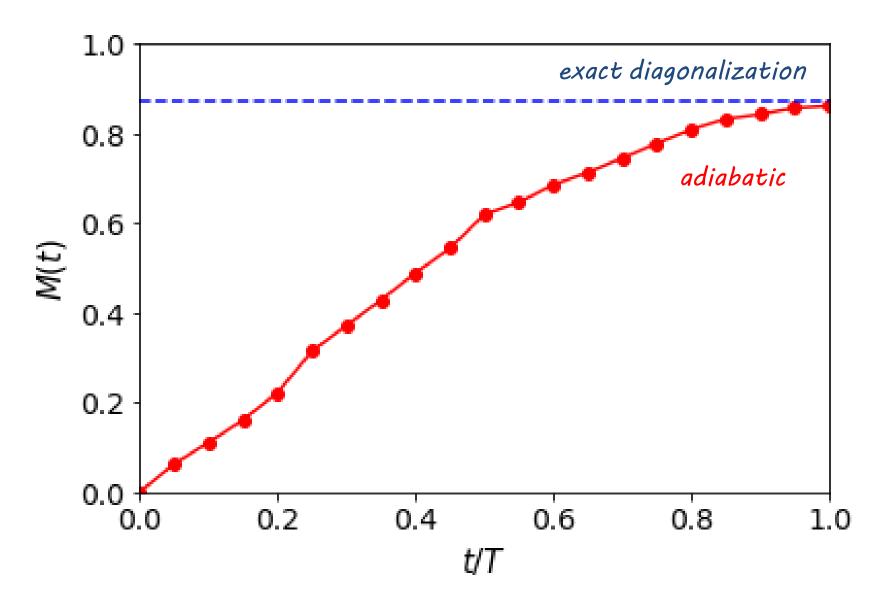
Transverse one is a bit more tricky:

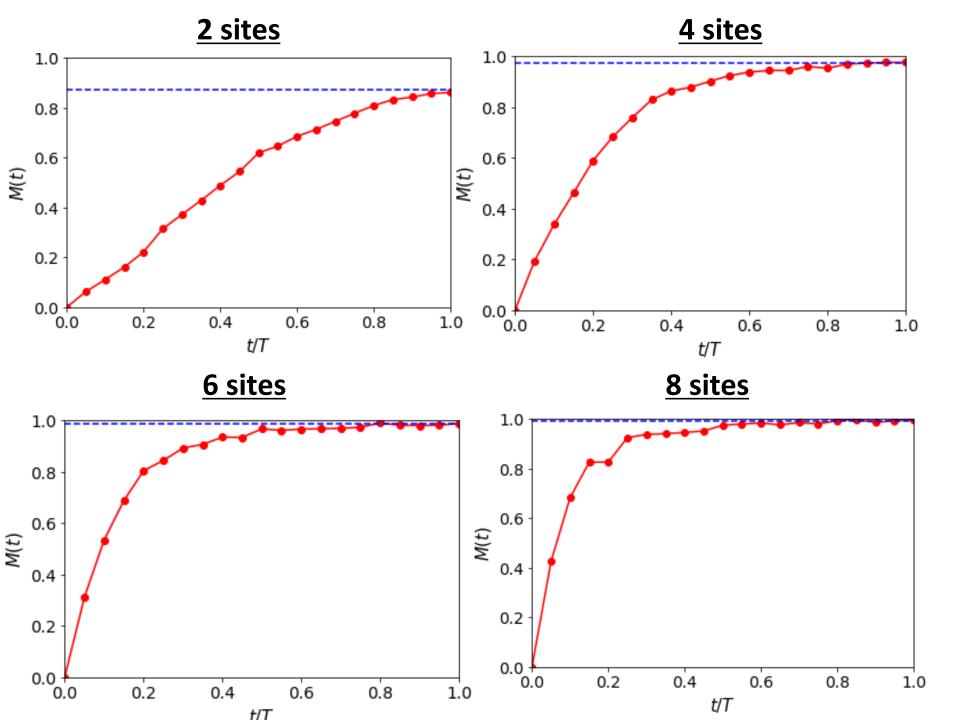
$$\frac{1}{N}\langle \operatorname{vac}|\sum_{n=1}^{N} X_{n}|\operatorname{vac}\rangle = \frac{1}{N}\langle \operatorname{vac}|\sum_{n=1}^{N} H^{(n)}Z_{n}H^{(n)}|\operatorname{vac}\rangle$$

$$= \frac{1}{N}\sum_{n=1}^{N}\sum_{i_{1}\cdots i_{N}=0,1} (-1)^{i_{n}} \left|\langle i_{1}\cdots i_{N}|H^{(n)}|\operatorname{vac}\rangle\right|^{2}$$

## Result by simulator (10000 shots)

2 sites,  $J = 1, h = 1, m = 1, T = 100, \delta t = 0.05, 2000$  time steps





## Renyi entropy

#### Dividing total Hilbert space as

$$\mathcal{H}_{\mathsf{tot}} = \mathcal{H}_A \otimes \mathcal{H}_B$$

reduced density matrix is defined as

$$\rho_A = \operatorname{tr}_{\mathcal{H}_B}(\rho_{\mathsf{tot}})$$

#### **Entanglement entropy:**

$$S_A = -\operatorname{tr}_{\mathcal{H}_A} \left( \rho_A \log \rho_A \right)$$

#### n-th Renyi entropy:

$$S_n = \frac{1}{1-n} \log \operatorname{tr}_{\mathcal{H}_A} (\rho_A^n) \qquad \left( S_A = \lim_{n \to 1} S_n \right)$$

### Quantum algorithm for 2nd Renyi entropy

Consider  $(N_A+N_B)$ -qubit system and the density matrix  $ho_{N_A+N_B}=|\Psi\rangle\langle\Psi|$ 

Let's divide the system into two systems:  $\mathcal{H}_{N_A+N_B}=\mathcal{H}_{N_A}\otimes\mathcal{H}_{N_B}$  & consider the 2nd Renyi entropy

$$S_2 = -\log \operatorname{tr}_{\mathcal{H}_{N_A}} \left( \rho_A^2 \right), \quad \rho_A = \operatorname{tr}_{\mathcal{H}_{N_B}} \left( \rho_{N_A + N_B} \right)$$

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$$S_2 = -\log \operatorname{tr}_{\mathcal{H}_{N_A}} \left( \rho_A^2 \right), \quad \rho_A = \operatorname{tr}_{\mathcal{H}_{N_B}} \left( \rho_{N_A + N_B} \right)$$

One can show (next slide)

[Hastings-Gonzalez-Kallin-Melko'10]

$$\operatorname{tr}_{\mathcal{H}_{N_A}}\left(\rho_A^2\right) = \langle \Psi | \otimes \langle \Psi | \operatorname{SWAP}_A | \Psi \rangle \otimes | \Psi \rangle$$

SWAP<sub>A</sub>: Exchange of A – part in  $|\Psi\rangle \otimes |\Psi\rangle$ 

#### Quantum algorithm for 2nd Renyi entropy (Cont'd)

$$\operatorname{tr}_{\mathcal{H}_{N_A}}\left(\rho_A^2\right) = \left\langle \Psi | \otimes \left\langle \Psi | \operatorname{SWAP}_A | \Psi \right\rangle \otimes \left| \Psi \right\rangle$$

#### Proof:

$$\langle \Psi | \otimes \langle \Psi | SWAP_A | \Psi \rangle \otimes | \Psi \rangle$$

$$= \sum_{k,\ell,k',\ell'} \bar{c}_{k\ell} \bar{c}_{k'\ell'} \langle \{k'\} \{\ell'\} | \otimes \langle \{k\} \{\ell\} | \sum_{i,j,i',j'} c_{ij} c_{i'j'} | \{i'\} \{j\} \rangle \otimes | \{i\} \{j'\} \rangle$$

$$= \sum_{i,j,i',j'} c_{ij} \bar{c}_{i'j} c_{i'j'} \bar{c}_{ij'}$$

$$(\rho_A)_{ii'} = \sum_{j} \langle \{i\}\{j\} | \rho_{N_A + N_B} | \{i'\}\{j\} \rangle = \sum_{j} c_{ij} \bar{c}_{i'j}$$

$$= \sum_{i,i'} (\rho_A)_{ii'} (\rho_A)_{i'i} = \operatorname{tr}_{\mathcal{H}_{N_A}} (\rho_A^2)$$

### <u>Demonstration: 2nd Renyi entropy of Bell state</u>

#### Bell state:

$$|B\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

#### Reduced density matrix:

$$\rho_{\text{red}} = \text{tr}_2 |B\rangle\langle B| = \frac{1}{2} (|0\rangle\langle 0| + |1\rangle\langle 1|)$$

#### 2nd Renyi entropy:

$$\operatorname{tr}\rho_{\text{red}}^2 = \operatorname{tr}\begin{pmatrix} 1/4 & 0\\ 0 & 1/4 \end{pmatrix} = \frac{1}{2}$$

$$S_2 = -\log \operatorname{tr} \rho_{\text{red}}^2 = \log 2$$

Let's reproduce it in IBM Quantum!

#### <u>Demonstration: 2nd Renyi entropy of Bell state (Cont'd)</u>

We know

$$\mathrm{tr}\rho_{\mathrm{red}}^2 = \langle B| \otimes \langle B| \; \mathsf{SWAP}^{(1,3)} \; |B\rangle \otimes |B\rangle$$

The Bell state is written as

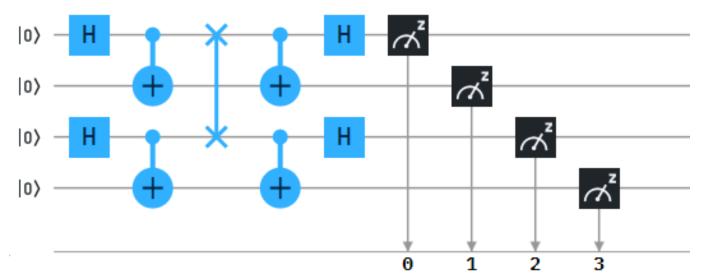
$$|0\rangle \qquad H \qquad = |B\rangle$$

Therefore,

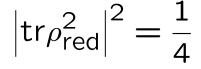
$$\operatorname{tr} \rho_{\mathrm{red}}^2 = \langle 0000 | U^{\dagger} \mathrm{SWAP}^{(1,3)} U | 0000 \rangle \quad (|B\rangle \otimes |B\rangle \equiv U | 0000 \rangle)$$

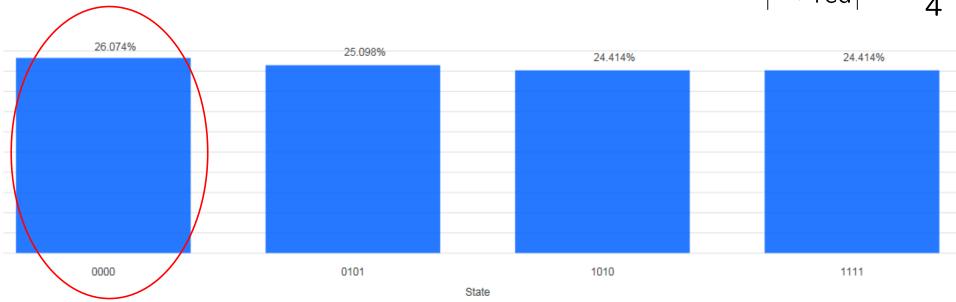
$$\left| \operatorname{tr} \rho_{\text{red}}^2 \right|^2 = \left| \langle 0000 | U^{\dagger} \text{SWAP}^{(1,3)} U | 0000 \rangle \right|^2$$

#### <u>Demonstration: 2nd Renyi entropy of Bell state (Cont'd)</u>

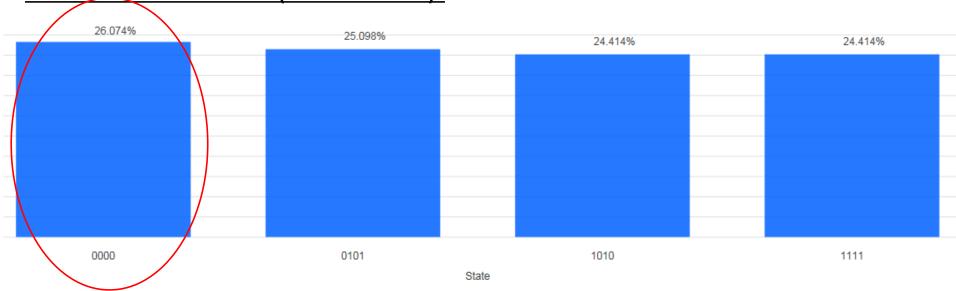




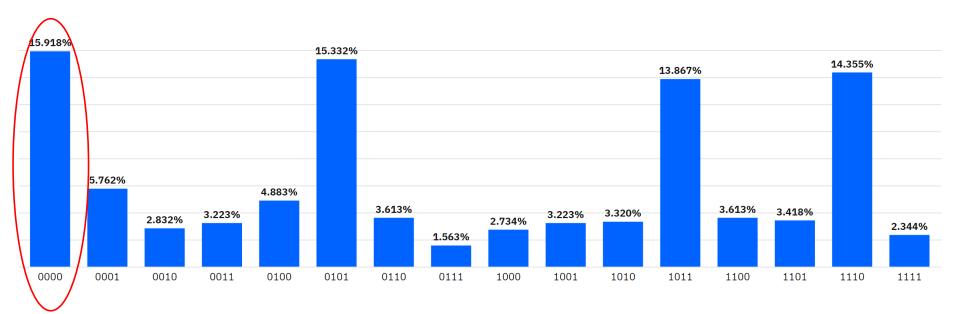




Result of simulator (1024 shots):



#### Result of quantum computer (1024 shots):



## More direct way?

#### We've directly computed

$$\left| \operatorname{tr} \rho_{\text{red}}^2 \right|^2 = \left| \langle 0000 | U^{\dagger} \text{SWAP}^{(1,3)} U | 0000 \rangle \right|^2$$

rather than itself:

$$\operatorname{tr} \rho_{\mathrm{red}}^2 = \langle 0000 | U^{\dagger} \mathrm{SWAP}^{(1,3)} U | 0000 \rangle$$

#### Can we directly compute it?

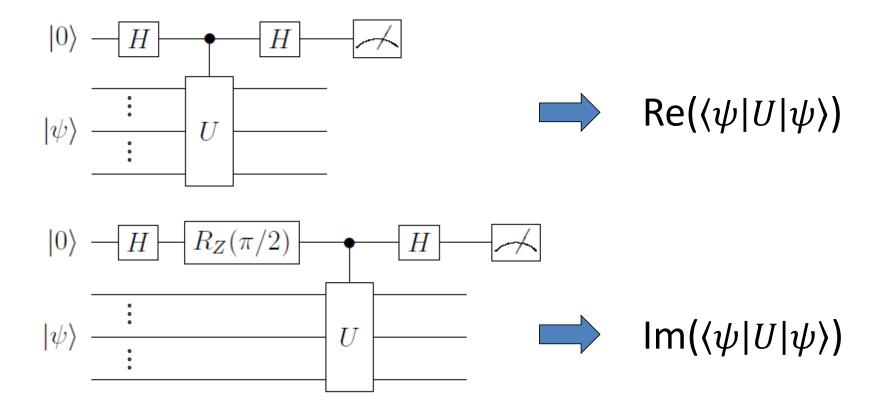
Yes, there is a way to compute expectation value of unitary op. under any state: (next slide)

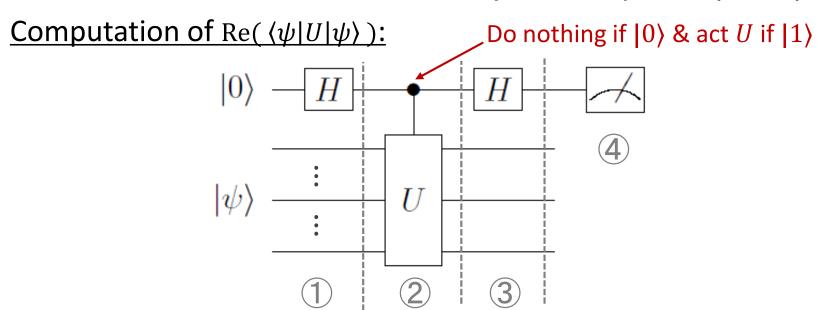
$$\langle \psi | U | \psi \rangle$$

1 Extend Hilbert space & consider the state

$$|0\rangle \otimes |\psi\rangle$$
"ancillary qubit"

② We can compute  $\langle \psi | U | \psi \rangle$  by using the 2 circuits: (next slide)





Computation of Re( $\langle \psi | U | \psi \rangle$ ): Do nothing if  $|0\rangle$  & act U if  $|1\rangle$   $|0\rangle \qquad H \qquad \qquad 4$   $|\psi\rangle \qquad \vdots \qquad \qquad U \qquad \qquad 3$ 

① 
$$H|0\rangle \otimes |\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle \otimes |\psi\rangle + \frac{1}{\sqrt{2}}|1\rangle \otimes |\psi\rangle$$

$$(2)$$
  $\frac{1}{\sqrt{2}}|0\rangle \otimes |\psi\rangle + \frac{1}{\sqrt{2}}|1\rangle \otimes U|\psi\rangle$ 

① 
$$H|0\rangle \otimes |\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle \otimes |\psi\rangle + \frac{1}{\sqrt{2}}|1\rangle \otimes |\psi\rangle$$

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(4) 
$$P_0 = \frac{1}{4} |(1+U)|\psi\rangle|^2 = \frac{1}{2} (1 + \text{Re}\langle\psi|U|\psi\rangle)$$
  
 $P_1 = \frac{1}{4} |(1-U)|\psi\rangle|^2 = \frac{1}{2} (1 - \text{Re}\langle\psi|U|\psi\rangle)$ 

Computation of Re( $\langle \psi | U | \psi \rangle$ ): Do nothing if  $|0\rangle$  & act U if  $|1\rangle$   $|0\rangle \qquad H \qquad \qquad 4$   $|\psi\rangle \qquad \vdots \qquad \qquad 1$   $2 \qquad 3$ 

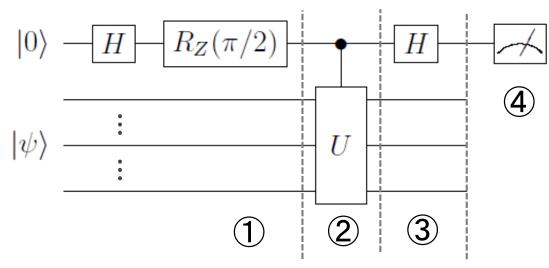
$$② \frac{1}{\sqrt{2}} |0\rangle \otimes |\psi\rangle + \frac{1}{\sqrt{2}} |1\rangle \otimes U|\psi\rangle$$

(4) 
$$P_0 = \frac{1}{4} |(1+U)|\psi\rangle|^2 = \frac{1}{2} (1 + \text{Re}\langle\psi|U|\psi\rangle)$$
  
 $P_1 = \frac{1}{4} |(1-U)|\psi\rangle|^2 = \frac{1}{2} (1 - \text{Re}\langle\psi|U|\psi\rangle)$ 



 $\operatorname{Re}\langle\psi|U|\psi\rangle = P_0 - P_1$ 

#### Computation of $Im(\langle \psi | U | \psi \rangle)$ :



$$\left(R_Z(\theta) = e^{-\frac{i\theta}{2}Z}\right)$$

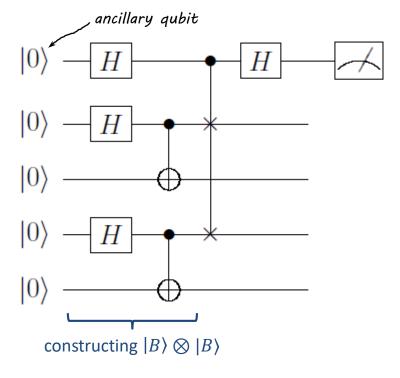
 $\operatorname{Im}\langle\psi|U|\psi\rangle = P_1 - P_0$ 

### Coming back to the Renyi entropy of Bell state

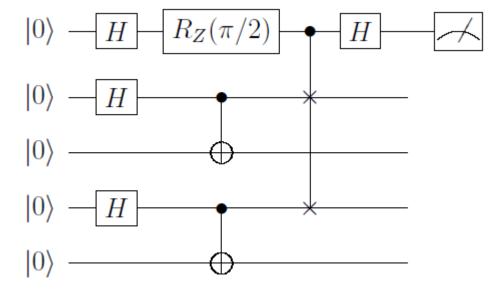
Taking  $|\psi\rangle = |B\rangle \otimes |B\rangle \otimes U = SWAP^{(1,3)}$ , we can directly compute

$$\operatorname{tr}\rho_{\mathrm{red}}^2 = \langle B | \otimes \langle B | \operatorname{SWAP}^{(1,3)} | B \rangle \otimes | B \rangle$$

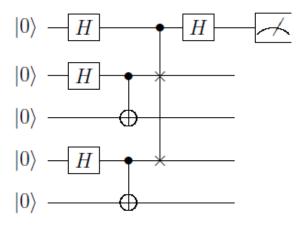
#### Real part:

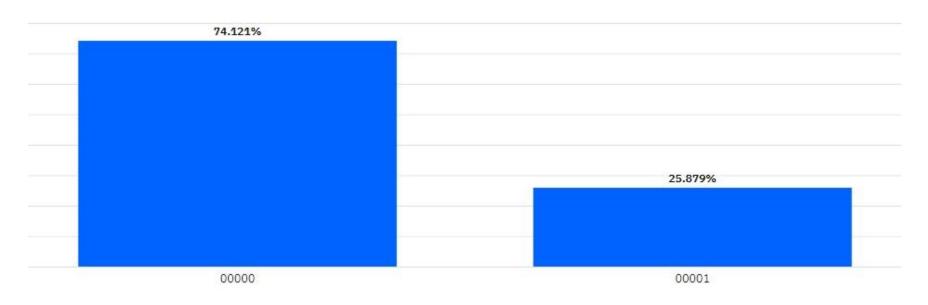


#### **Imaginary part:**



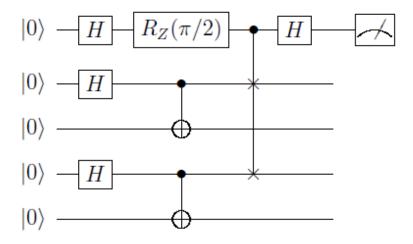
### Result of simulator (real part, 1024 shots)

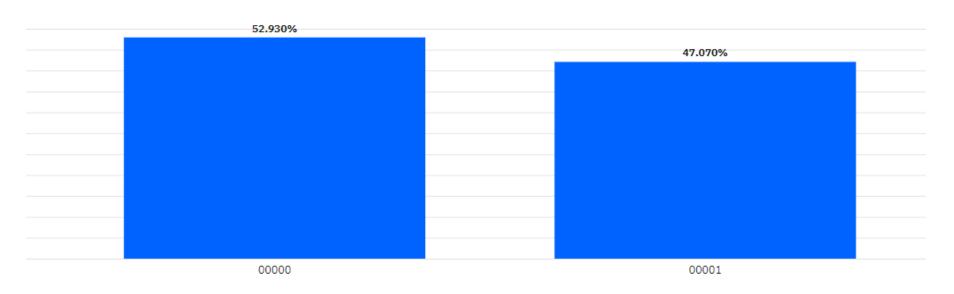




Expectation: 
$$P_0 - P_1 = \text{Re tr} \rho_{\text{red}}^2 = \frac{1}{2}$$

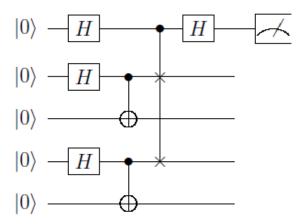
#### Result of simulator (imaginary part, 1024 shots)

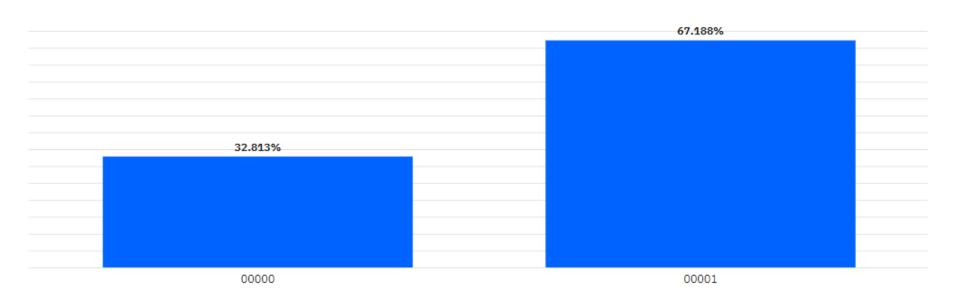




Expectation:  $P_1 - P_0 = \text{Im tr} \rho_{\text{red}}^2 = 0$ 

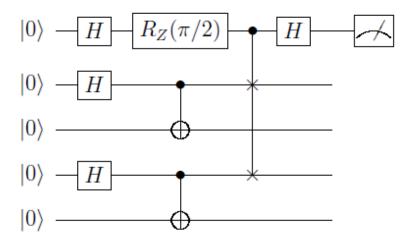
#### Result of quantum computer (real part, 1024 shots)

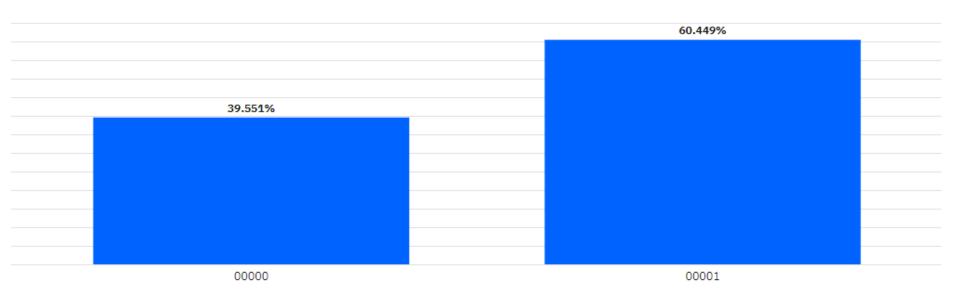




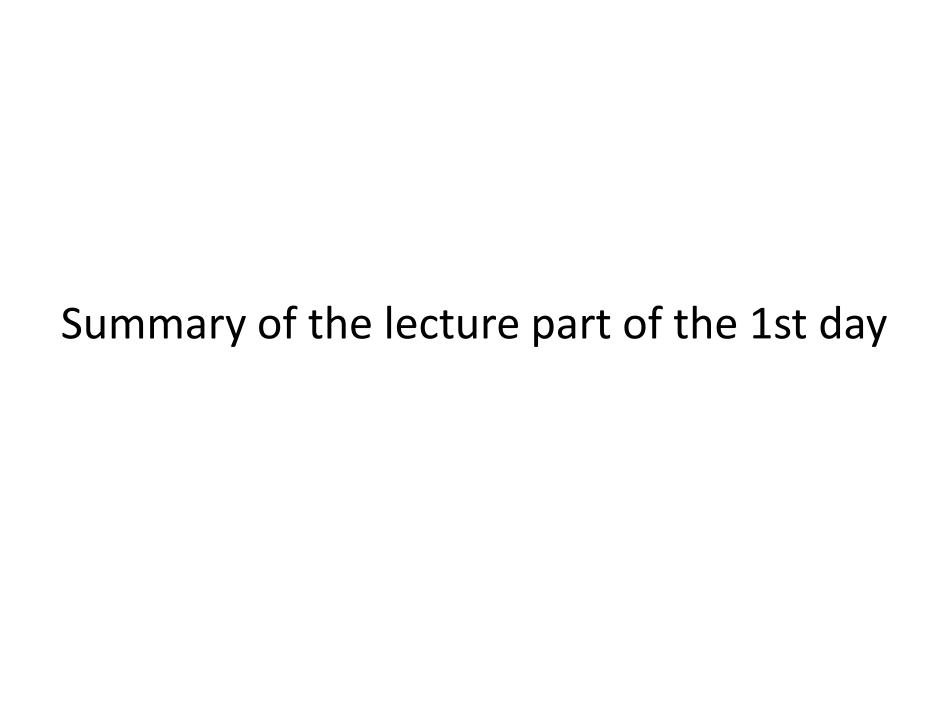
Expectation: 
$$P_0 - P_1 = \text{Re tr} \rho_{\text{red}}^2 = \frac{1}{2}$$

#### Result of quantum computer (imaginary part, 1024 shots)





Expectation:  $P_1 - P_0 = \text{Im tr} \rho_{\text{red}}^2 = 0$ 



## <u>Summary</u>

- Quantum computation is suitable for operator formalism which is free from sign problem
- Instead we have to deal with huge vector space.
   Quantum computers in future may do this job.
- "Rule" of quantum computation
  - = Do something interesting by a combination of acting unitary op. & measurement
- Real quantum computer has errors
- Quantum error correction is important

## Hands-on 1

#### Download a file from my github:

https://github.com/masazumihonda/lectures/tree/main/2023\_Niiga ta QC

# Appendix

### What if we replace *T* by something else?

$$T = e^{\frac{i\pi}{8}} R_Z(\pi/4) \qquad \qquad T' \equiv R_Z(\phi) ??$$

We have the identity:

$$T'HT'H = R_{\vec{n}}(\theta)$$

where

$$\vec{n} = \frac{1}{\sqrt{1 + \cos^2(\phi/2)}} \begin{pmatrix} \cos(\phi/2) \\ \sin(\phi/2) \\ \cos(\phi/2) \end{pmatrix} & \mathbf{\&} \quad \cos(\theta/2) \equiv \cos^2(\phi/2)$$

We can approximate any single qubit gate by combining H & T' if  $\theta/2\pi$  is irrational