Application of Quantum Computation to Quantum Field Theory

- Basics & Spin system -

Masazumi Honda

(本多正純)





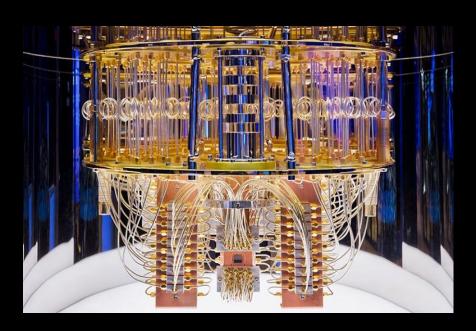


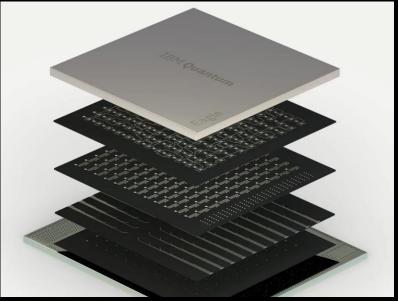






Quantum computer sounds growing well...





Article

Evidence for the utility of quantum computing before fault tolerance

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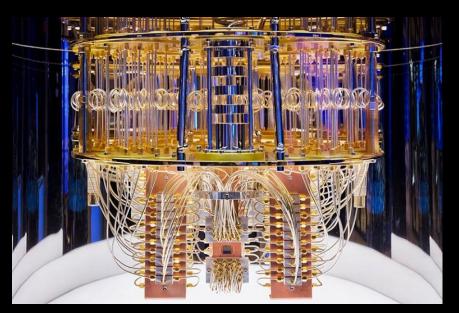
Accepted: 18 April 2023

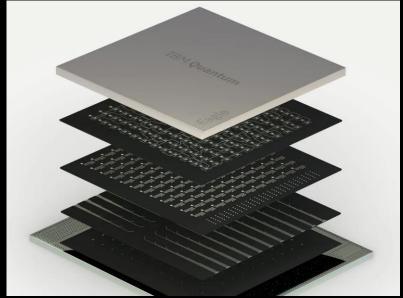
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Quantum computing promises to offer substantial speed-ups over its classical

Quantum computer sounds growing well...



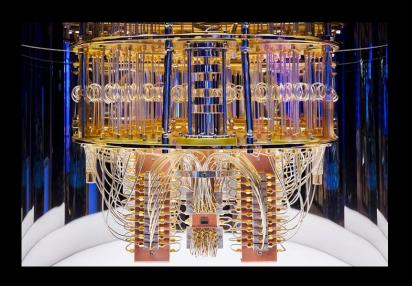


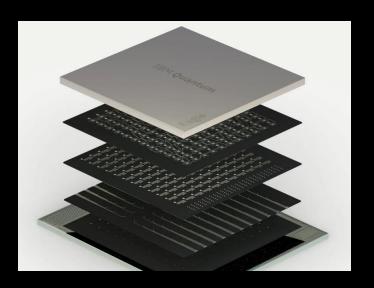
Article

Evidence for the utility of quantum computing before fault tolerance

How can we use it for us?

Applications mentioned in media?





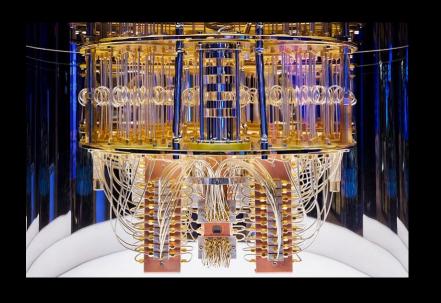


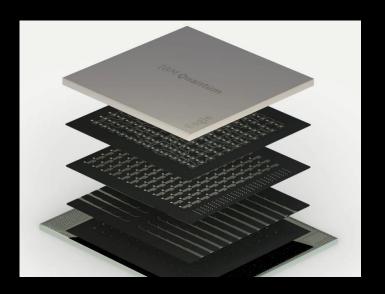






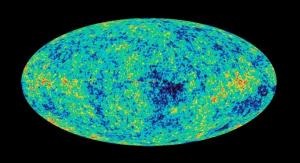
In my mind...













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

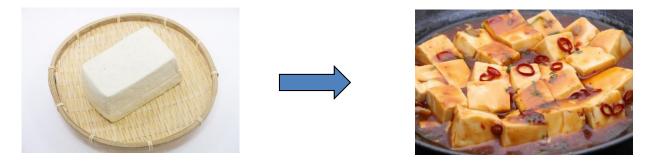
→ Liberation from infamous sign problem in Monte Carlo?

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:

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

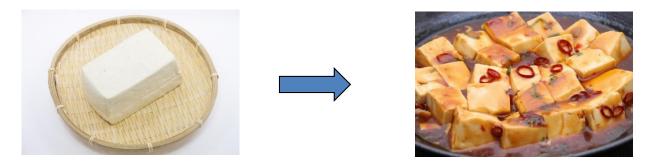


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② Numerically Evaluate it by (Markov Chain) Monte Carlo method regarding the Boltzmann factor as a probability:

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

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

Sign problem in Monte Carlo simulation (Cont'd)

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Examples w/ sign problem:

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

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?

Should we care now as "users"?

Quantum computers don't have sufficient powers yet.

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

I personally think:

³ 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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$$R_X(\theta) = e^{-\frac{i\theta}{2}X}, \quad R_Y(\theta) = e^{-\frac{i\theta}{2}Y}, \quad R_Z(\theta) = e^{-\frac{i\theta}{2}Z}$$

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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

<u>2 qubits – 4 dim. Hilbert space:</u>

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

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

N qubits – 2^N 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

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

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

Two qubit gates used here

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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:

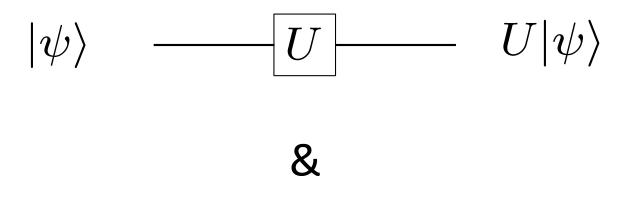
$$\mathsf{SWAP}|\psi\rangle\otimes|\phi\rangle=|\phi\rangle\otimes|\psi\rangle$$

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

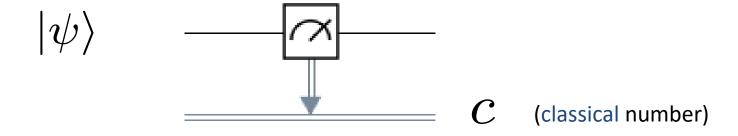
We'll see this is useful to compute Renyi entropy

Rule of the game

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

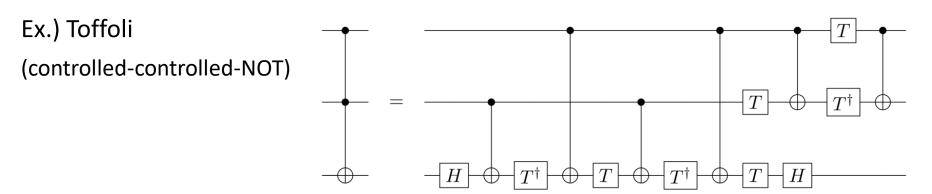


measurements:



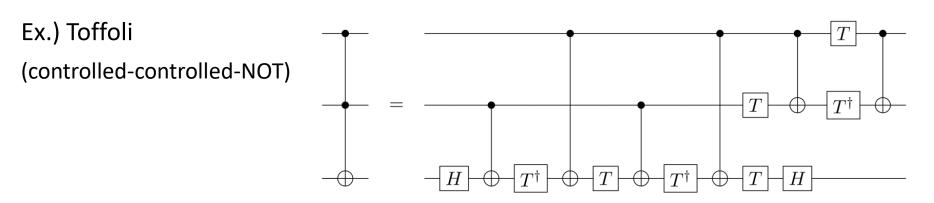
Universality

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



Universality

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

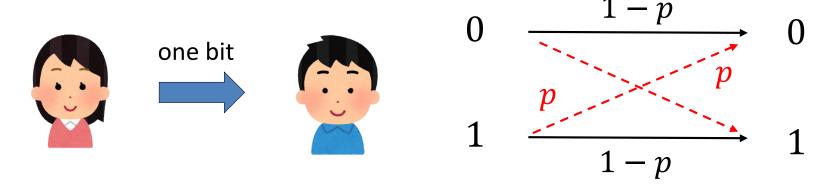
(4) Approximate \forall single qubit gate: $R_{\vec{n}}(\alpha)R_{\vec{m}}(\beta)$ $R_{\vec{n}}(\gamma)$ (To achieve accuracy ϵ , it requires $\mathcal{O}(\log^c(1/\epsilon))$ gates w/ $c\sim 2$) [Solovay '95, Kitaev '97]

Errors in classical computers

Computer interacts w/ environment error/noise

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Computer interacts w/ environment error/noise

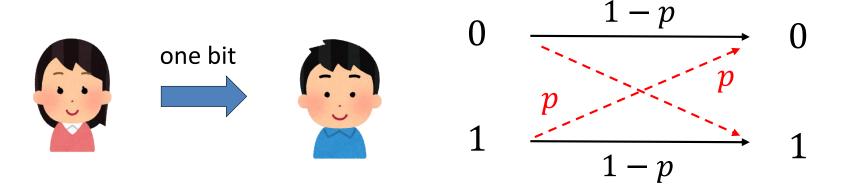


Suppose we send a bit but have "error" in probability p

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

Computer interacts w/ environment error/noise

(In addition to decoherence & measurement errors)

Unknown unitary operators are multiplied:

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

~ major obstruction of the development

(We will come back to this point on the 3rd day)

(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)

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Short summary

- Qubit = Quantum bit
- Important gates:

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

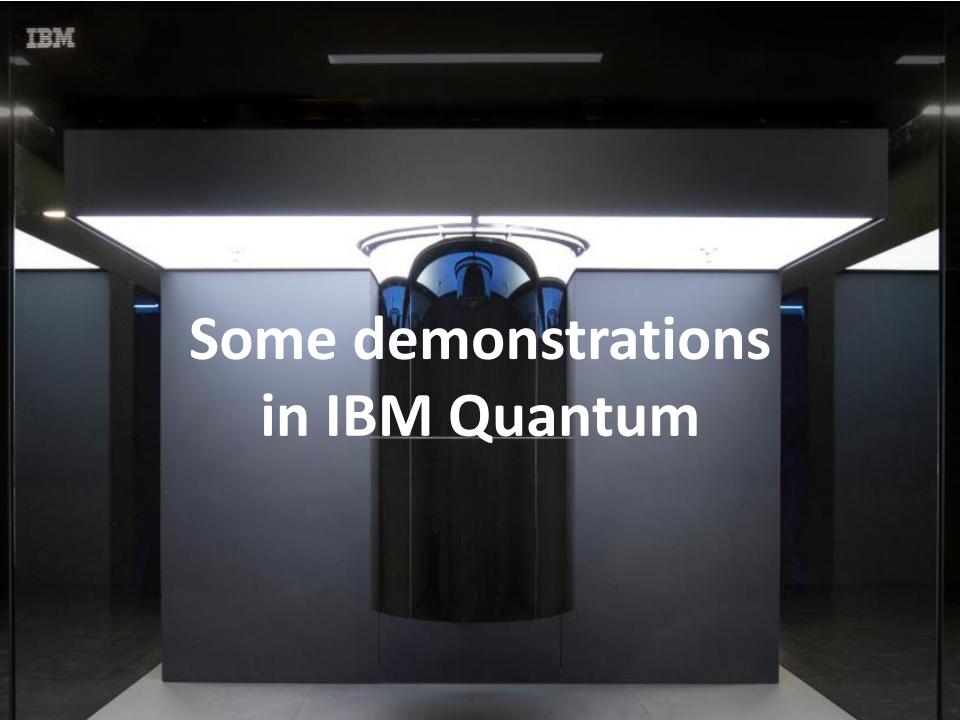
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$$CX|0\rangle \otimes |\psi\rangle = |0\rangle \otimes |\psi\rangle, \quad CX|1\rangle \otimes |\psi\rangle = |1\rangle \otimes X|\psi\rangle$$

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

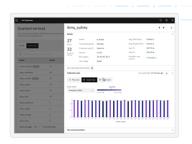
$$T = e^{\frac{\pi i}{8}} R_Z \left(\frac{\pi}{4}\right) = \begin{pmatrix} 1 & 0\\ 0 & e^{\frac{i\pi}{4}} \end{pmatrix}$$

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



Real quantum computers. Right at your fingertips.

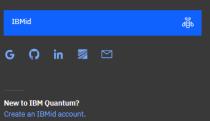
IBM offers cloud access to the most advanced quantum computers available. Learn, develop, and run programs with our quantum applications and systems.



View quantum system details

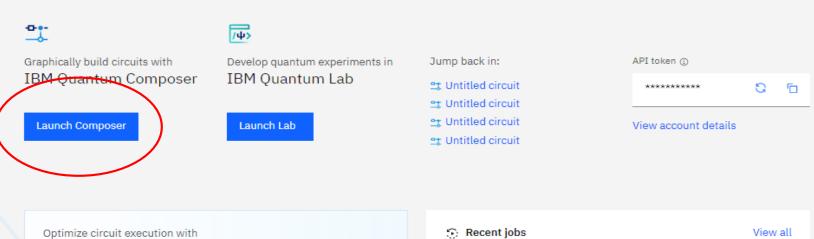
Check out the status, topology, calibration data, and access details of your IBM quantum systems.

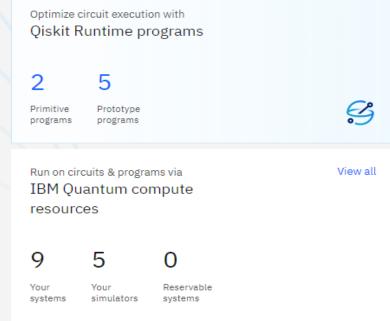
Sign in to IBM Quantum

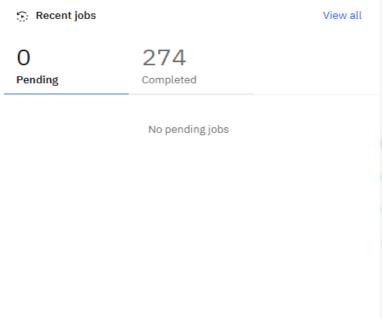


Having trouble signing in:

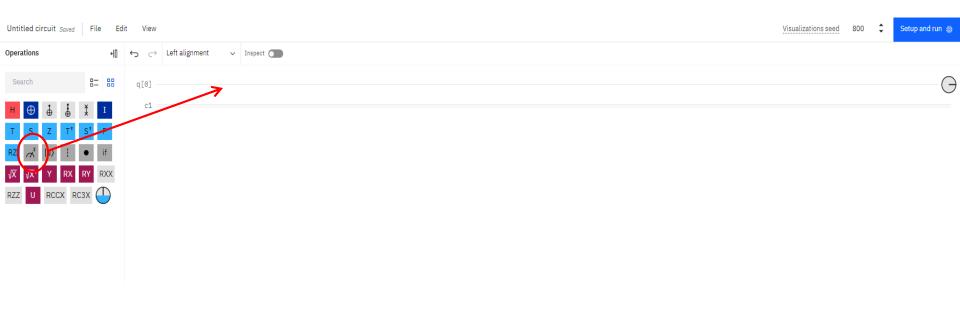
Welcome, Honda Masazumi



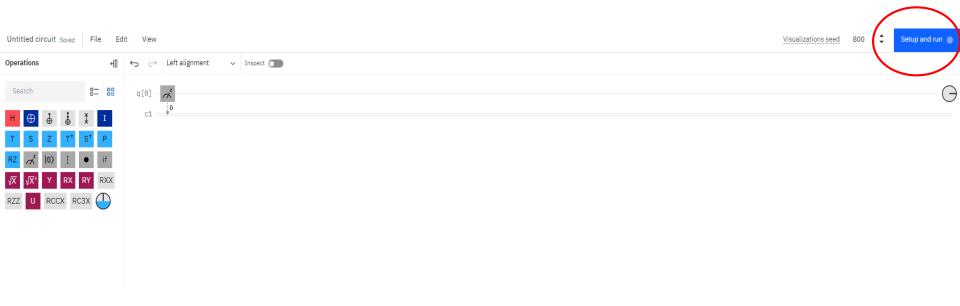




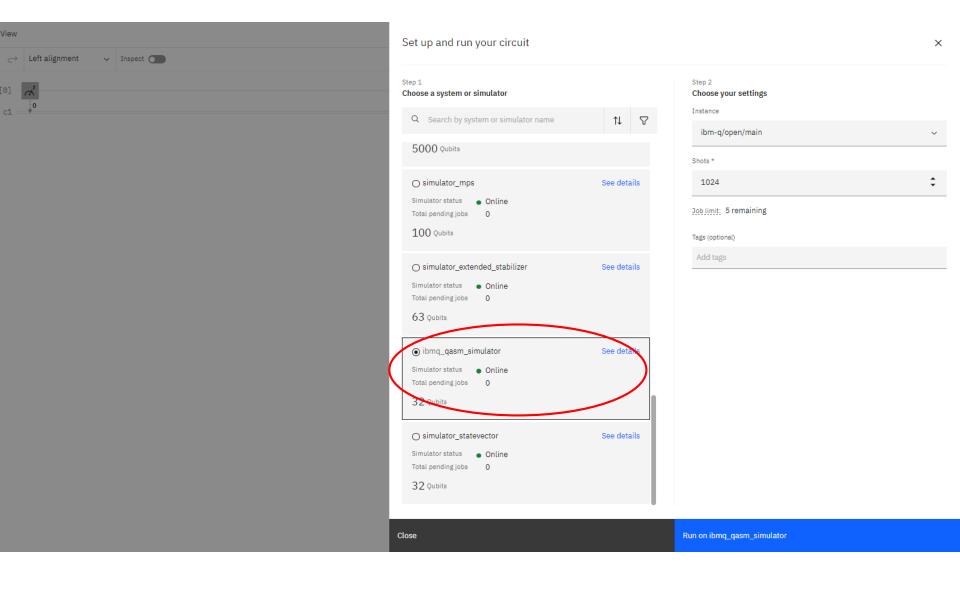
A trivial problem: measure |0|



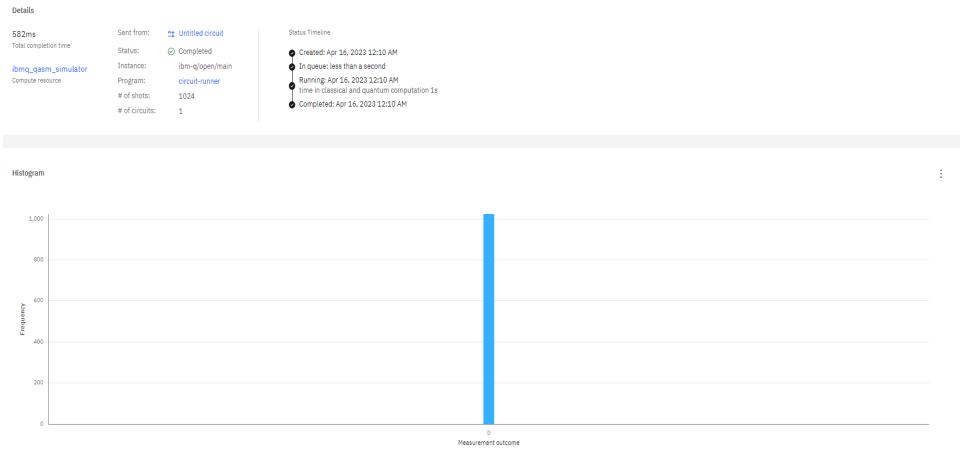
A trivial problem: measure $|0\rangle$ (Cont'd)



Measure 1024 times in simulator

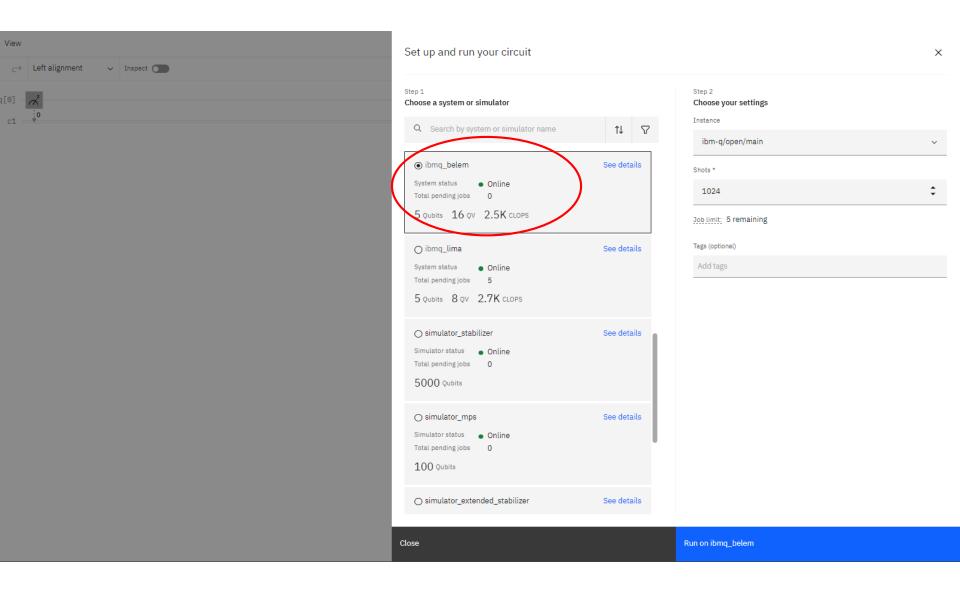


Trivial result

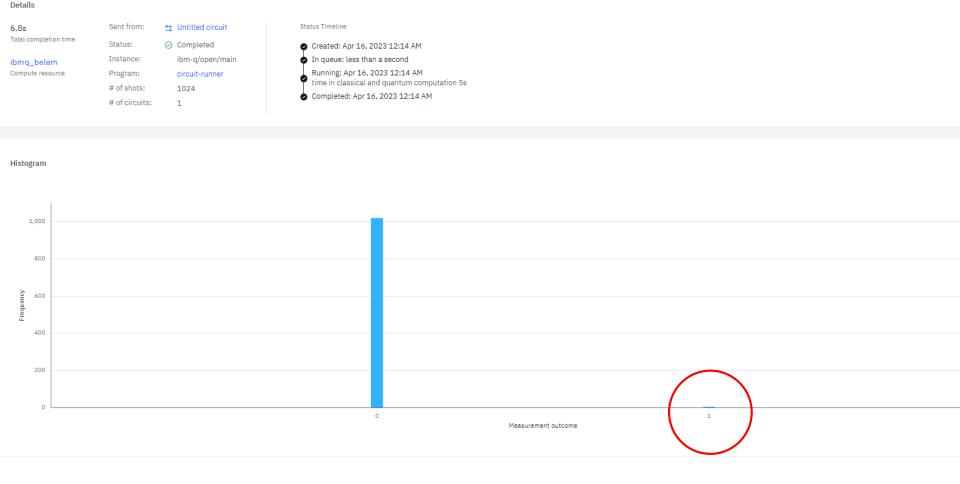


Of Course!

Measure 1024 times in quantum computer

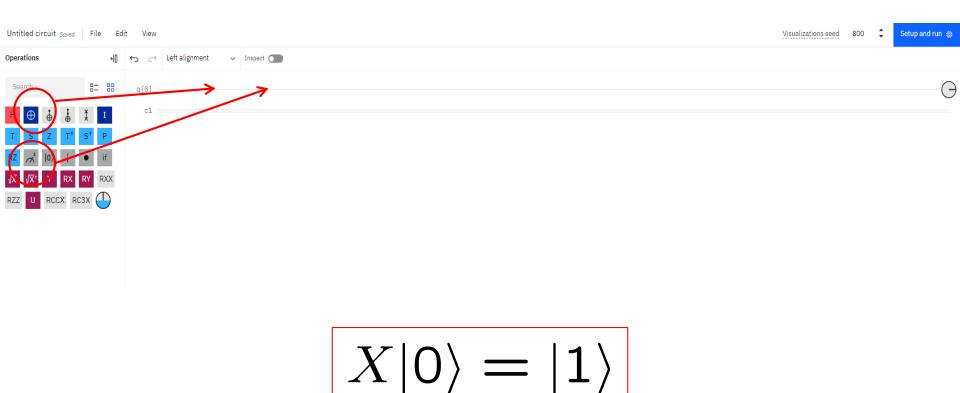


Result of quantum computer?

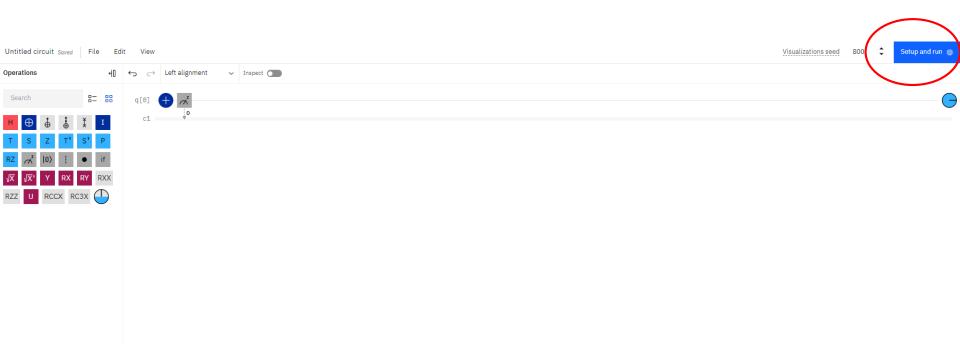


This is the error!

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

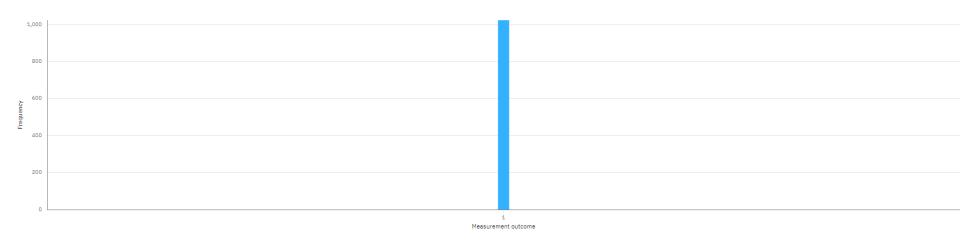
 # of circuits:
 1

■ 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

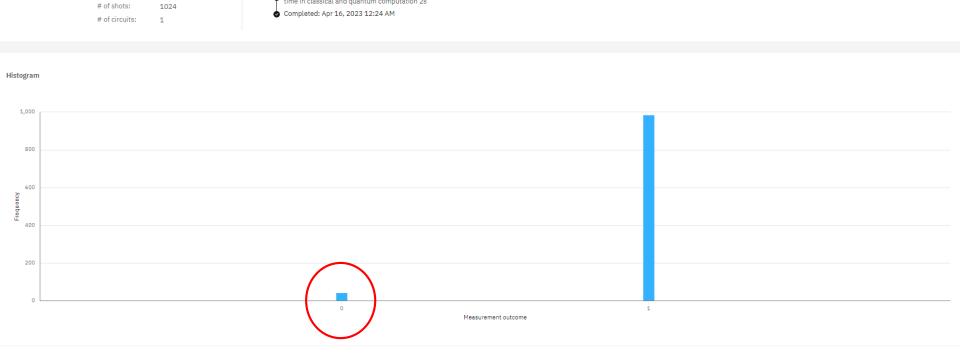
Oreated: Apr 16, 2023 12:24 AM

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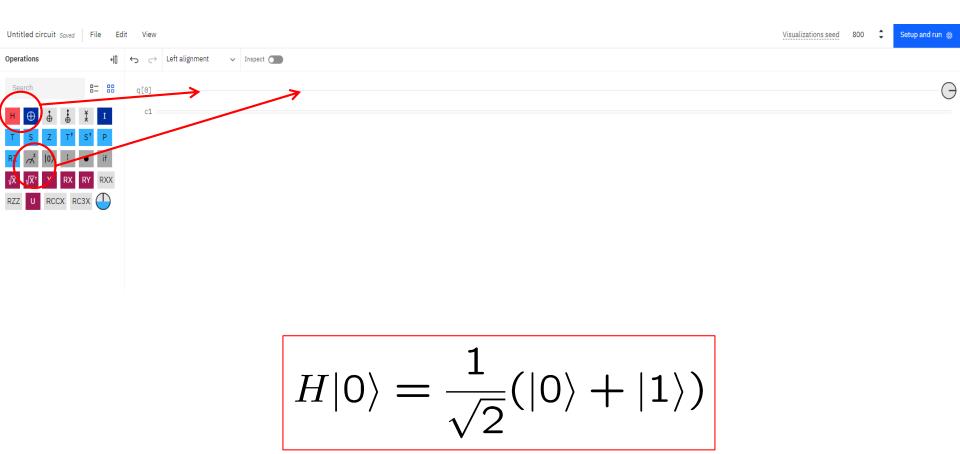
Error again

time in classical and quantum computation 2s

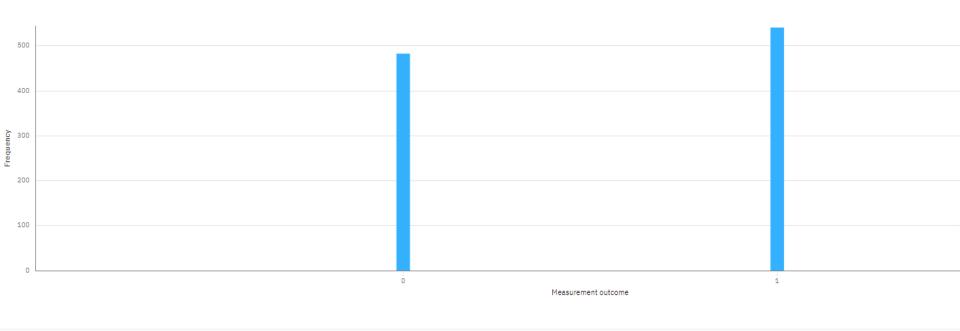
In queue: less than a second



The simplest nontrivial problem: Hadamard gate

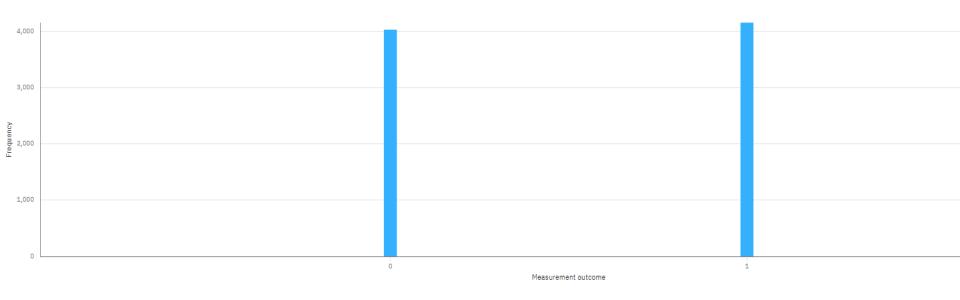


Result of simulator (1024 shots)



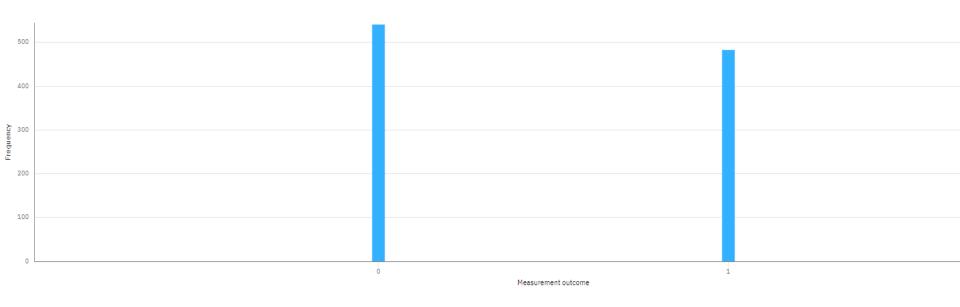
Not exactly 50:50 because of statistical errors

Result of simulator (8192 shots)



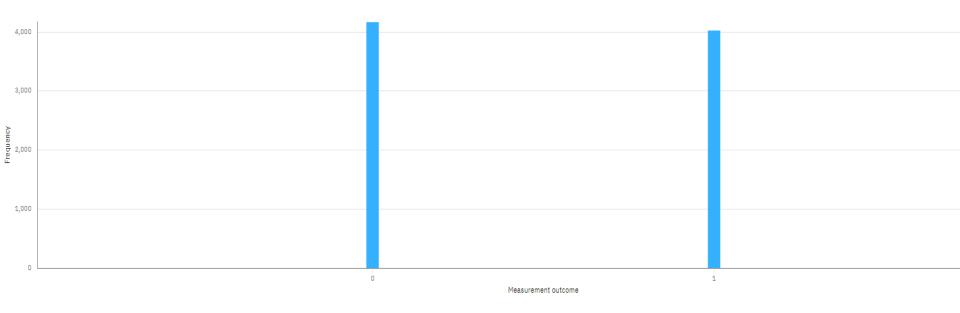
Improved!

Result of quantum computer (1024 shots)



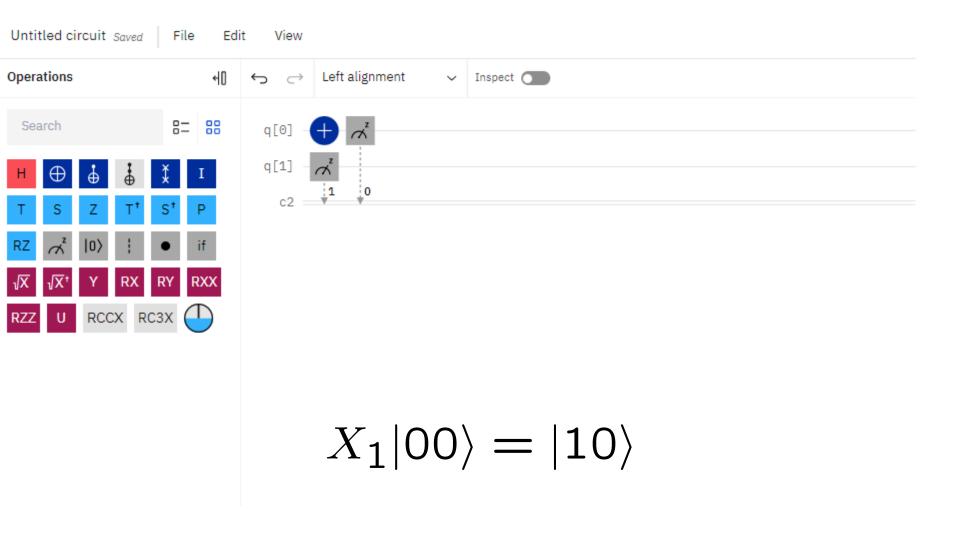
∃ Both errors & statistical errors

Result of quantum computer (8192 shots)



Statistical errors are improved

A trivial problem for 2 qubits



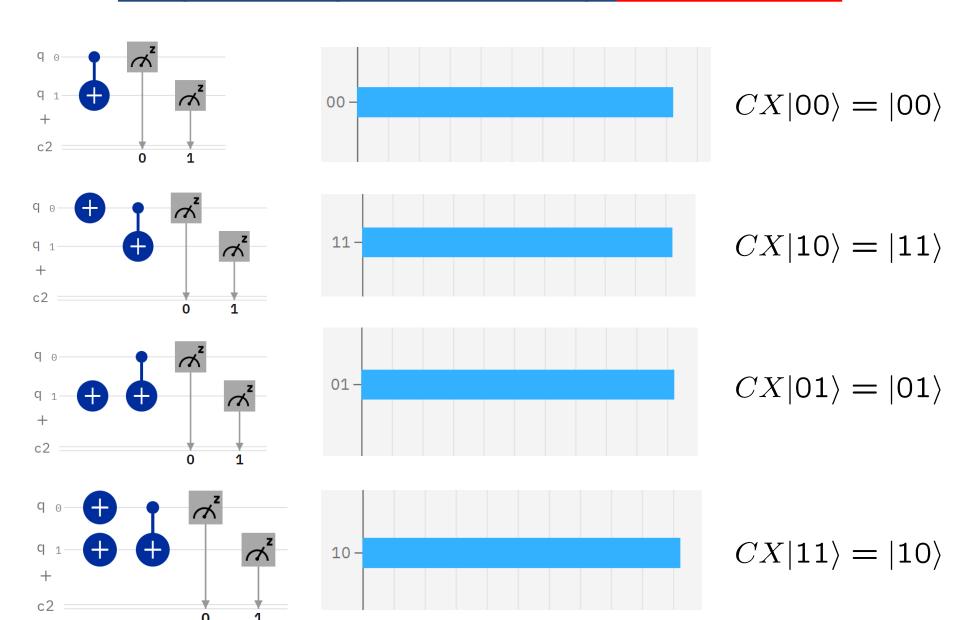
Result of simulator (1024 shots)

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

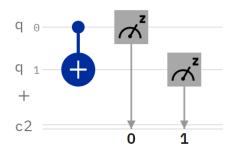


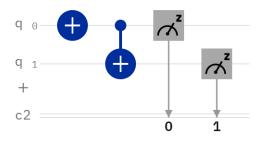
Note that notation is different from the ket notation

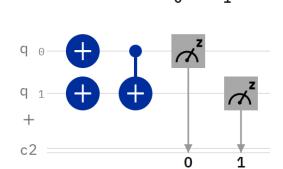
2 qubit operation by simulator



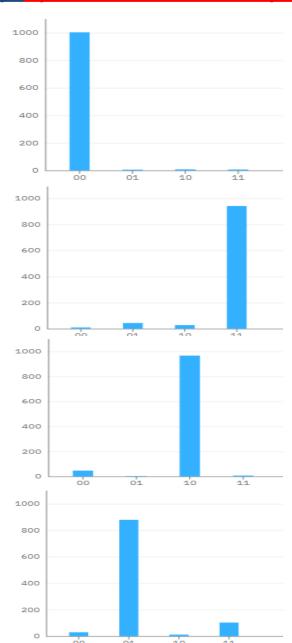
2 qubit operation by quantum computer (1024 shots)







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:

(³ 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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$$e^{-iH_X \frac{t}{M}} = e^{-i\frac{ht}{M}X_2} e^{-i\frac{ht}{M}X_1} = R_X^{(2)} \left(\frac{2ht}{M}\right) R_X^{(1)} \left(\frac{2ht}{M}\right)$$

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:

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

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

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

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

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

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

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

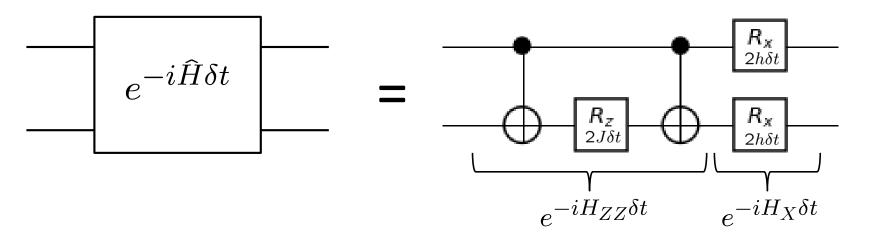
Thus,

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

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:

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

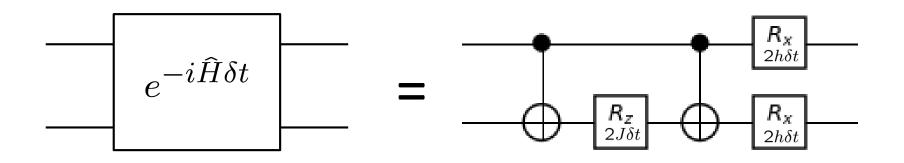
$$= \left| \langle 00 | H^{(2)}H^{(1)}e^{-i\hat{H}t}H^{(2)}H^{(1)} | 00 \rangle \right|^{2}$$

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

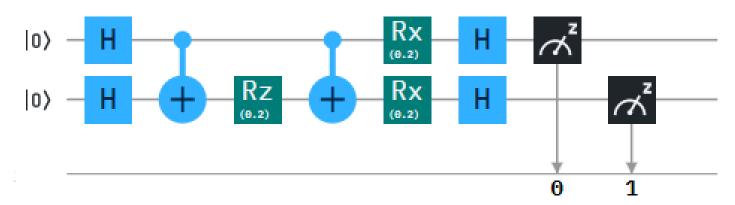
$$P(t) = \left| \langle + + | e^{-i\hat{H}t} | + + \rangle \right|^2 = \left| \langle 00 | H^{(2)} H^{(1)} e^{-i\hat{H}t} H^{(2)} H^{(1)} | 00 \rangle \right|^2$$



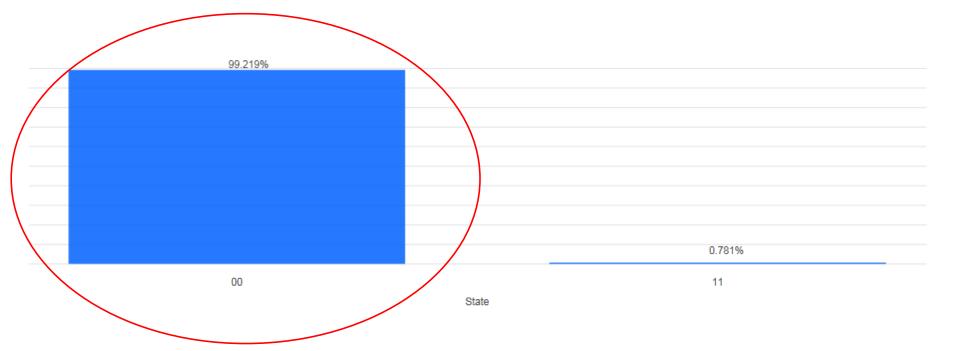
Let's compute it for J = 1, h = 1, t = 0.1, M = 1

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

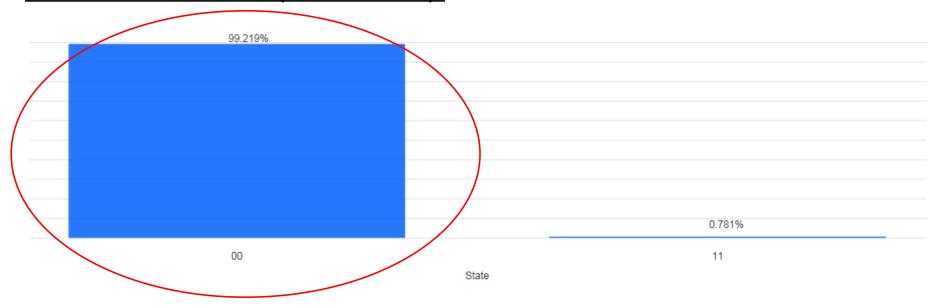
Demonstration for the survival probability (Cont'd)



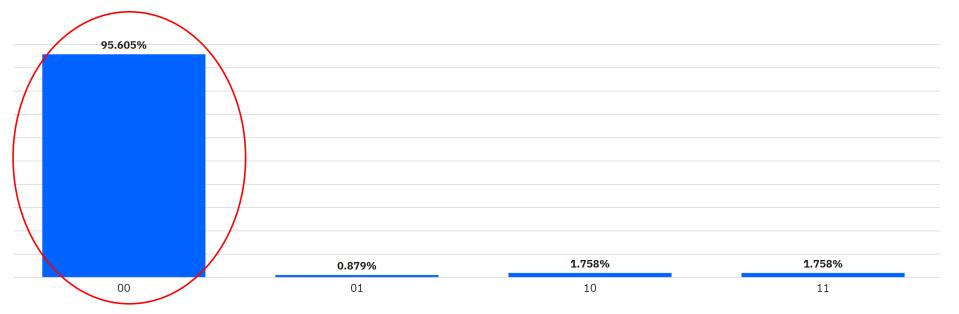
Result by simulator w/ 1024 shots:



Result of simulator (1024 shots):

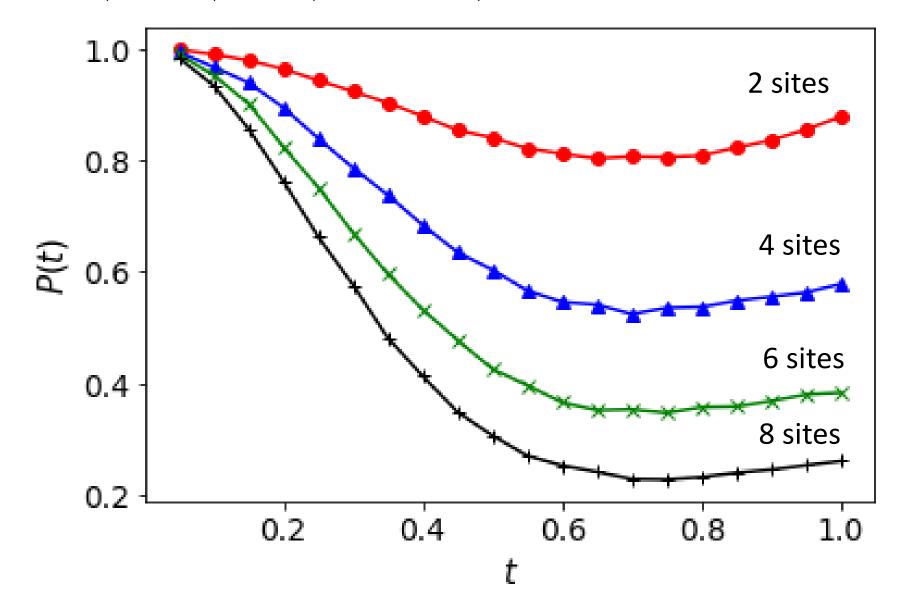


Result of quantum computer (1024 shots):



More serious computation

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



Computational costs for large size system

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

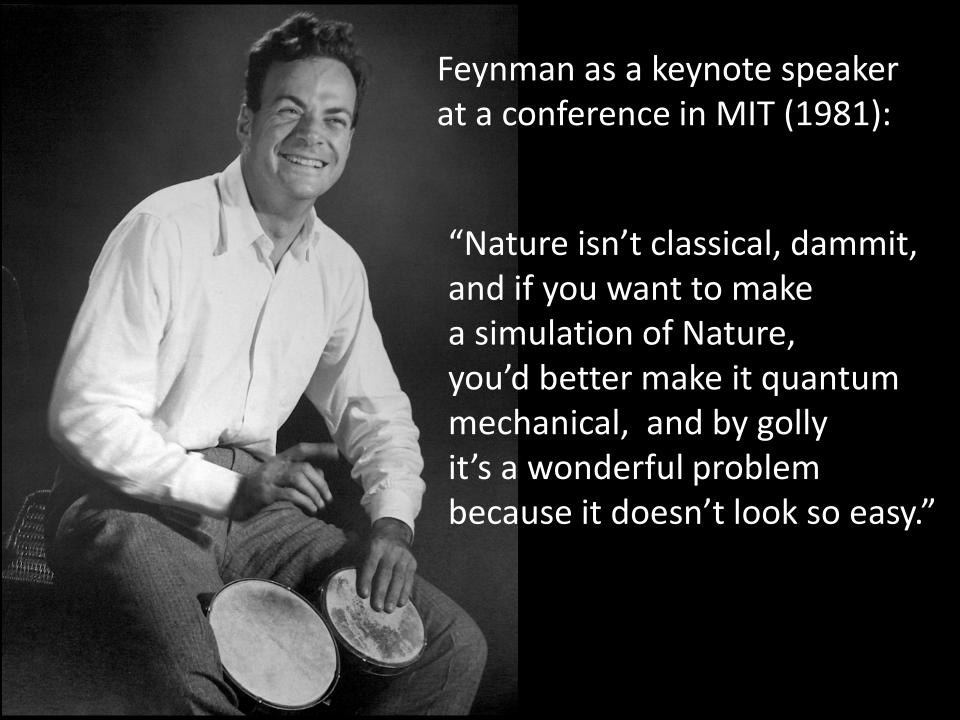
Classical computer

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)

[∃]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>:

Adiabatic state preparation of vacuum

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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_{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:

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

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

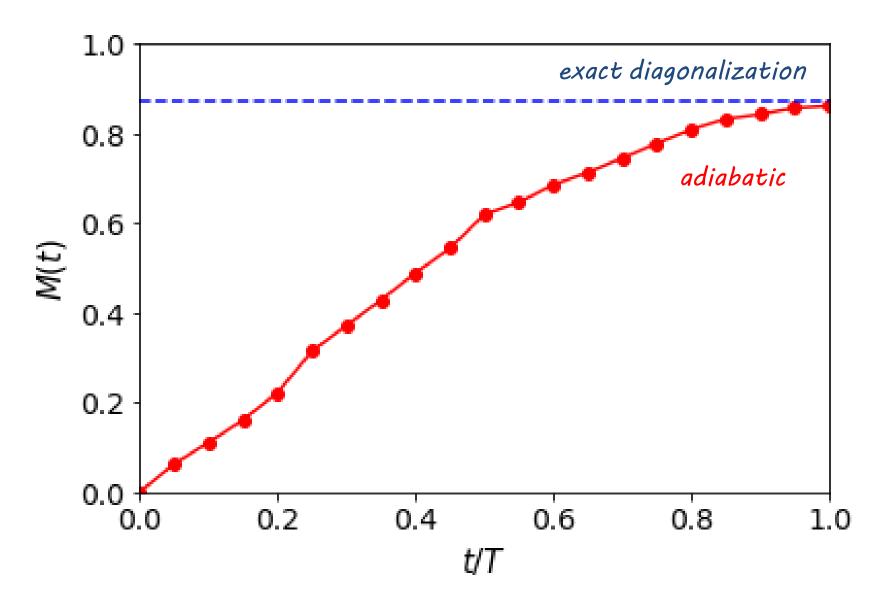
Transverse one is a bit more tricky:

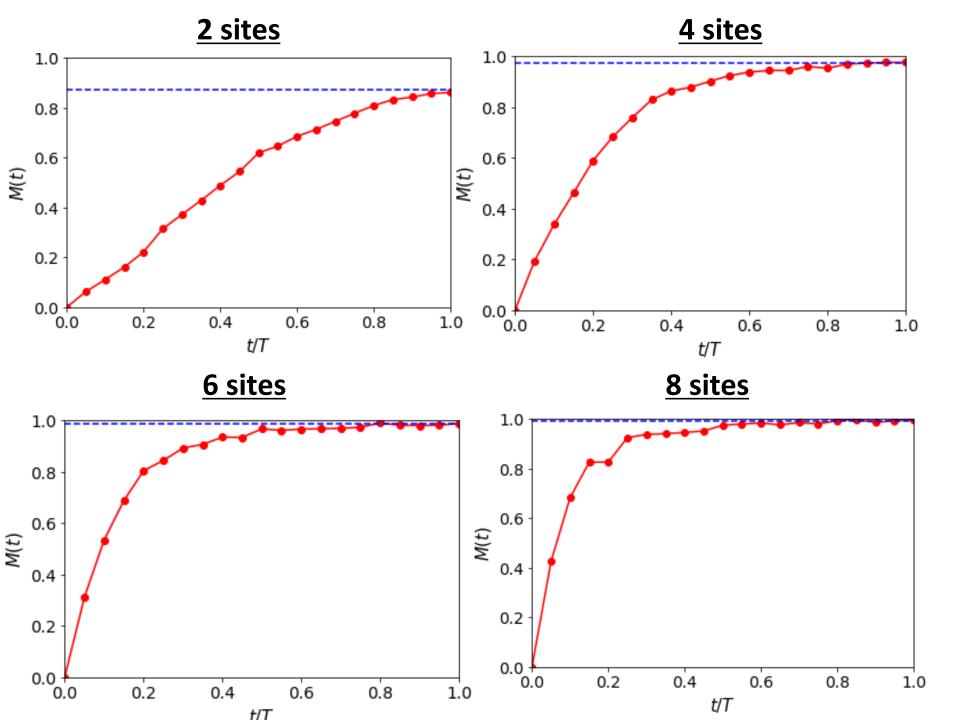
$$\frac{1}{N}\langle \operatorname{vac}|\sum_{n=1}^{N} X_{n}|\operatorname{vac}\rangle = \frac{1}{N}\langle \operatorname{vac}|\sum_{n=1}^{N} H^{(n)}Z_{n}H^{(n)}|\operatorname{vac}\rangle$$

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

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_A: 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

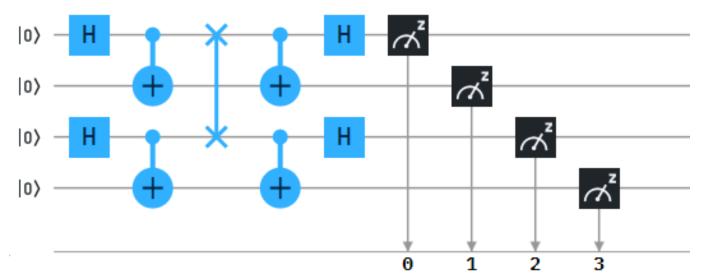
$$|0\rangle \qquad H \qquad = |B\rangle$$

Therefore,

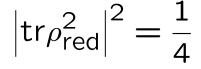
$$\operatorname{tr} \rho_{\mathrm{red}}^2 = \langle 0000 | U^{\dagger} \mathrm{SWAP}^{(1,3)} U | 0000 \rangle \quad (|B\rangle \otimes |B\rangle \equiv U | 0000 \rangle)$$

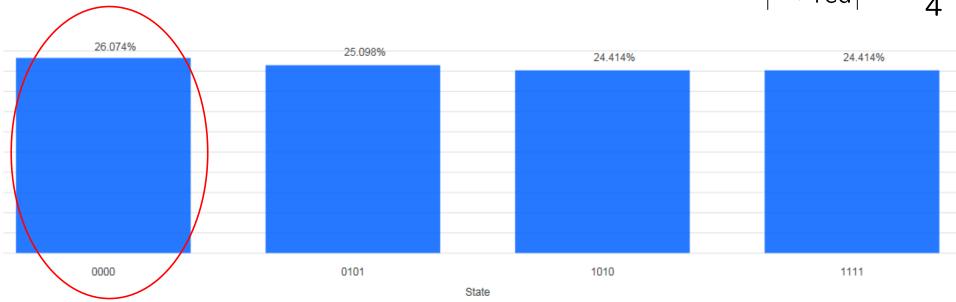
$$\left| \operatorname{tr} \rho_{\text{red}}^2 \right|^2 = \left| \langle 0000 | U^{\dagger} \text{SWAP}^{(1,3)} U | 0000 \rangle \right|^2$$

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

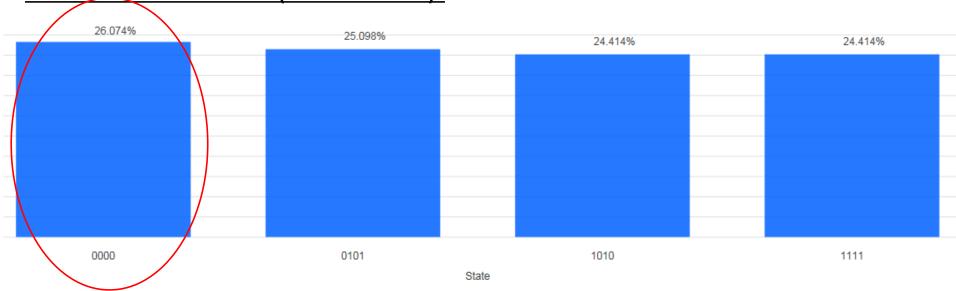




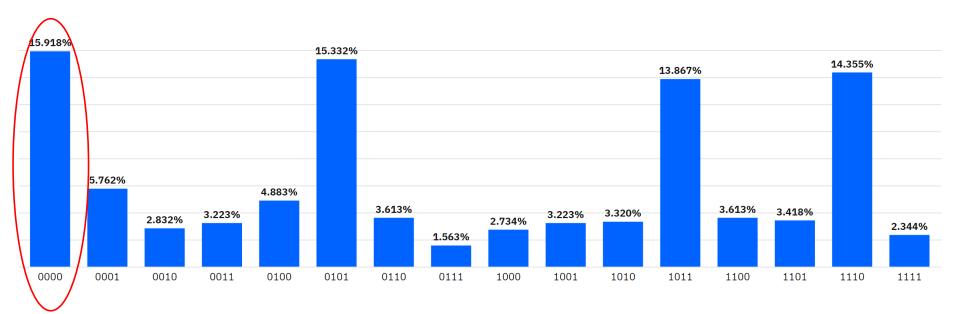




Result of simulator (1024 shots):



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?

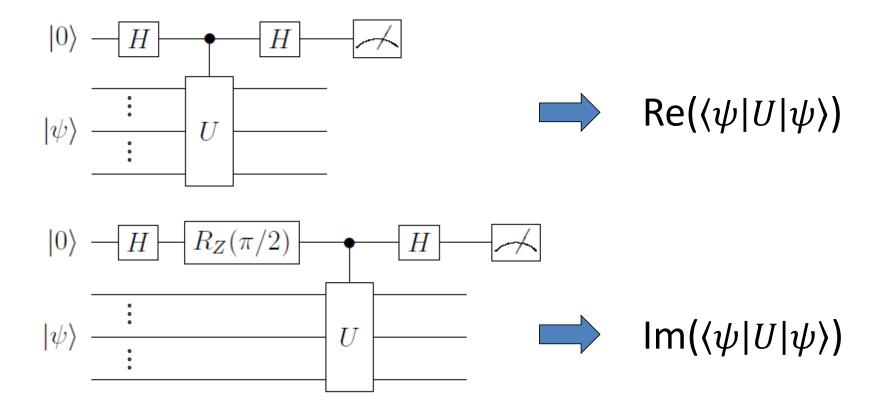
Yes, there is a way to compute expectation value of unitary op. under any state: (next slide)

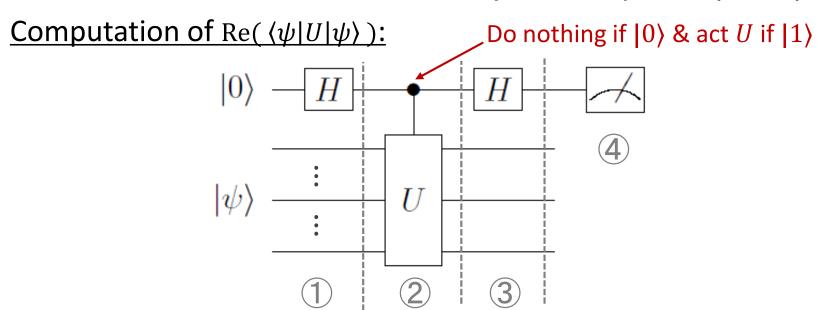
$$\langle \psi | U | \psi \rangle$$

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 $|1\rangle$ $|0\rangle \qquad H \qquad \qquad 4$ $|\psi\rangle \qquad \vdots \qquad \qquad 1$ $2 \qquad 3$

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

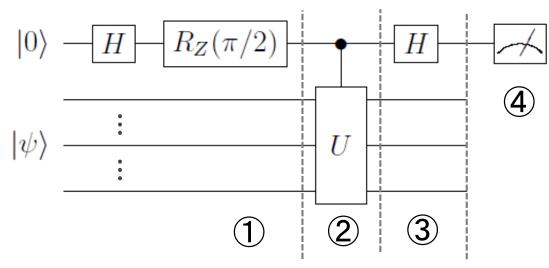
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$$P_0 = \frac{1}{4} |(1+U)|\psi\rangle|^2 = \frac{1}{2} (1 + \text{Re}\langle\psi|U|\psi\rangle)$$

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



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

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



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

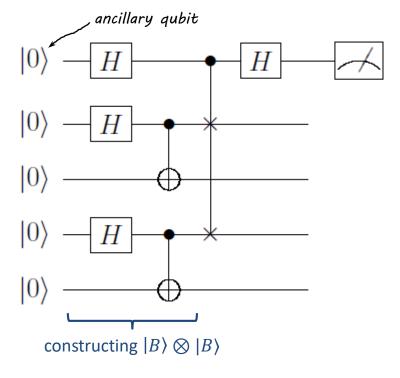
 $\operatorname{Im}\langle\psi|U|\psi\rangle = P_1 - P_0$

Coming back to the Renyi entropy of Bell state

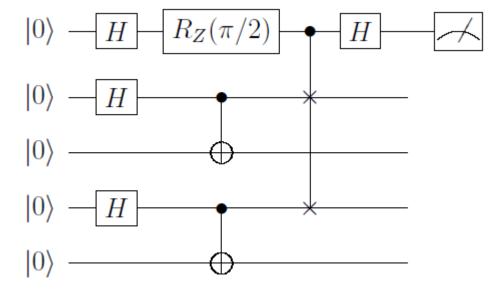
Taking $|\psi\rangle = |B\rangle \otimes |B\rangle \otimes U = SWAP^{(1,3)}$, we can directly compute

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

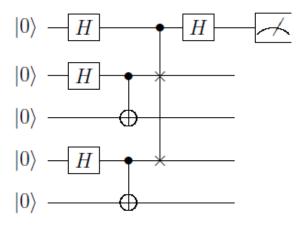
Real part:

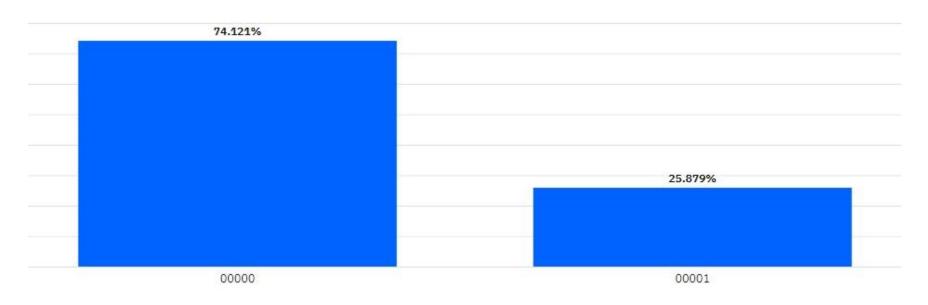


Imaginary part:



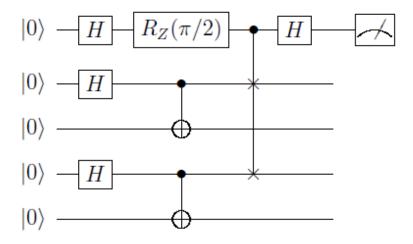
Result of simulator (real part, 1024 shots)

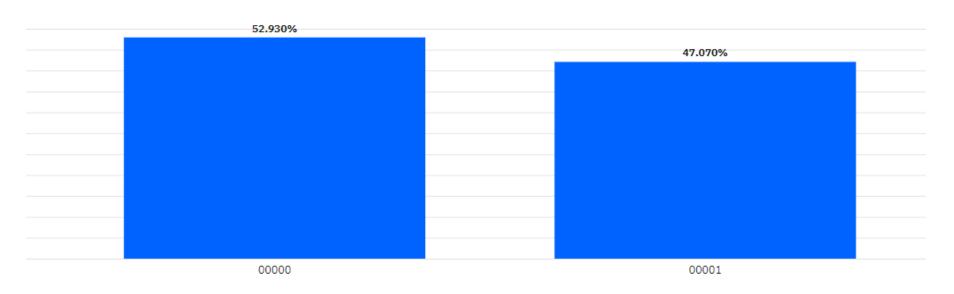




Expectation:
$$P_0 - P_1 = \text{Re tr} \rho_{\text{red}}^2 = \frac{1}{2}$$

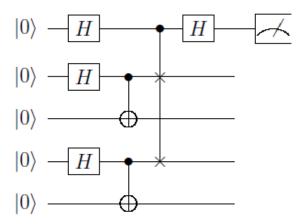
Result of simulator (imaginary part, 1024 shots)

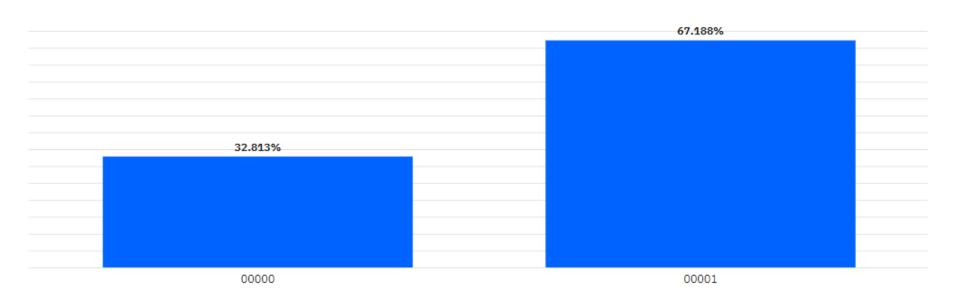




Expectation: $P_1 - P_0 = \text{Im tr} \rho_{\text{red}}^2 = 0$

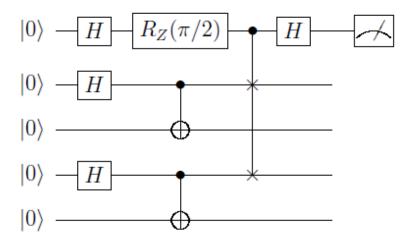
Result of quantum computer (real part, 1024 shots)

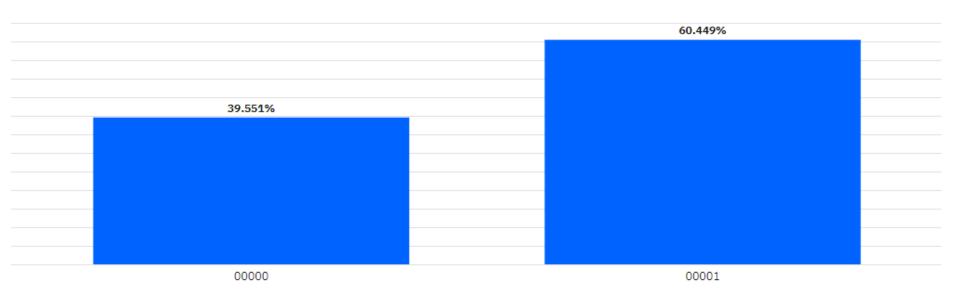




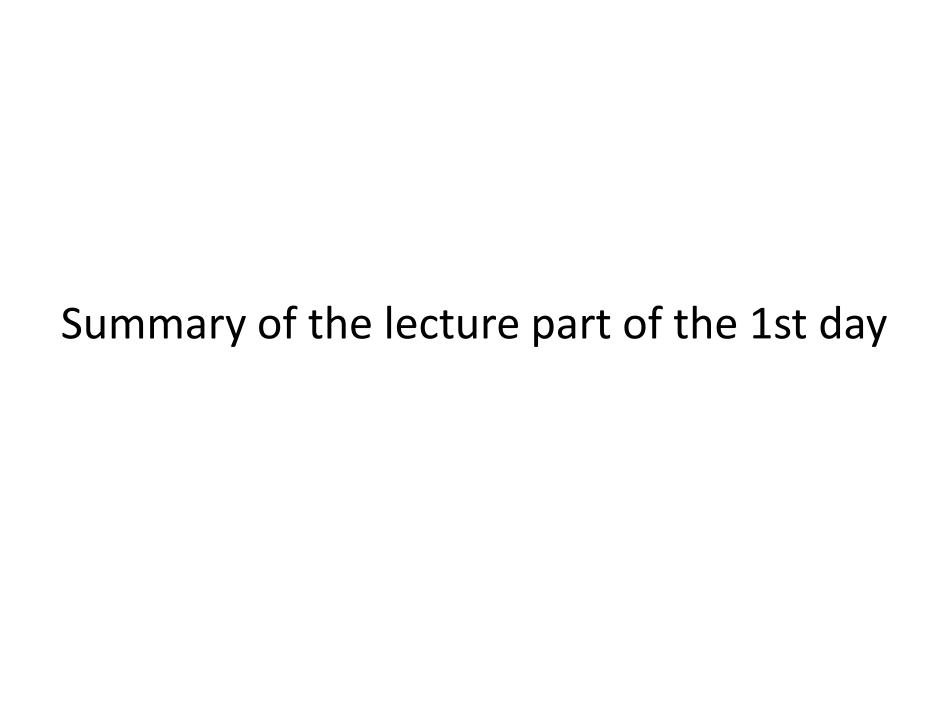
Expectation:
$$P_0 - P_1 = \text{Re tr} \rho_{\text{red}}^2 = \frac{1}{2}$$

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