素粒子物理学のための量子計算入門
～基礎＆スピン系編～

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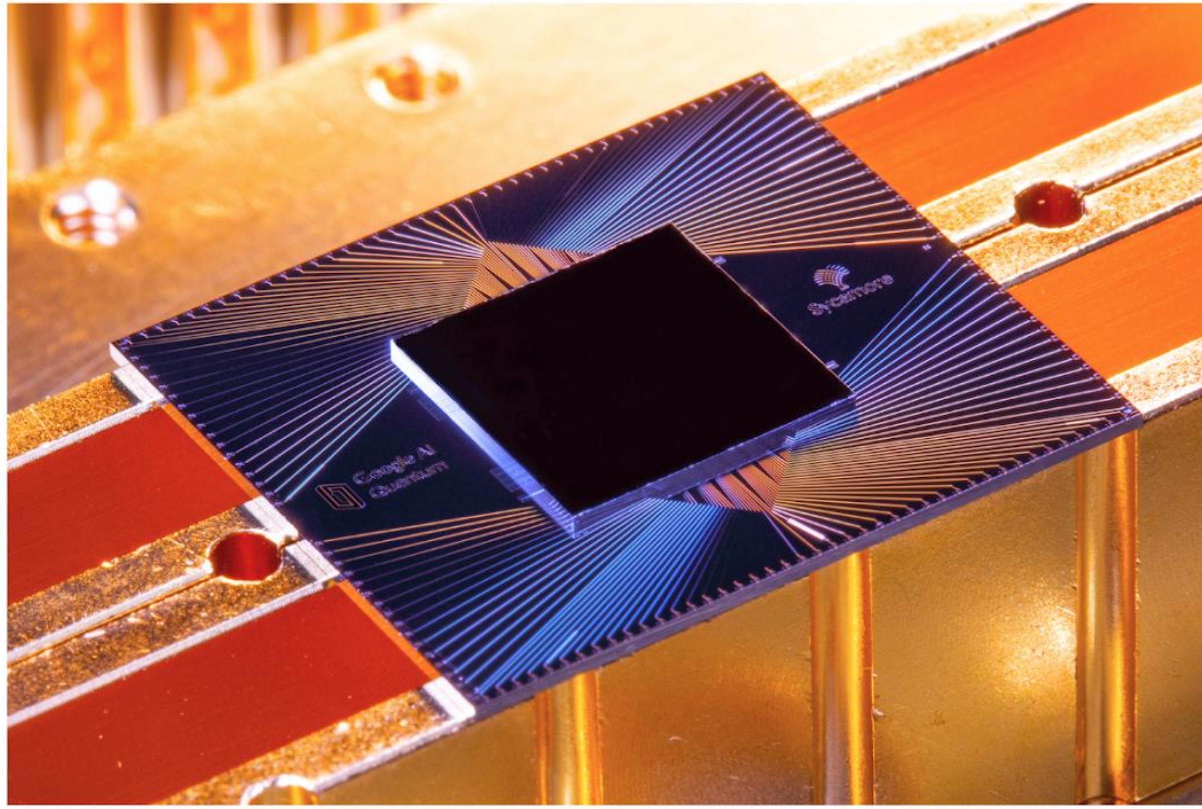
第11回HPC-Phys勉強会

※zoomにて録画予定

Quantum computer sounds growing well…

[Credit: Forest Stearns, Google AI Quantum Artist in Residence (CC BY-ND 4.0)]

[Credit: Erik Lucero, Research Scientist and Lead Production Quantum Hardware, Google (CC BY-ND 4.0)]



Article

Quantum supremacy using a programmable superconducting processor

https://doi.org/10.1038/s41586-019-1666-5

Frank Arute[1], Kunal Arya[1], Ryan Babbush[1], Dave Bacon[1], Joseph C. Bardin[1,2], Rami Barends[1],

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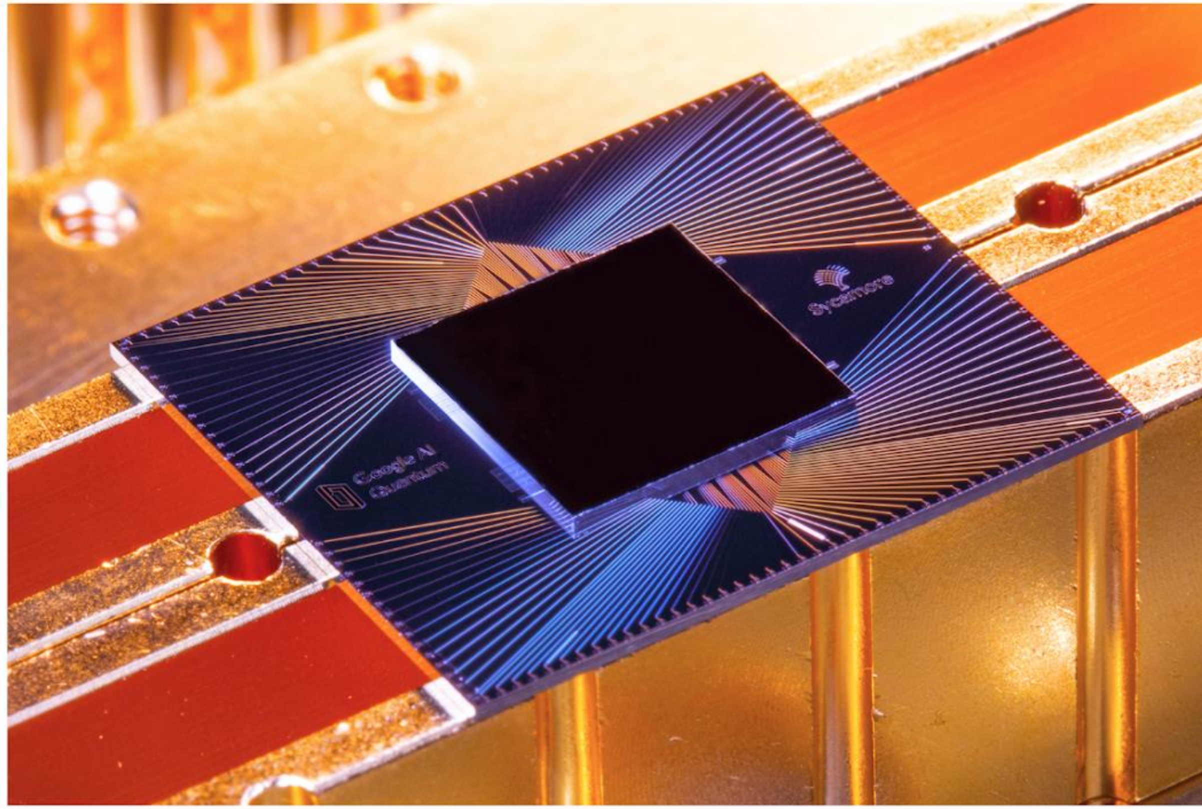
[Credit: Erik Lucero, Research Scientist and Lead Production Quantum Hardware, Google (CC BY-ND 4.0)]



Article

Quantum supremacy using a programmable superconducting processor

This lecture = How can we use it for particle physics?

This lecture is a preparation for

Application of Quantum Computation
to
Quantum Field Theory (QFT)

- <u>Generic motivation:</u>

  simply would like to use powerful computers?

- <u>Specific motivation:</u>

This lecture is a preparation for

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 Hamiltonian formalism

$\longrightarrow$ Liberation from infamous sign problem in Monte Carlo?

(next slide)

Sign problem in Monte Carlo simulation

Conventional approach to simulate QFT:

(this point is explained to give a motivation & isn't essential to understand main contents of the lectures)

① Discretize Euclidean spacetime by lattice:

& make path integral finite dimensional:

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

②

Sign problem in Monte Carlo simulation

Conventional approach to simulate QFT:

(this point is explained to give a motivation & isn't essential to understand main contents of the lectures)

① Discretize Euclidean spacetime by lattice:

& make path integral finite dimensional:

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

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

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

Sign problem in Monte Carlo simulation (Cont'd)

Markov Chain Monte Carlo:

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

problematic when Boltzmann factor isn't $\mathbf{R}_{\geqq 0}$ & 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 Hamiltonian formalism,

sign problem is absent from the beginning

($^{\exists}$various approaches within framework of path integral formalism but I'll skip it)

Cost of Hamiltonian 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:

$^{\exists}$ Many things to do even now in various contexts

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

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)

- $^{\exists}$ only 1 example so far to take a serious continuum limit

[Chakraborty-MH-Kikuchi-Izubuchi-Tomiya '20]

Some good news…

- If you have google or facebook account,
  you can immediately use IBM's quantum computer for free

- Algorithms for simulating quantum system are much easier than ones for generic purpose (e.g. Shor's algorithm for prime factorization)

- Simple code can be made by drug & drop in IBM's website and serious code is made by python

- I am beginner of both python and quantum computation (started on June, 2019)

- It's fun!!

Plan

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:

$$\alpha|0\rangle + \beta|1\rangle \qquad \text{w/} \quad |\alpha|^2 + |\beta|^2 = 1$$

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:** $|\psi\rangle \rightarrow U|\psi\rangle$ (multiplying 2x2 unitary matrix)

  In quantum circuit notation,

$$|\psi\rangle \quad -\!\!\!-\!\!\!-\boxed{U}-\!\!\!-\!\!\!- \quad U|\psi\rangle$$

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

Single qubit operations

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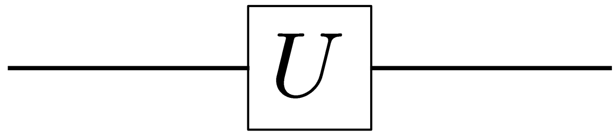
In quantum circuit notation,

$|\psi\rangle$

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



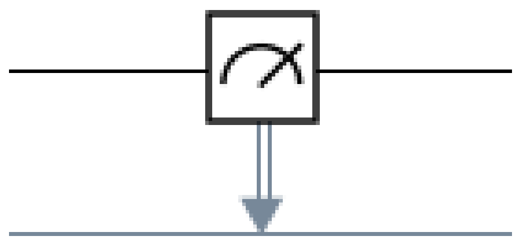
$U|\psi\rangle$

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

- Measurement:

$|\psi\rangle$

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



c (classical number)

$$\begin{cases} c = 0 \text{ w/ probability } |\alpha|^2 \\ c = 1 \text{ w/ probability } |\beta|^2 \end{cases}$$

Single qubit gates used here

$\underline{X, Y, Z \text{ gates :}}$ (just Pauli matrices)

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

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

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R_X, R_Y, R_Z gates :

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

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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:

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

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

N qubits – 2^N dim. Hilbert space:

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

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

Two qubit gates used here

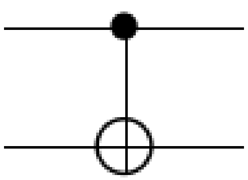
Controlled X (NOT) gate:

$$\begin{cases} CX|00\rangle = |00\rangle, & CX|01\rangle = |01\rangle, \\ CX|10\rangle = |11\rangle, & CX|11\rangle = |10\rangle \end{cases}$$

or equivalently

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

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



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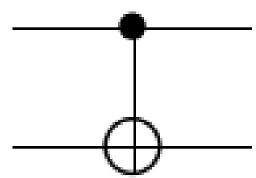
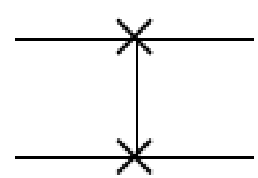


SWAP gate:

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

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



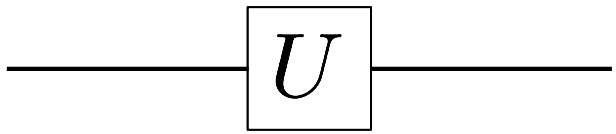
We'll see this is useful to compute Renyi entropy

Rule of the game

Do something interesting by a combination of

action of Unitary operators:

$|\psi\rangle$

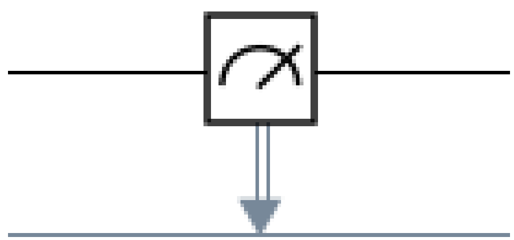


$U|\psi\rangle$

&

measurements:

$|\psi\rangle$



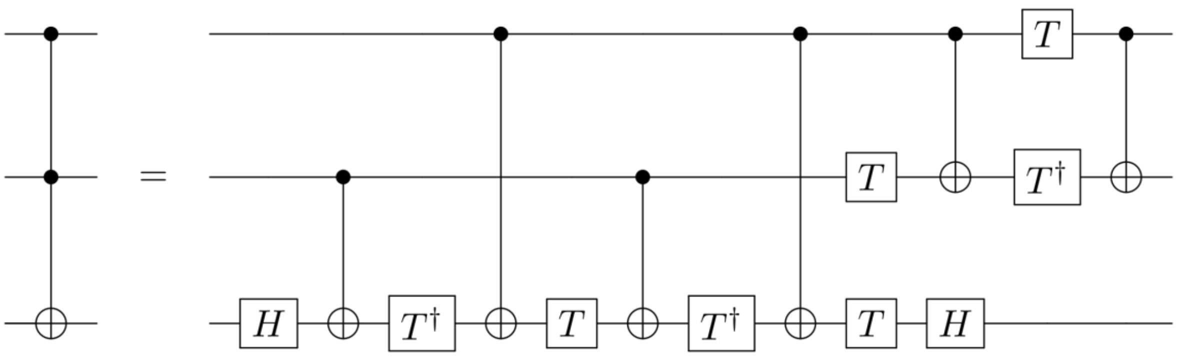
c (classical number)

Universality

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

Ex.) Toffoli

(controlled-controlled-NOT)



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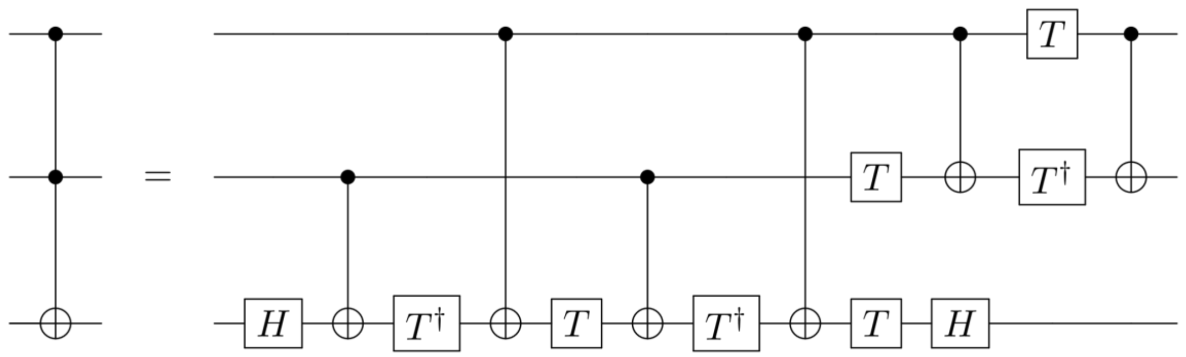

- Any single qubit gate is approximated by a combination of H & T in arbitrary precision

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

- H, T & CX are universal

Errors in Quantum computer

In real quantum computer,

Qubits in quantum circuit ≠ isolated system

➡ Interactions w/ environment cause errors/noises

We need to include "quantum error corrections" which seem to require a huge number of qubits

(∼ major obstruction of the development)

This lecture won't discuss quantum error corrections but it can be taken into account in an independent way of details of algorithm

(Classical) simulator for Quantum computer

Quantum computation $\subset$ 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:

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

$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \equiv |+\rangle, \quad H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \equiv |-\rangle$$

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

- 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

Some demonstrations in IBM Quantum Experience

IBM Quantum Experience is quantum on the cloud

Accelerate your research and applications with the next generation of the leading quantum cloud services and software platform.

Try it out now

Powerful software for the most powerful hardware

Put quantum to work

Run experiments on IBM Q systems and simulators available to the public and IBM Q Network.

Develop and deploy

Explore quantum applications in areas such as chemistry, optimization, finance, and AI.

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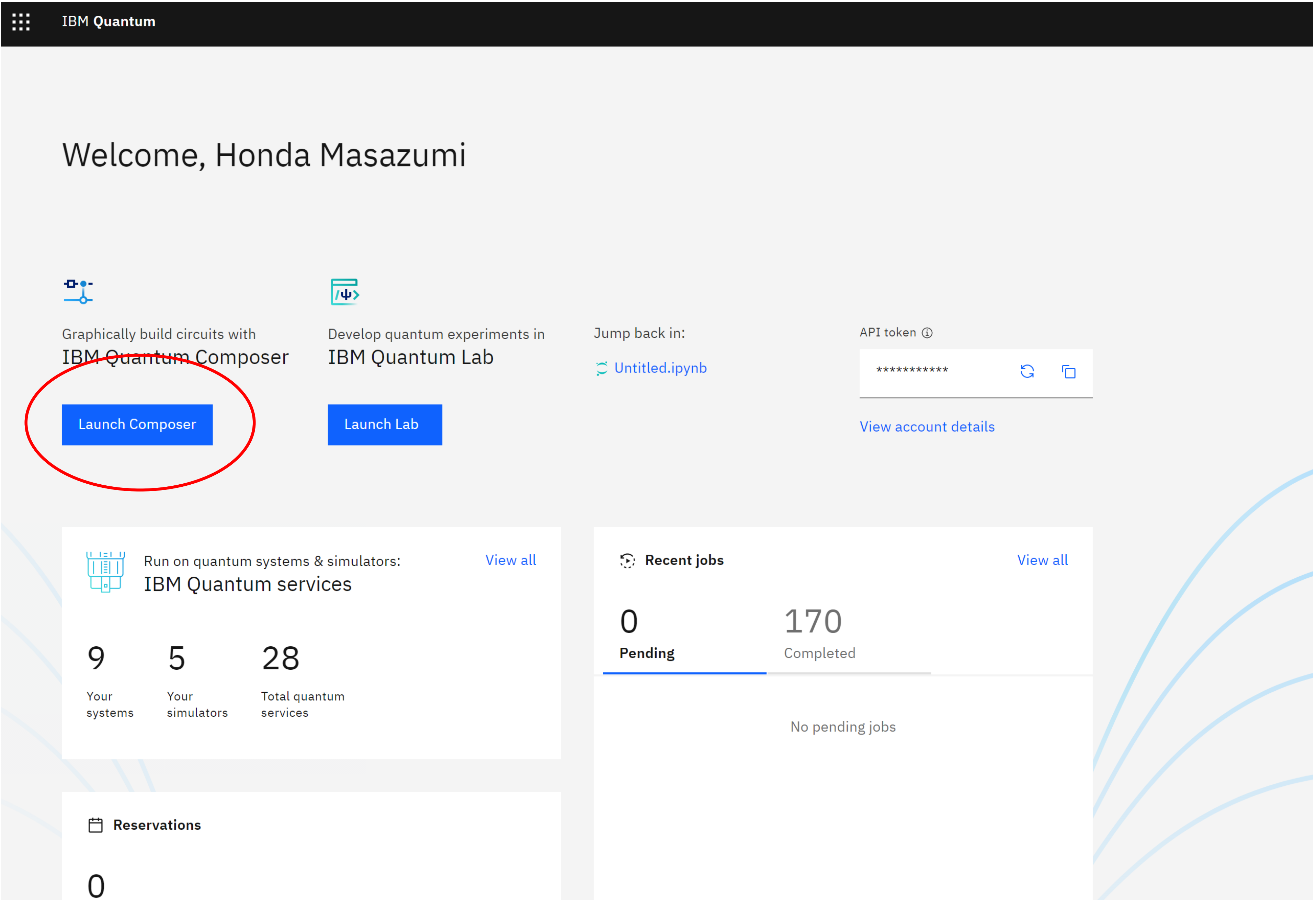
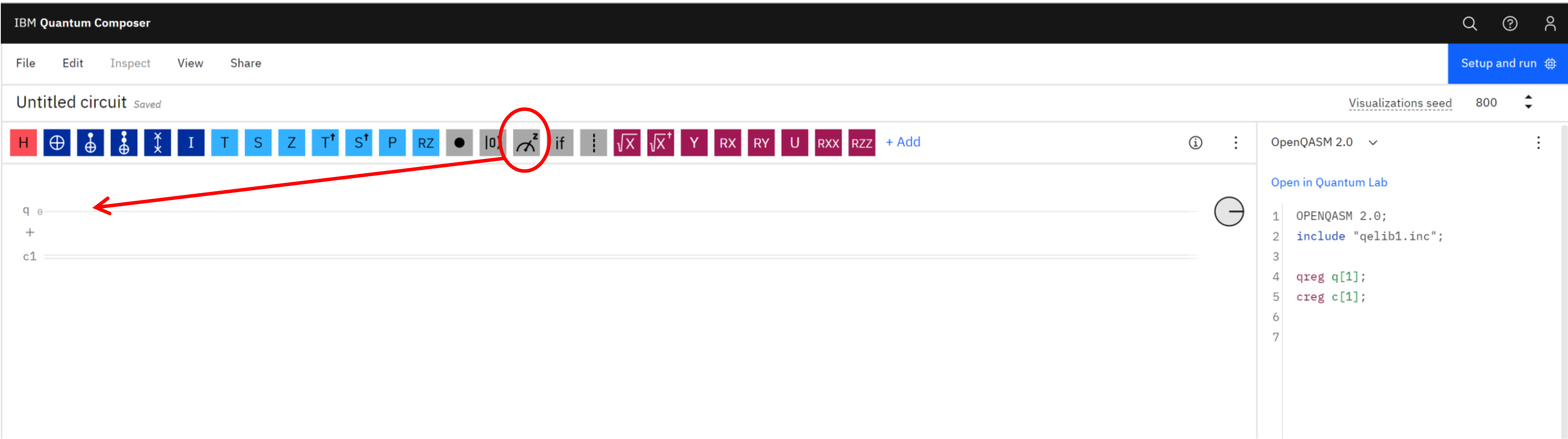
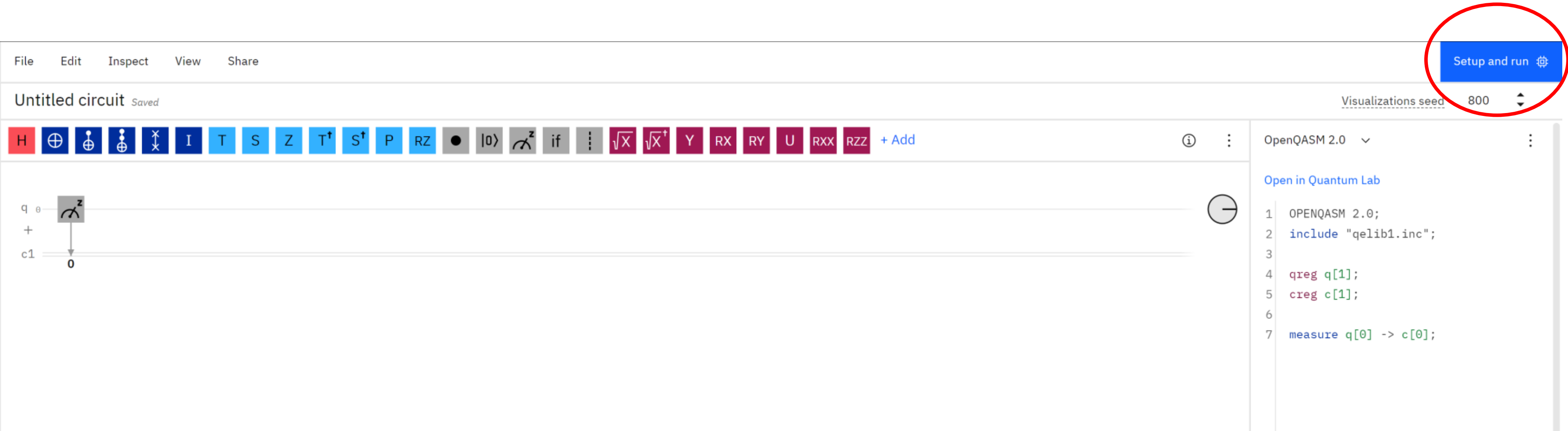

IBM Quantum
Welcome, Honda Masazumi
Graphically build circuits with
IBM Quantum Composer
Launch Composer
Develop quantum experiments in
IBM Quantum Lab
Launch Lab
Jump back in:
Untitled.ipynb
API token
****
View account details
Run on quantum systems & simulators:
IBM Quantum services
View all
9
Your systems
5
Your simulators
28
Total quantum services
Recent jobs
View all
0
Pending
170
Completed
No pending jobs
Reservations
0

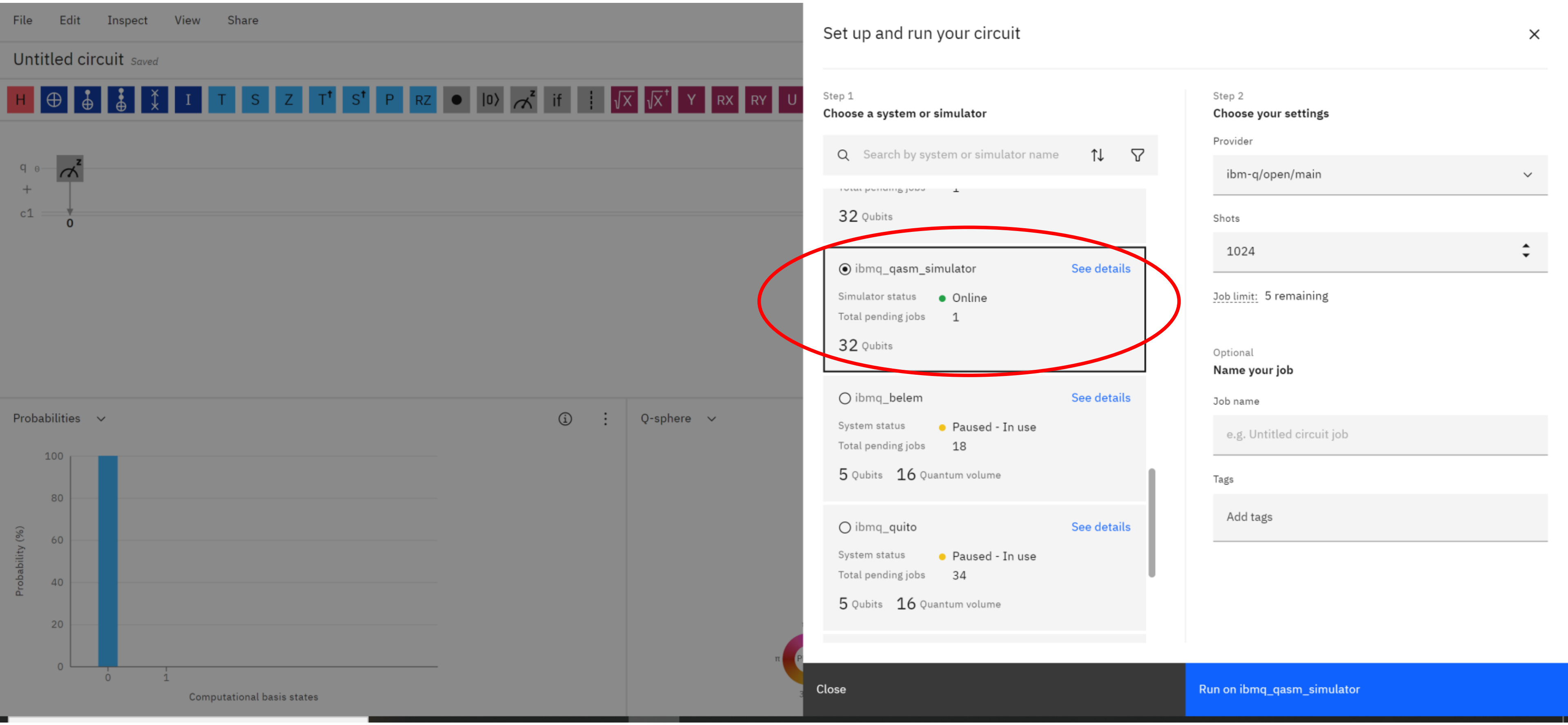
A trivial problem: measure $|0\rangle$



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



Measure 1024 times in simulator



Trivial result

Details

3.4s
Total completion time

ibmq_qasm_simulator
System

Sent from	Untitled circuit
Created on	Jun 09, 2021 5:08 PM
Sent to queue	Jun 09, 2021 5:08 PM
Provider	ibm-q/open/main
Run mode	fairshare
# of shots	1024
# of circuits	1

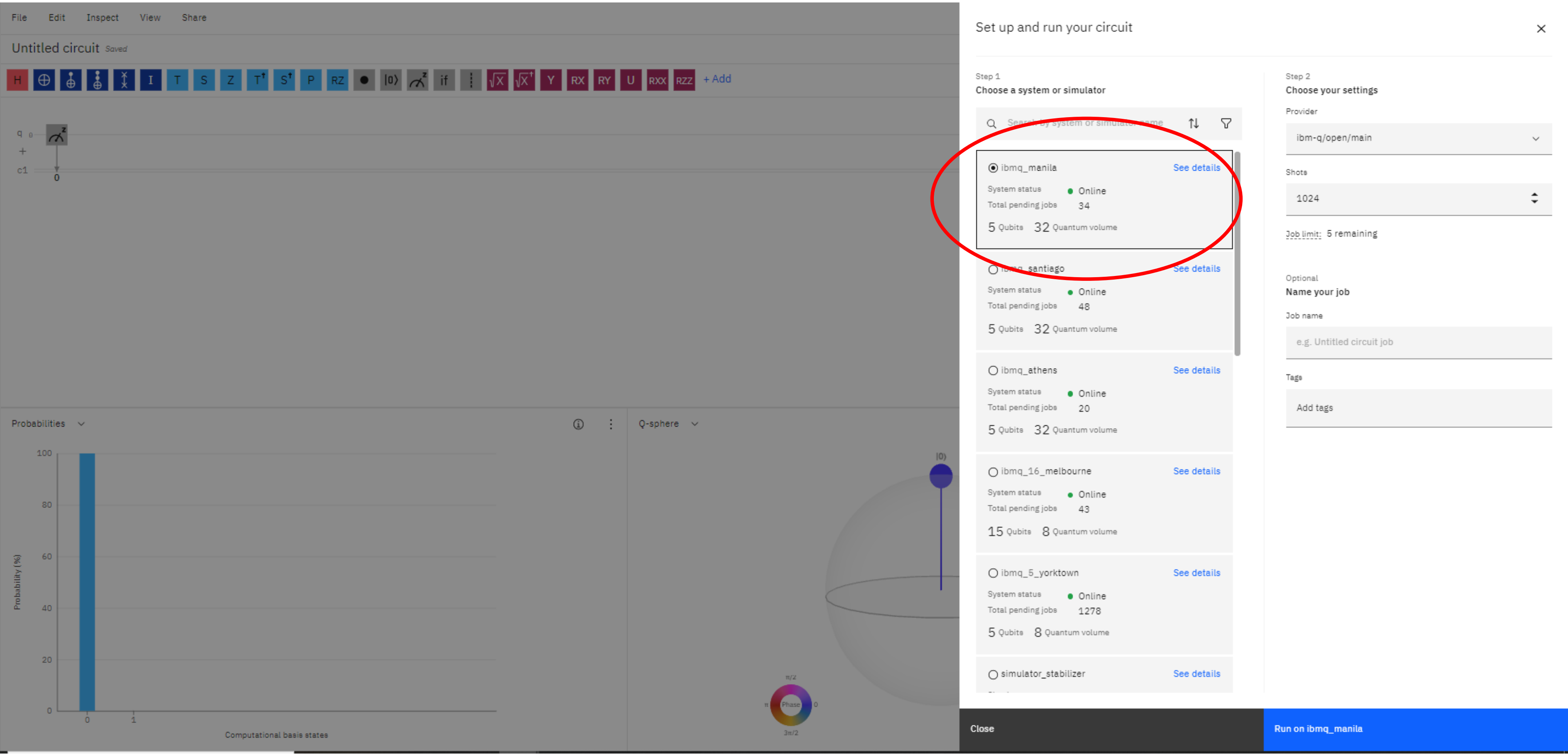
Status Timeline

- Created: Jun 09, 2021 5:08 PM
- Transpiling: 679ms
- Validating: 791ms
- In queue: 99ms
- Running: 1.5s
  approx. time in system 1.1s
- Completed: Jun 09, 2021 5:08 PM

Histogram

Of Course!

Measure 1024 times in quantum computer



Result of quantum computer?

Details

55m 53.3s
Total completion time

ibmq_manila
System

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Created on	Jun 09, 2021 6:57 PM
Sent to queue	Jun 09, 2021 6:57 PM
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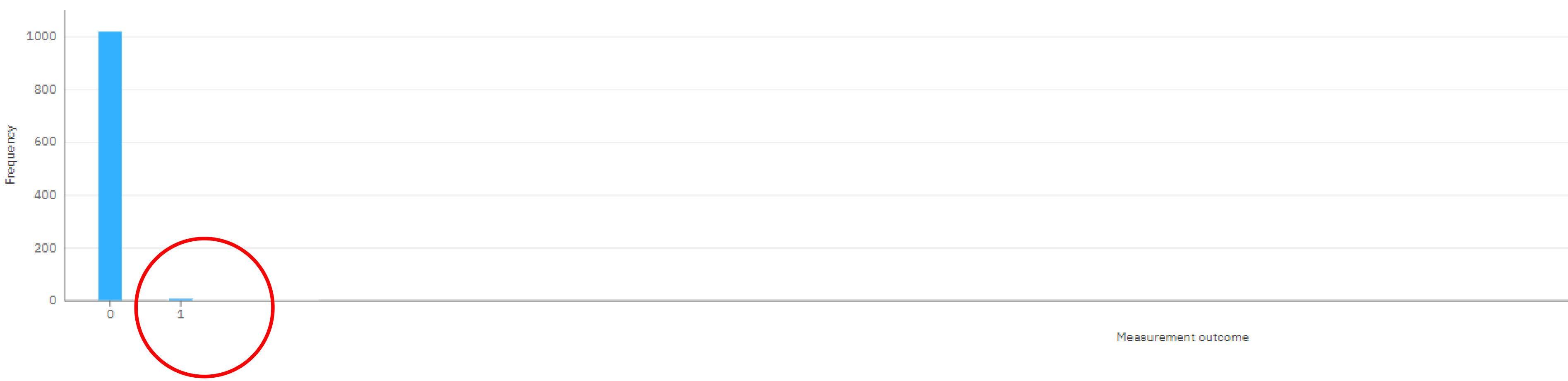
Run mode	fairshare
# of shots	1024
# of circuits	1

Status Timeline

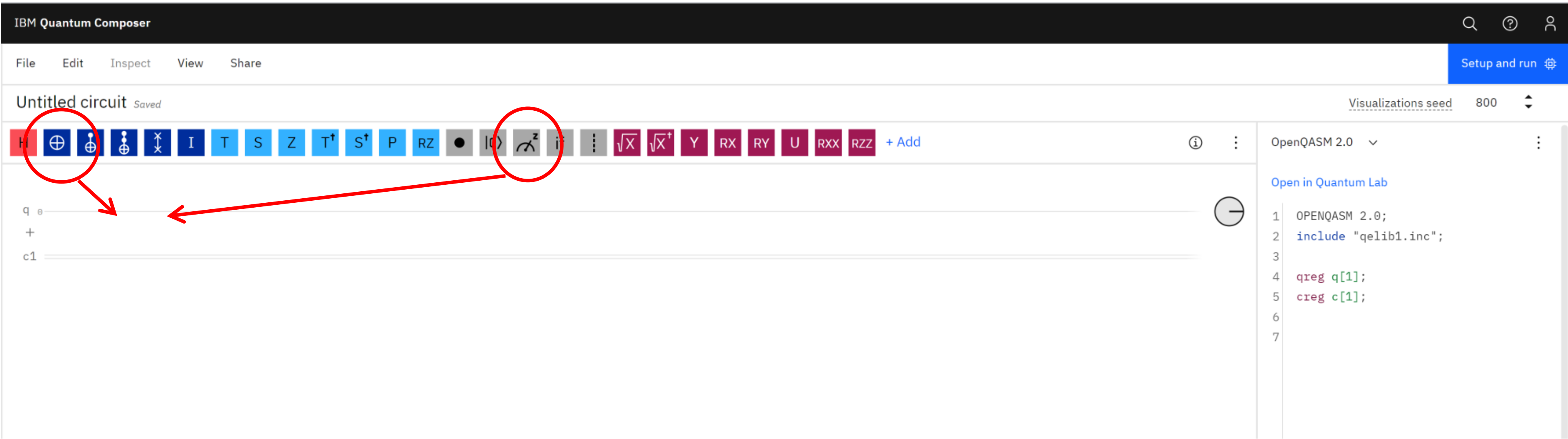
- Created: Jun 09, 2021 6:57 PM
- Transpiling: 571ms
- Validating: 728ms
- In queue: 55m 40.2s
- Running: 11.3s
  approx. time in system 10.9s
- Completed: Jun 09, 2021 7:53 PM

Histogram



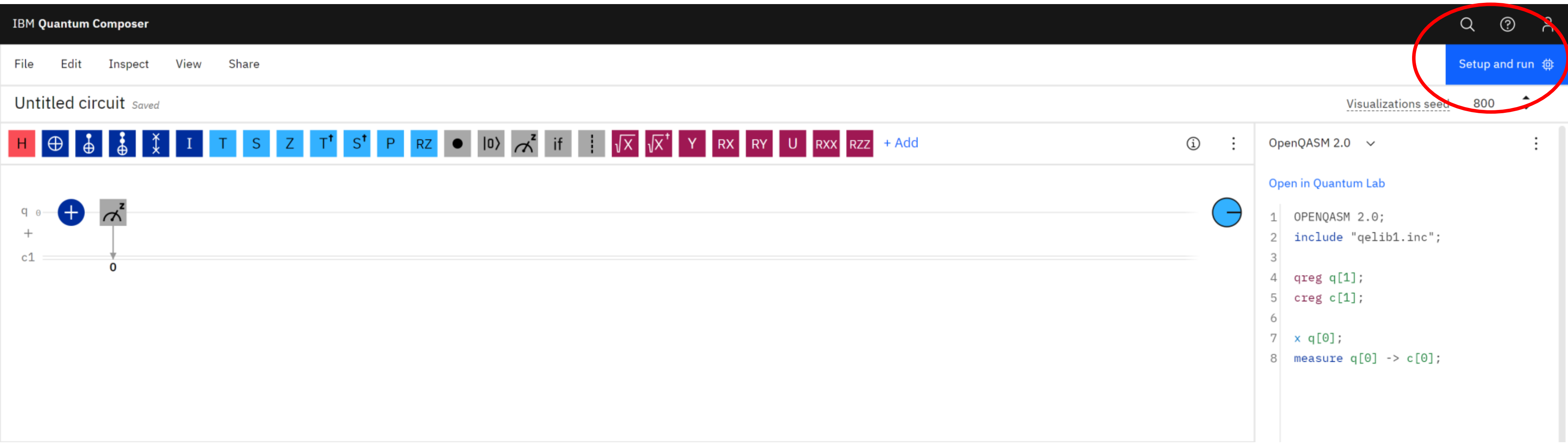
This is the error!

Another trivial problem: measure |1⟩



$$\boxed{X|0\rangle = |1\rangle}$$

Another trivial problem: measure $|1\rangle$ (Cont'd)



Result of simulator (1024 shots)

Details

3s
Total completion time

ibmq_qasm_simulator
System

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Sent to queue	Jun 09, 2021 5:26 PM
Provider	ibm-q/open/main
Run mode	fairshare
# of shots	1024
# of circuits	1

Status Timeline

- Created: Jun 09, 2021 5:26 PM
- Transpiling: 522ms
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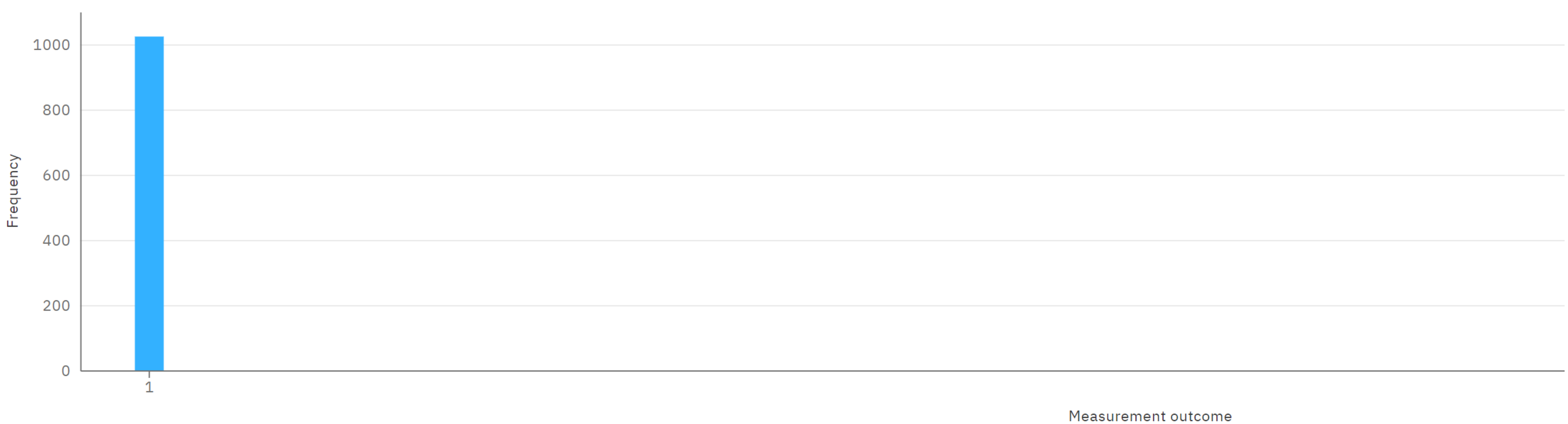
- In queue: 301ms
- Running: 1.1s
  approx. time in system 835ms
- Completed: Jun 09, 2021 5:26 PM

Histogram



Result of quantum computer (1024shots)

Details

56m 26.5s
Total completion time

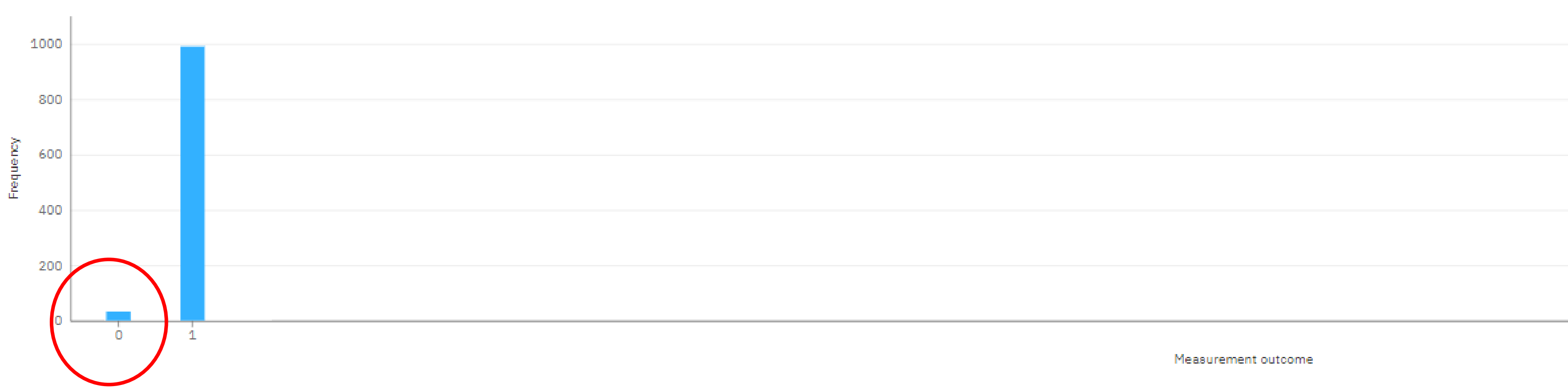
ibmq_manila
System

Sent from	Untitled circuit
Created on	Jun 09, 2021 6:57 PM
Sent to queue	Jun 09, 2021 6:57 PM
Provider	ibm-q/open/main
Run mode	fairshare
# of shots	1024
# of circuits	1

Status Timeline

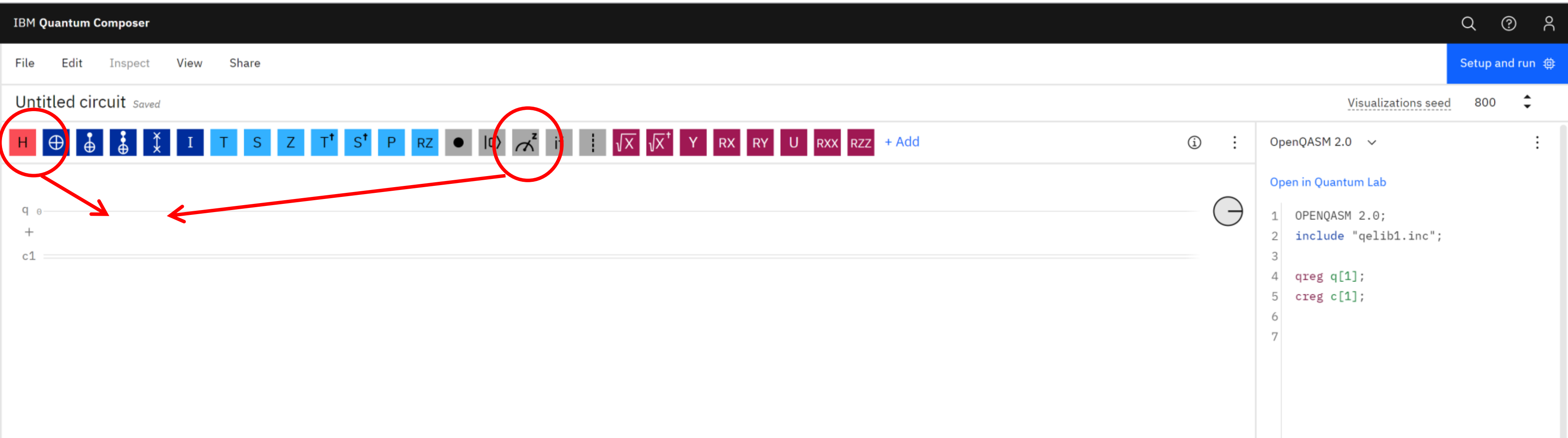
- Created: Jun 09, 2021 6:57 PM
- Transpiling: 745ms
- Validating: 1.1s
- In queue: 56m 7.3s
- Running: 17s
  approx. time in system 16.3s
- Completed: Jun 09, 2021 7:53 PM

Histogram



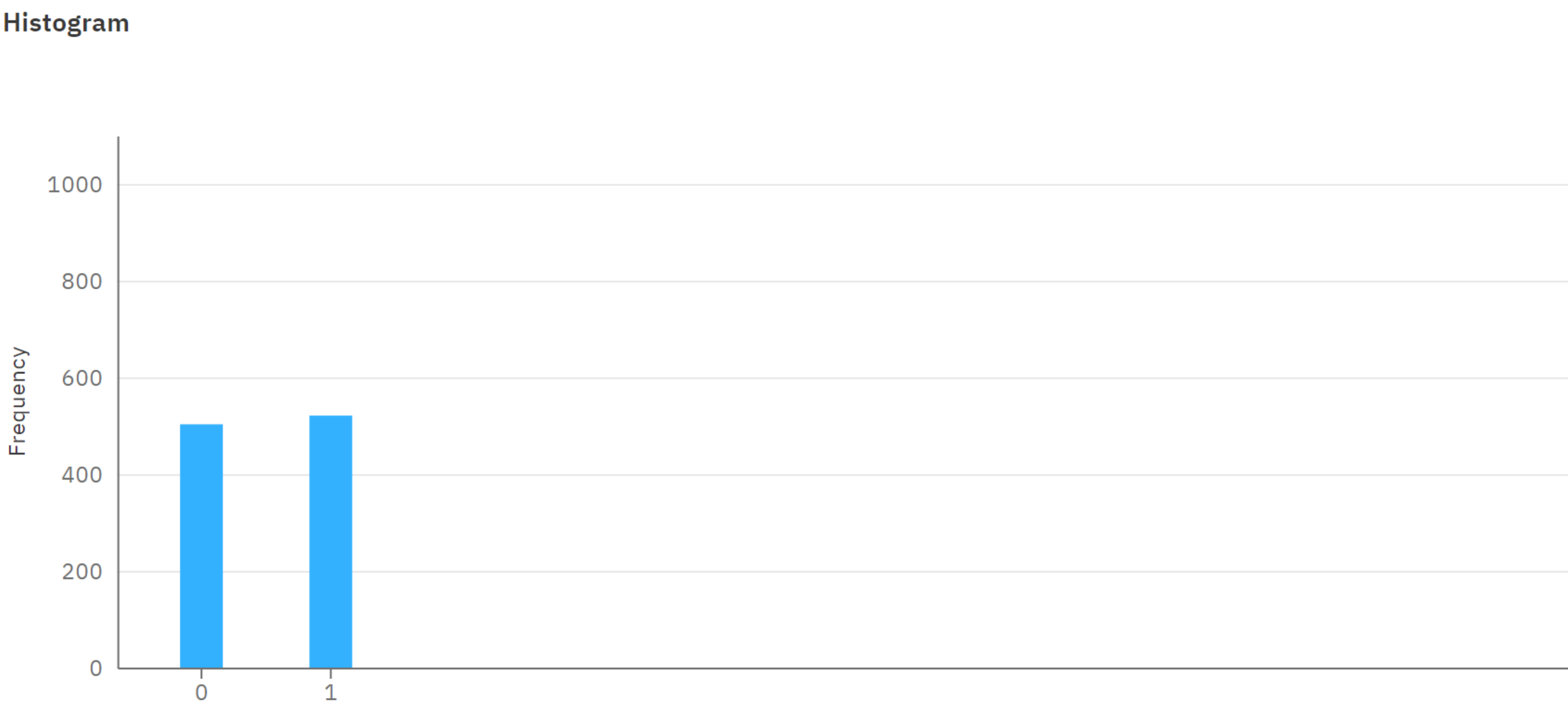
Error again

The simplest nontrivial problem: Hadamard gate



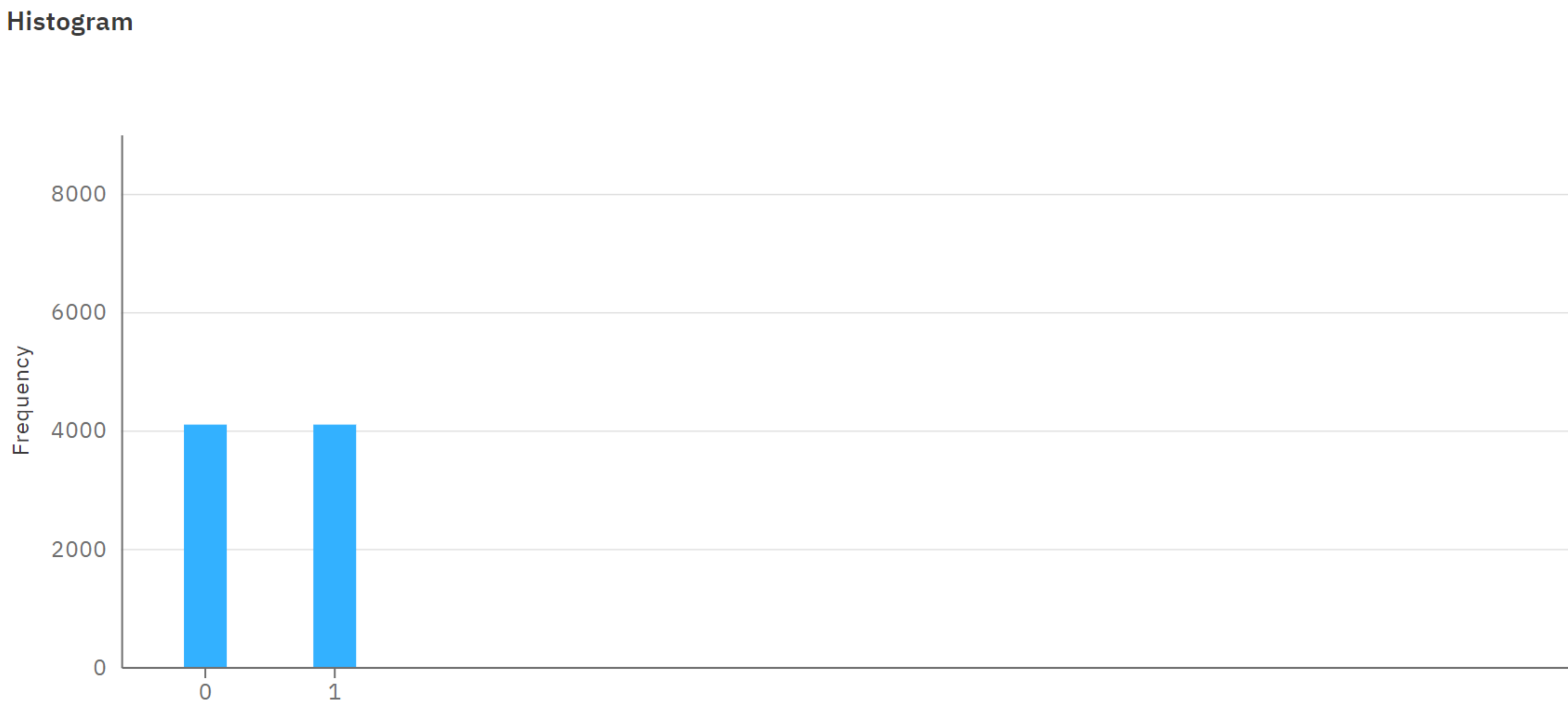
$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

Result of simulator (1024 shots)



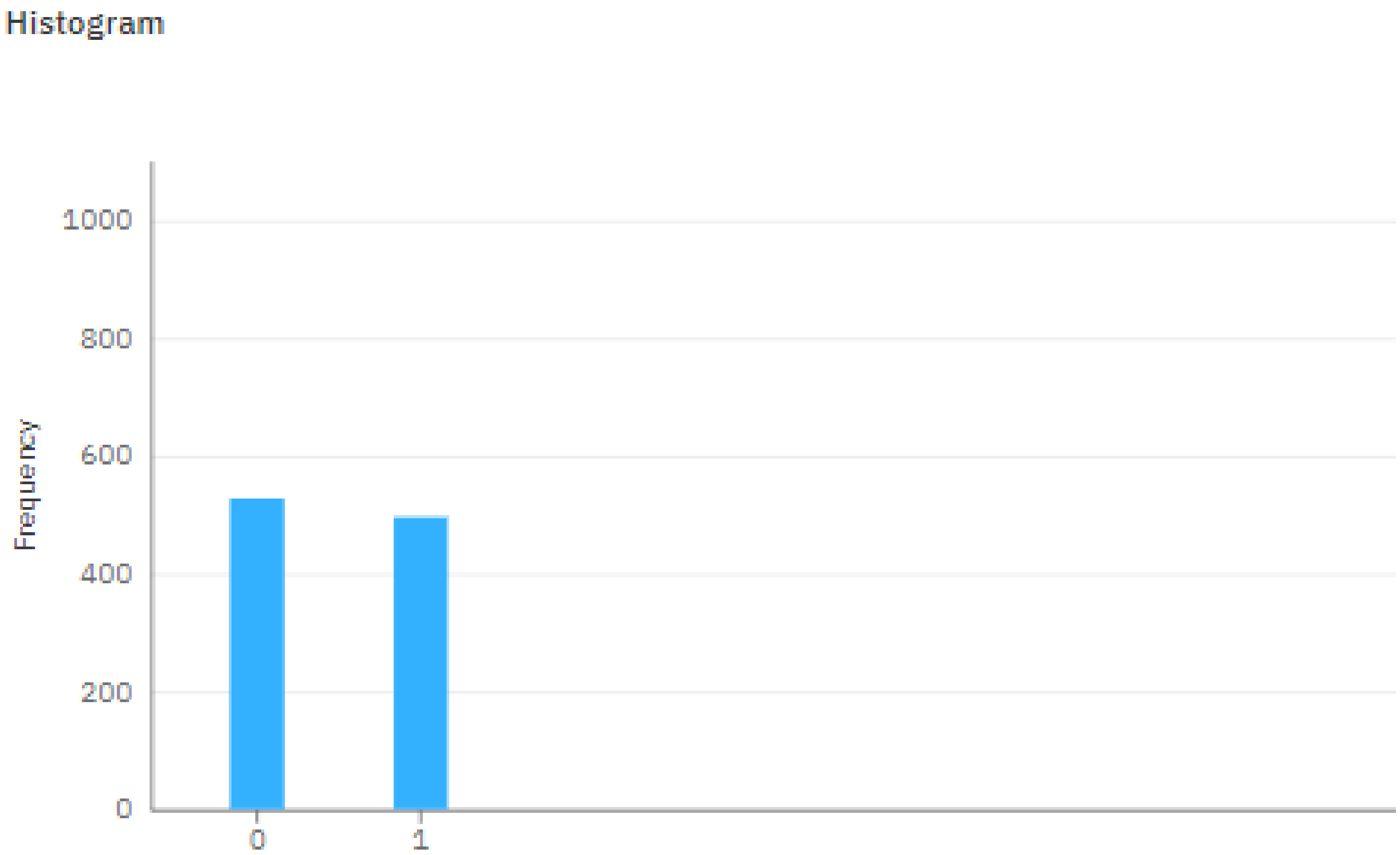
Not exactly 50:50 because of **statistical errors**

Result of simulator (8192 shots)



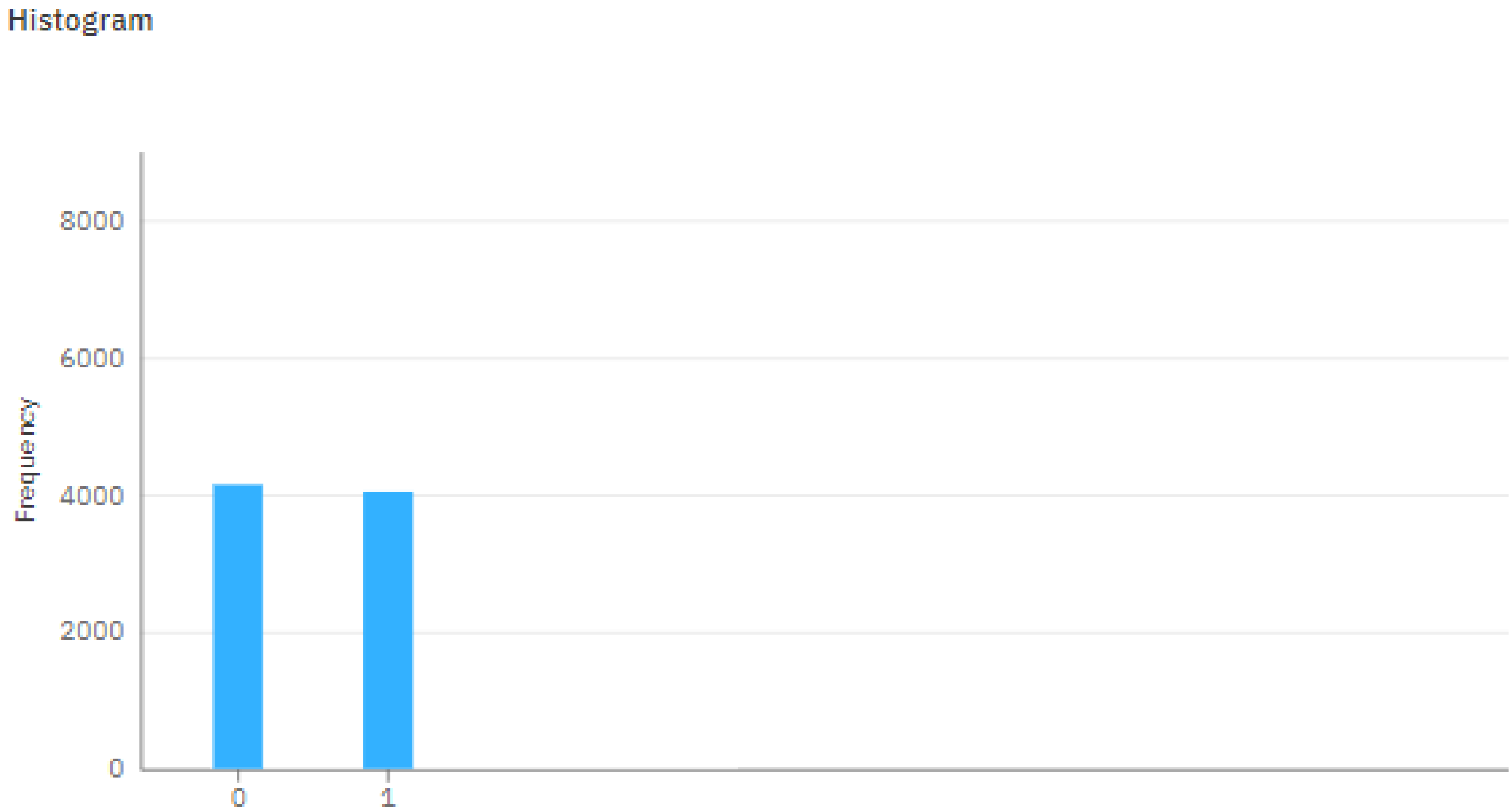
Improved!

Result of quantum computer (1024 shots)



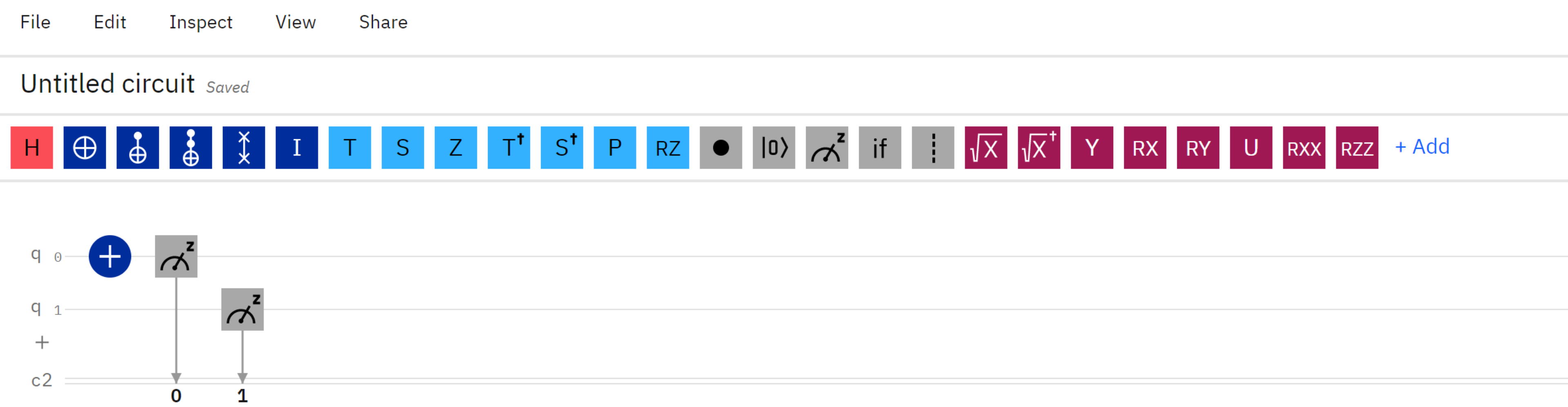
∃ Both errors & statistical errors

Result of quantum computer (8192 shots)



Statistical errors are improved

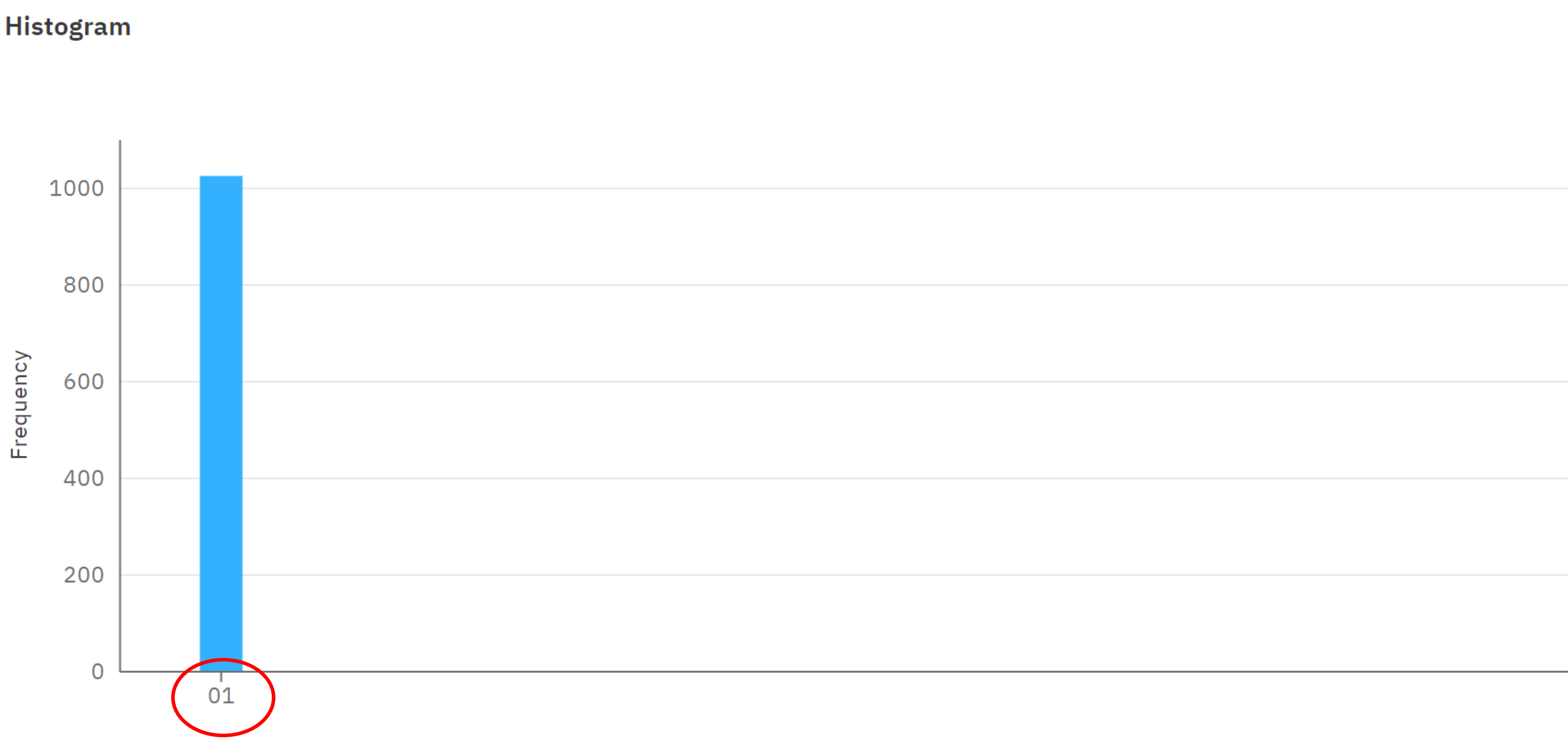
A trivial problem for 2 qubits



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

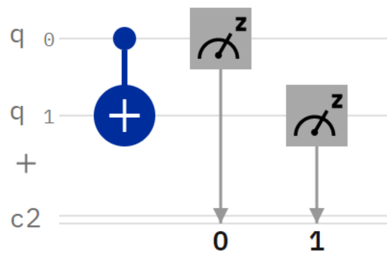
Result of simulator (1024 shots)

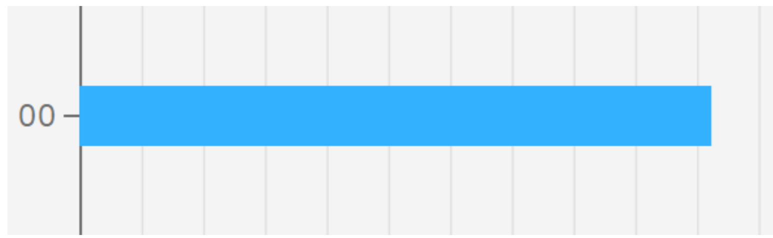
$$\boxed{X_1|00\rangle = |10\rangle}$$



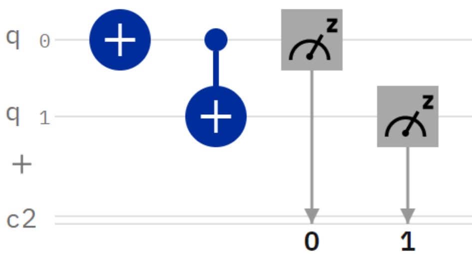
Note that notation is different from the ket notation

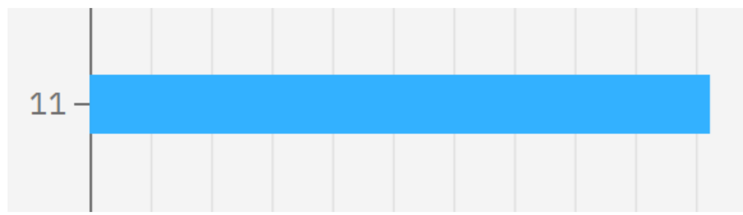
2 qubit operation by simulator



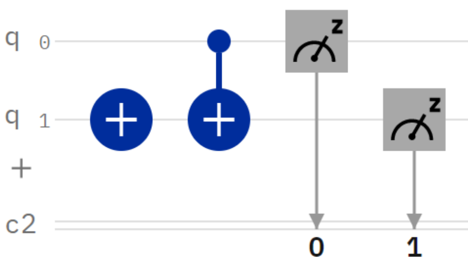


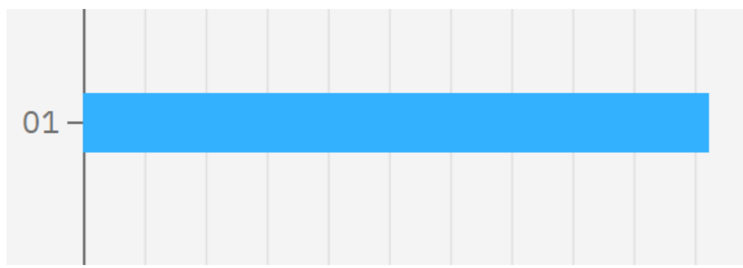
$$CX|00\rangle = |00\rangle$$



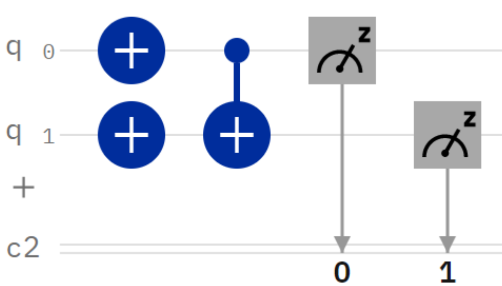


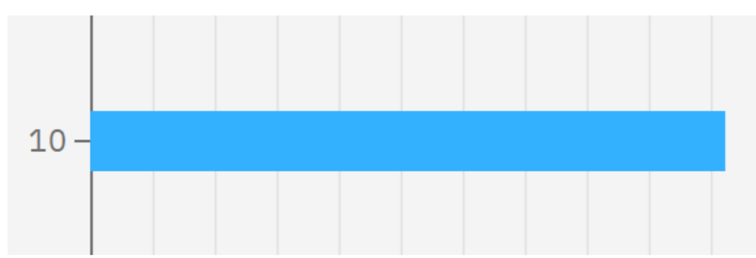
$$CX|10\rangle = |11\rangle$$





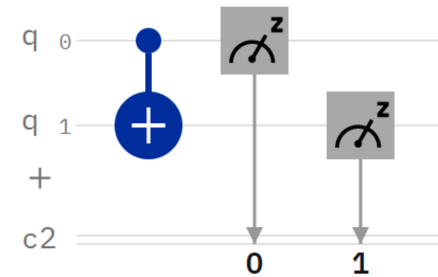
$$CX|01\rangle = |01\rangle$$

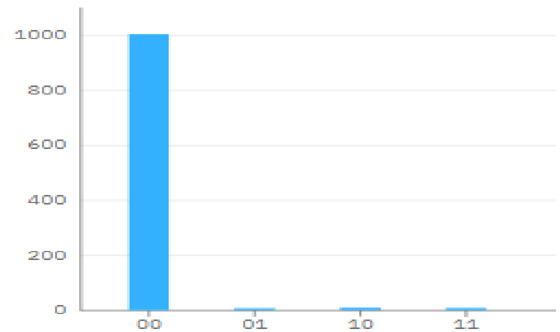




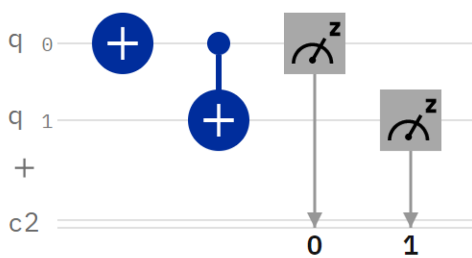
$$CX|11\rangle = |10\rangle$$

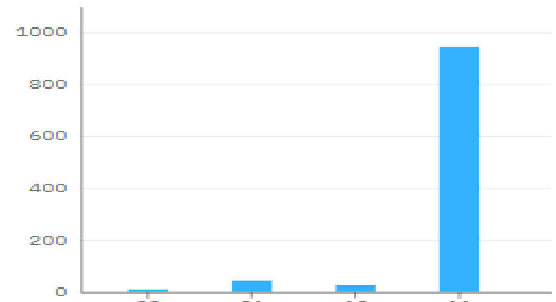
2 qubit operation by quantum computer (1024 shots)



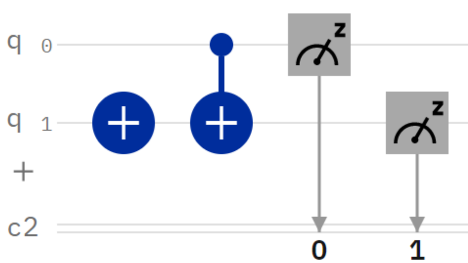


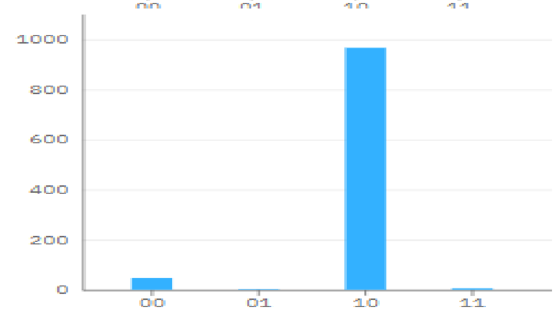
$$CX|00\rangle = |00\rangle$$



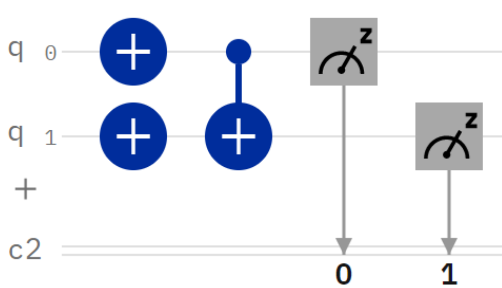


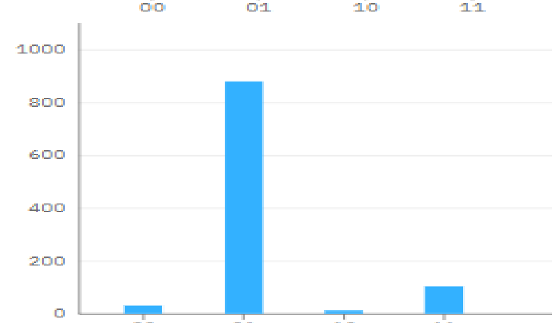
$$CX|10\rangle = |11\rangle$$





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





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

Quantum simulation of Spin system

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:

($\exists$ 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)

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

The 1st one is trivial:

acting on qubit 2 acting on qubit 1

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

Time evolution operator (Cont'd)

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

The 1st one is trivial:

acting on qubit 2 acting on qubit 1

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

The 2nd one is nontrivial:

$$e^{-iH_{ZZ}\frac{t}{M}} = e^{-i\frac{Jt}{M}Z_1 Z_2} = \cos\frac{Jt}{M} - iZ_1 Z_2 \sin\frac{Jt}{M}$$

One can show (see next slide)

$$e^{-i\frac{Jt}{M}Z_1 Z_2} = CX R_Z^{(2)}\left(\frac{2Jt}{M}\right) CX$$

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,

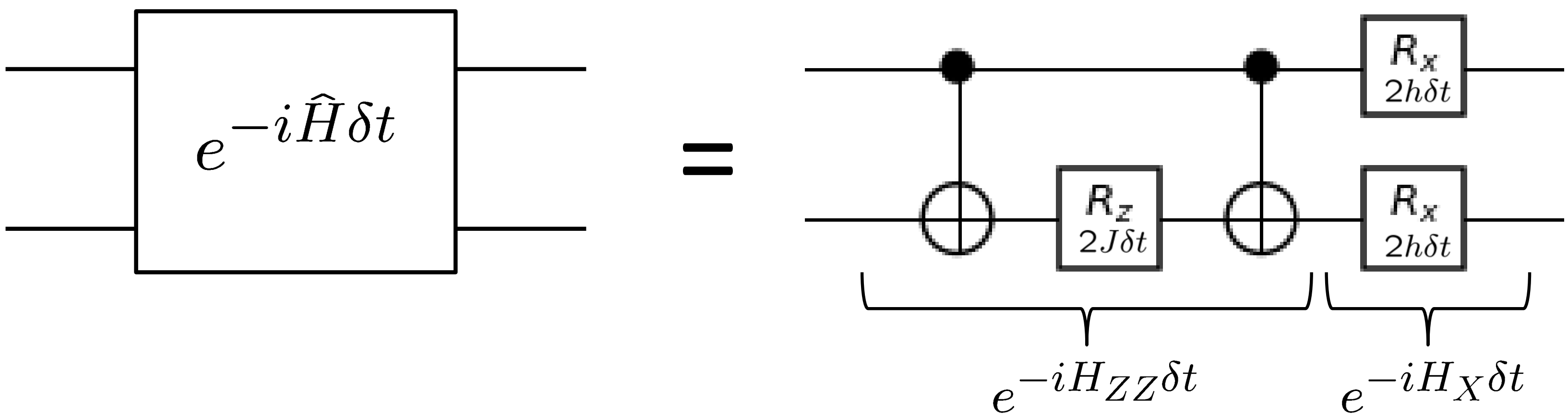
$$CXR_Z^{(2)}(2c)CX|\varphi\rangle \otimes |\psi\rangle = \cos c|\varphi\rangle \otimes |\psi\rangle - i\sin c\; Z|\varphi\rangle \otimes Z|\psi\rangle$$

$$= e^{-icZ_1Z_2}|\varphi\rangle \otimes |\psi\rangle$$

Quantum circuit for time evolution op.

$$H_X = -h(X_1 + X_2), \qquad H_{ZZ} = -J Z_1 Z_2$$

$$\delta t = \frac{t}{M} \ll 1$$



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

Survival probability of free vacuum

For J=0, 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:

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

Toy version of Schwinger effect

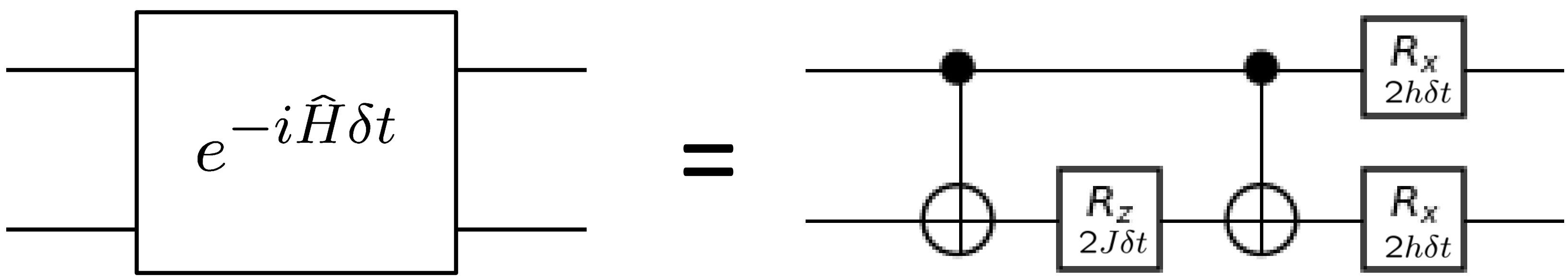
$$= \left| \langle 00 | H^{(2)} H^{(1)} e^{-i\hat{H}t} H^{(2)} H^{(1)} |00\rangle \right|^2$$

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

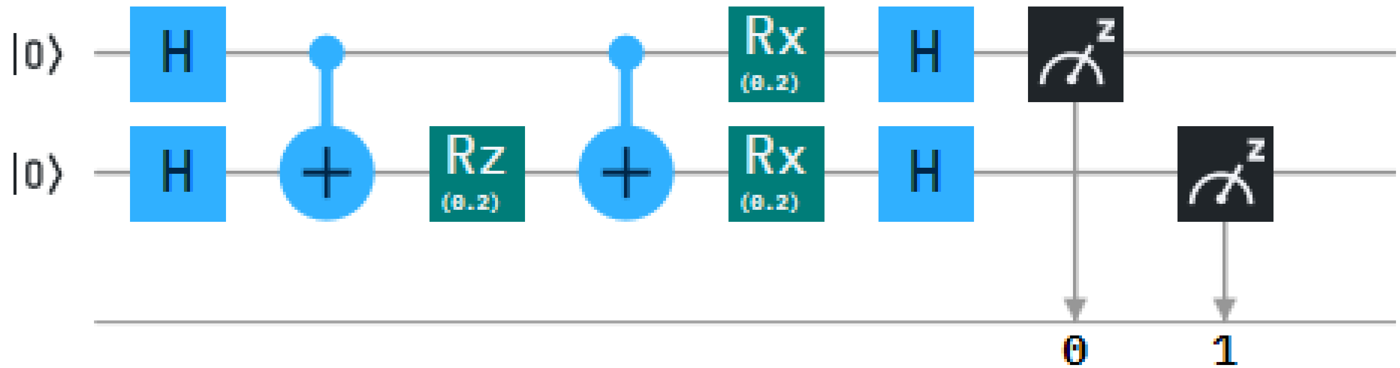
$$P(t) = \left|\langle ++|e^{-i\hat{H}t}|++\rangle\right|^2 = \left|\langle 00|H^{(2)}H^{(1)}e^{-i\hat{H}t}H^{(2)}H^{(1)}|00\rangle\right|^2$$



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

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

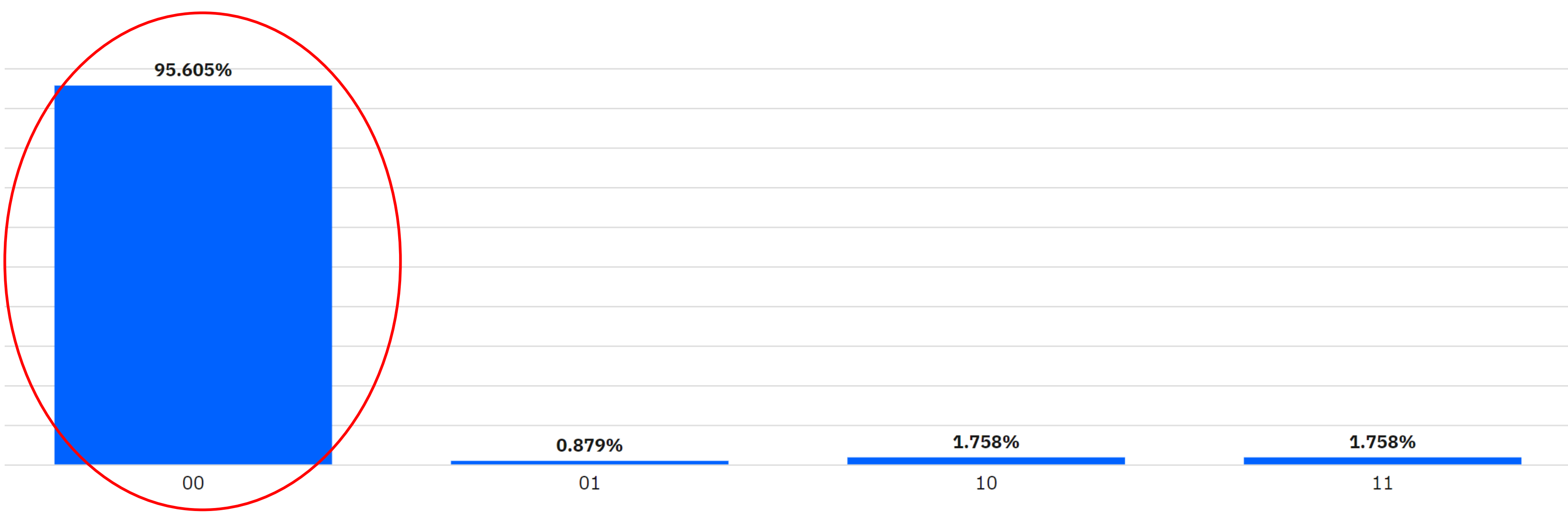
Demonstration for the survival probability (Cont'd)



Result by simulator w/ 1024 shots:

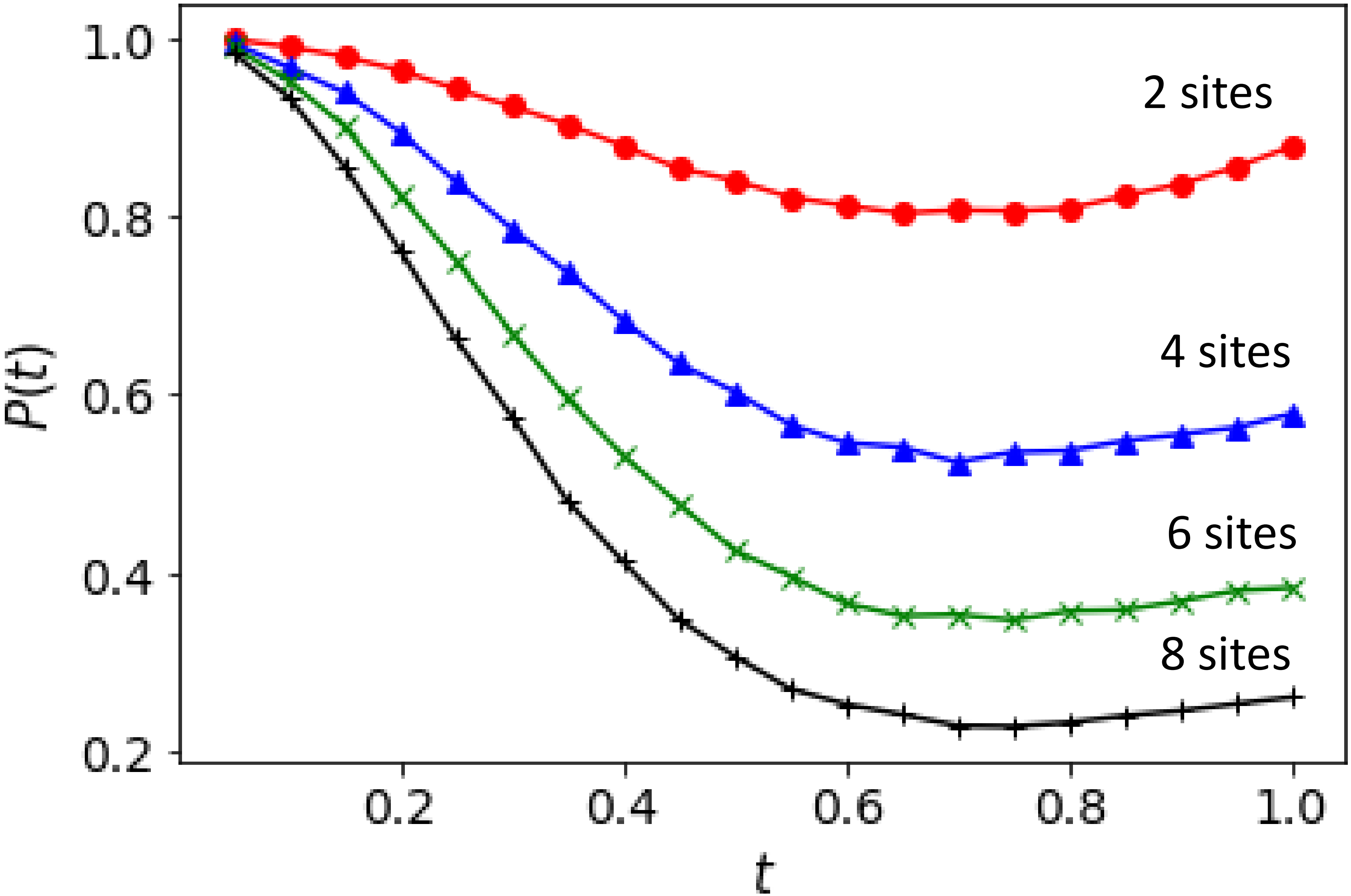
Result of simulator (1024 shots):

Result of quantum computer (1024 shots):



More serious computation

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



Adiabatic state preparation of vacuum

Step 1: Choose an initial Hamiltonian H_0 of a simple system whose ground state $|\mathrm{vac}_0\rangle$ is known and unique

Step 2:

Step 3:

Adiabatic state preparation of vacuum

Step 1: Choose an initial Hamiltonian H_0 of a simple system whose ground state $|\mathrm{vac}_0\rangle$ is known and unique

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

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

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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

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

For transverse Ising model

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

Choose

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

Discretize the integral:

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

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:

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

It is easiest to compute magnetization:

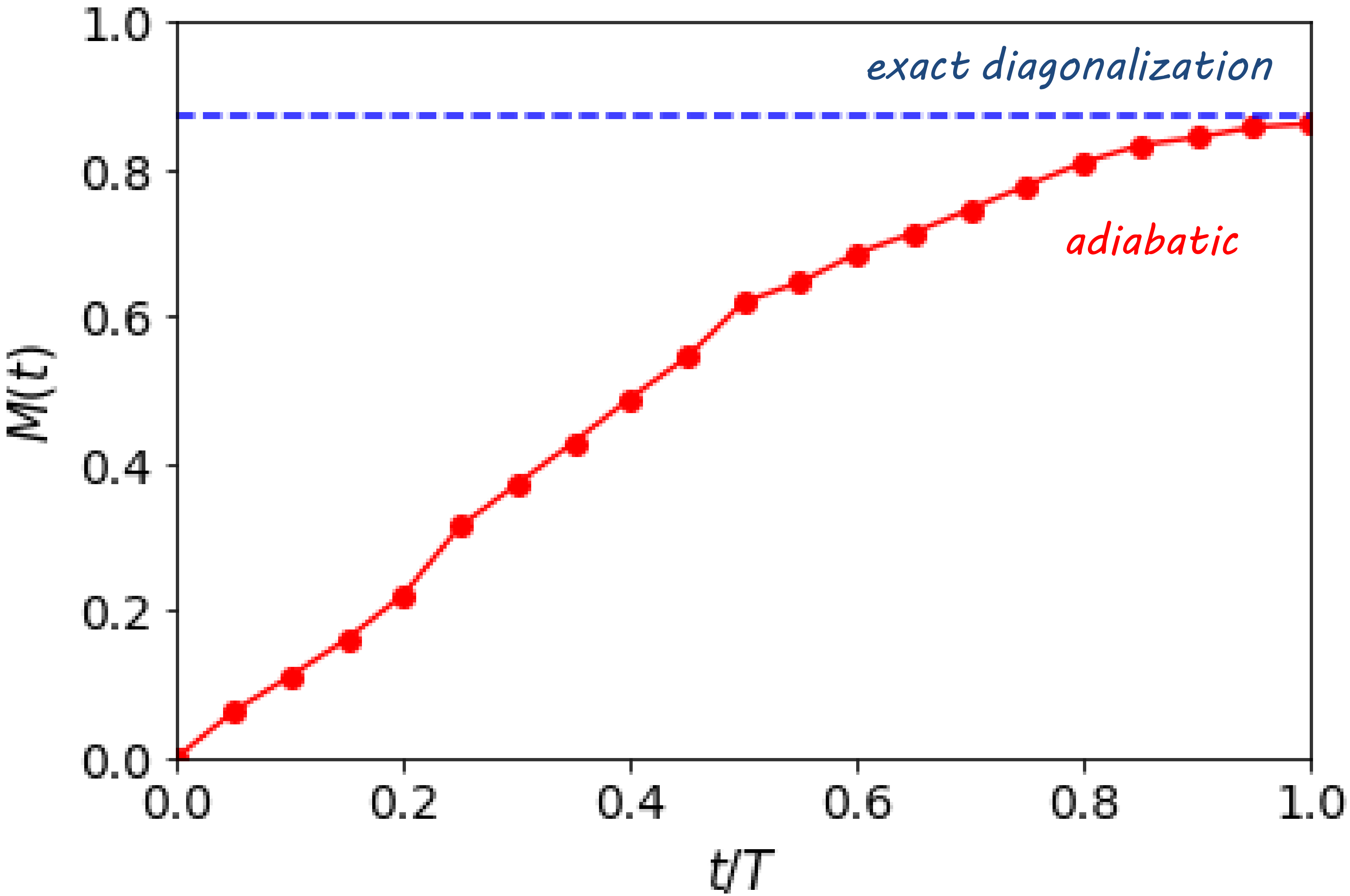
$$\frac{1}{N}\langle \text{vac}|\sum_{n=1}^{N} Z_n|\text{vac}\rangle = \frac{1}{N}\sum_{n=1}^{N}\sum_{i_1\cdots i_N=0,1}\langle \text{vac}|Z_n|i_1\cdots i_N\rangle\langle i_1\cdots i_N|\text{vac}\rangle$$

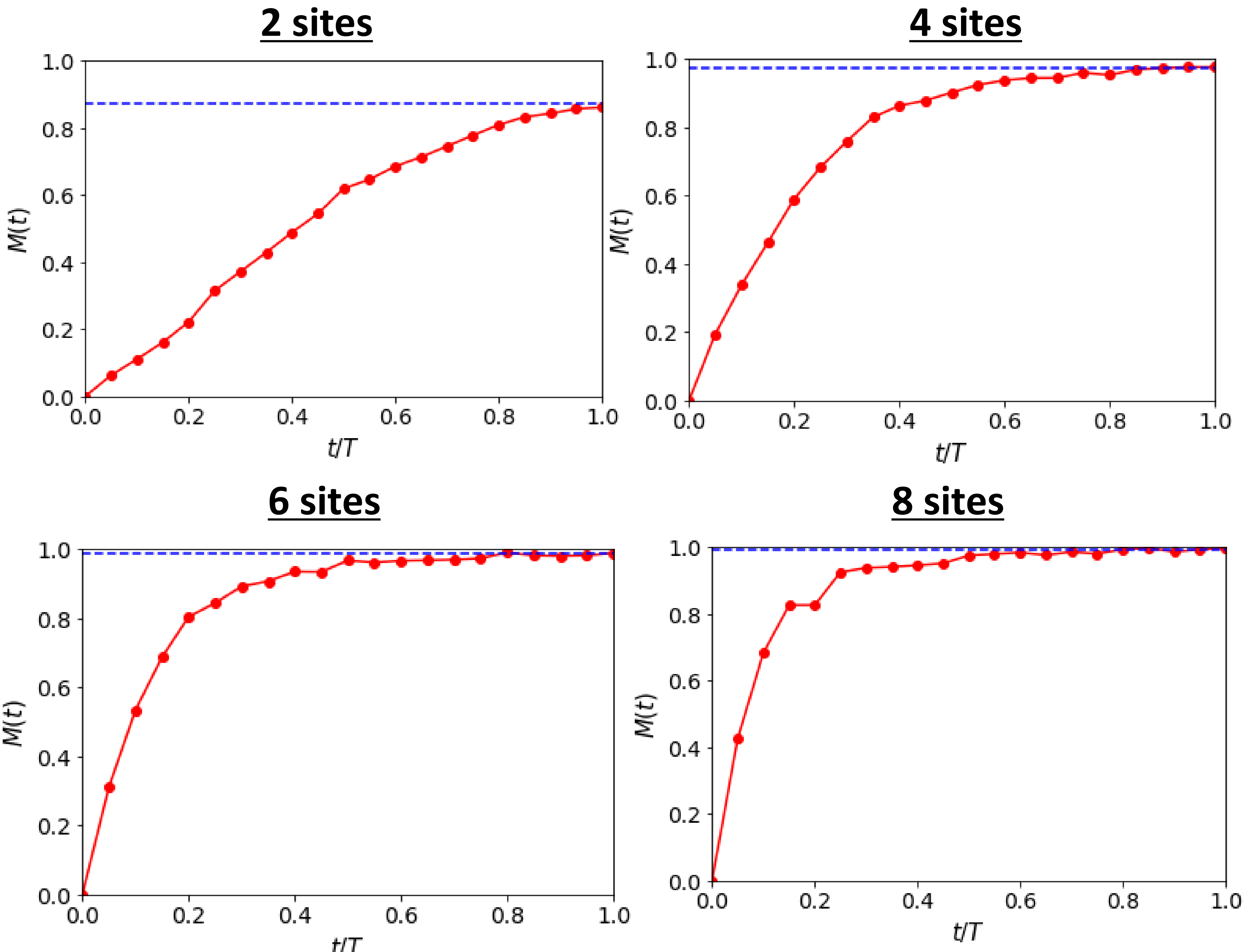
$$= \frac{1}{N}\sum_{n=1}^{N}\sum_{i_1\cdots i_N=0,1}(-1)^{i_n}\left|\langle i_1\cdots i_N|\text{vac}\rangle\right|^2$$

$$\left(\begin{array}{l} \text{Transverse one is a bit more tricky:} \\ \dfrac{1}{N}\langle \text{vac}|\displaystyle\sum_{n=1}^{N} X_n|\text{vac}\rangle = \dfrac{1}{N}\langle \text{vac}|\displaystyle\sum_{n=1}^{N} H^{(n)}Z_nH^{(n)}|\text{vac}\rangle \\ \qquad = \dfrac{1}{N}\displaystyle\sum_{n=1}^{N}\sum_{i_1\cdots i_N=0,1}(-1)^{i_n}\left|\langle i_1\cdots i_N|H^{(n)}|\text{vac}\rangle\right|^2 \end{array}\right)$$

Result by simulator (10000 shots)

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





2 sites
4 sites
6 sites
8 sites
M(t)
t/T
0.0
0.2
0.4
0.6
0.8
1.0

Renyi entropy

Dividing total Hilbert space as

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

reduced density matrix is defined as

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

Entanglement entropy:

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

n-th Renyi entropy:

$$S_n = \frac{1}{1-n} \log \text{tr}_{\mathcal{H}_A}(\rho_A^n)$$

Quantum algorithm for 2nd Renyi entropy

Consider $(N_A + N_B)$-qubit system and the density matrix

$$\rho_{N_A+N_B} = |\Psi\rangle\langle\Psi|$$

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

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

Quantum algorithm for 2nd Renyi entropy

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

One can show (next slide) [Hastings-Gonzalez-Kallin-Melko'10]

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

$$\mathrm{SWAP}_A : \text{Exchange of } A-\text{part in } |\Psi\rangle \otimes |\Psi\rangle$$

$$\left(\begin{array}{l} \text{For } \ |\Psi\rangle = \sum_{i,j} c_{ij} |i_1 \cdots i_{N_A} j_1 \cdots j_{N_B}\rangle, \\ \mathrm{SWAP}_A |\Psi\rangle \otimes |\Psi\rangle \equiv \sum_{i,j,i',j'} c_{ij} c_{i'j'} |i'_1 \cdots i'_{N_A} j_1 \cdots j_{N_B}\rangle \otimes |i_1 \cdots i_{N_A} j'_1 \cdots j'_{N_B}\rangle \end{array} \right)$$

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

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

Proof:

$$\langle\Psi| \otimes \langle\Psi|\ \mathsf{SWAP}_A\ |\Psi\rangle \otimes |\Psi\rangle$$

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

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

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

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

Demonstration: 2nd Renyi entropy of Bell state

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:

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

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

Let’s reproduce it in IBM Q Experience

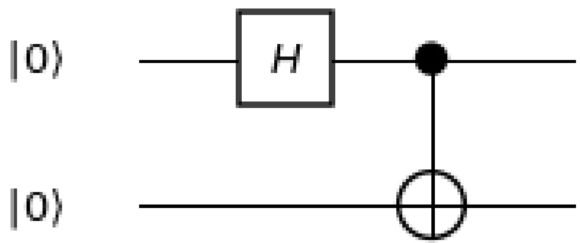
Demonstration: 2nd Renyi entropy of Bell state (Cont'd)

We know

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

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

The Bell state is written as



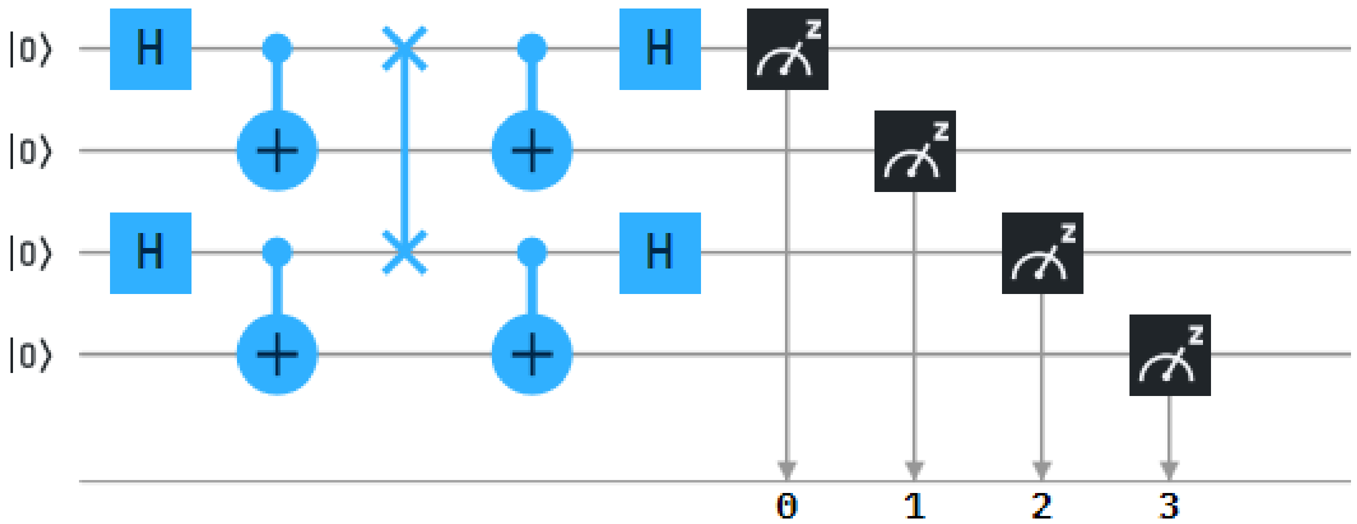
$$= |B\rangle$$

Therefore,

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

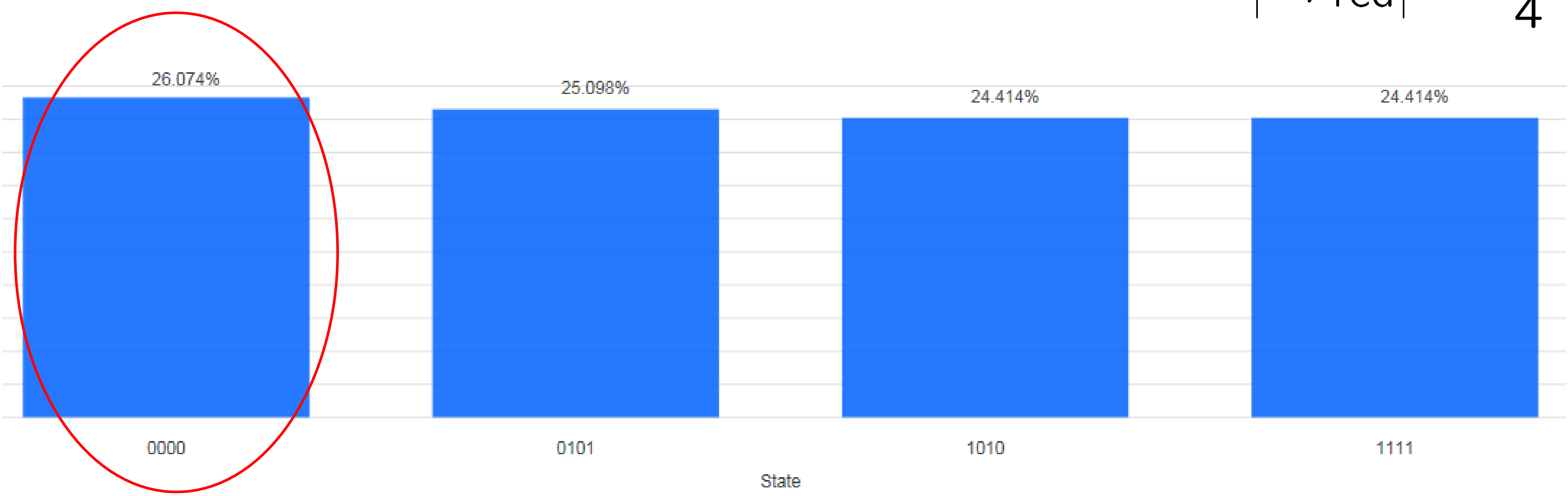
$$\left|\mathrm{tr}\rho_{\mathrm{red}}^2\right|^2 = \left|\langle 0000| \ U^\dagger \mathsf{SWAP}^{(1,3)} U \ |0000\rangle\right|^2$$

Demonstration: 2nd Renyi entropy of Bell state (Cont'd)

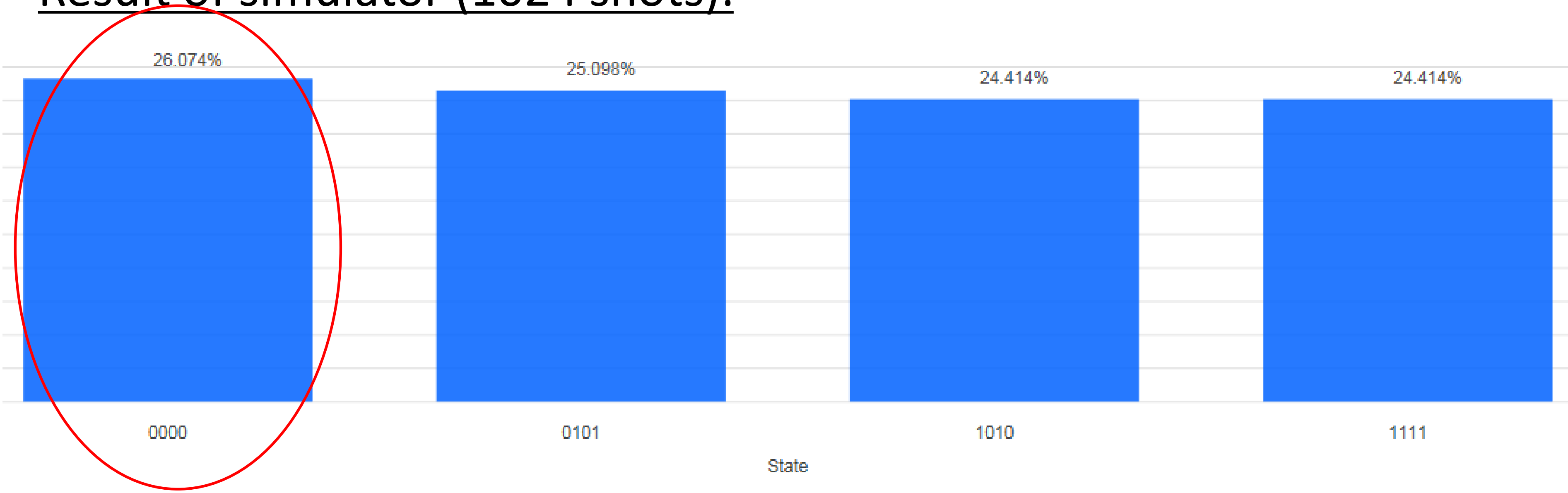


Result of simulator (1024 shots):

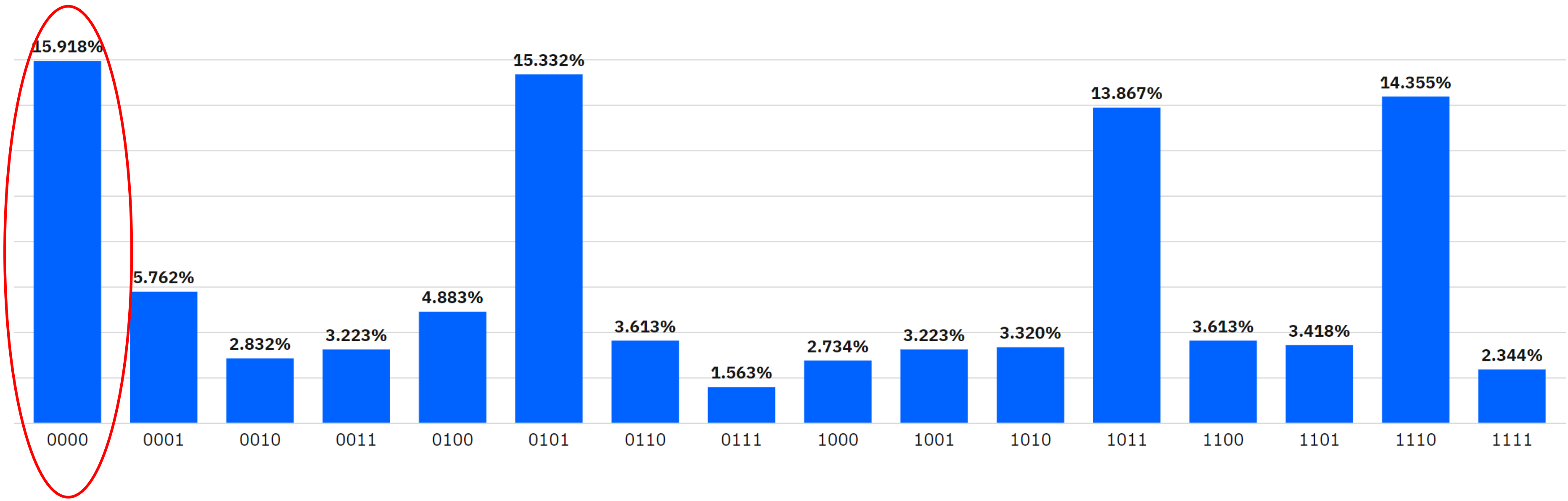
$$\left|\mathrm{tr}\rho_{\mathrm{red}}^{2}\right|^{2}=\frac{1}{4}$$



Result of simulator (1024 shots):



Result of quantum computer (1024 shots):



More direct way?

We've directly computed

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

rather than itself:

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

Can we directly compute it?

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

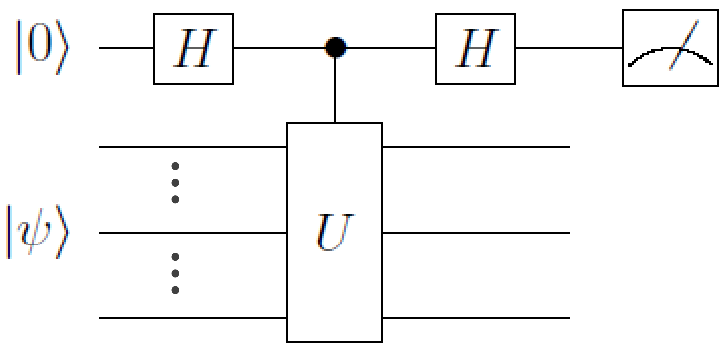
$$\langle\psi|\ \mathrm{U}\ |\psi\rangle$$

“Hadamard test”: standard way to compute $\langle\psi|\, U \,|\psi\rangle$

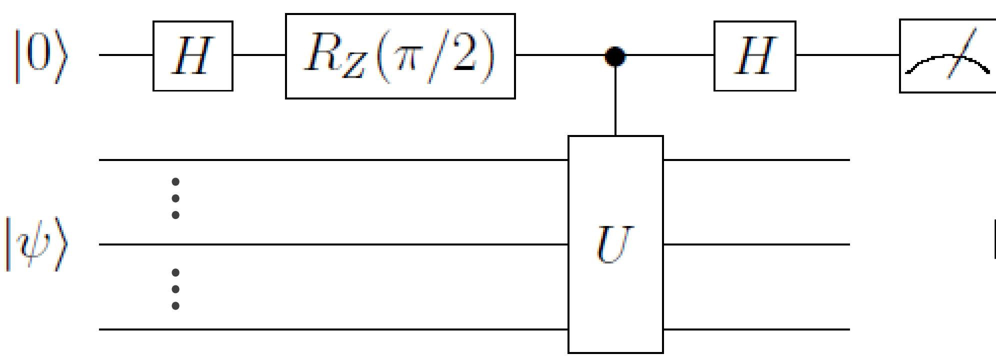
① Extend Hilbert space & consider the state

$$\underbrace{|0\rangle}_{\text{“ancillary qubit”}} \otimes |\psi\rangle$$

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



$\mathrm{Re}(\langle\psi|U|\psi\rangle)$

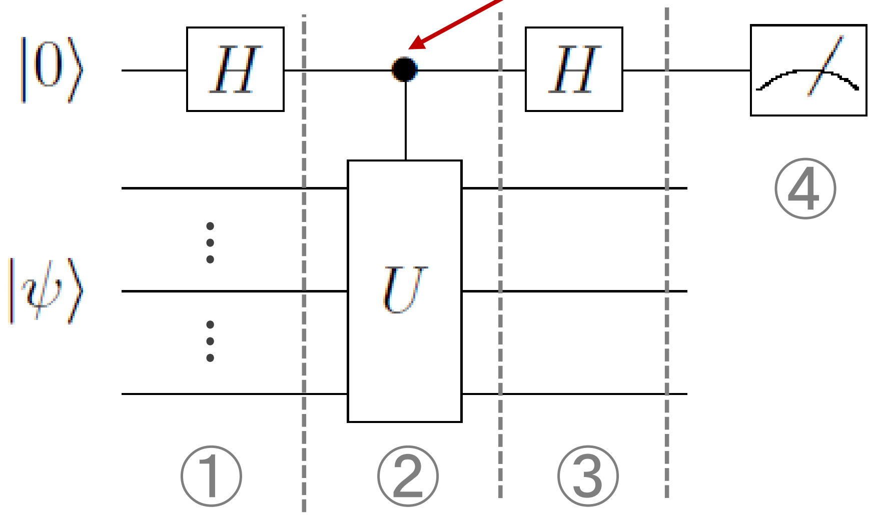


$\mathrm{Im}(\langle\psi|U|\psi\rangle)$

“Hadamard test”: standard way to compute $\langle\psi|\ U\ |\psi\rangle$ (Cont’d)

Computation of $\mathrm{Re}(\ \langle\psi|U|\psi\rangle\ )$:

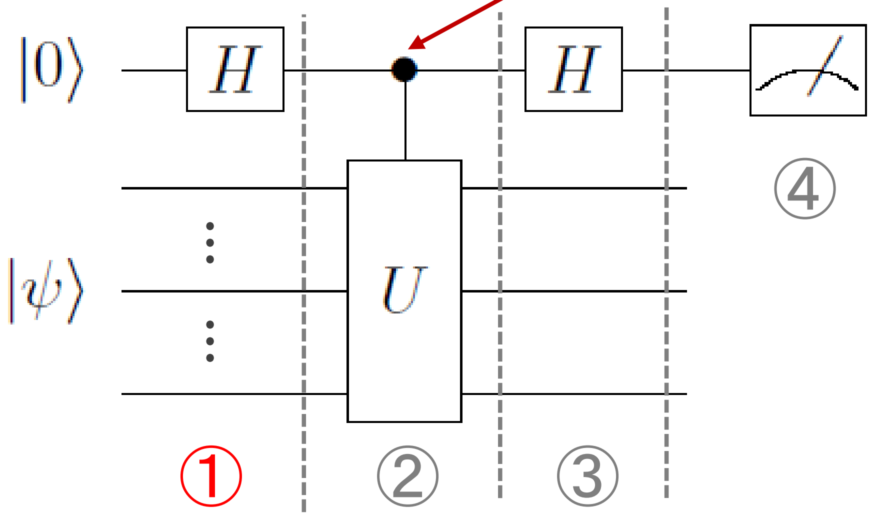
Do nothing if $|0\rangle$ & act U if $|1\rangle$



“Hadamard test”: standard way to compute $\langle\psi|\ U\ |\psi\rangle$ (Cont’d)

Computation of $\mathrm{Re}(\ \langle\psi|U|\psi\rangle\ )$:

Do nothing if $|0\rangle$ & act U if $|1\rangle$

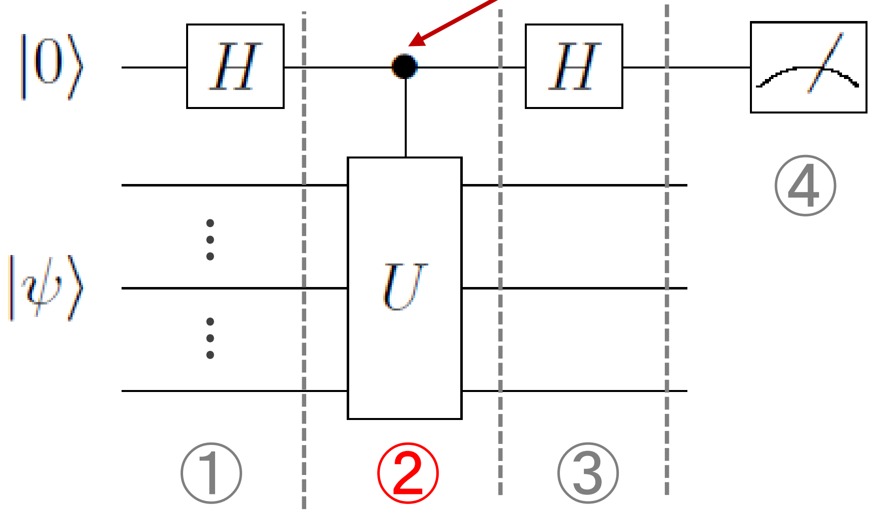


① $H|0\rangle \otimes |\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle \otimes |\psi\rangle\ + \frac{1}{\sqrt{2}}|1\rangle \otimes |\psi\rangle$

"Hadamard test": standard way to compute $\langle\psi|\ \mathrm{U}\ |\psi\rangle$ (Cont'd)

Computation of $\mathrm{Re}(\ \langle\psi|U|\psi\rangle\ )$:

Do nothing if $|0\rangle$ & act U if $|1\rangle$

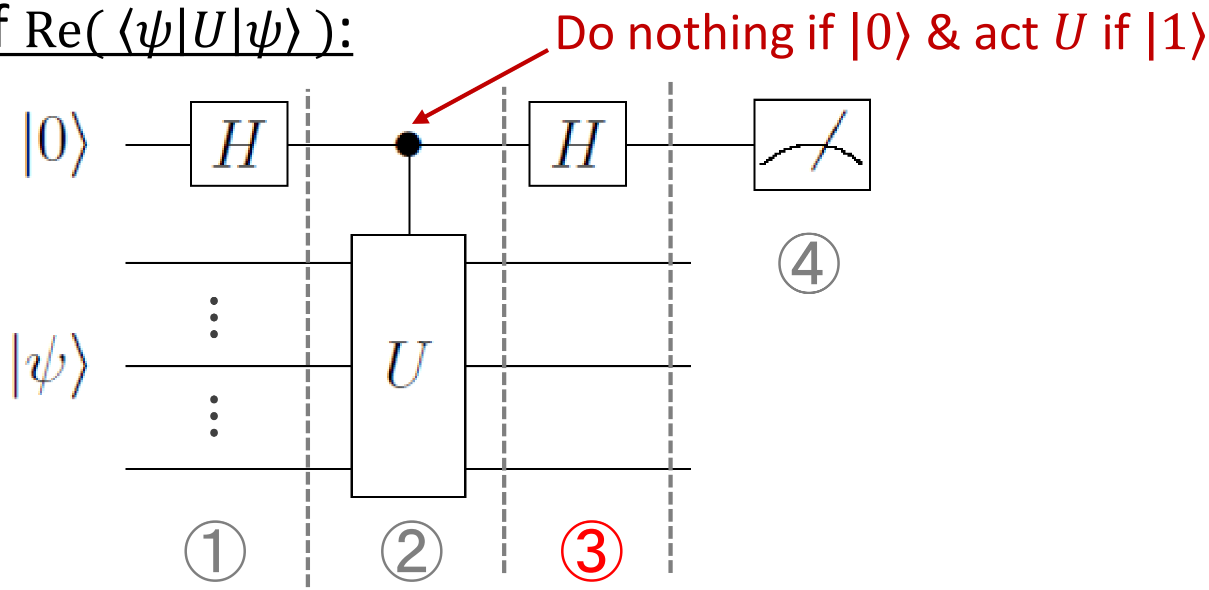


① $H|0\rangle \otimes |\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle \otimes |\psi\rangle + \frac{1}{\sqrt{2}}|1\rangle \otimes |\psi\rangle$

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

"Hadamard test": standard way to compute $\langle\psi| \mathrm{U} |\psi\rangle$ (Cont'd)

Computation of $\mathrm{Re}(\langle\psi|U|\psi\rangle)$:



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

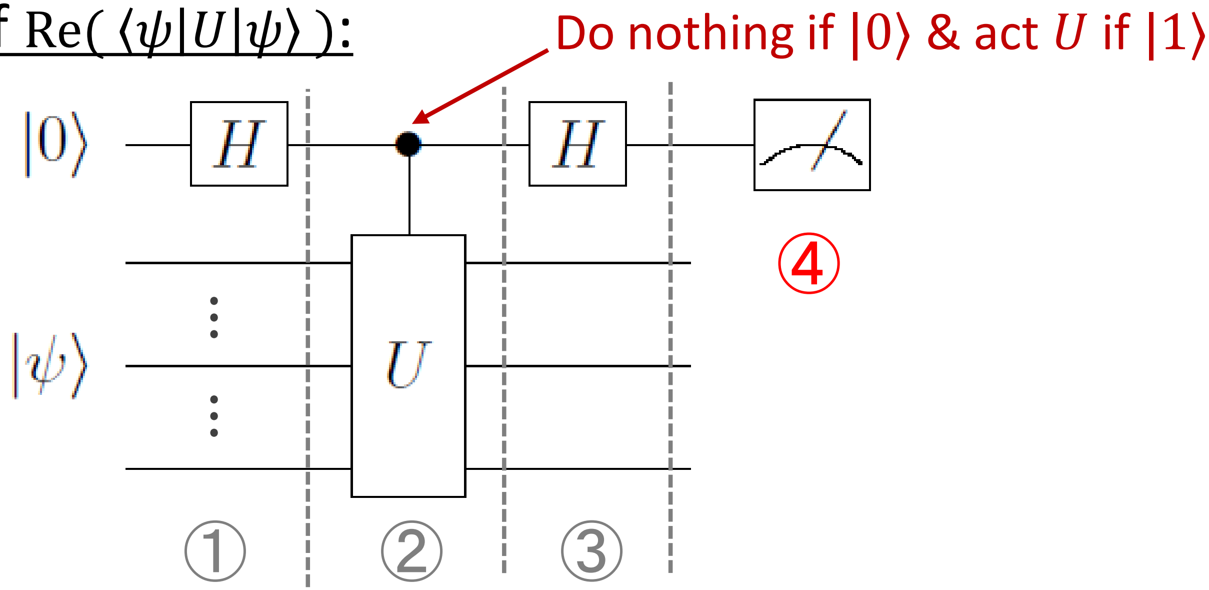
② $\frac{1}{\sqrt{2}}|0\rangle \otimes |\psi\rangle + \frac{1}{\sqrt{2}}|1\rangle \otimes U|\psi\rangle$

③ $\frac{1}{2}(|0\rangle + |1\rangle) \otimes |\psi\rangle + \frac{1}{2}(|0\rangle - |1\rangle) \otimes U|\psi\rangle$

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

"Hadamard test": standard way to compute $\langle\psi|\ U\ |\psi\rangle$ (Cont'd)

Computation of $\mathrm{Re}(\ \langle\psi|U|\psi\rangle\ )$:



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

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

③ $\frac{1}{2}(|0\rangle + |1\rangle) \otimes |\psi\rangle \ + \frac{1}{2}(|0\rangle - |1\rangle) \otimes U|\psi\rangle$

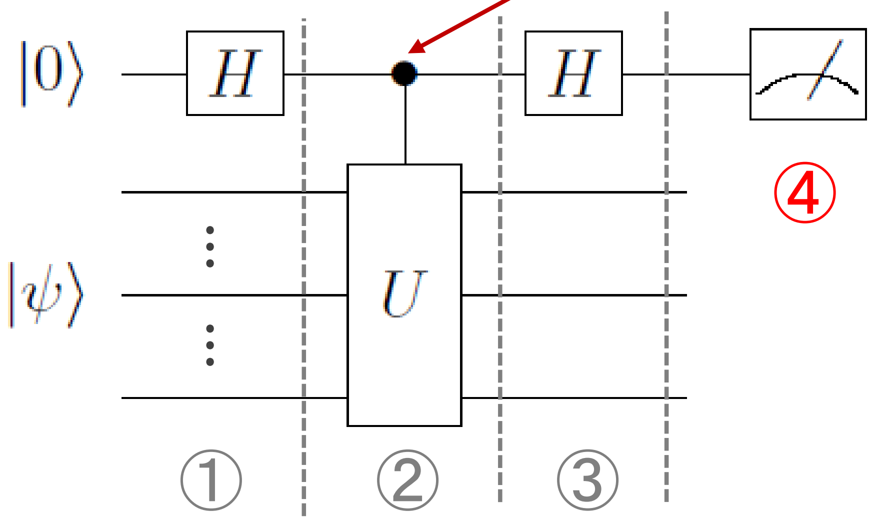
$= \frac{1}{2}|0\rangle \otimes (1+U)|\psi\rangle \ + \frac{1}{2}|1\rangle \otimes (1-U)|\psi\rangle$

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

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

"Hadamard test": standard way to compute $\langle\psi|\, U\, |\psi\rangle$ (Cont'd)

Computation of $\mathrm{Re}(\langle\psi|U|\psi\rangle)$:



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

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

③ $\frac{1}{2}(|0\rangle + |1\rangle) \otimes |\psi\rangle + \frac{1}{2}(|0\rangle - |1\rangle) \otimes U|\psi\rangle$

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

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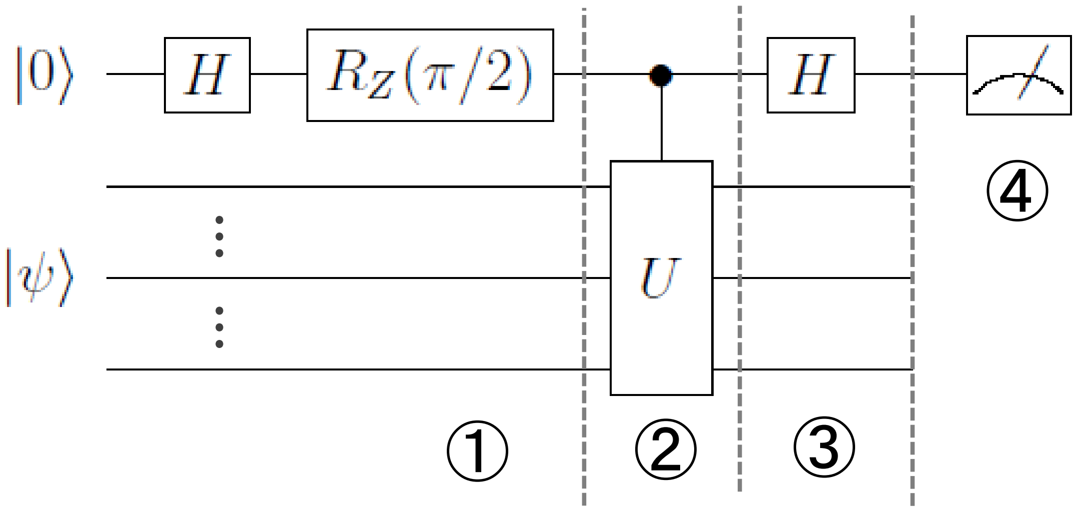
$P_1 = \frac{1}{4}|(1-U)|\psi\rangle|^2 = \frac{1}{2}(1 - \mathrm{Re}\langle\psi|U|\psi\rangle)$

$\Rightarrow$ $\boxed{\mathrm{Re}\langle\psi|U|\psi\rangle = P_0 - P_1}$

“Hadamard test”: standard way to compute $\langle\psi|\ U\ |\psi\rangle$ (Cont’d)

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

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



① $\mathrm{R_Z}(\pi/2)H|0\rangle \otimes |\psi\rangle = \frac{e^{-\frac{\pi i}{4}}}{\sqrt{2}}|0\rangle \otimes |\psi\rangle + \frac{e^{+\frac{\pi i}{4}}}{\sqrt{2}}|1\rangle \otimes |\psi\rangle$

② $\frac{e^{-\frac{\pi i}{4}}}{\sqrt{2}}|0\rangle \otimes |\psi\rangle + \frac{e^{+\frac{\pi i}{4}}}{\sqrt{2}}|1\rangle \otimes U|\psi\rangle$

③ $\frac{e^{-\frac{\pi i}{4}}}{2}|0\rangle \otimes (1 + iU)|\psi\rangle + \frac{e^{-\frac{\pi i}{4}}}{2}|1\rangle \otimes (1 - iU)|\psi\rangle$

④ $P_0 = \frac{1}{4}|(1 + iU)|\psi\rangle|^2 = \frac{1}{2}(\ 1 - \mathrm{Im}\langle\psi|U|\psi\rangle\ )$

$P_1 = \frac{1}{4}|(1 - iU)|\psi\rangle|^2 = \frac{1}{2}(\ 1 + \mathrm{Im}\langle\psi|U|\psi\rangle\ )$

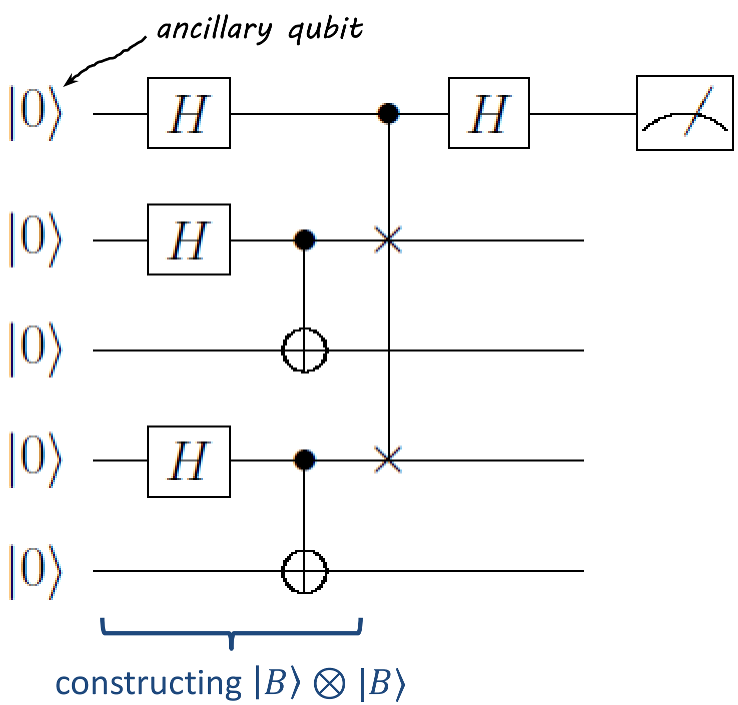
$$\boxed{\mathrm{Im}\langle\psi|U|\psi\rangle = P_1 - P_0}$$

Coming back to the Renyi entropy of Bell state

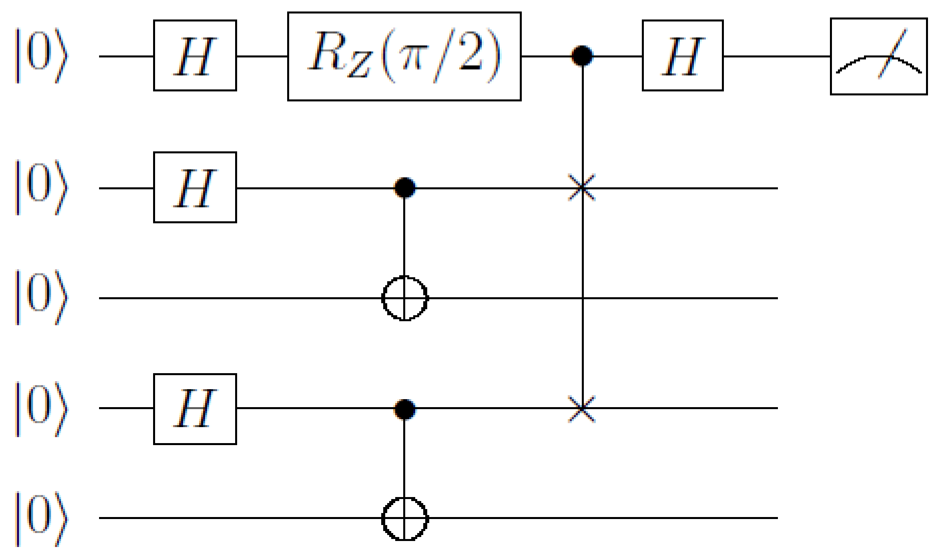
Taking $|\psi\rangle = |B\rangle \otimes |B\rangle$ & $U = \mathrm{SWAP}^{(1,3)}$, we can directly compute

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

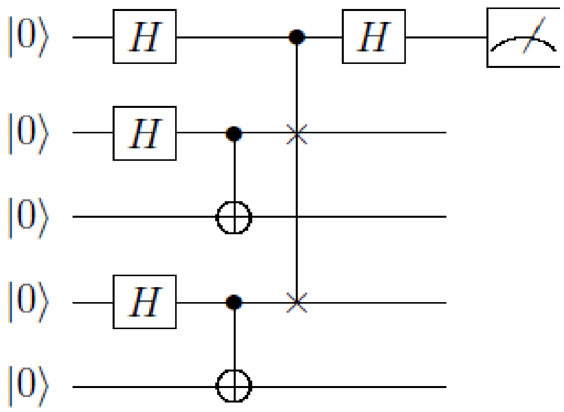
Real part:

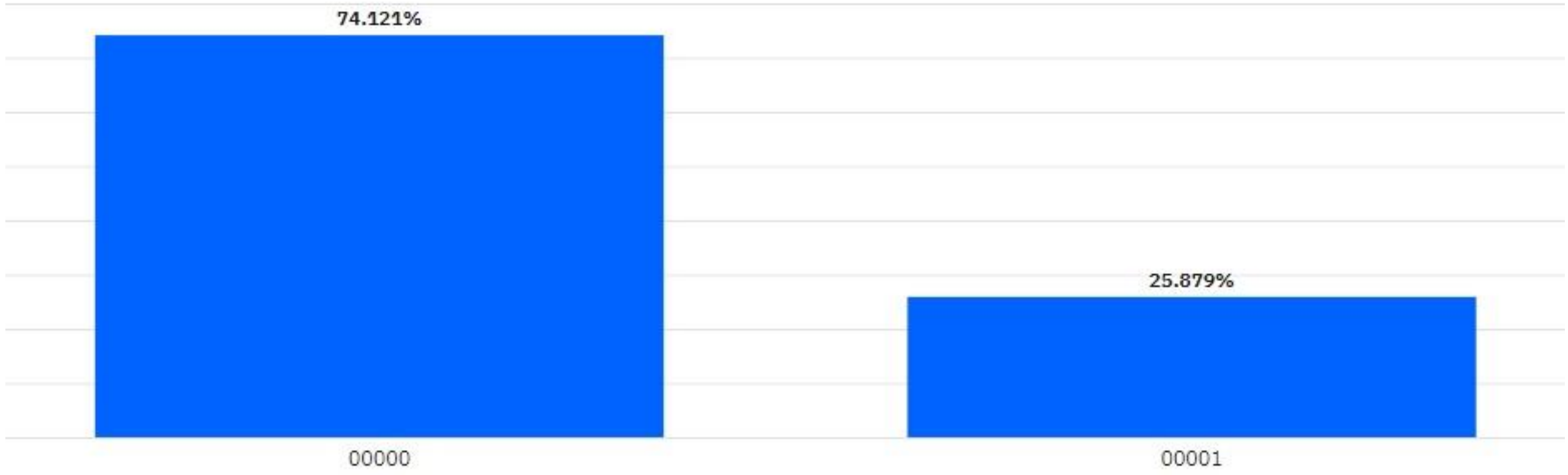


Imaginary part:



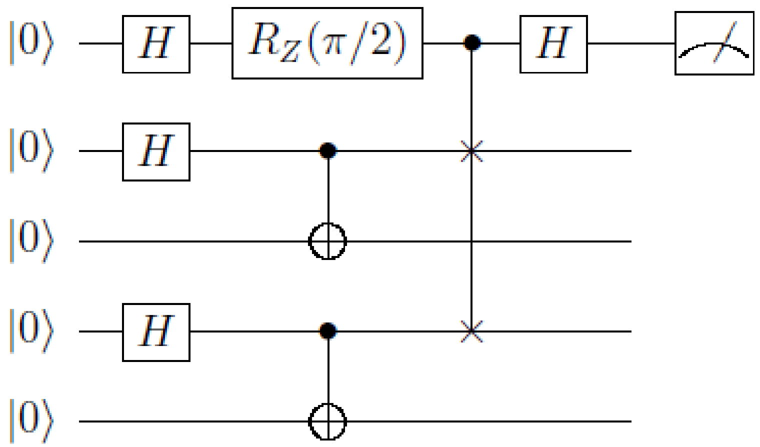
Result of simulator (real part, 1024 shots)

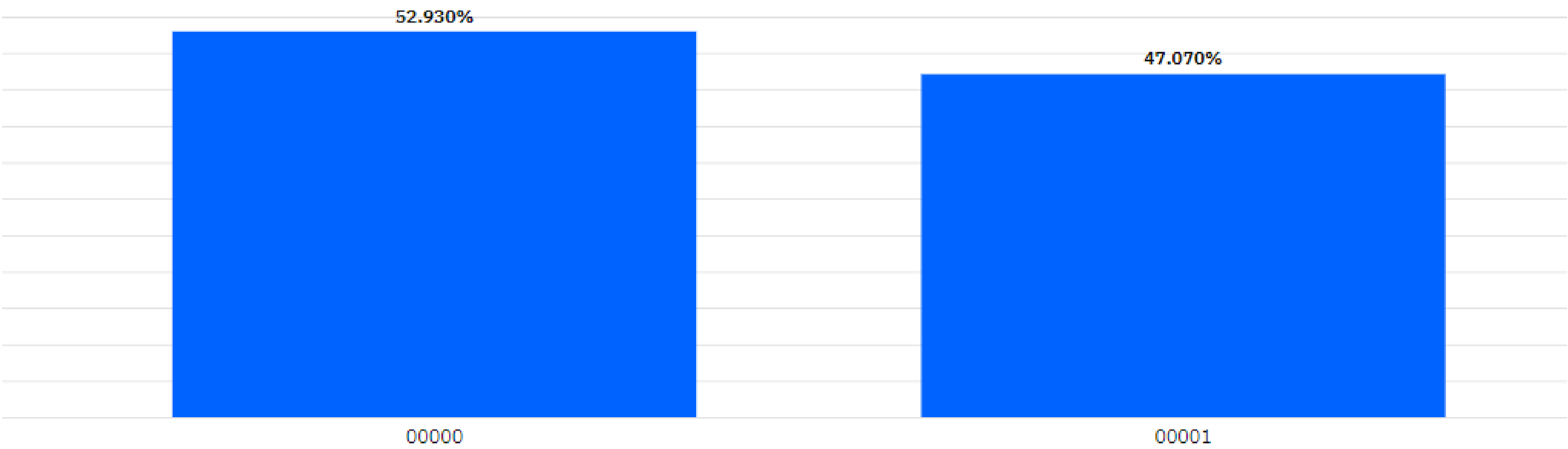




Expectation: $P_0 - P_1 = \mathrm{Re}\,\mathrm{tr}\rho_{\mathrm{red}}^2 = \dfrac{1}{2}$

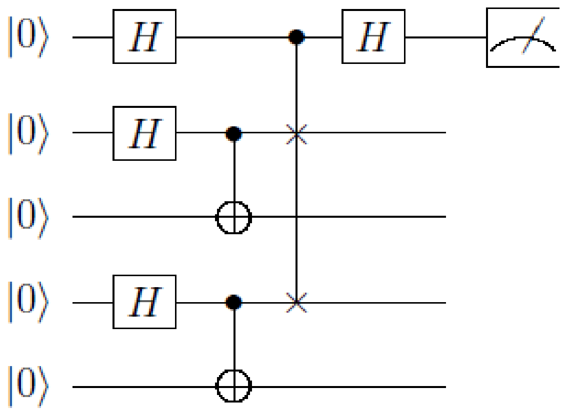
Result of simulator (imaginary part, 1024 shots)

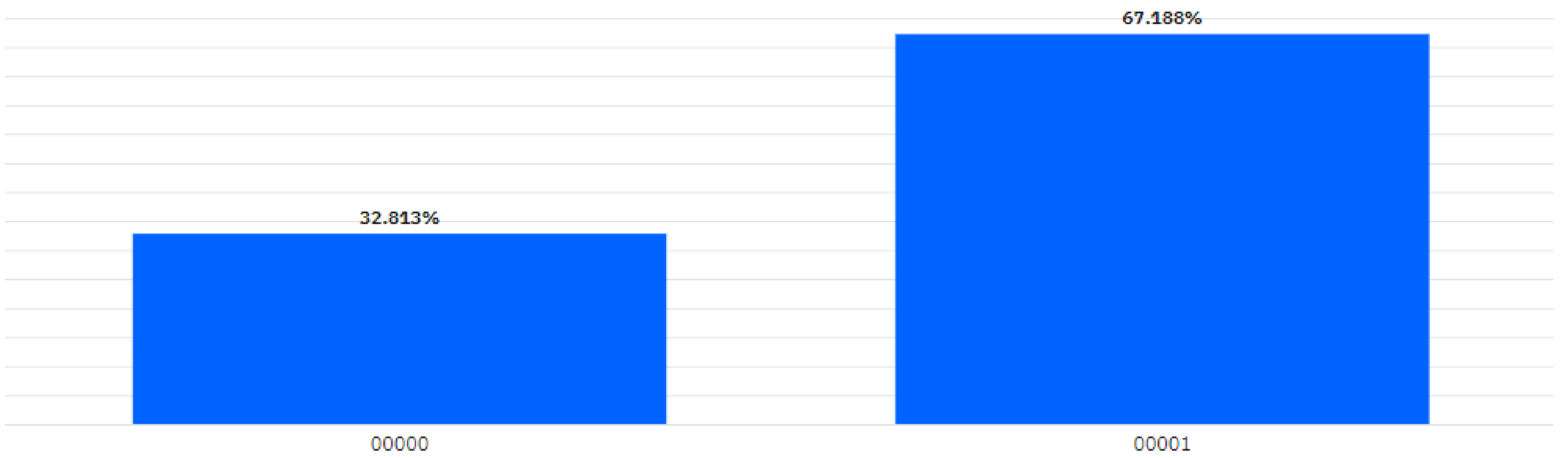




Expectation: $P_1 - P_0 = \mathrm{Im}\ \mathrm{tr}\rho_{\mathrm{red}}^2 = 0$

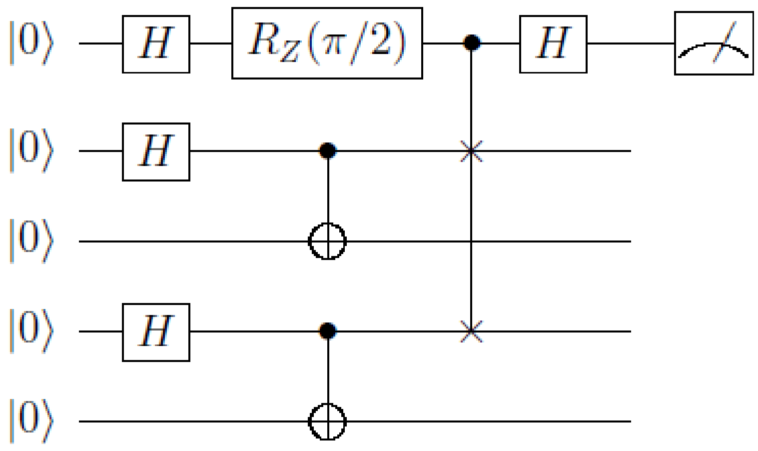
Result of quantum computer (real part, 1024 shots)

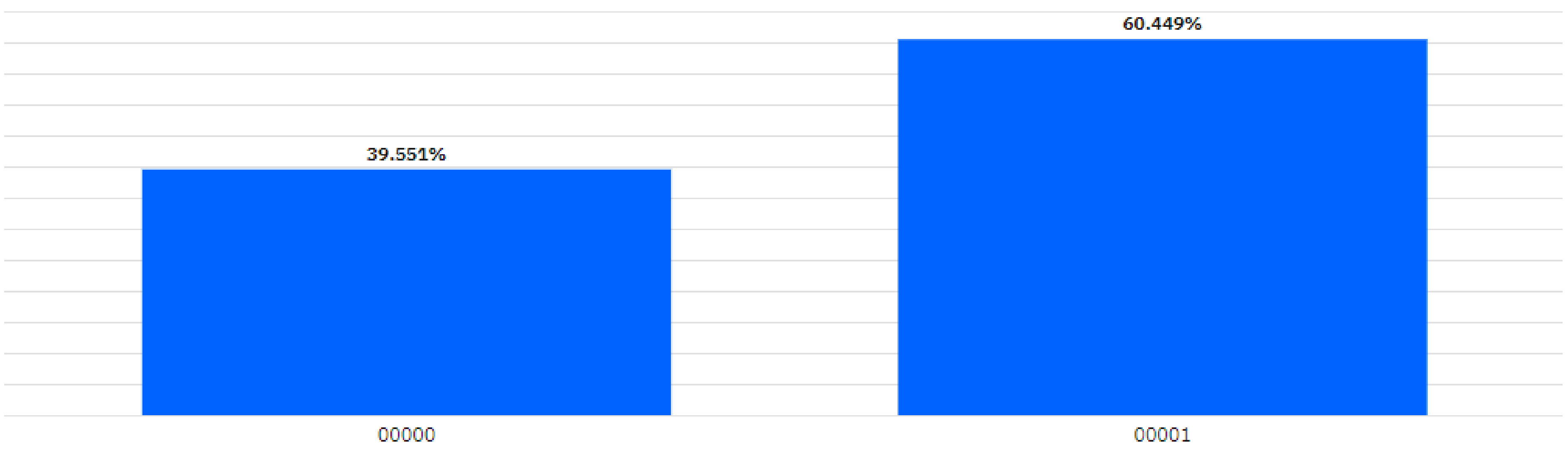




Expectation: $P_0 - P_1 = \mathrm{Re}\,\mathrm{tr}\rho_{\mathrm{red}}^2 = \dfrac{1}{2}$

Result of quantum computer (imaginary part, 1024 shots)





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

Summary

Summary

fun & $^{\exists}$many things to do even now

- Quantum computation is suitable for Hamiltonian formalism which is free from sign problem

- Instead we have to deal with huge vector space. Quantum computers in future may do this job.

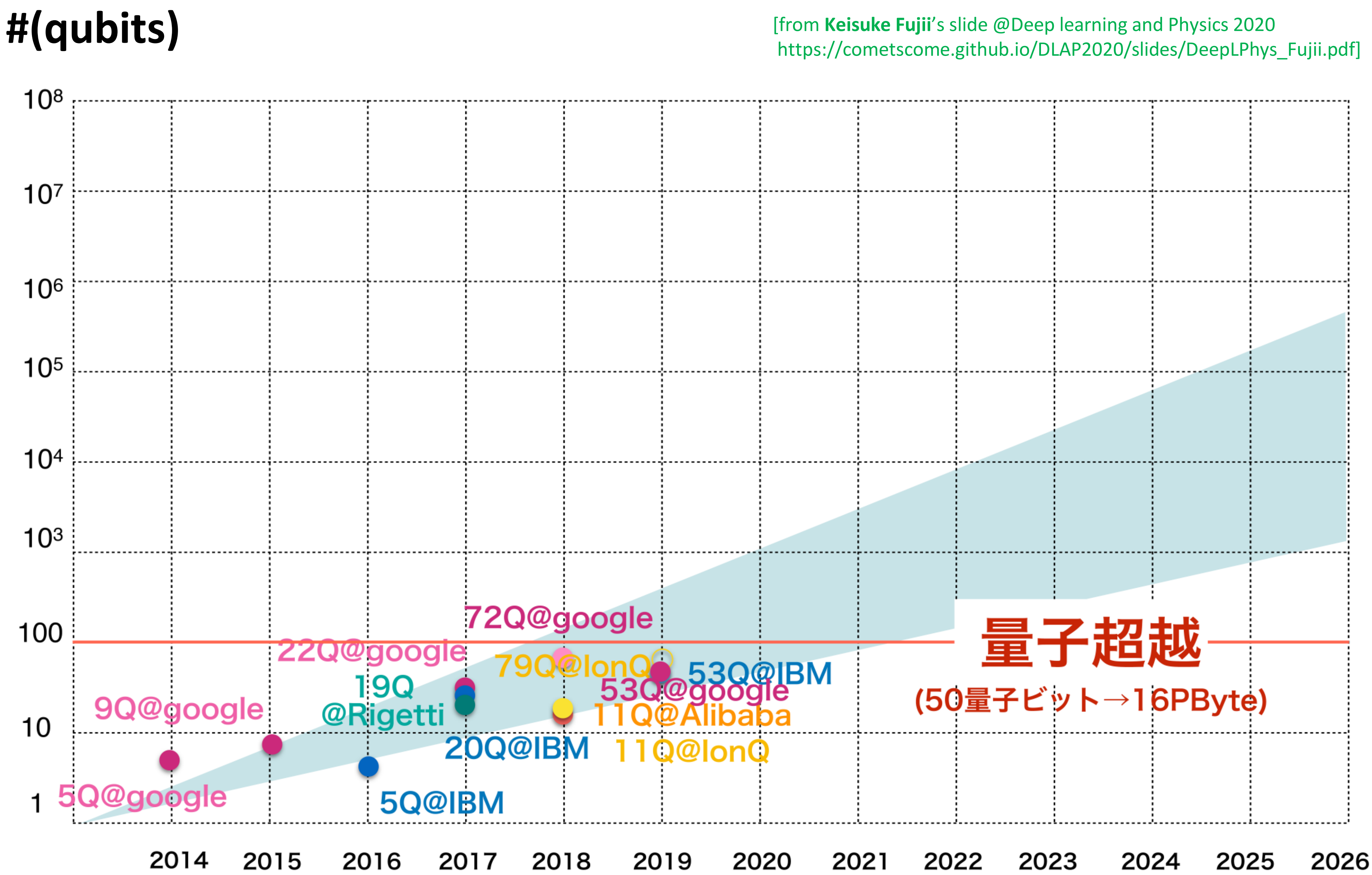
- "Rule" of quantum computation
  = Do something interesting by a combination of
  acting unitary op. & measurement

- Real quantum computer has errors

- Quantum error correction is important

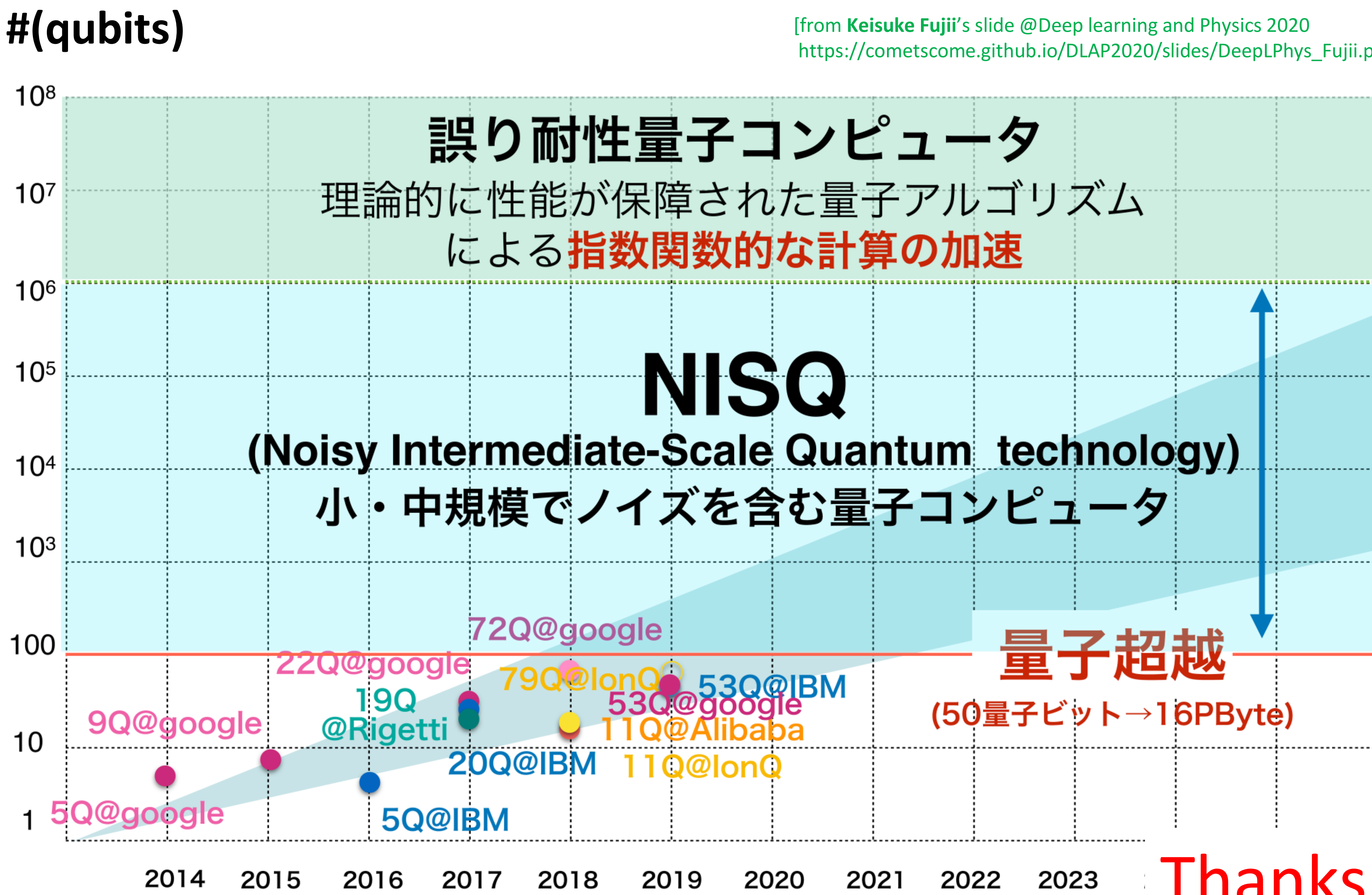
“Quantum” Moore’s law?

[from **Keisuke Fujii**’s slide @Deep learning and Physics 2020
https://cometscome.github.io/DLAP2020/slides/DeepLPhys_Fujii.pdf]



“Quantum” Moore’s law?

[from **Keisuke Fujii**’s slide @Deep learning and Physics 2020
https://cometscome.github.io/DLAP2020/slides/DeepLPhys_Fujii.pdf]



Thanks!

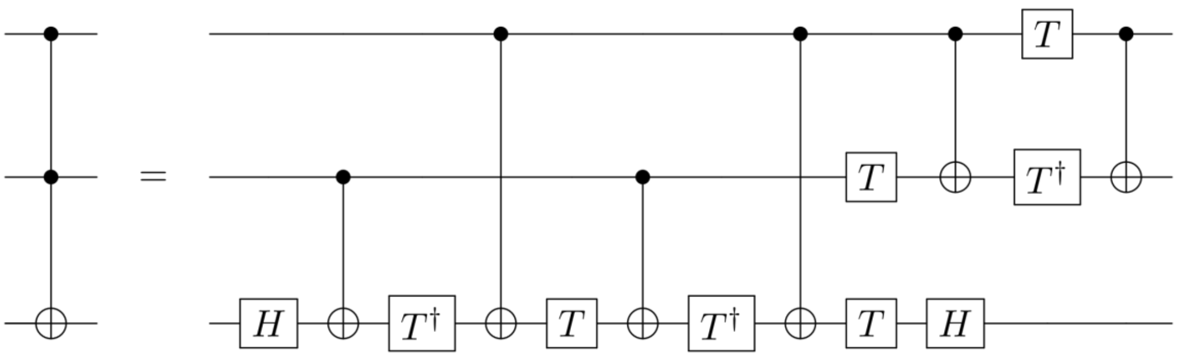
Appendix

Universality

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

Ex.) Toffoli

(controlled-controlled-NOT)



- Any single qubit gate is approximated by a combination of H & T in arbitrary precision

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

- H, T & CX are universal

Approximation of single qubit gate by H & T

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

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

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

where

$$\vec{n} = \frac{1}{\sqrt{1+\cos^2(\pi/8)}} \begin{pmatrix} cos(\pi/8) \\ \sin(\pi/8) \\ cos(\pi/8) \end{pmatrix} \quad \& \quad \underbrace{\cos(\theta/2)}_{2\pi \times (\text{irrational})!} \equiv \cos^2(\pi/8)$$

② Use Weyl's uniform distribution theorem:

$\theta \boldsymbol{Z}$ is uniformly distributed mod 1 $\Rightarrow$ approximate $R_{\vec{n}}(\alpha)$ for $\forall\alpha$

③ Construct rotation around another axis:

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

④ Approximate $\forall$single qubit gate: $R_{\vec{n}}(\alpha)R_{\vec{m}}(\beta)\, R_{\vec{n}}(\gamma)$

What if we replace T by something else?

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

We have the identity:

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

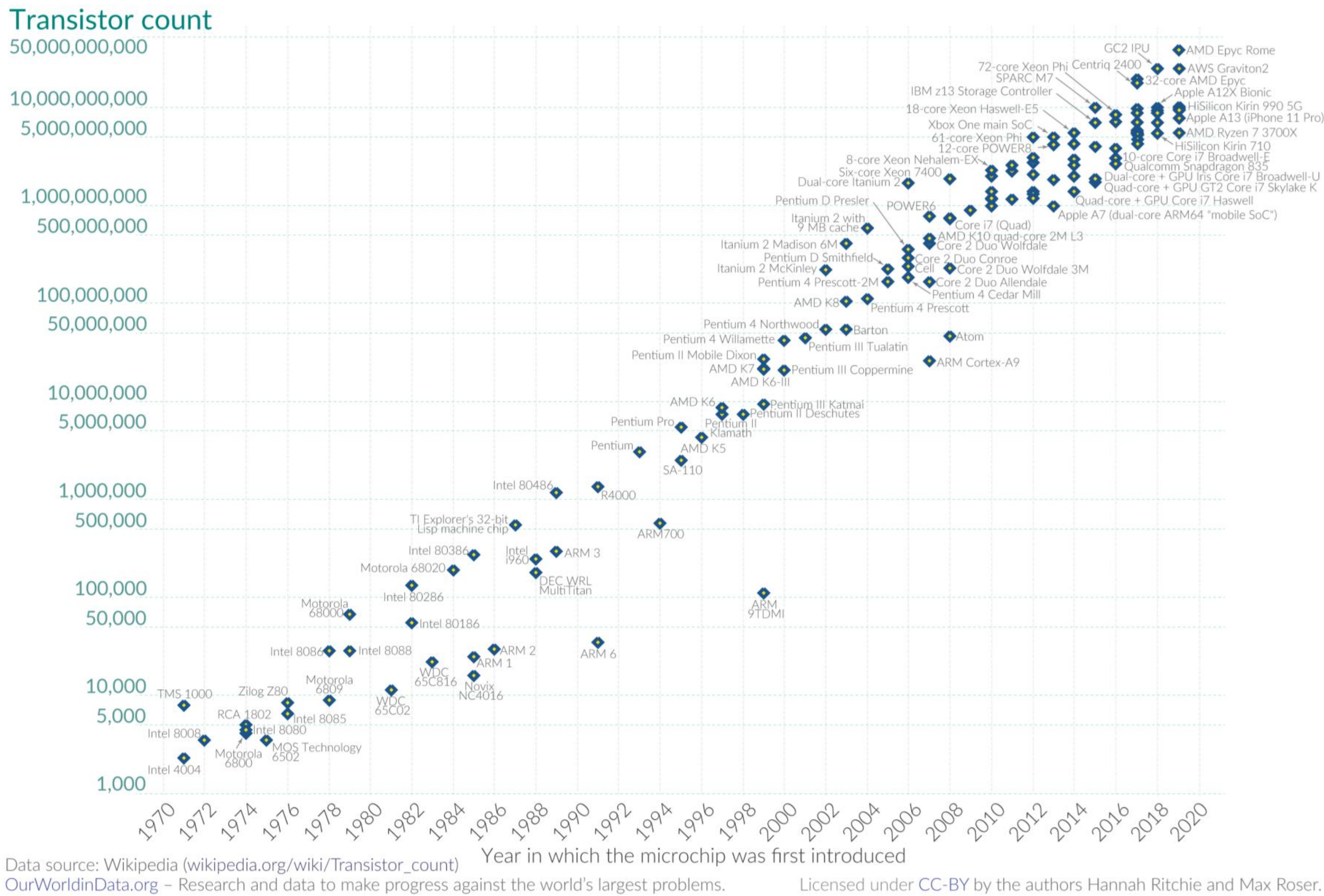
where

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

We can approximate any single qubit gate

by combining H & T' if $\theta/2\pi$ is irrational

Moore’s law



[by Max Roser, Hannah Ritchie, https://ourworldindata.org/uploads/2020/11/Transistor-Count-over-time.png]