

# Efficient Optimization on neutral atoms Quantum Computers

Or... “The unbearable pain of running  
quantum algorithms in the 2020’s”

Quminars @ UNIBO 16/04/2024  
Simone Tibaldi, University of Bologna

**INDICO** page:

<https://agenda.infn.it/event/41198/>



# Efficient Optimization on neutral atoms Quantum Computers

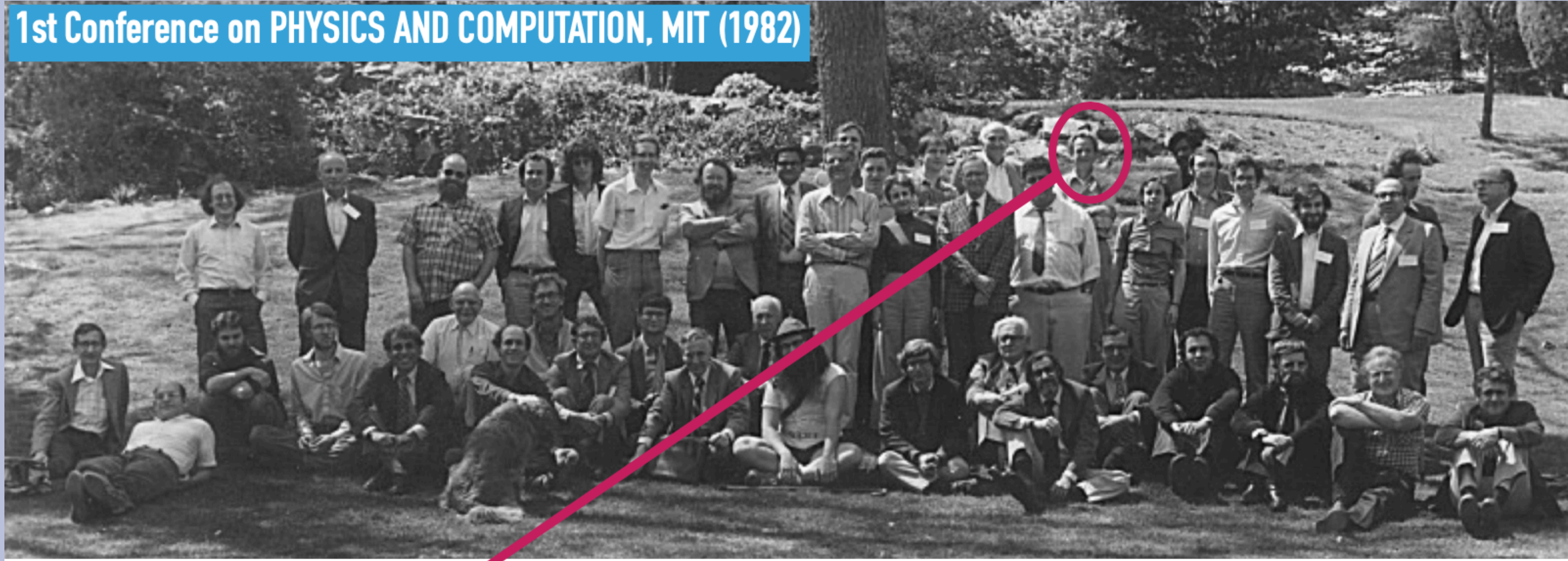
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## From THIS ...

### 1st Conference on PHYSICS AND COMPUTATION, MIT (1982)



Now, what kind of physics are we going to imitate? First, I am going to describe the possibility of simulating physics in the classical approximation, a thing which is usually described by local differential equations. But the physical world is quantum mechanical, and therefore the proper problem is the simulation of quantum physics—which is what I really want to talk about, but I'll come to that later. So what kind of simulation do I mean?

I want to talk about the possibility that there is to be an *exact* simulation, that the computer will do *exactly* the same as nature.

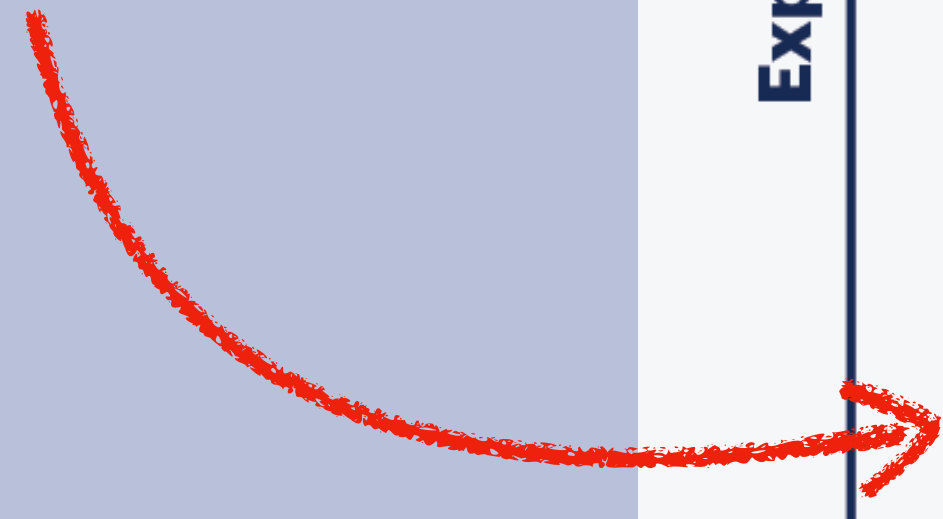
*International Journal of Theoretical Physics, Vol. 21, Nos. 6/7, 1982*

... to THIS

# Hype Cycle for Emerging Technologies, 2021



We made it!

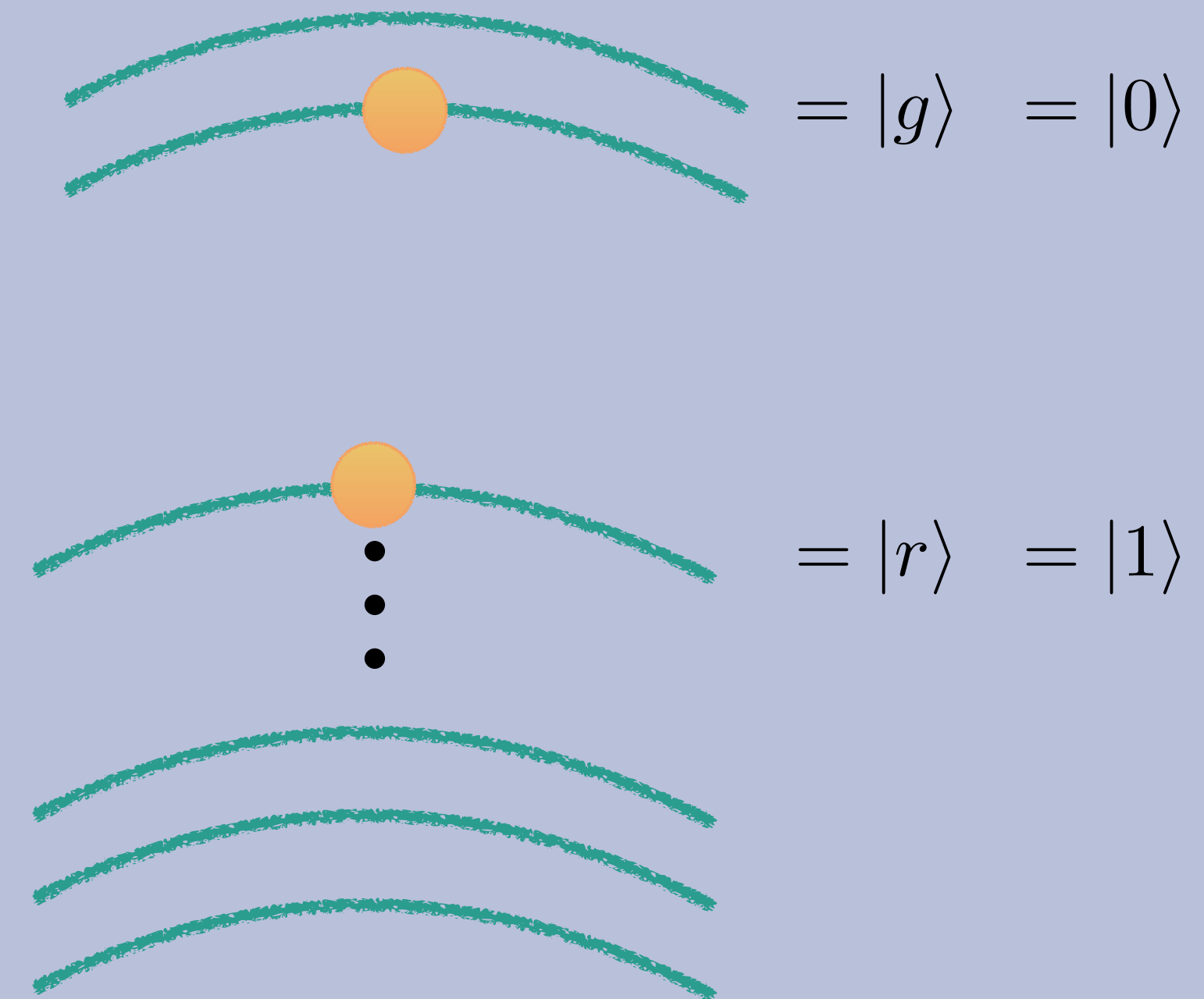
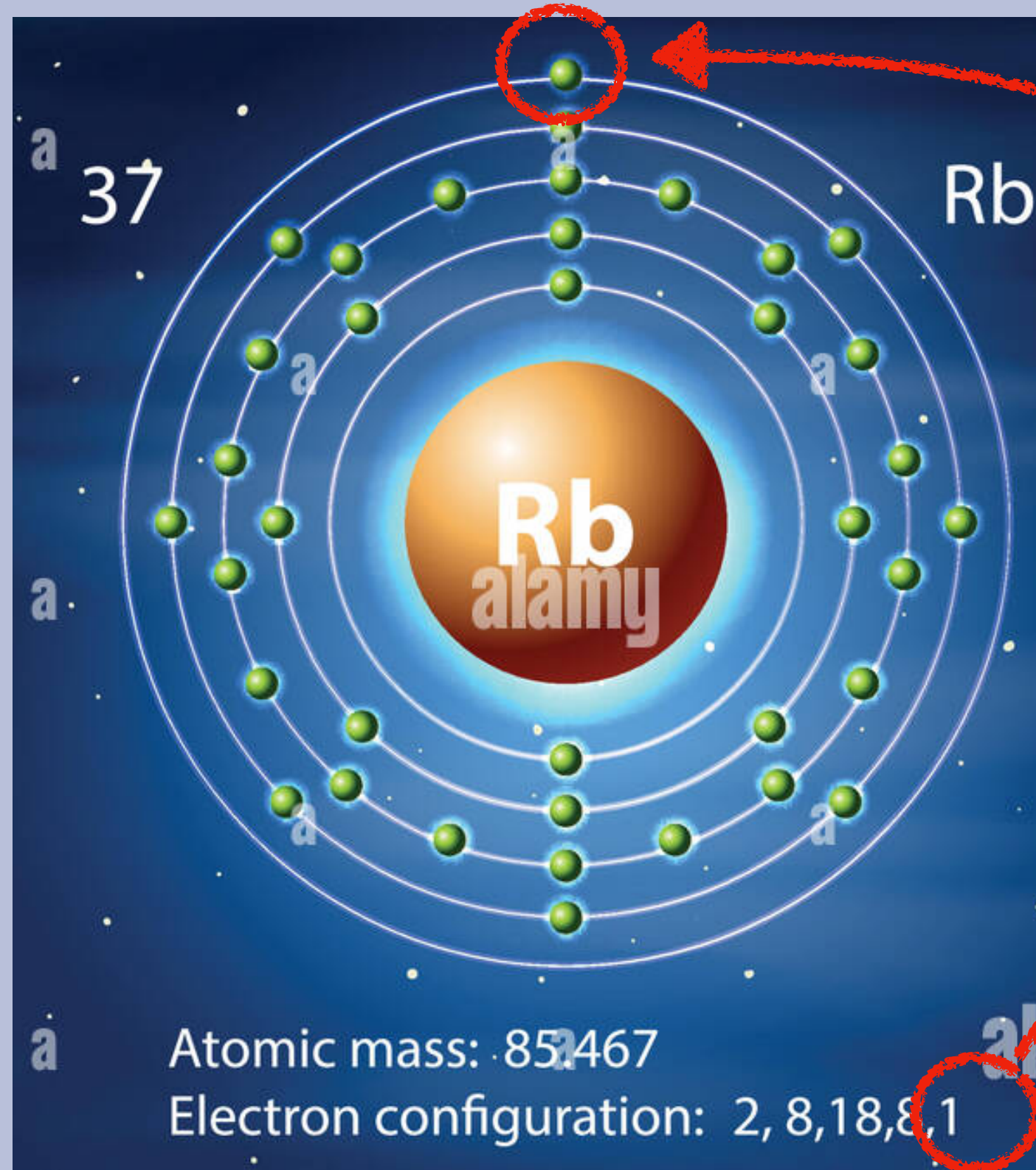


[gartner.com](https://www.gartner.com)

Source: Gartner  
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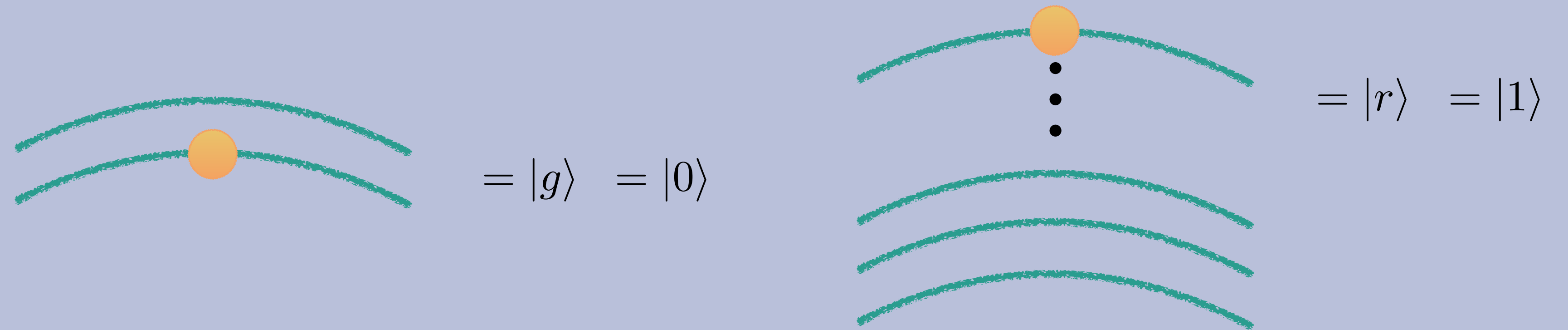
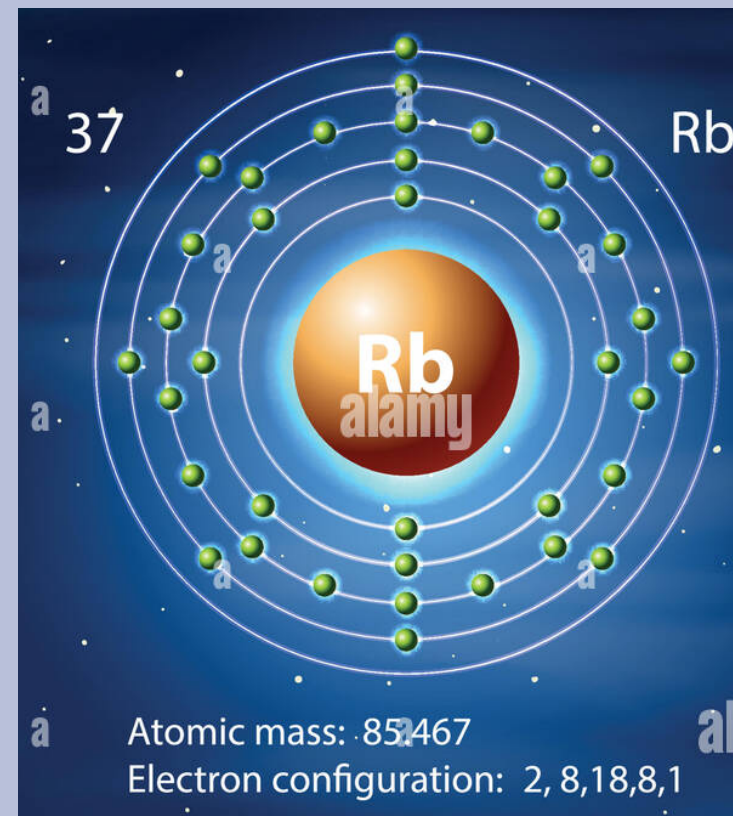
**Gartner**

Let's create one

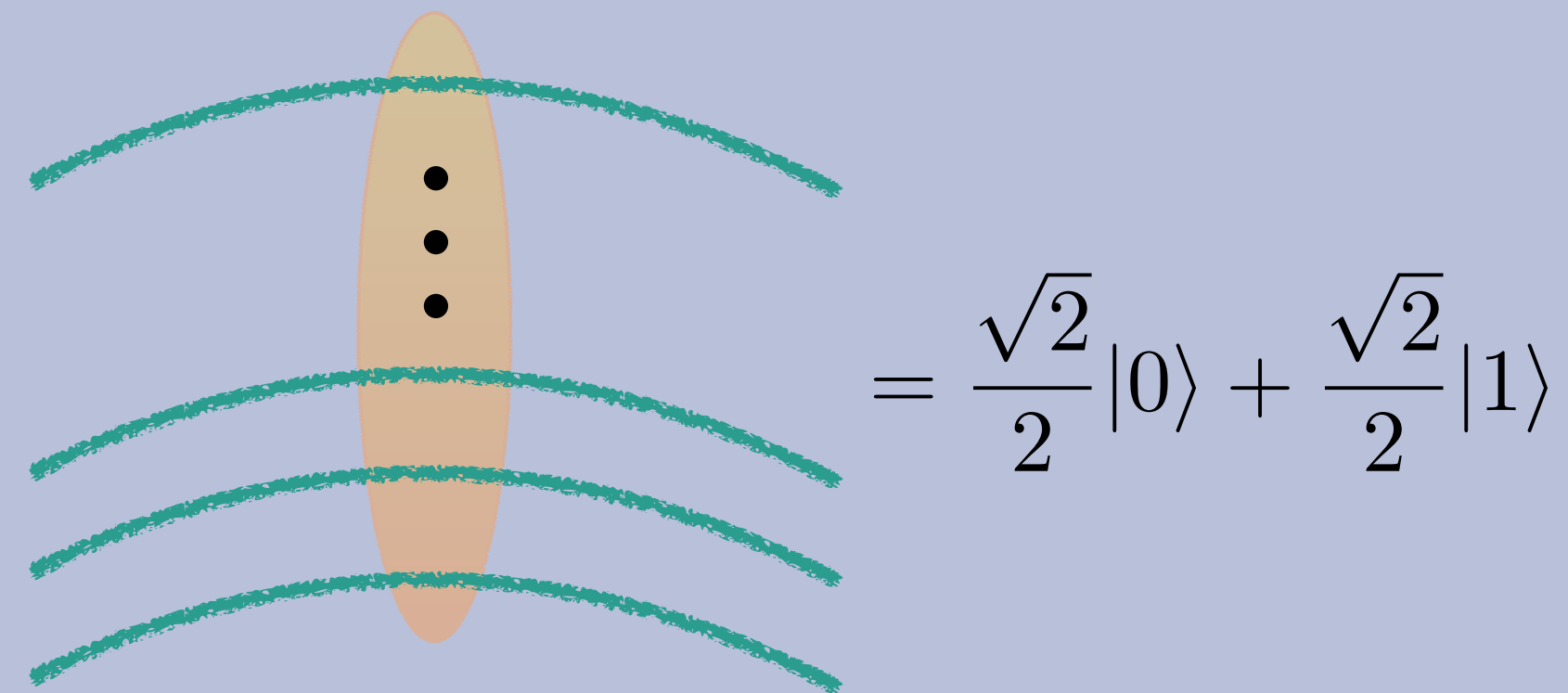


We can control the state with a laser set to a specific frequency

# Let's create one



By applying a specific pulse we can create a superposition



Each state with probability of being populated of:

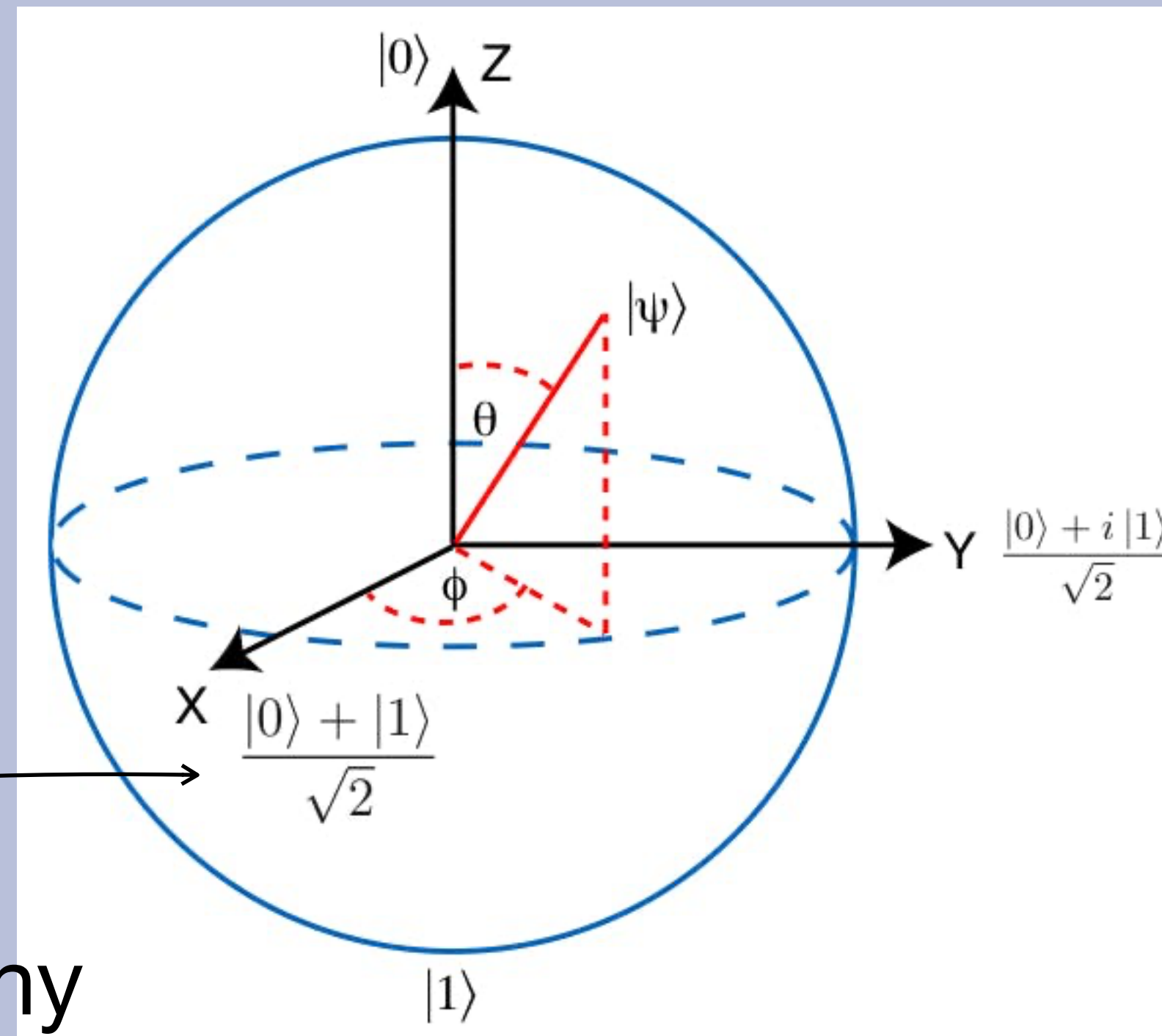
$$\left(\frac{\sqrt{2}}{2}\right)^2 + \left(\frac{\sqrt{2}}{2}\right)^2 = \frac{1}{2} + \frac{1}{2} = 1$$

And we can do much more

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$|\Psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha|0\rangle + \beta|1\rangle$$

$$|\alpha|^2 + |\beta|^2 = 1$$



This is one of infinitely many possible superposition states

This is a qubit

Rotating the qubit is like applying (quantum) gates

$$\boxed{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

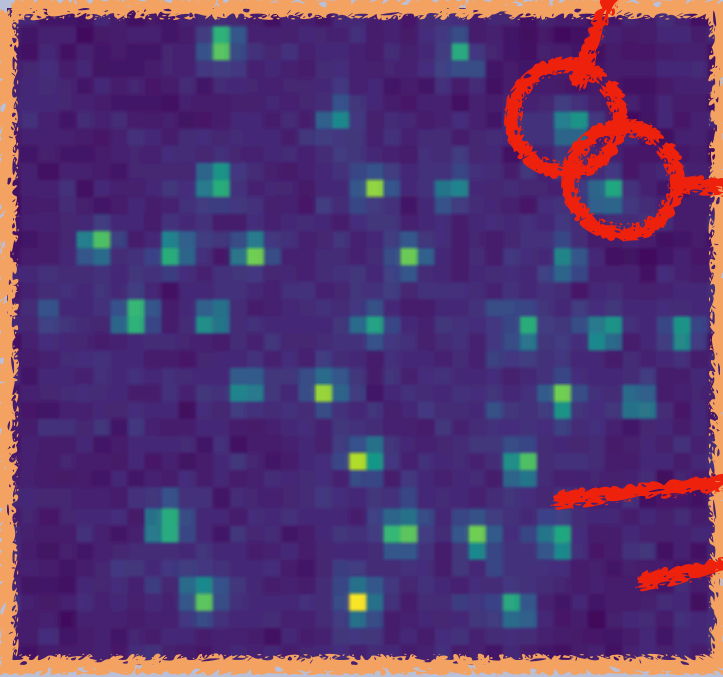
$$\boxed{R_z} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$$

Example:  $H|\Psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

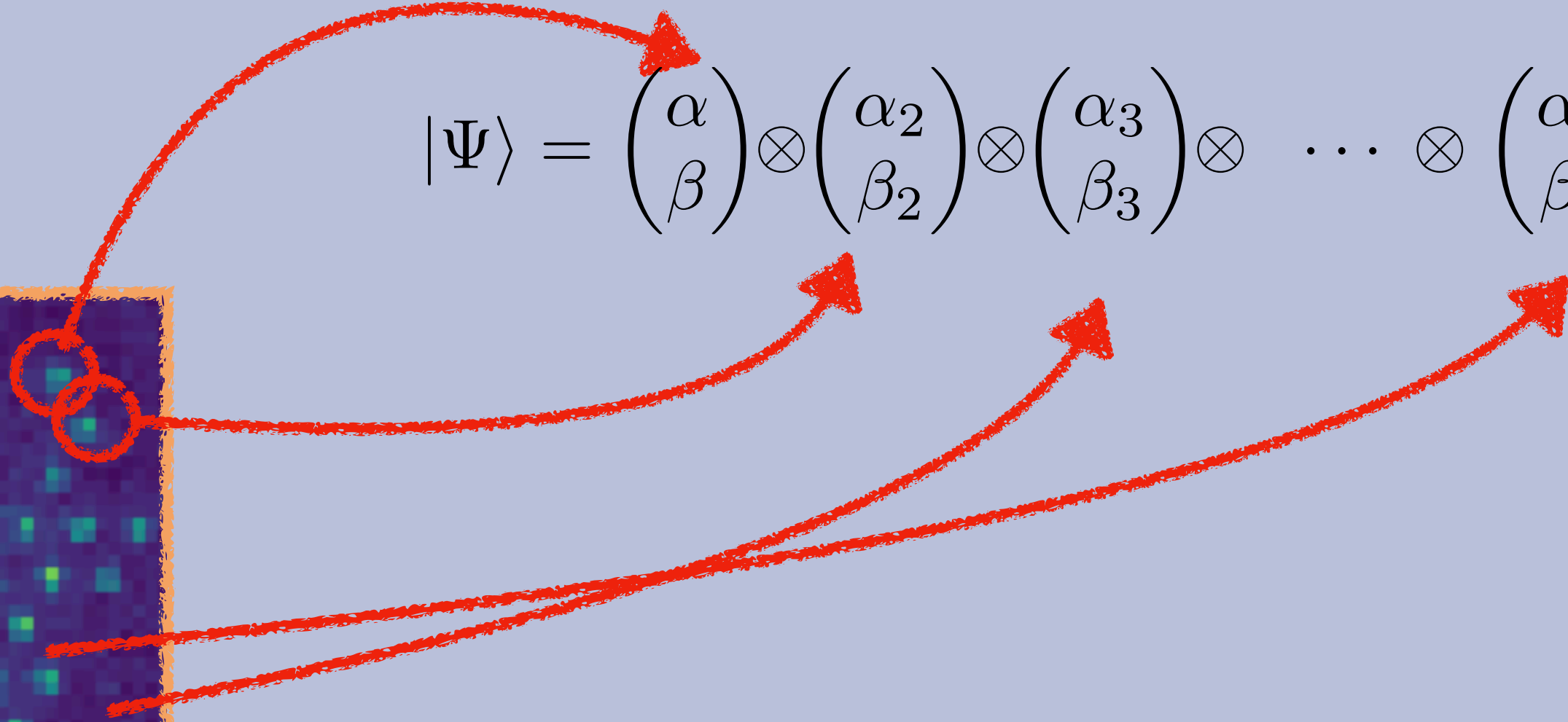
And we can add more qubits as well...



$$\begin{pmatrix} \alpha_1 \\ \beta_1 \end{pmatrix} \otimes \begin{pmatrix} \alpha_2 \\ \beta_2 \end{pmatrix} = \begin{pmatrix} \alpha_1 \alpha_2 \\ \alpha_1 \beta_2 \\ \beta_1 \alpha_2 \\ \beta_1 \beta_2 \end{pmatrix} = \alpha_1 \alpha_2 |00\rangle + \alpha_1 \beta_2 |01\rangle + \beta_1 \alpha_2 |10\rangle + \beta_1 \beta_2 |11\rangle$$

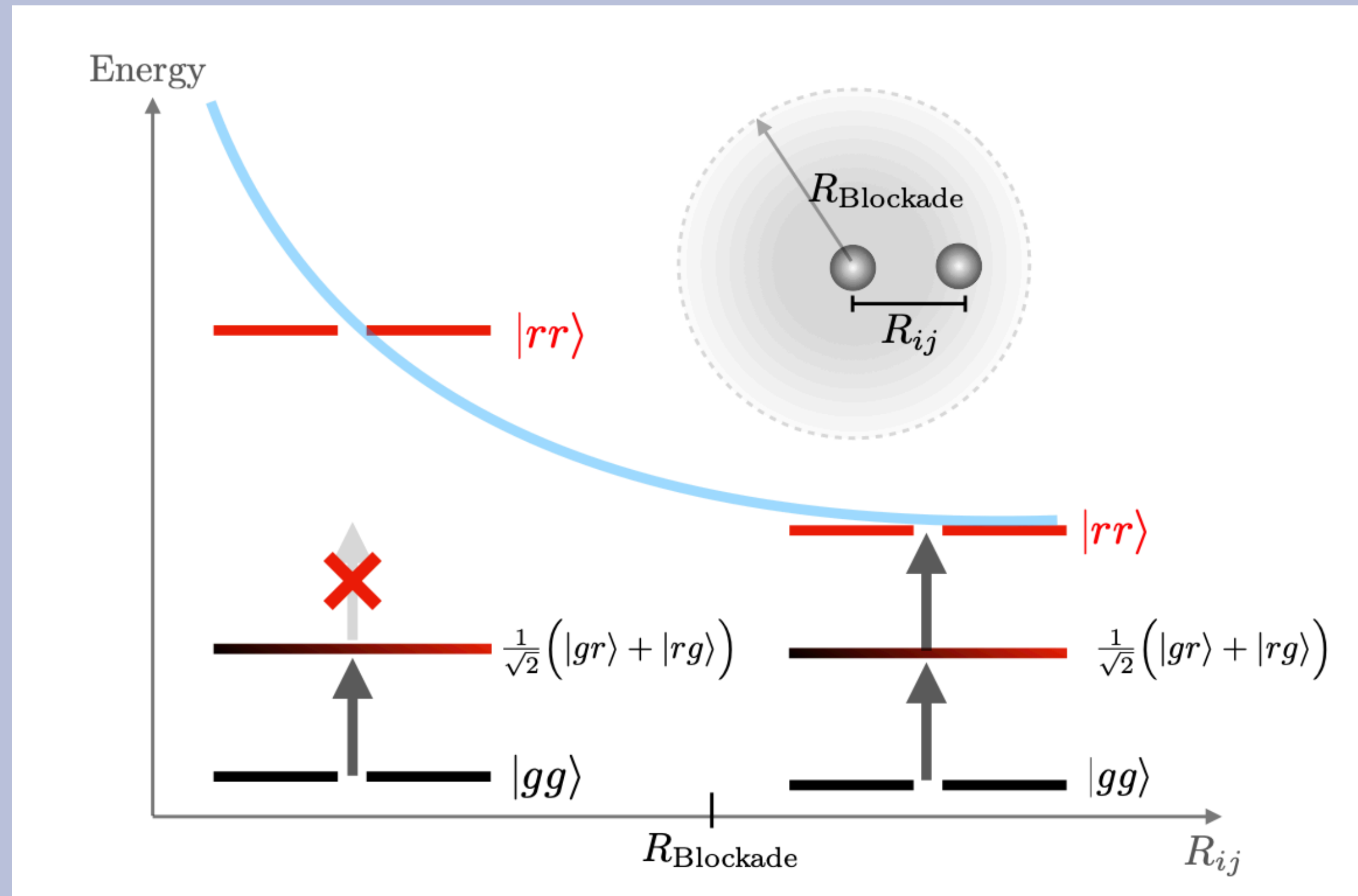


$$|\Psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \otimes \begin{pmatrix} \alpha_2 \\ \beta_2 \end{pmatrix} \otimes \begin{pmatrix} \alpha_3 \\ \beta_3 \end{pmatrix} \otimes \dots \otimes \begin{pmatrix} \alpha_N \\ \beta_N \end{pmatrix} = \begin{pmatrix} \alpha_1 \alpha_2 \alpha_3 \dots \alpha_N \\ \alpha_1 \alpha_2 \alpha_3 \dots \beta_N \\ \vdots \\ \beta_1 \beta_2 \beta_3 \dots \beta_N \end{pmatrix} = 2^N$$





With 2 qubits we can also create entanglement...



... exploiting the Rydberg blockade.

When two atoms are close enough, electrons cannot be excited to  $|r\rangle$  at the same time

The result:

Far apart:

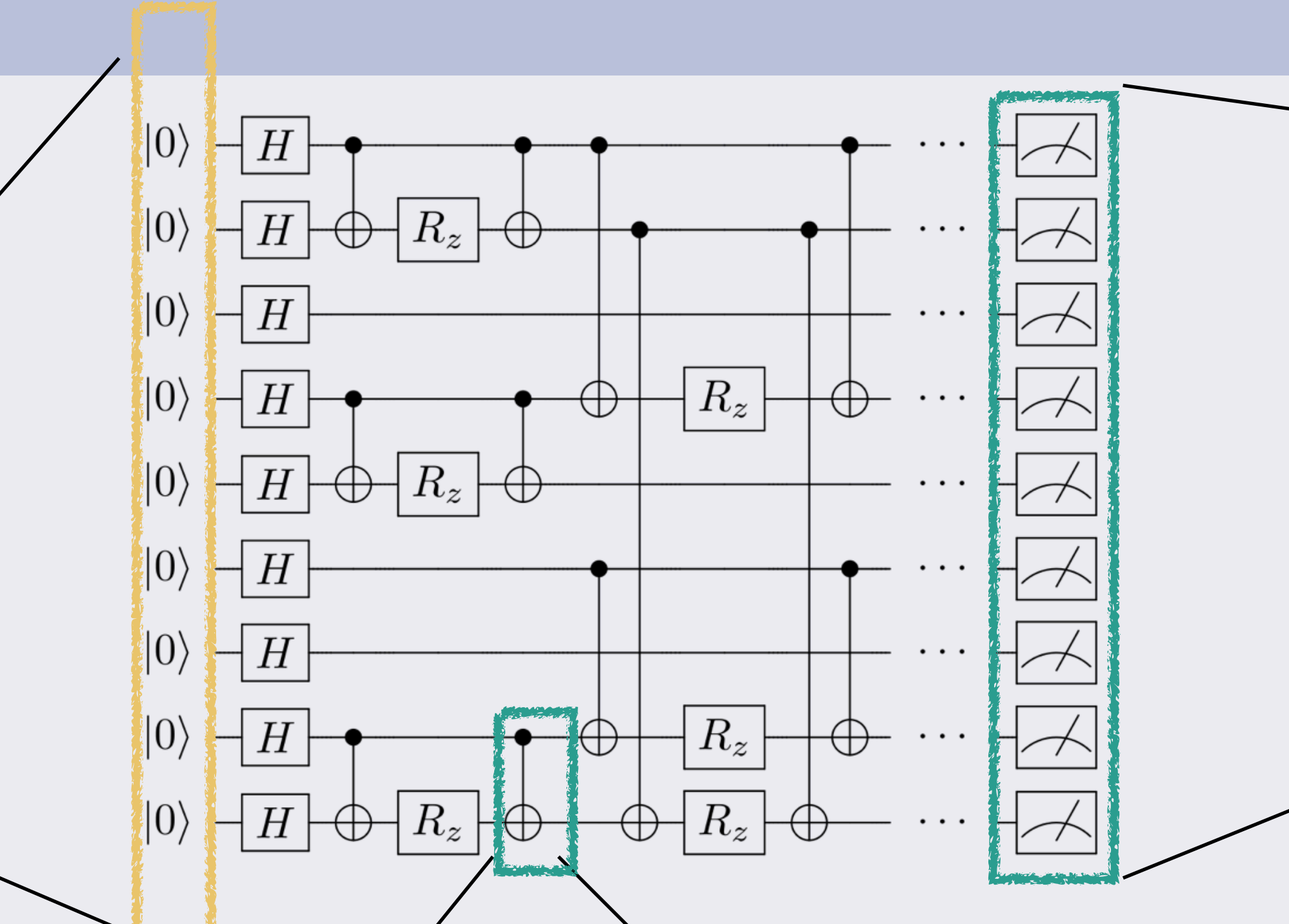
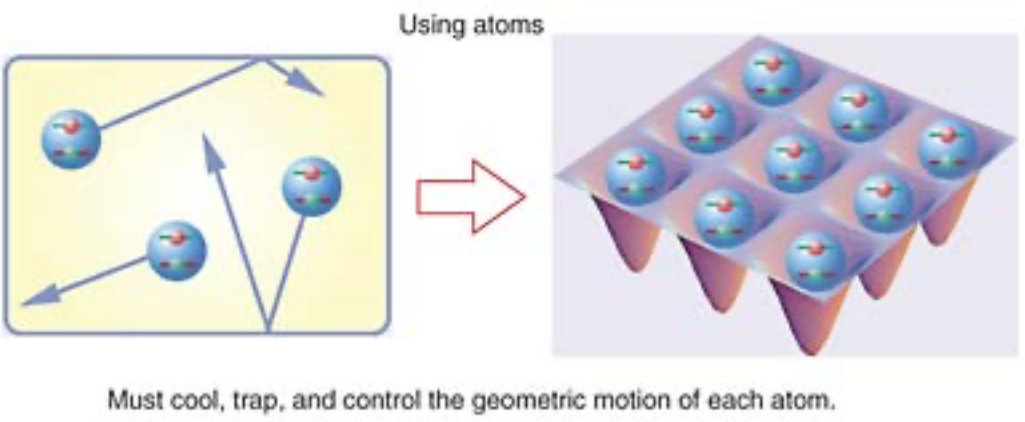
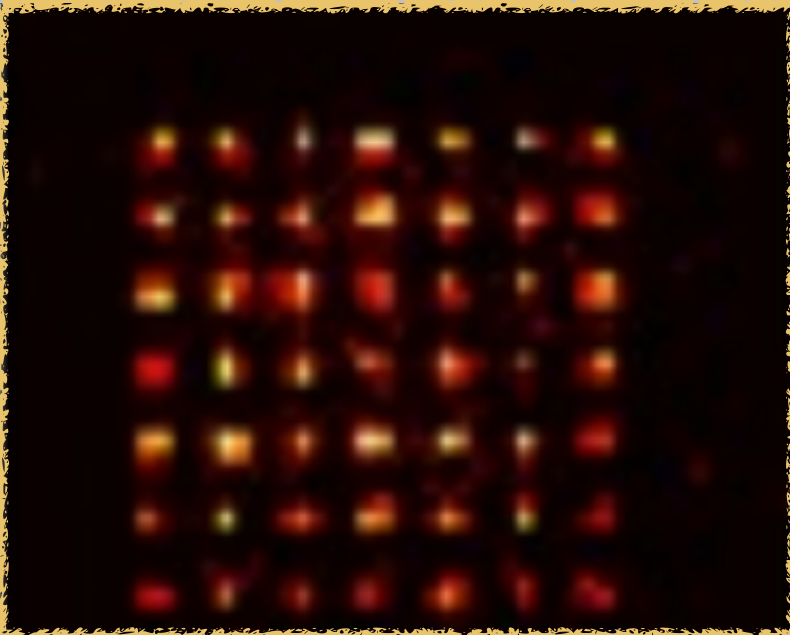
$$|gg\rangle \rightarrow \frac{1}{2}(|gg\rangle + |gr\rangle + |rg\rangle + |rr\rangle) = \frac{1}{\sqrt{2}}(|g\rangle + |r\rangle) \otimes \frac{1}{\sqrt{2}}(|g\rangle + |r\rangle)$$

Closer than R

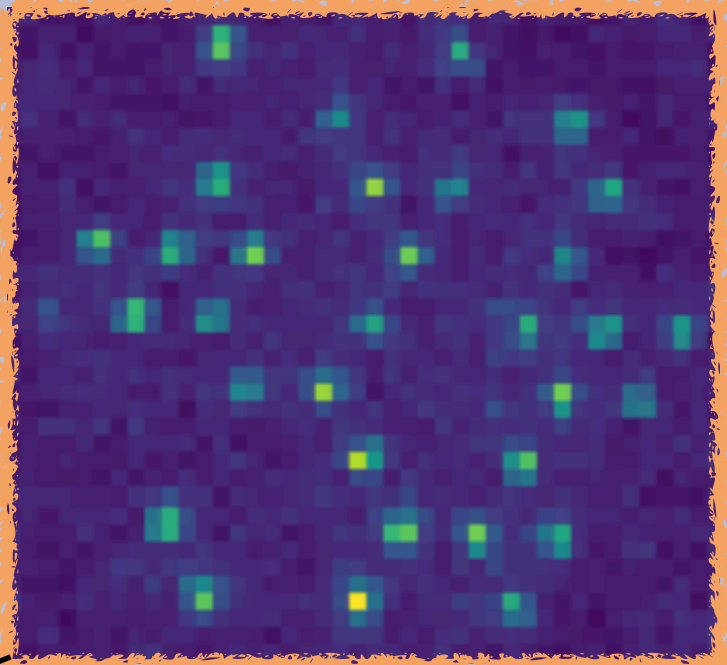
$$|gg\rangle \rightarrow \frac{1}{2}(|gg\rangle + |gr\rangle + |rg\rangle - |rr\rangle) \quad \text{Two electrons are entangled!}$$

# Rotating a qubit + entanglement = quantum computation

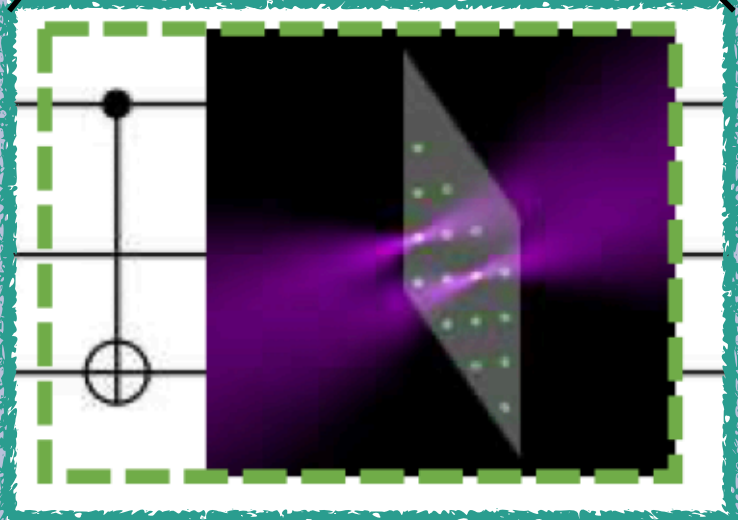
Prepare a state



Measure

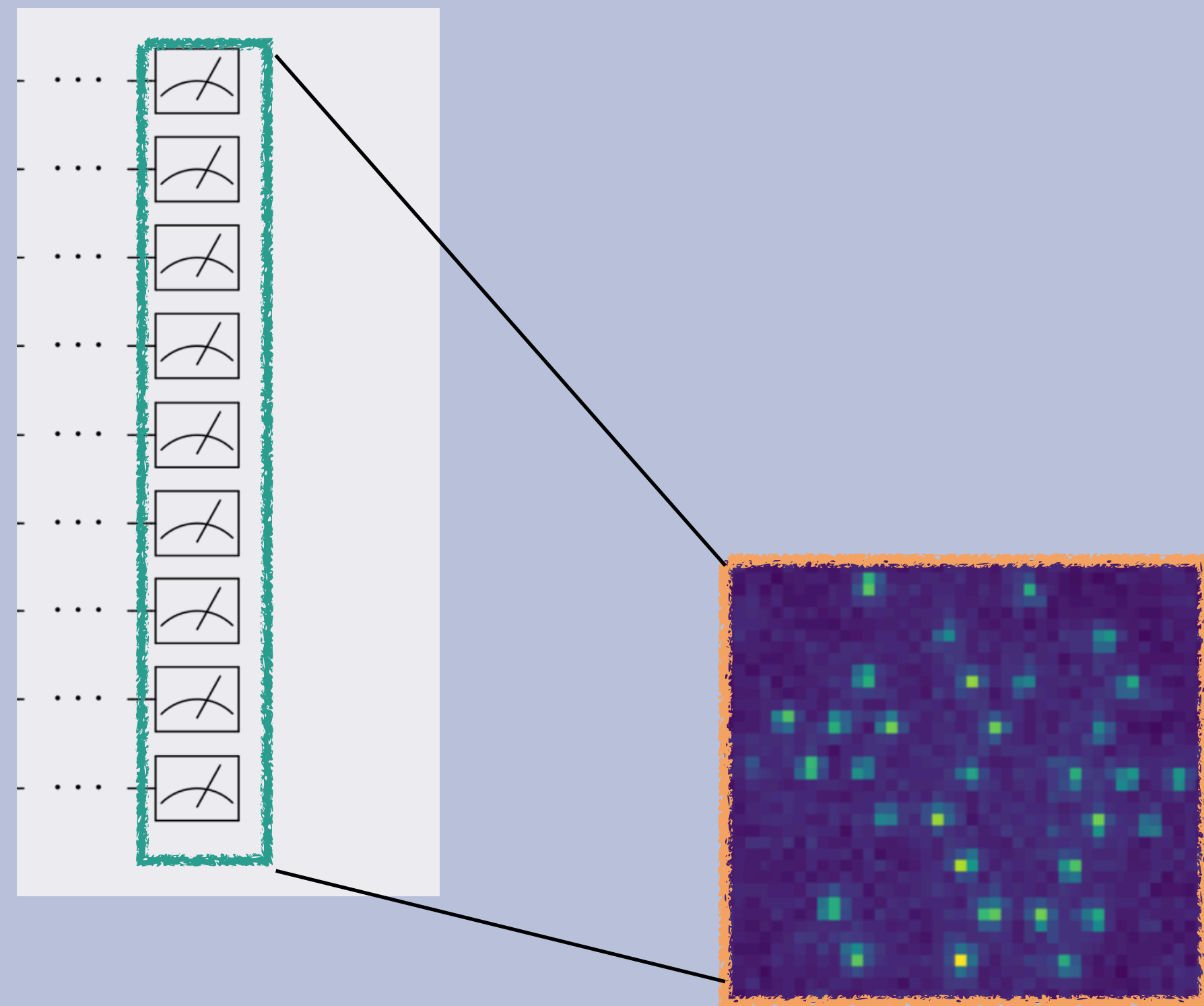


Apply gates



This is called  
DIGITAL MODE

The measurement problem is central in every type of QC because measuring means destroying a state.

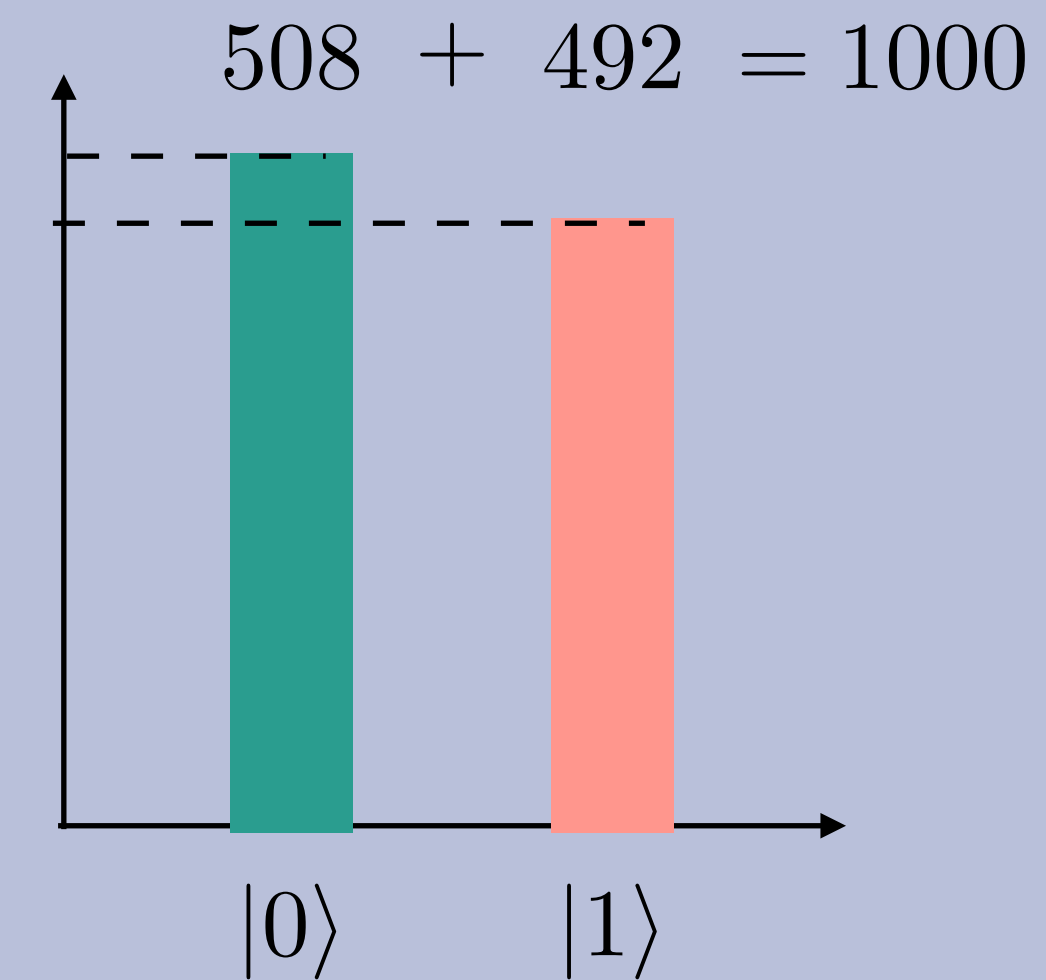


A camera flashes the qubits and erases the ones in  $|r\rangle$

## Example

$$|+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\left(\frac{\sqrt{2}}{2}\right)^2 = \frac{1}{2} = p_0 = p_1$$



## DIGITAL MODE

What can we do with digital?

Any algorithm, all of them.

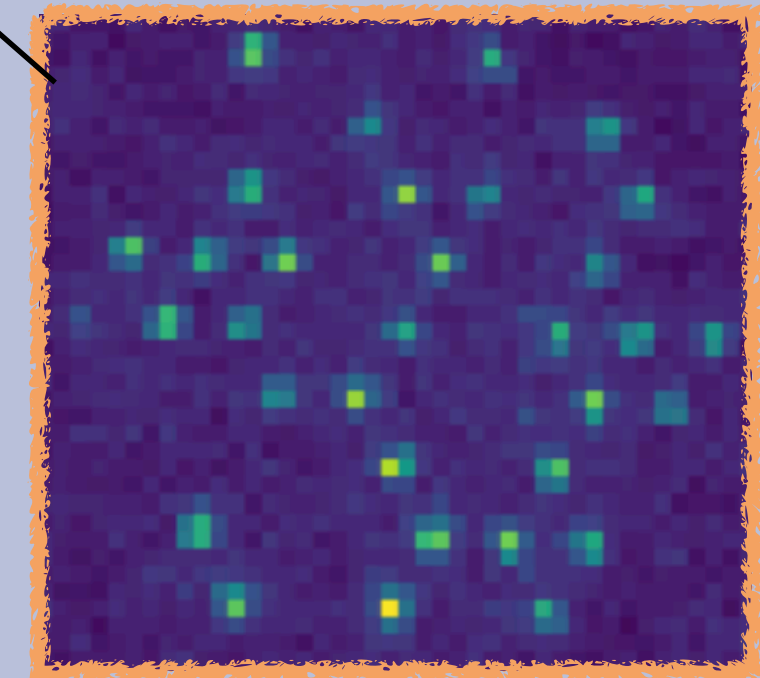
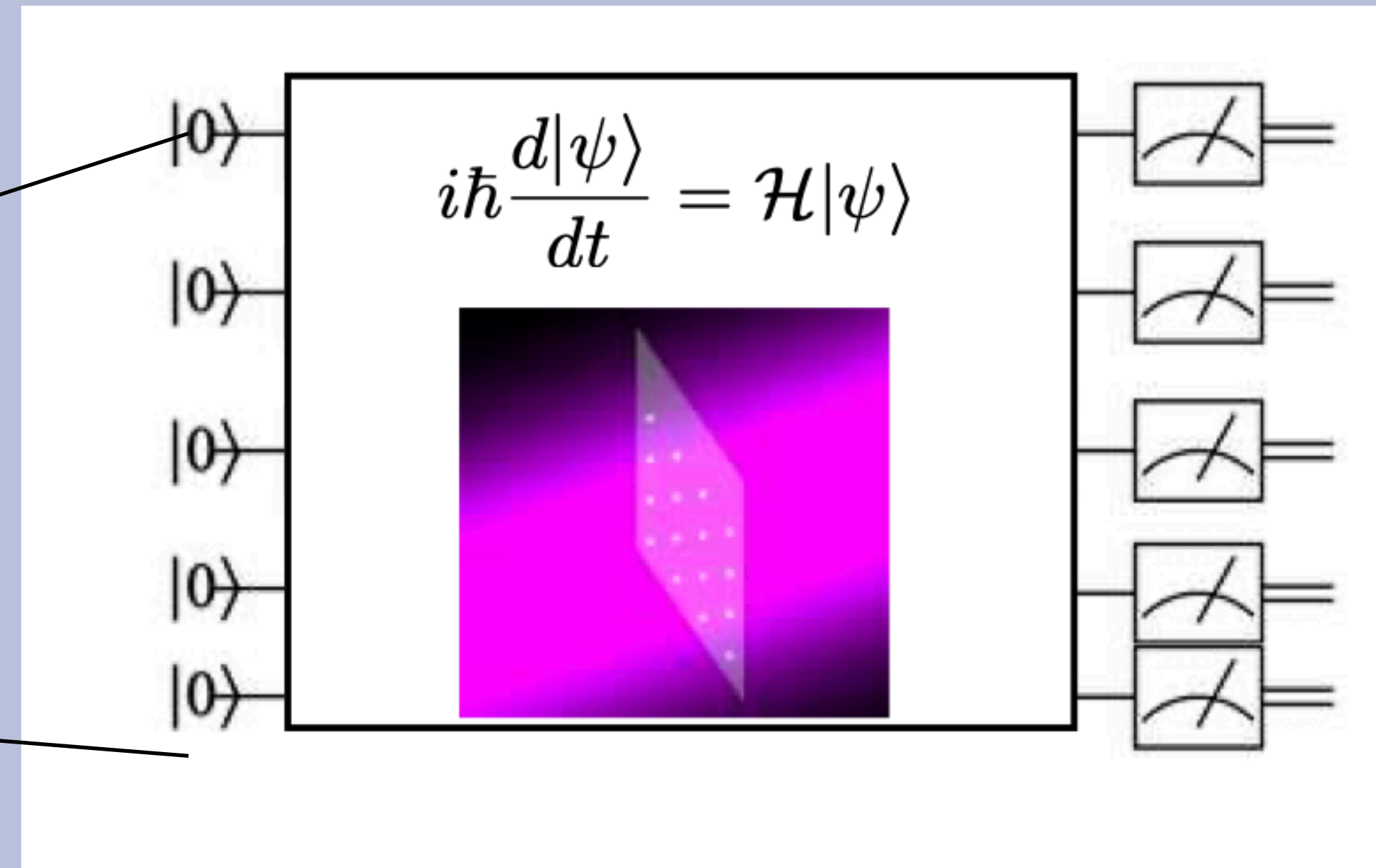
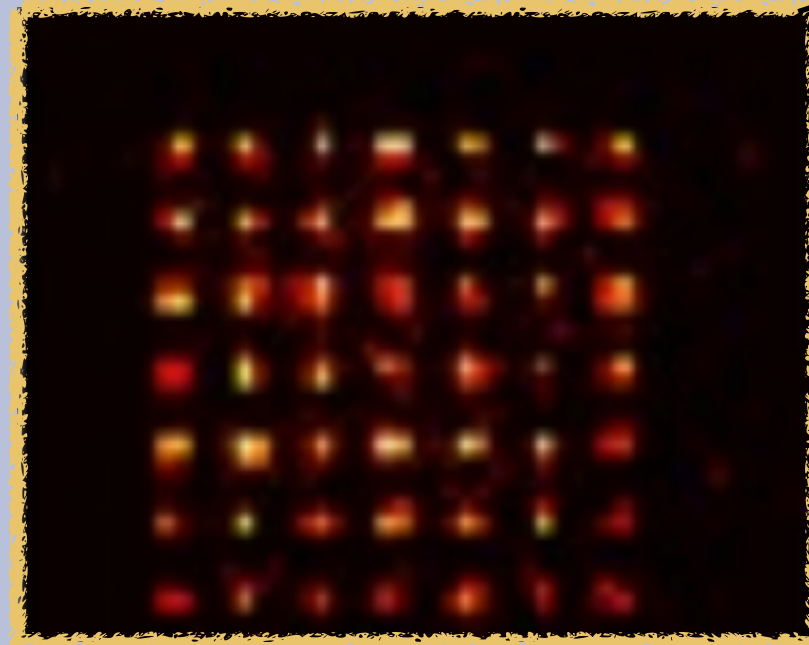
Ex: Shor, quantum neural networks ...

Why isn't everything digital?

It's difficult :(

# An “easier” approach: Analog Quantum Computation

Prepare a state



What can we do?

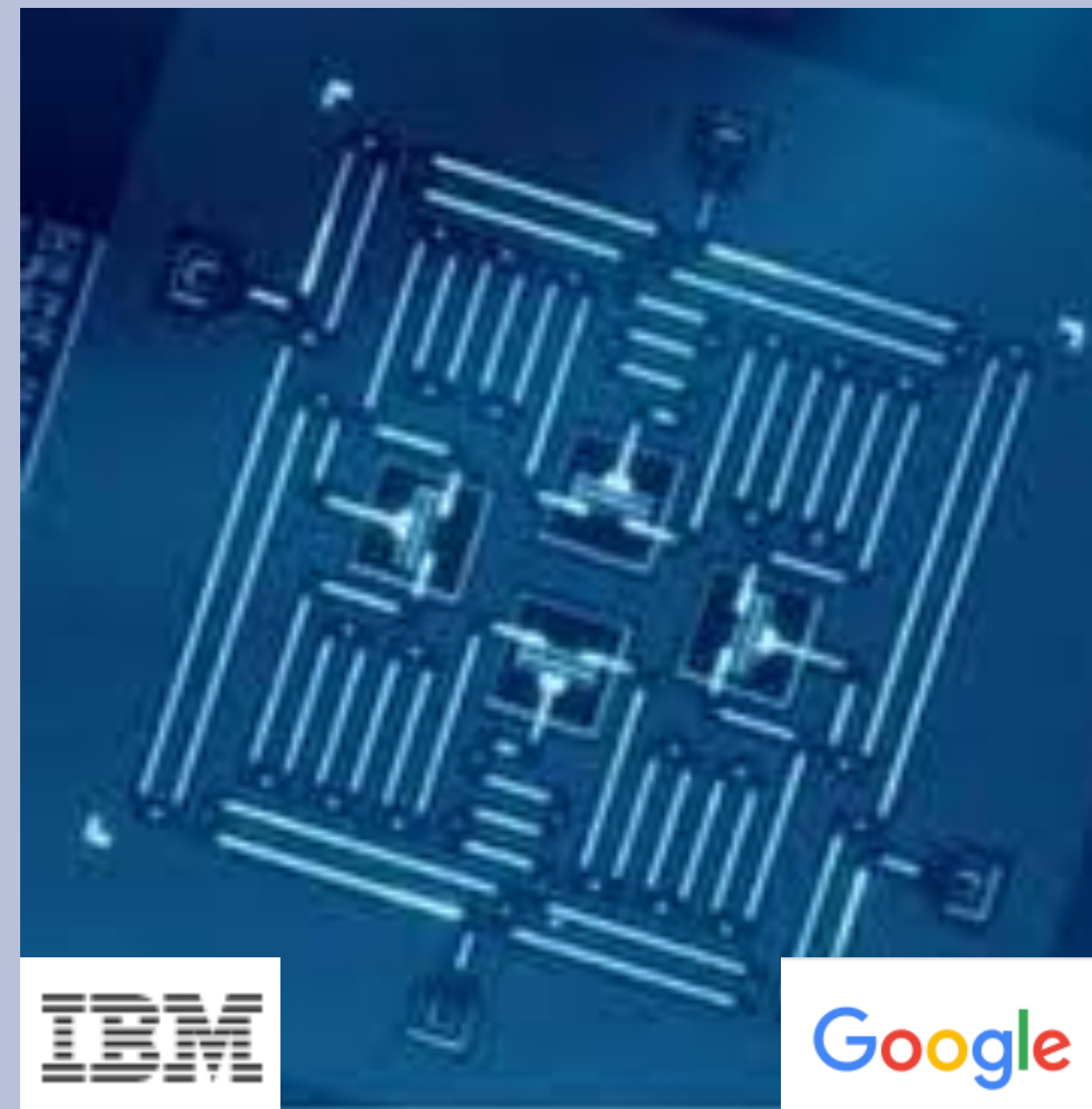
Almost every algorithm.

Are there other ways to create a QC?

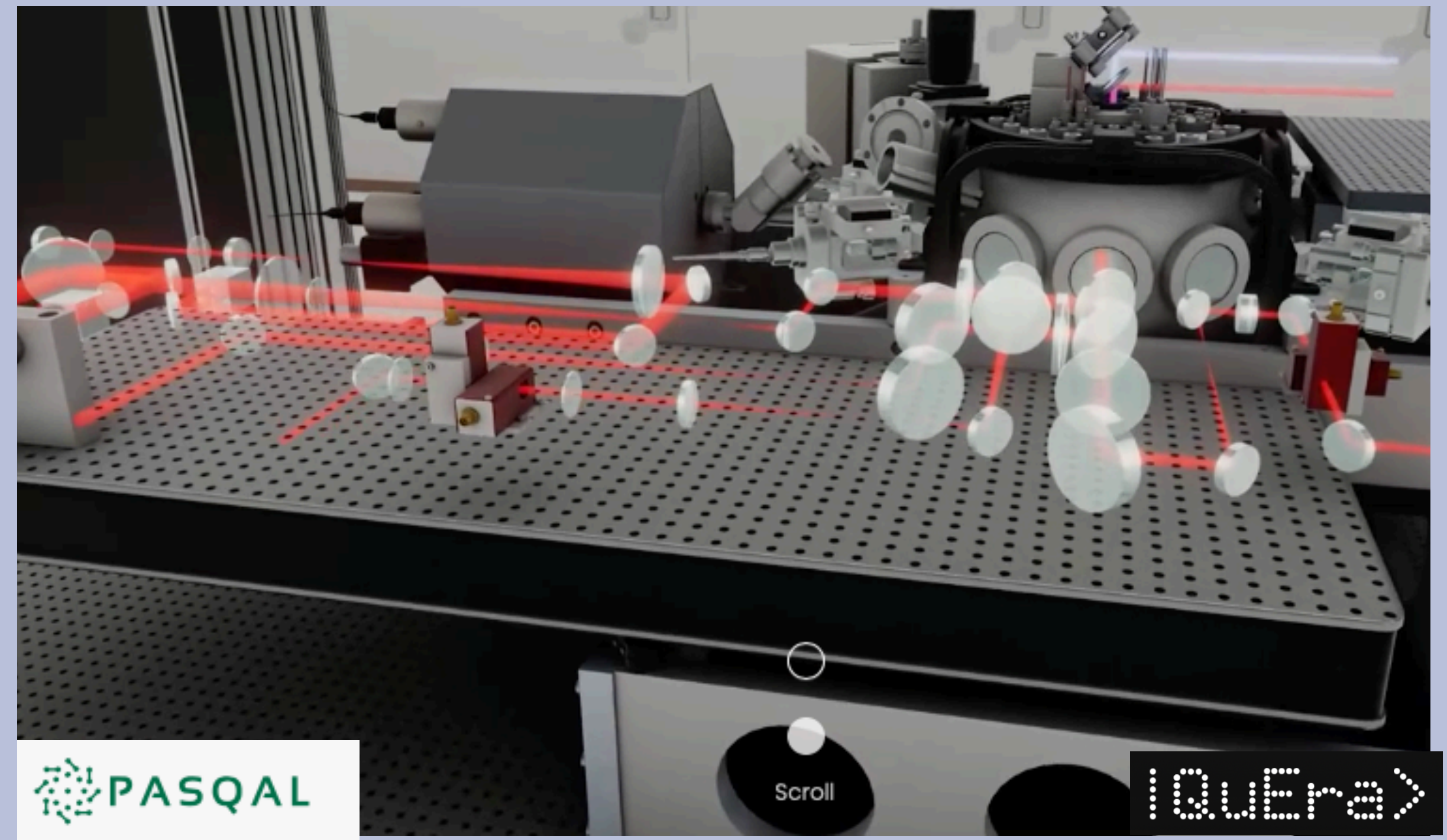
Yes, a few people are working on it



analog QC,  
superconducting  
technology



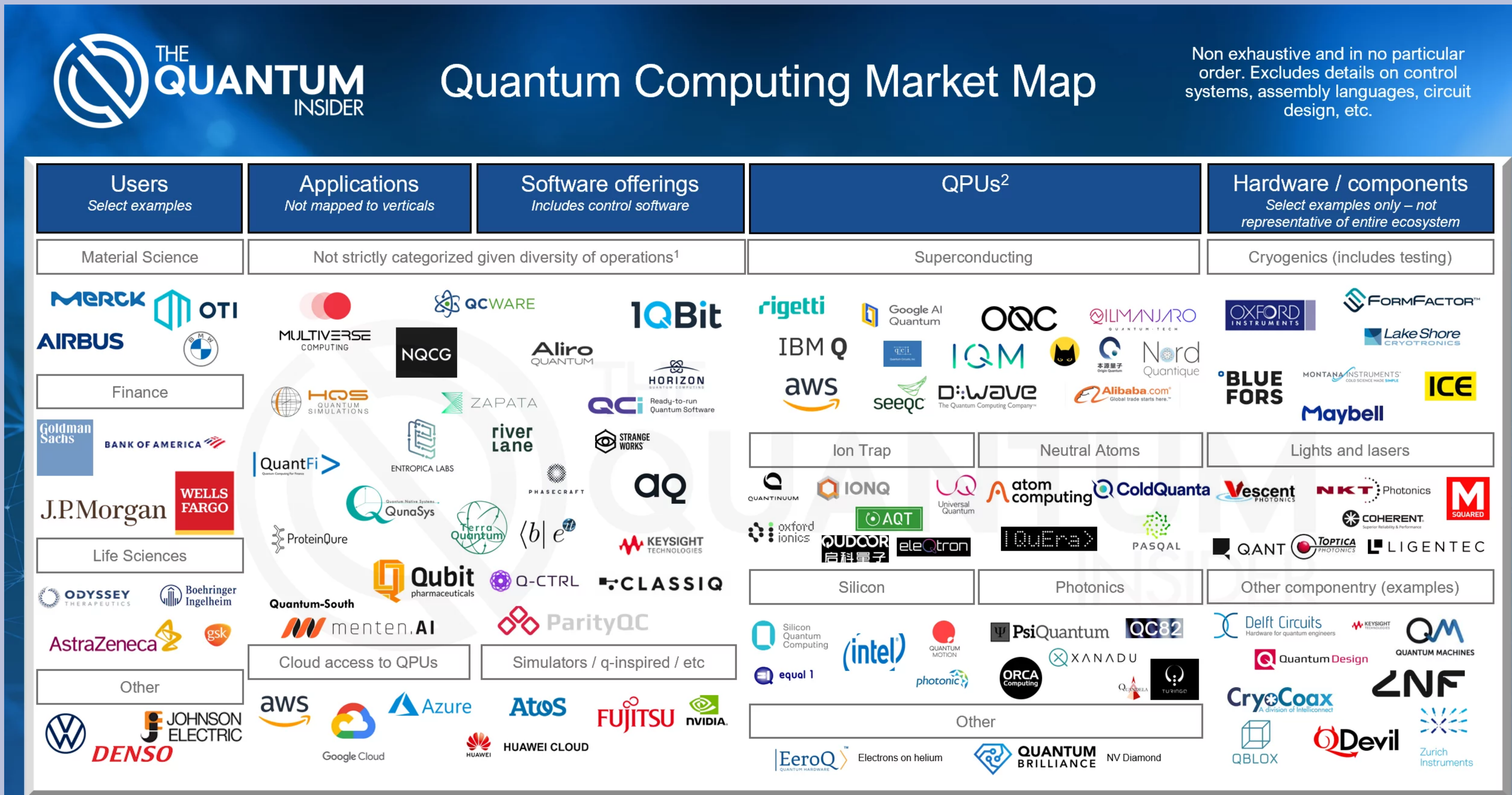
digital QC,  
superconducting  
technology



analogue/digital QC,  
Rydberg atom  
technology

# Are there other ways to create a QC?

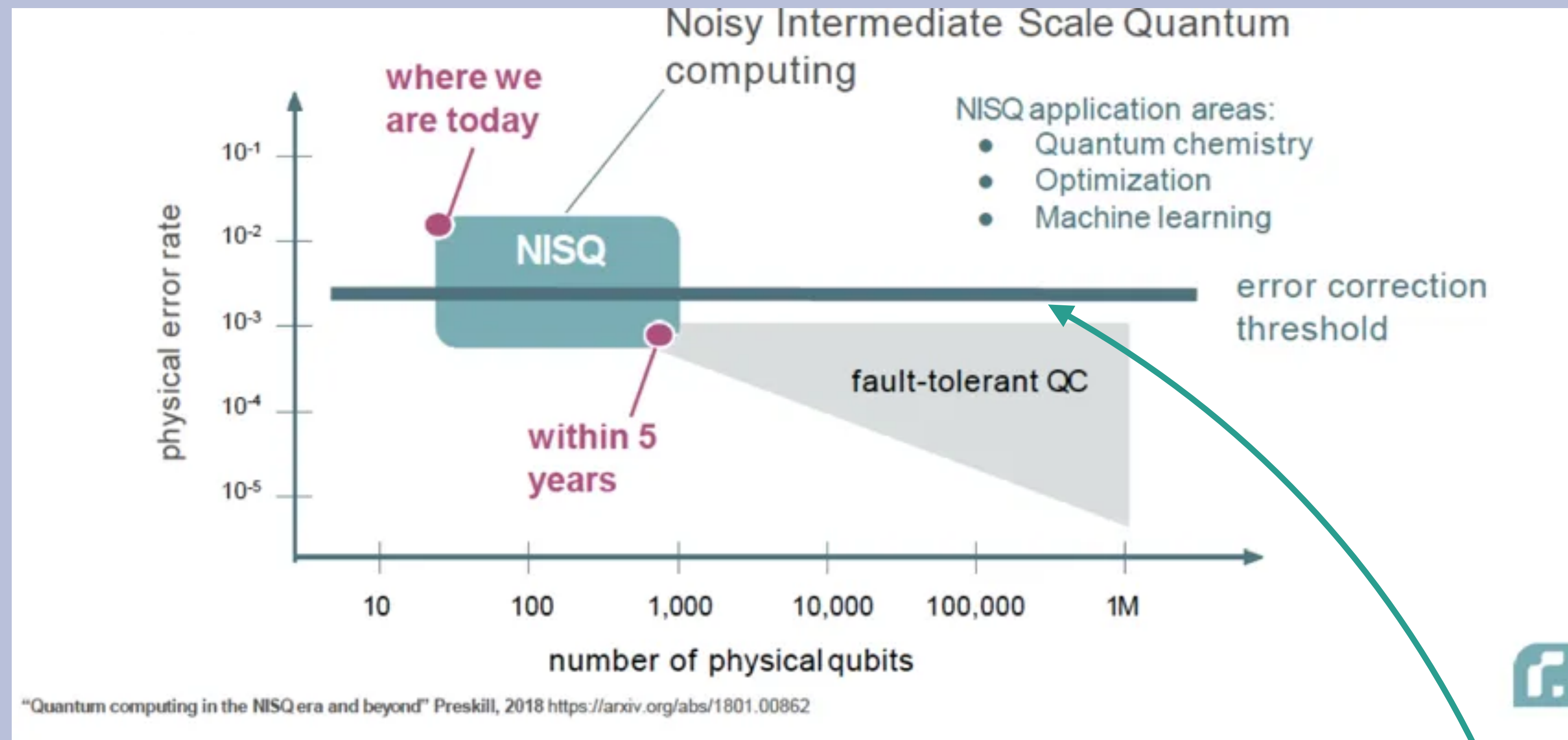
## Probably more than a few



<sup>1</sup> Software offerings can be further classified into SDKs, firmware / enablers, algorithms / applications, simulators etc. but many companies are offering a mixture across the stack  
<sup>2</sup> Many QPU providers are offering full stack services (e.g. Pasqal acquired Qu&Co, Quantinuum was originally CQC prior to merger with HQS, etc.)

Is any technology better than other?

Two main ways to tell: no. of qubits and noise



Each company/university/research center has a roadmap (path) inside this graph over time



Lets run an algorithm

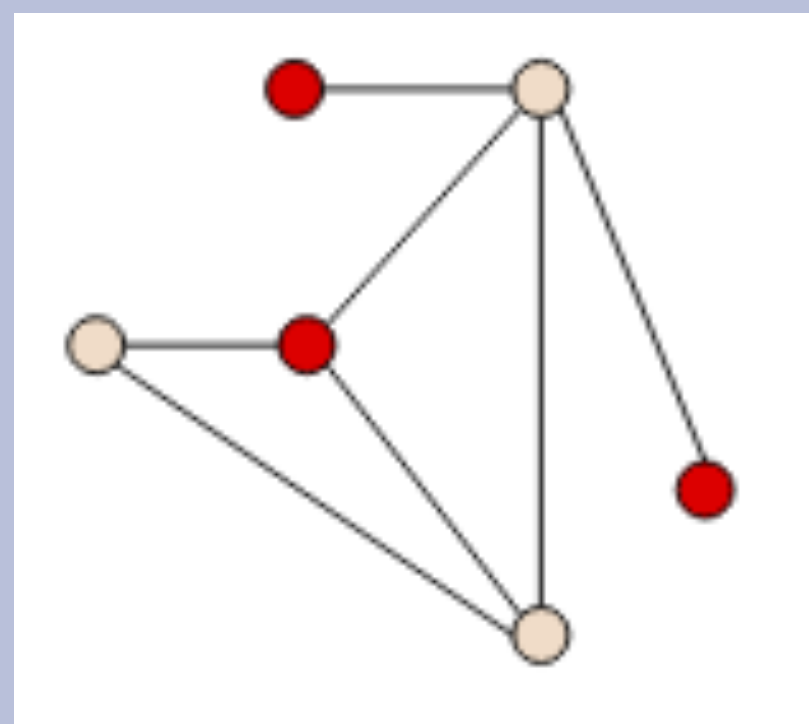
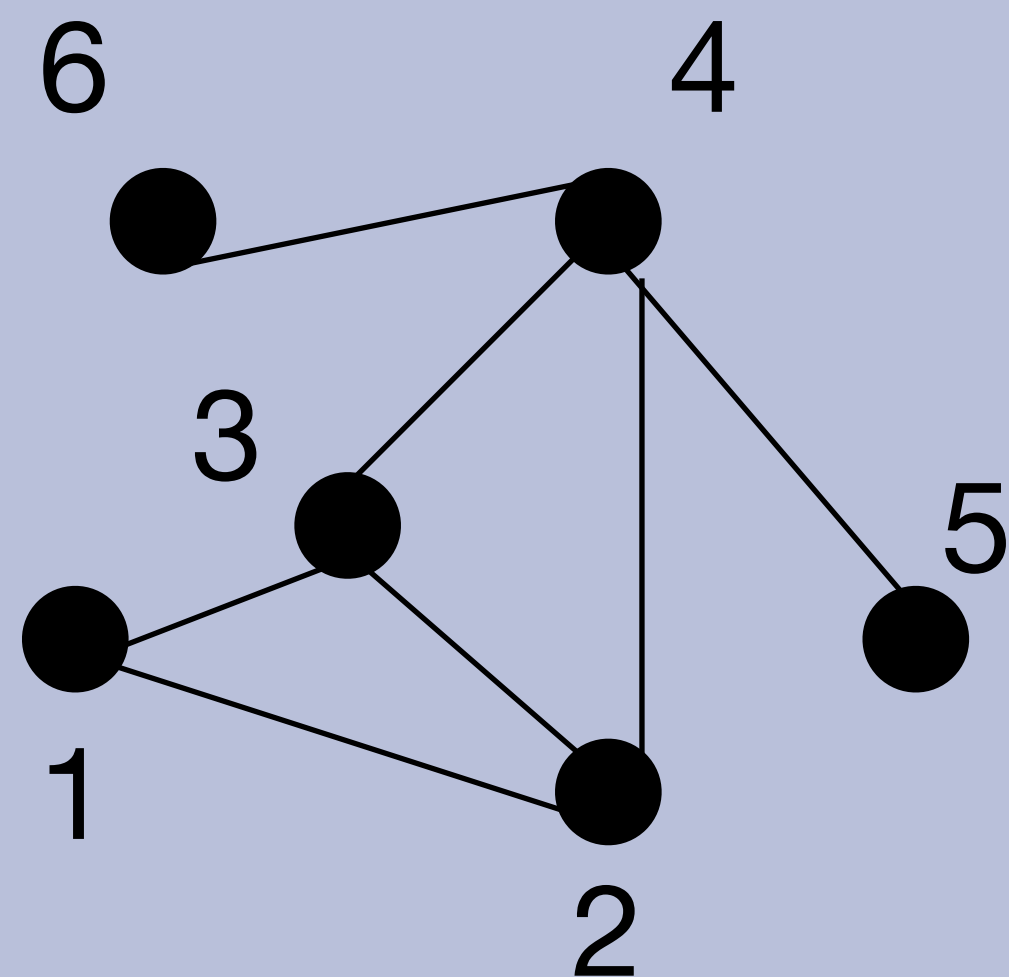
Pick an architecture: neutral atoms

Pick a method: analog, no choice

Pick a classical problem: combinatorial

Pick an algorithm: variational quantum circuit

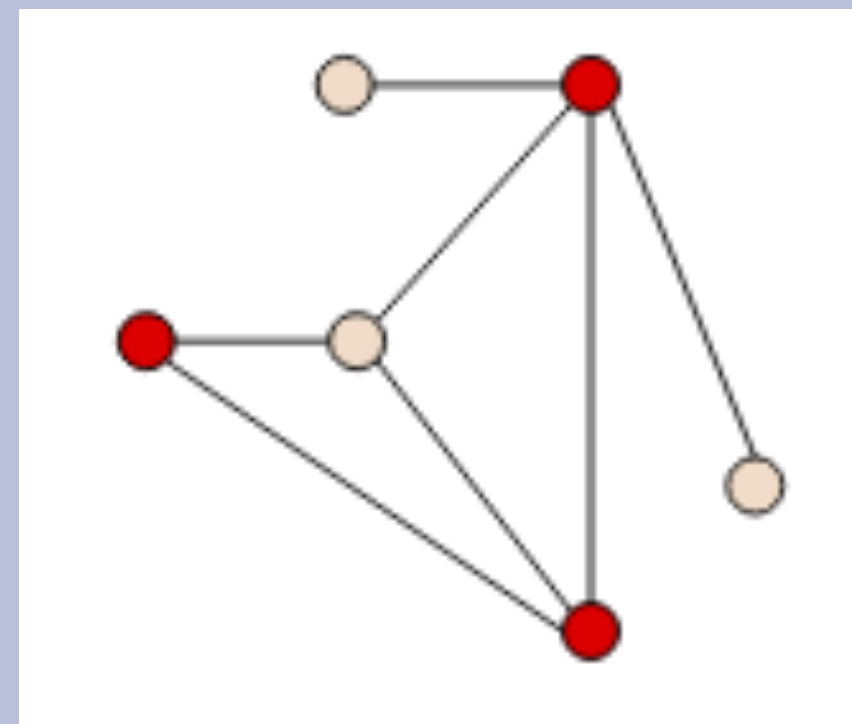
# THE MIS problem



001011

Is a solution

$$E = -3$$



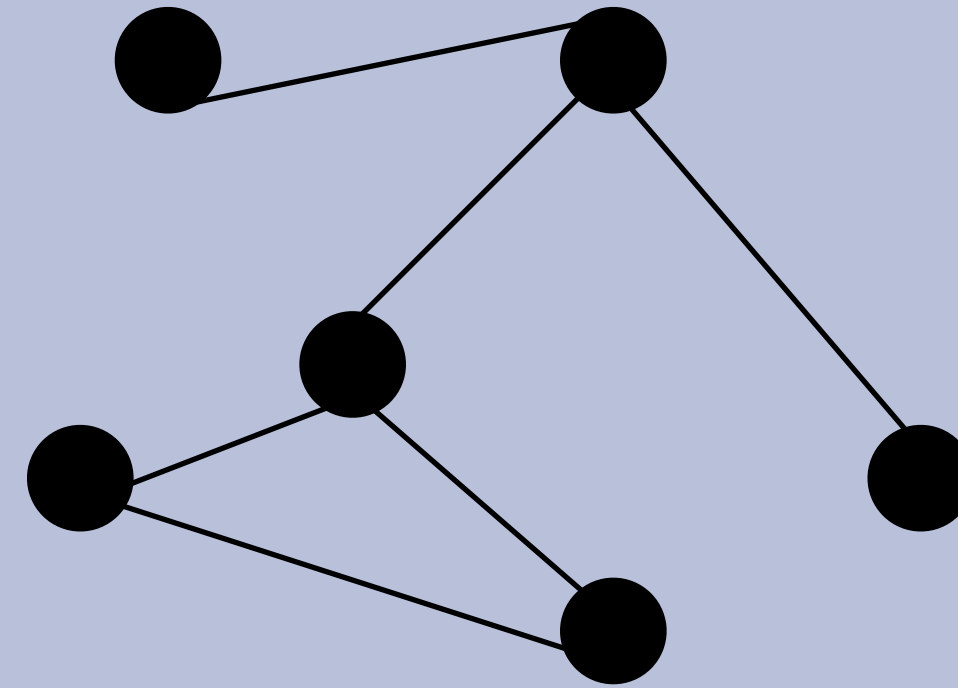
110100

It's not a solution

$$E = -3 + 2 = -1$$

$$E = -\sum_i x_i + \sum_{i,j} x_i x_j$$

# Why MIS?



First: Ubiquitous

Second: Ising encoding

$$E = - \sum_{i \in G} x_i + \sum_{(i,j) \in E} x_i x_j$$

$x_i \in \{0, 1\}$

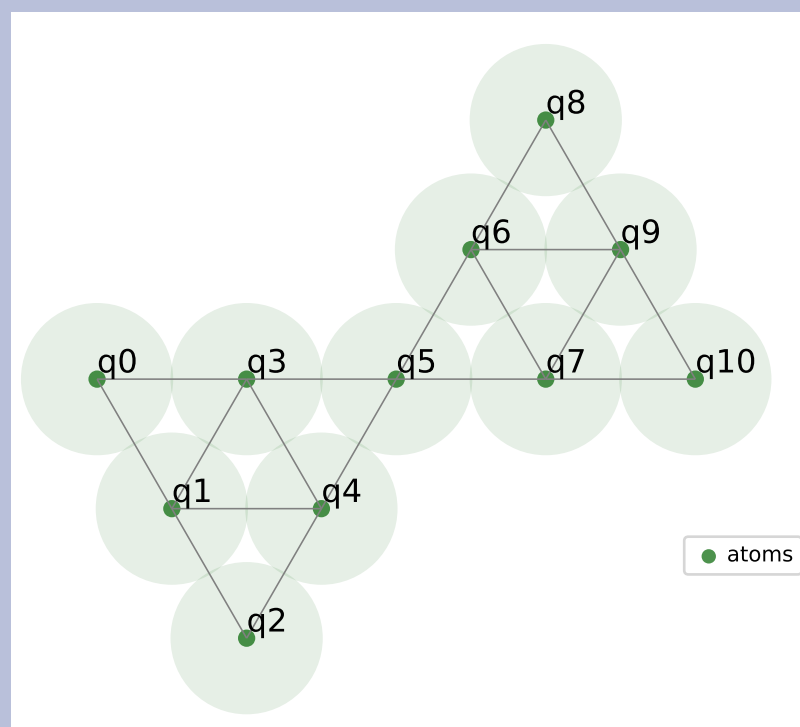


$$H = \sum_{i \in G} Z_i + \sum_{(i,j) \in E} (1 - Z_i)(1 - Z_j)$$

$$Z_i |1\rangle = -1 |1\rangle$$

$$Z_i |0\rangle = +1 |0\rangle$$

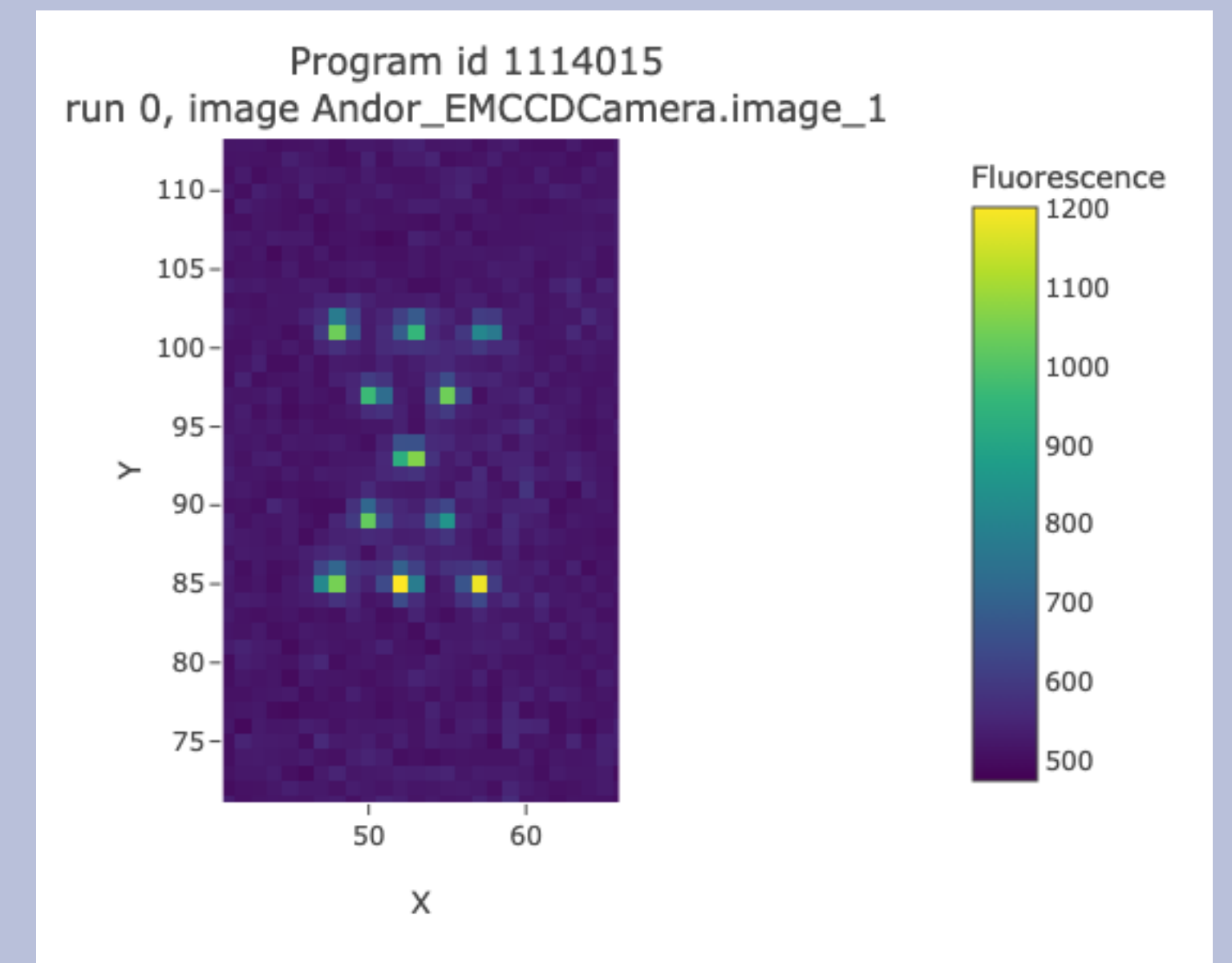
Third: spatial dependency



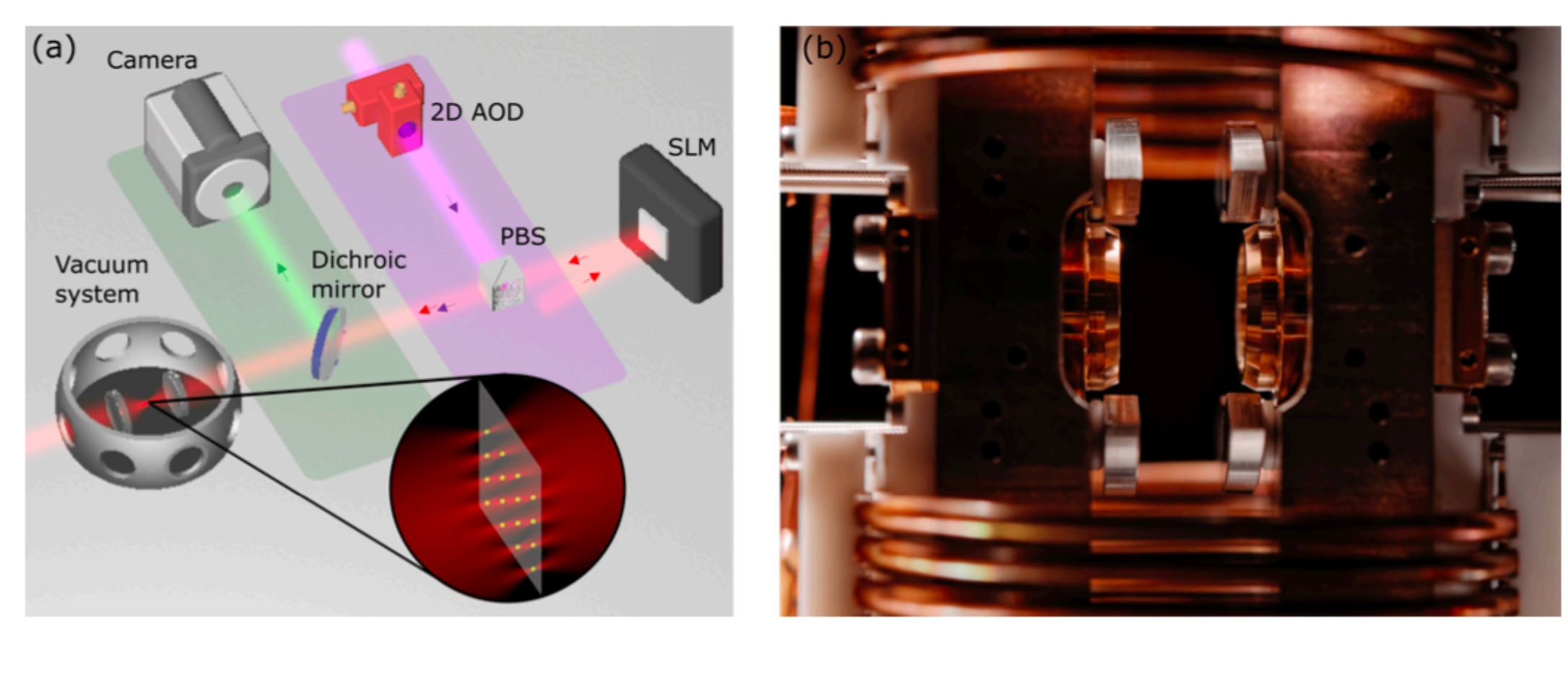
Equivalence between graph problem



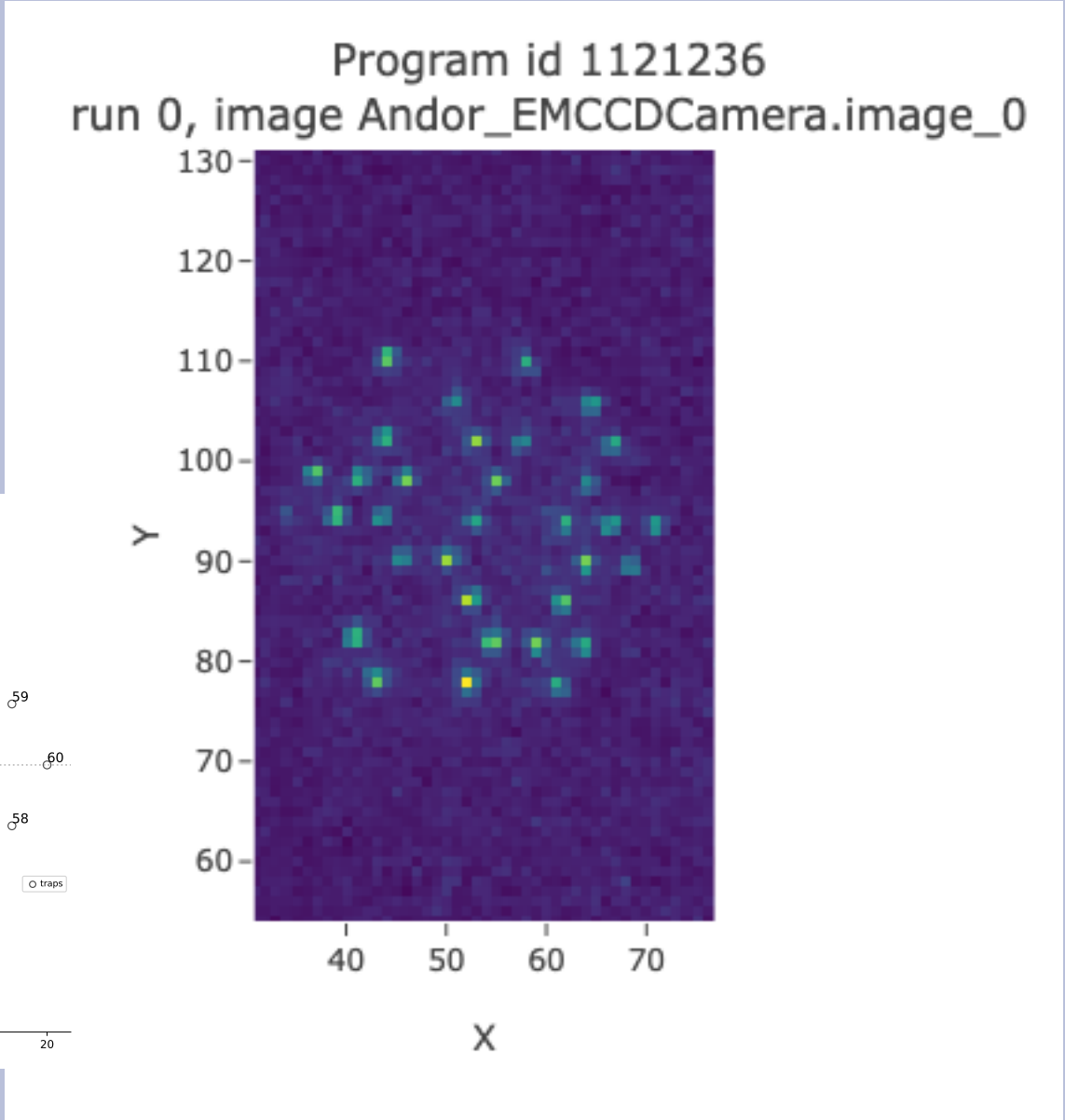
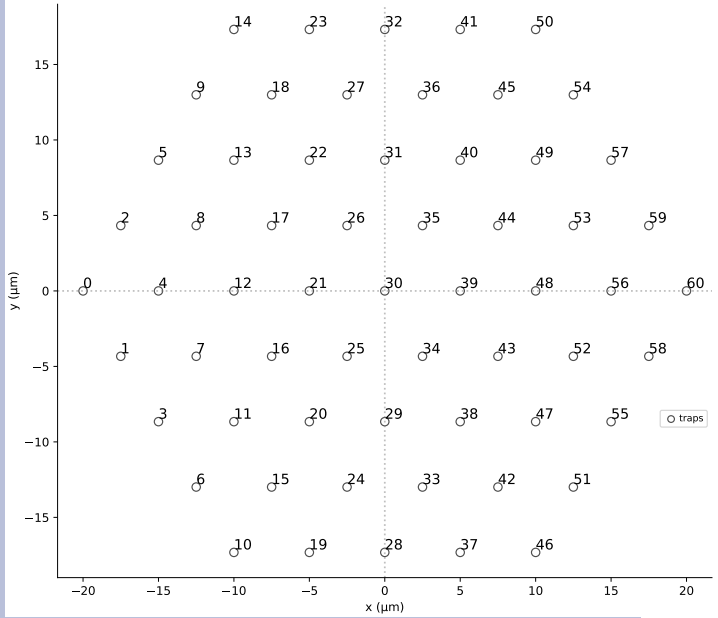
and atoms positions



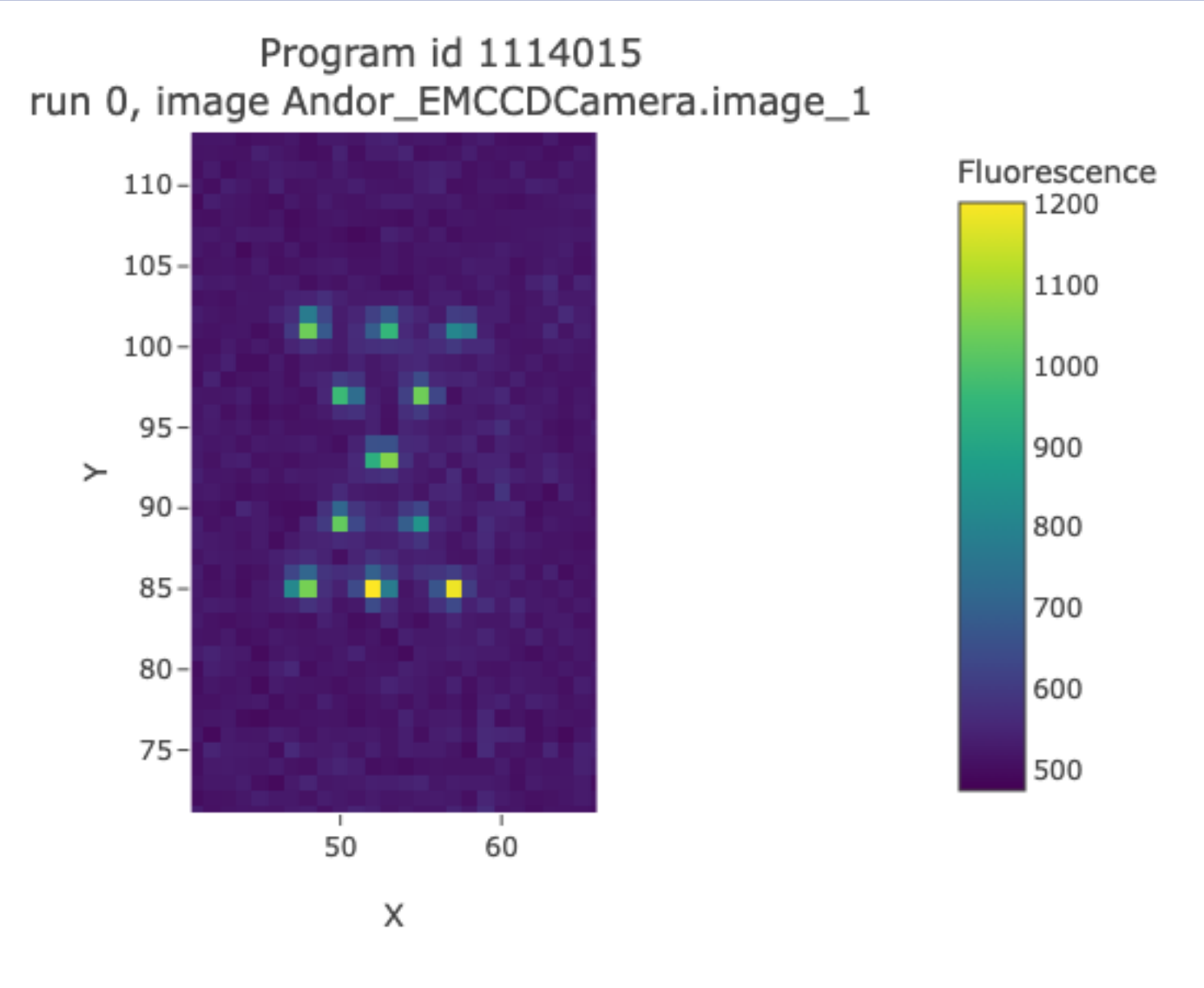
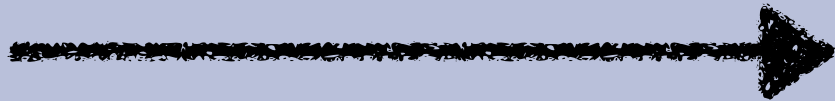
# HOW TO RUN AN ANALOG ALGORITHM: 1. Load the graph



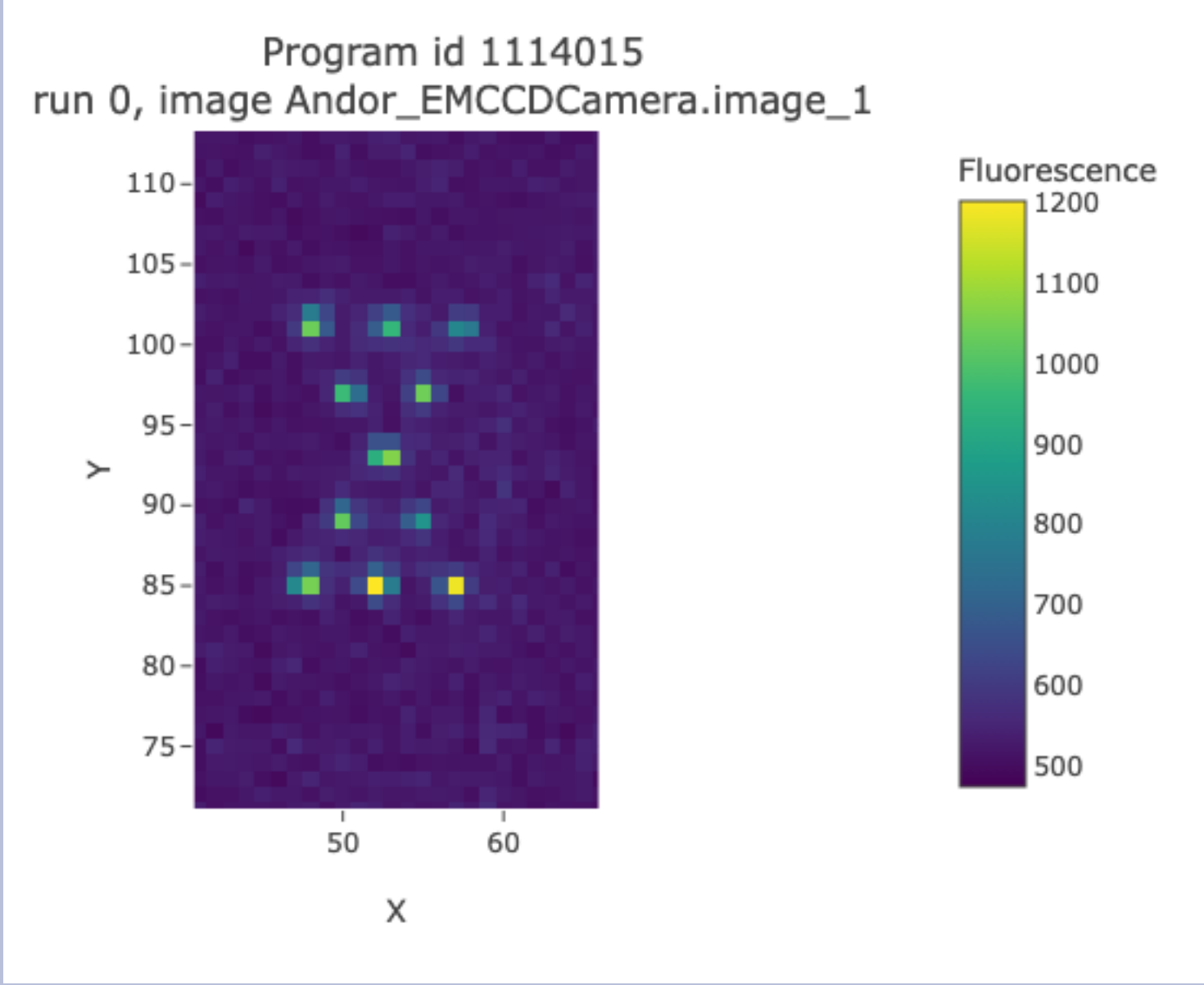
First:  
load randomly



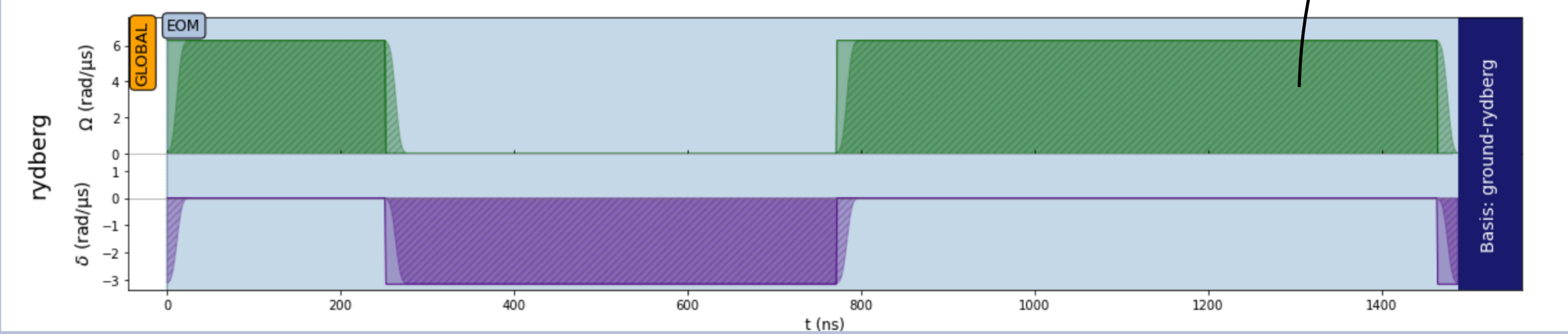
Then, readjust



# HOW TO RUN AN ANALOG ALGORITHM: 2. Apply pulses for random times



This durations are initially random



Applies phase according to the energy of the problem

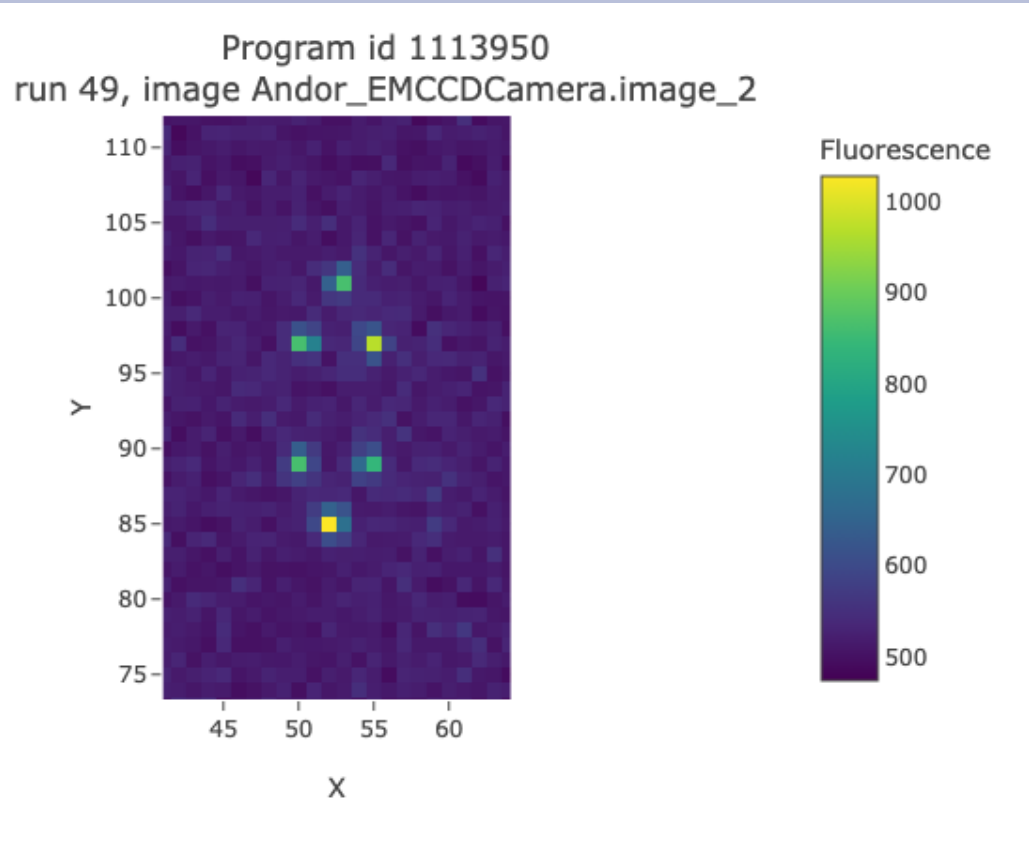
Rotates qubits from  $|0\rangle$  to  $|1\rangle$

$$H_M = \Omega(t) \sum_i \sigma_i^x$$

$$H_C = -\delta(t) \sum_i n_i + U_{i,j} \sum_{(i,j) \in E} n_i n_j$$

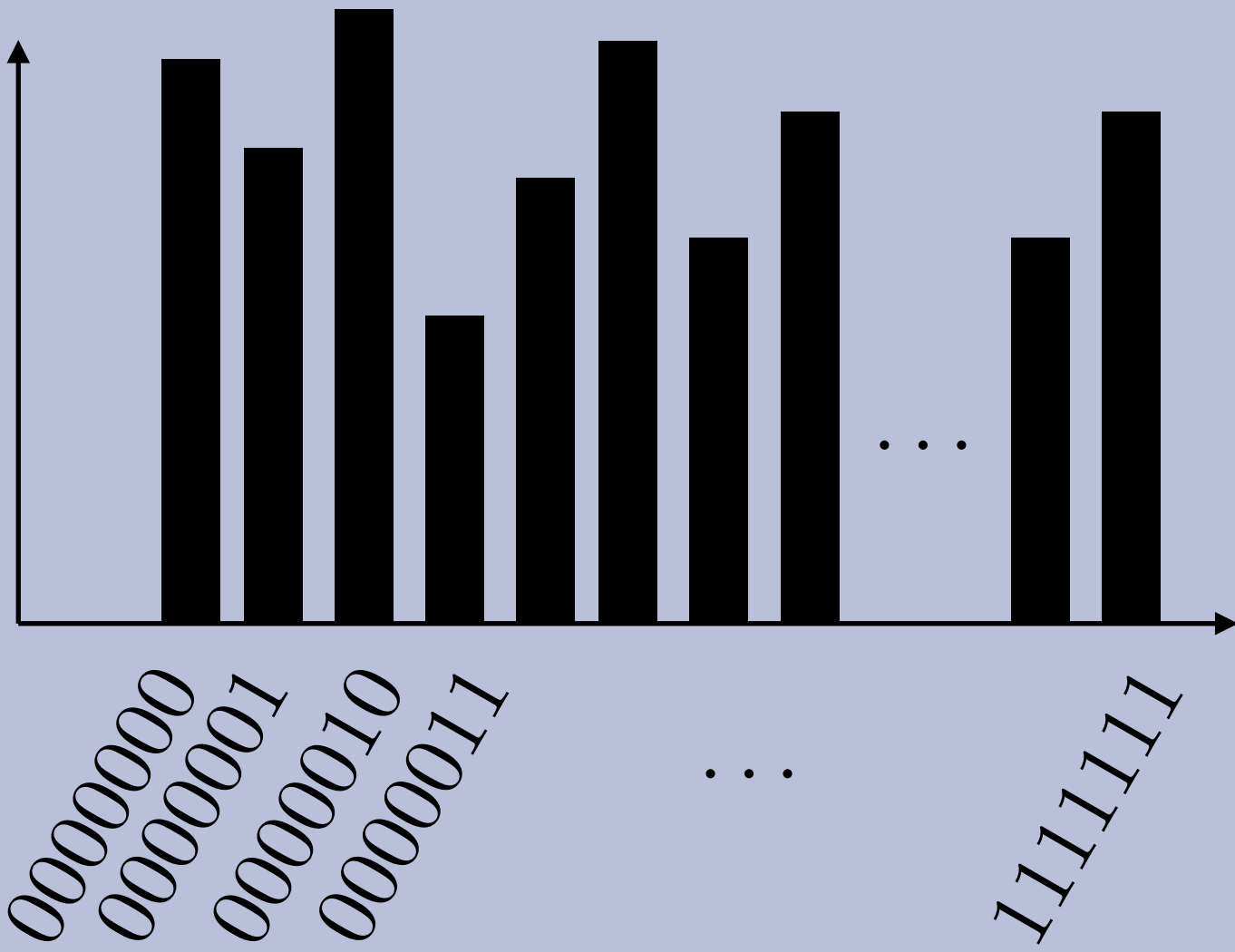
# HOW TO RUN AN ANALOG ALGORITHM: 3. Measure and repeat

We measure, obtain a bitstring, repeat N times

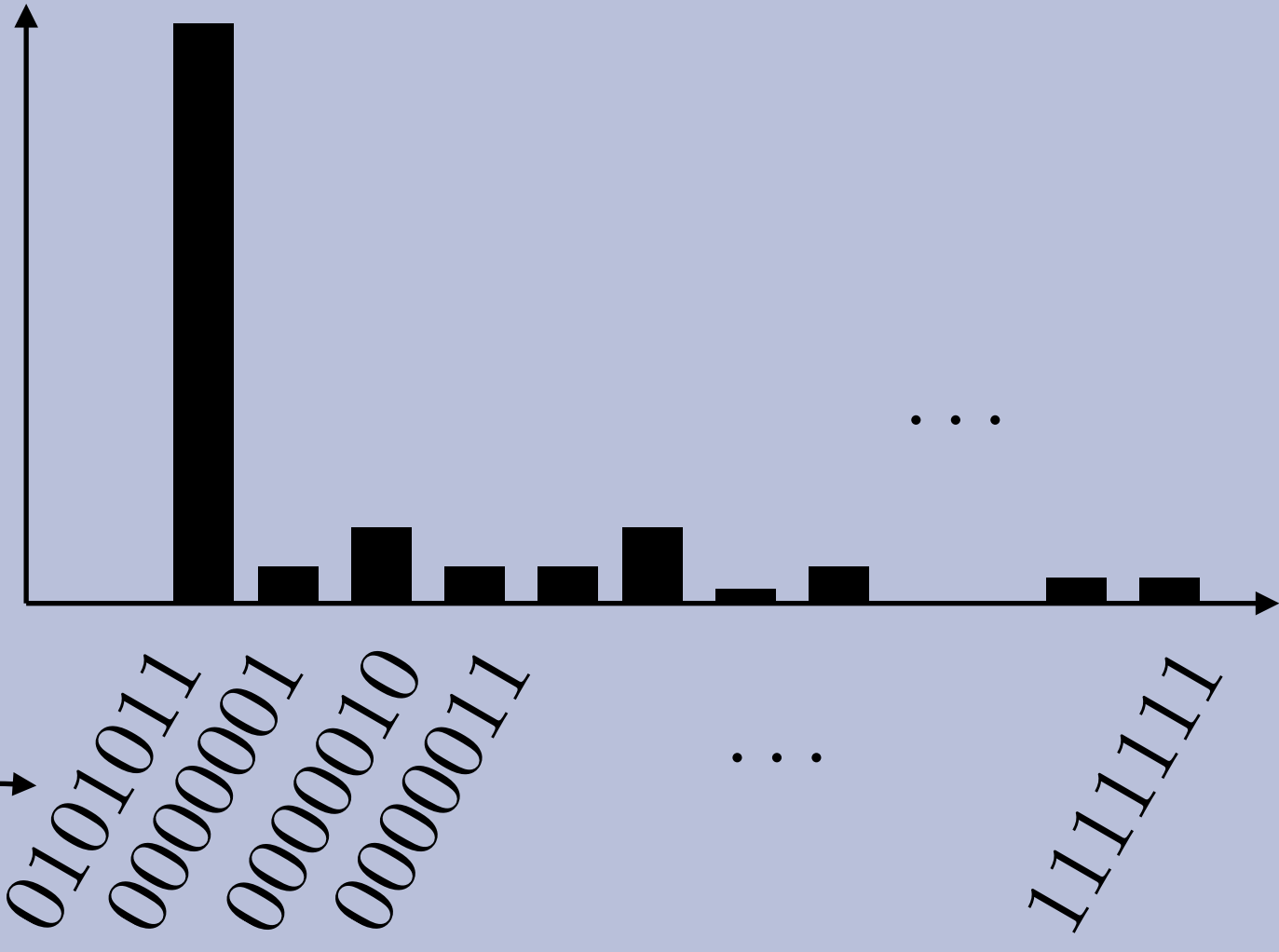


An example of a measured solution

How do we go from

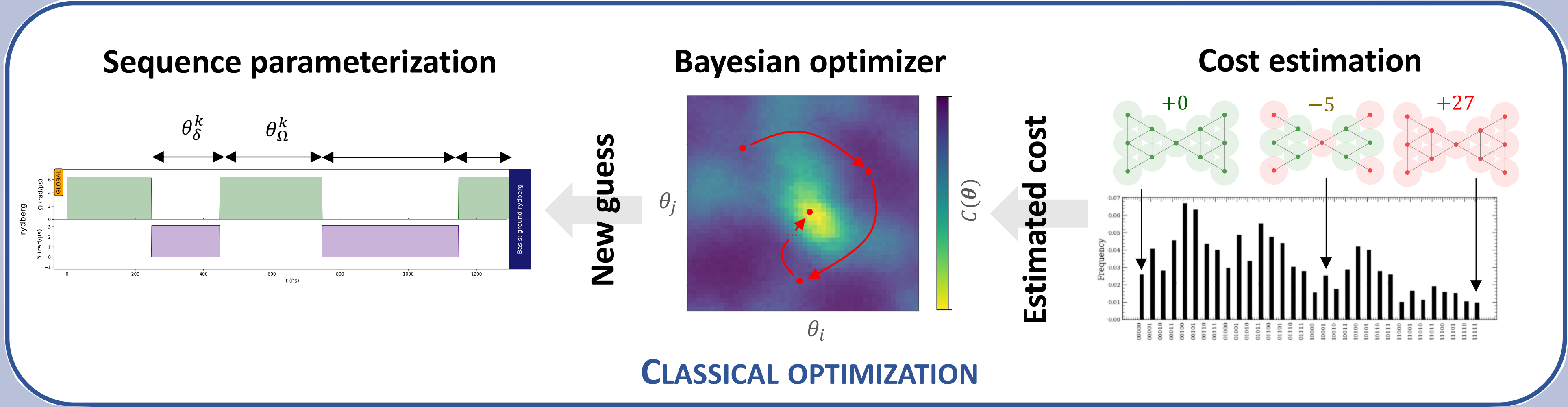
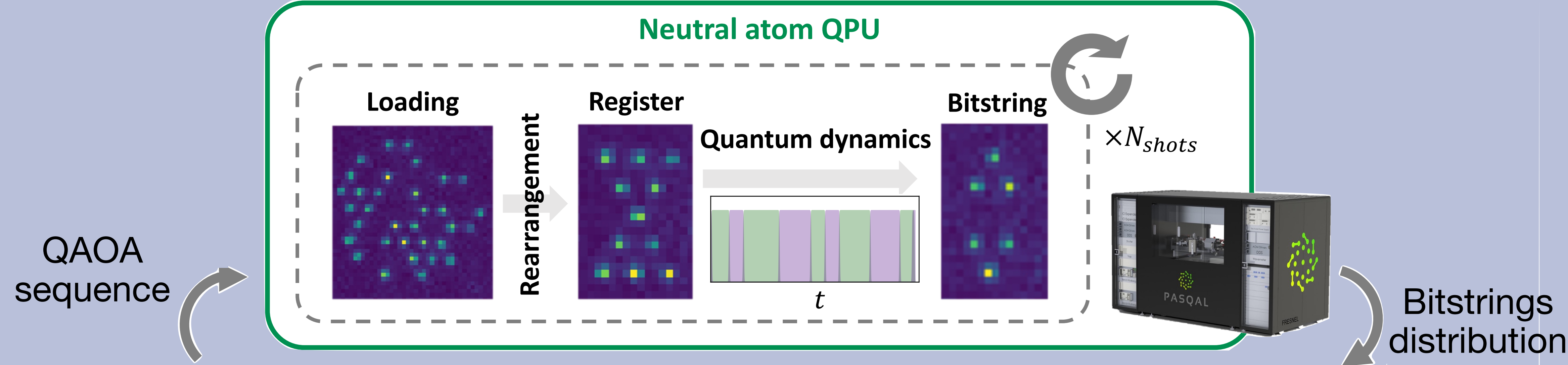


→



Solution

# How do we solve it: QAOA



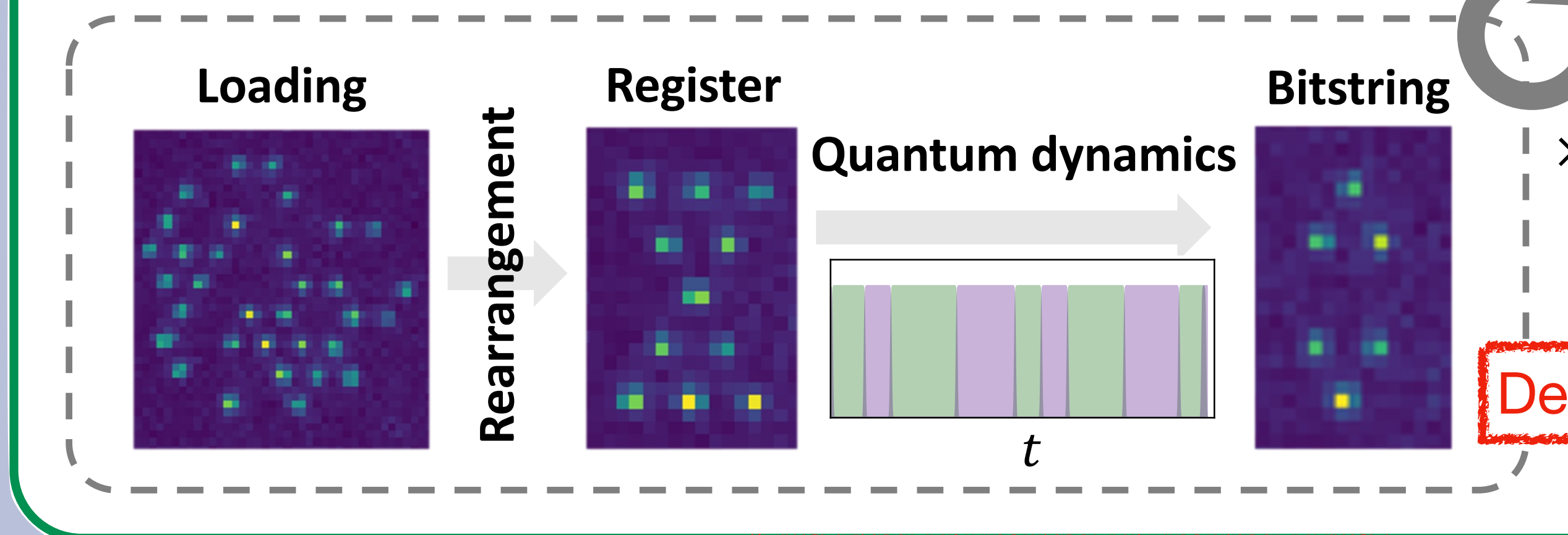
# How do we solve it: QAOA

Rearrangement takes 95% of computation time

Dynamic errors:  
Doppler shift  
waist/amplitude fluctuations  
rephrasing  
depolarisation

Measurement errors  
5~8% false positive  
8~10% false negative

Loading has 50% succes rate per atom



Low repetition rate  
~1 Hz (very bad!!)

Descrutive measurement!

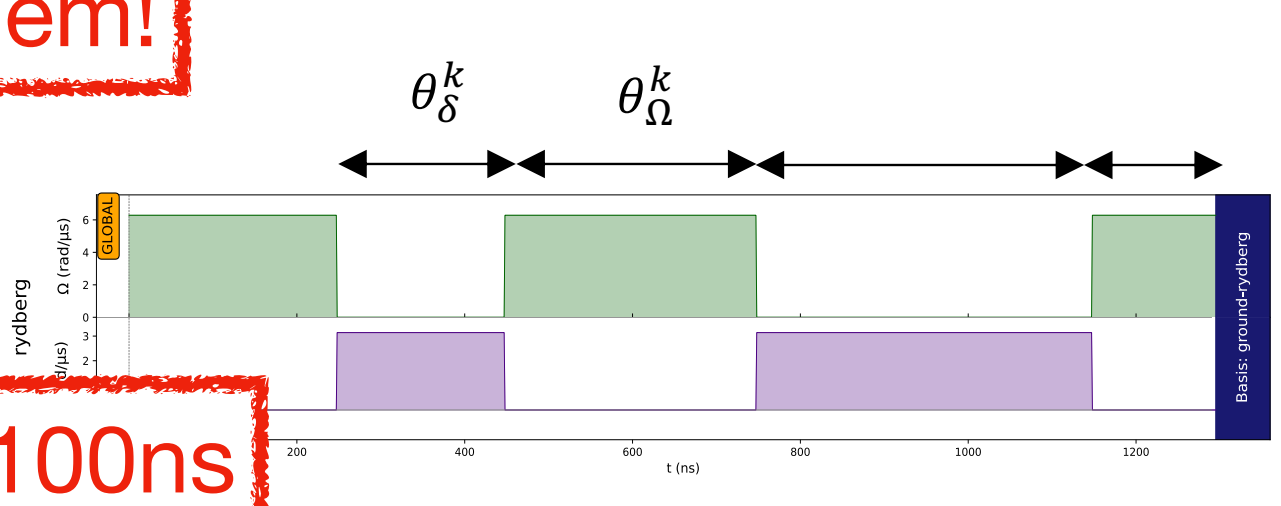


Bitstrings distribution

Optimizer needs to converge in a few steps

## Sequence parameterization

Ramp Problem!



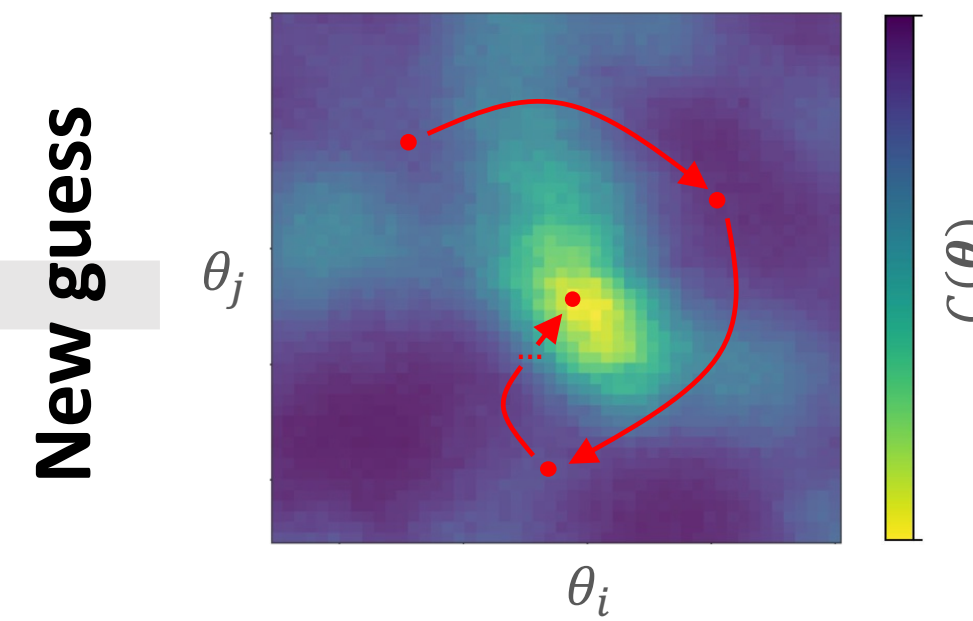
Min duration 100ns

Error on durations!

Square signal approximation

Decoherence time!  
Max duration 5000ns

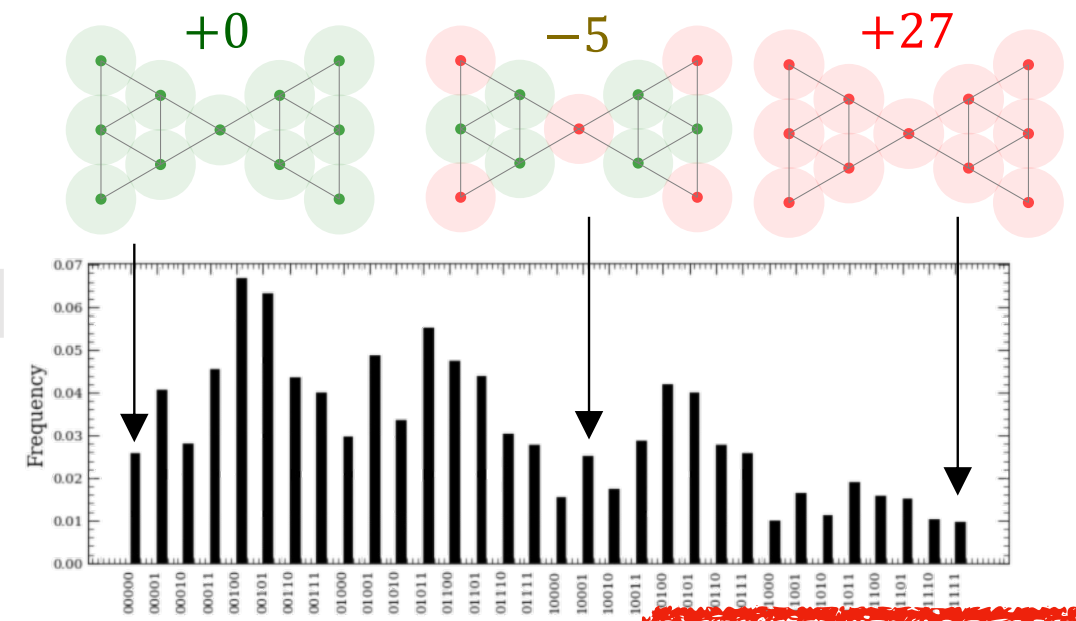
## Bayesian optimizer



## CLASSICAL OPTIMIZATION

Can't exploit the gradient

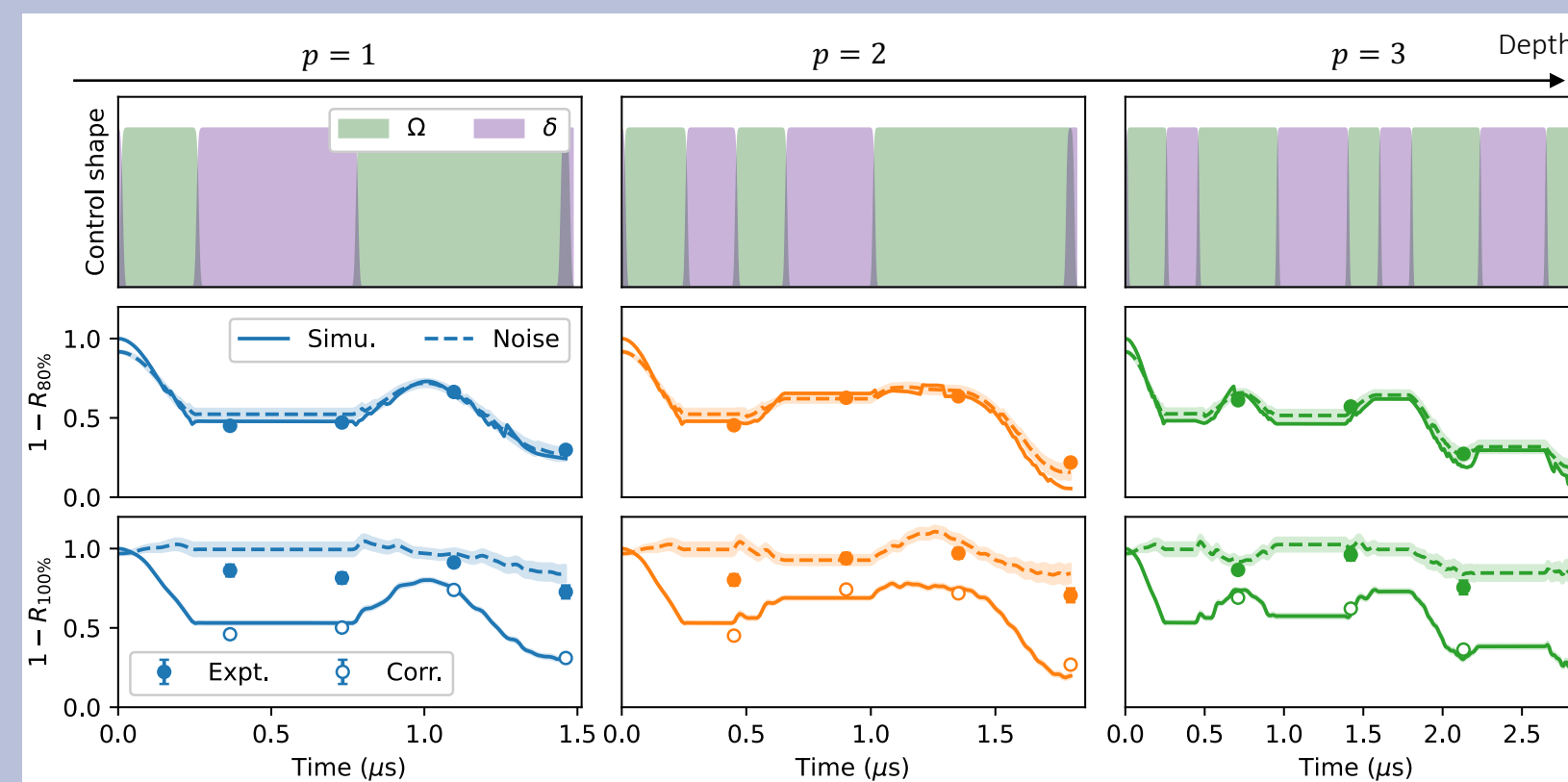
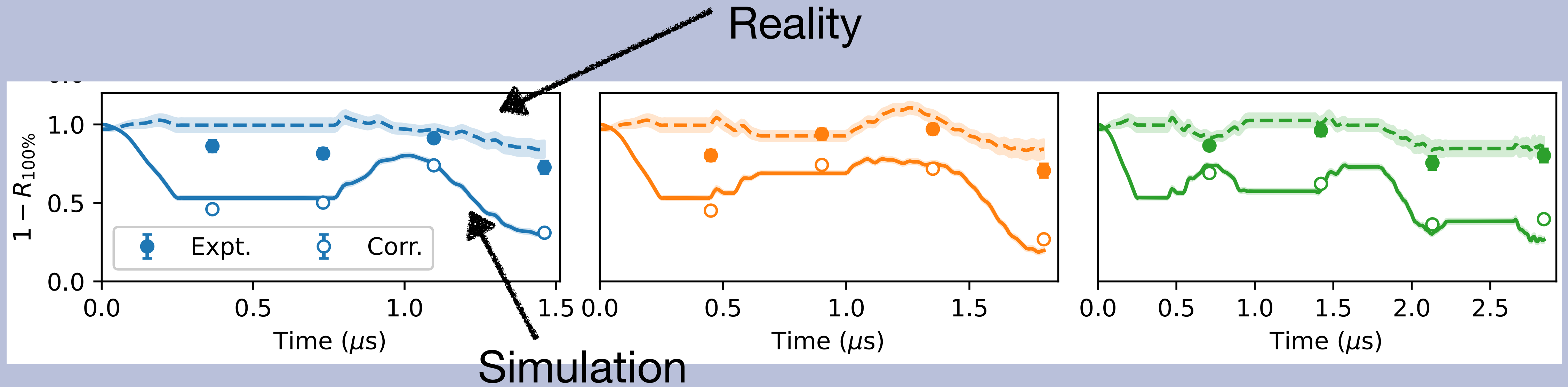
## Cost estimation



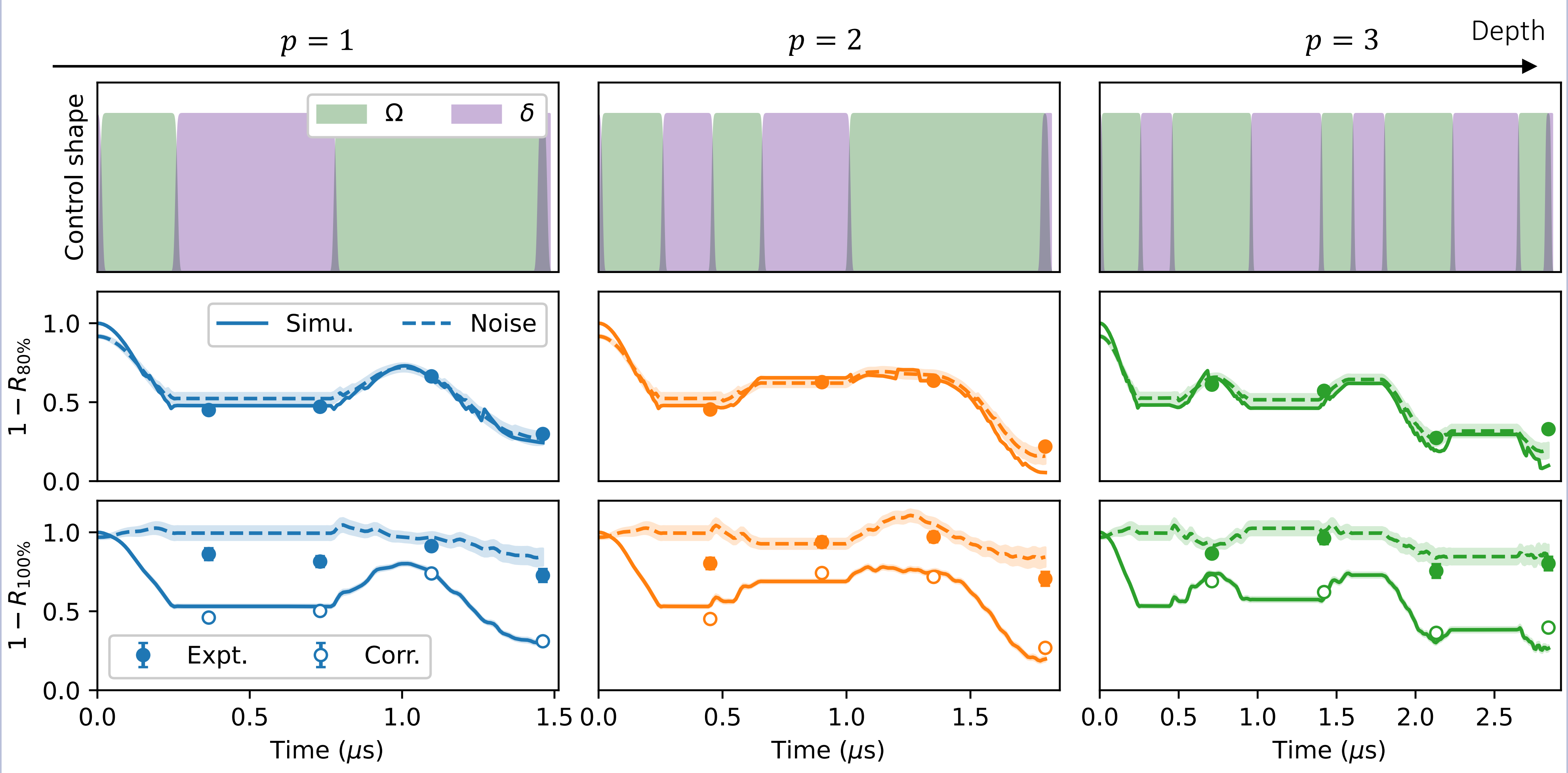
Very noisy and imprecise energy estimate



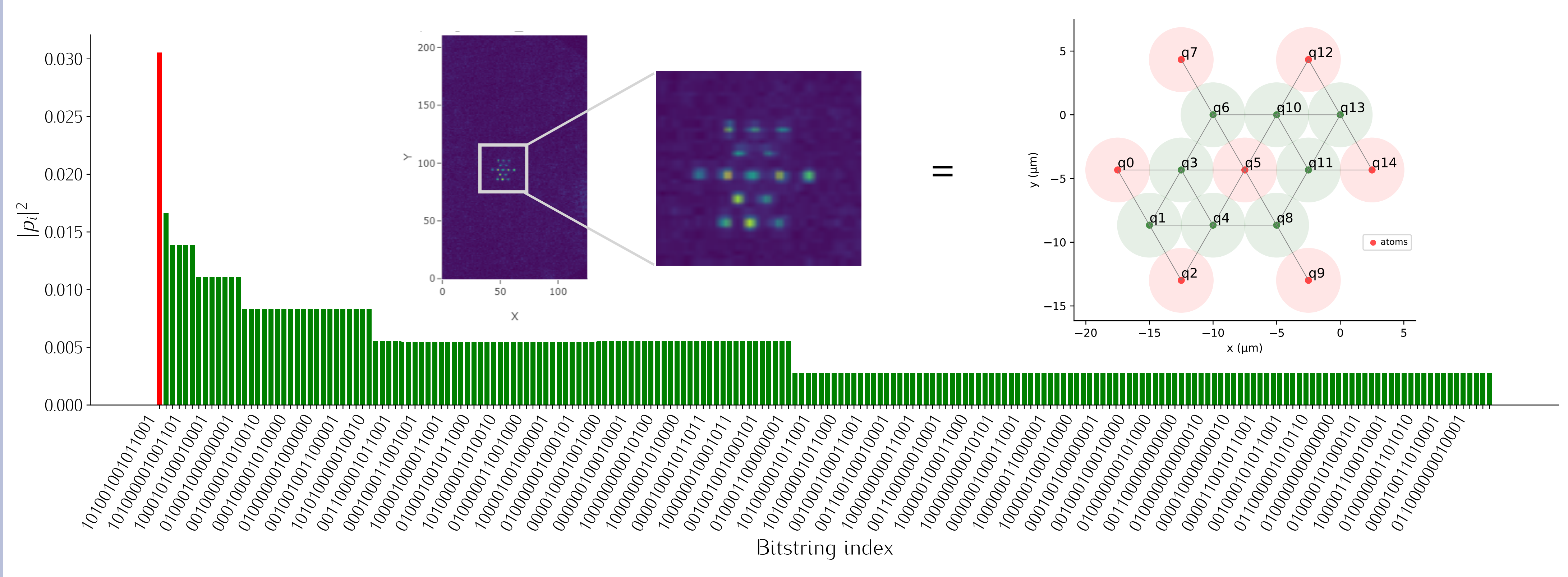
As a results



# So nothing works?



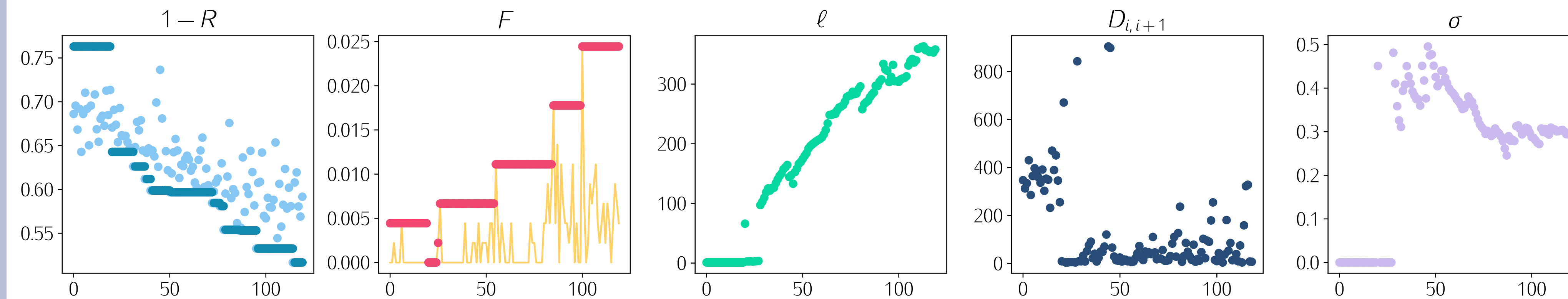
# Conclusions



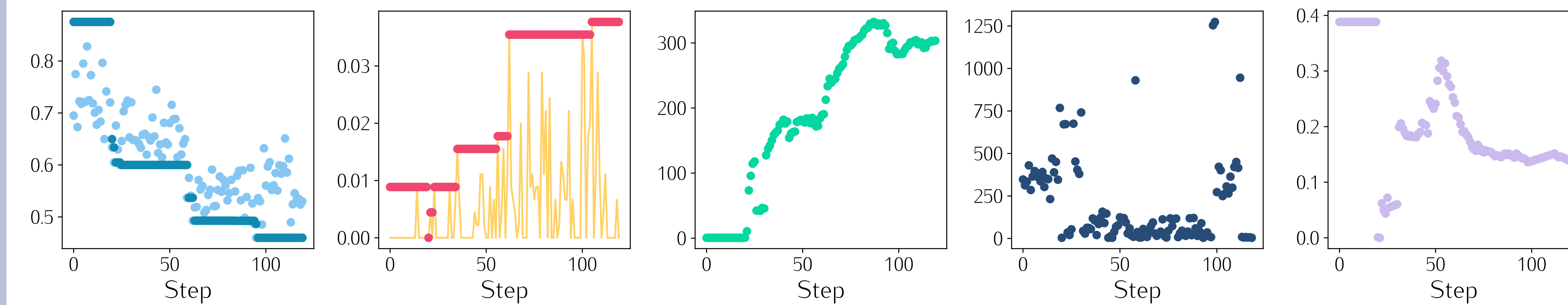
Be careful but be hopeful

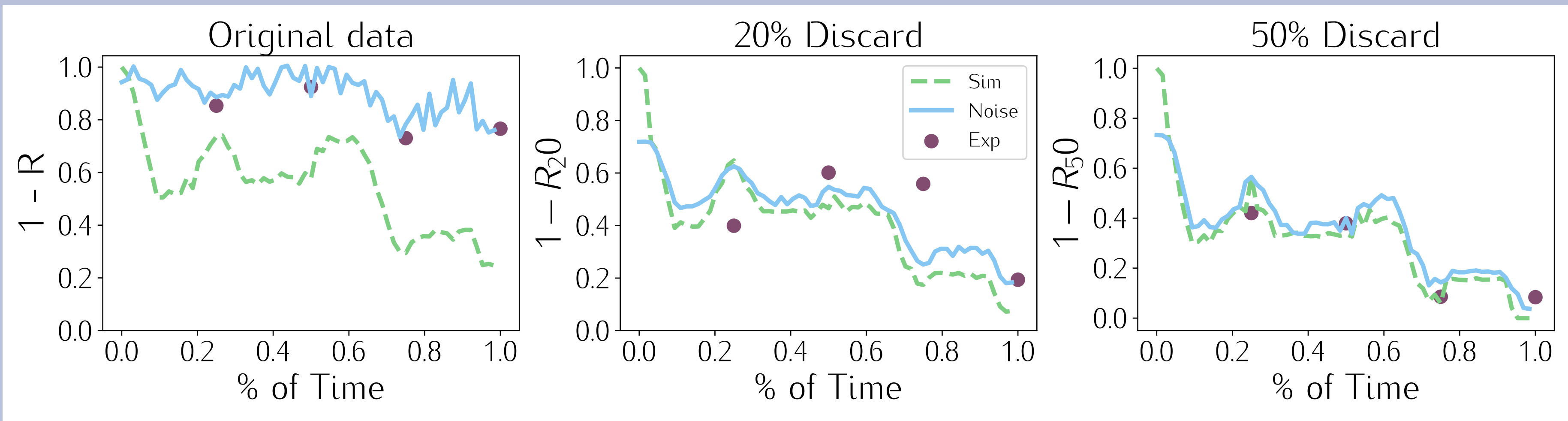
Thank you

(a) Experiment



(b) Simulation



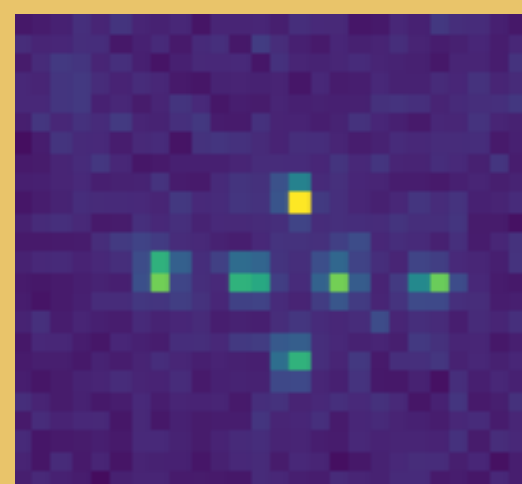


# BENCHMARK CORRECTING FOR SPAM: ONE WAY

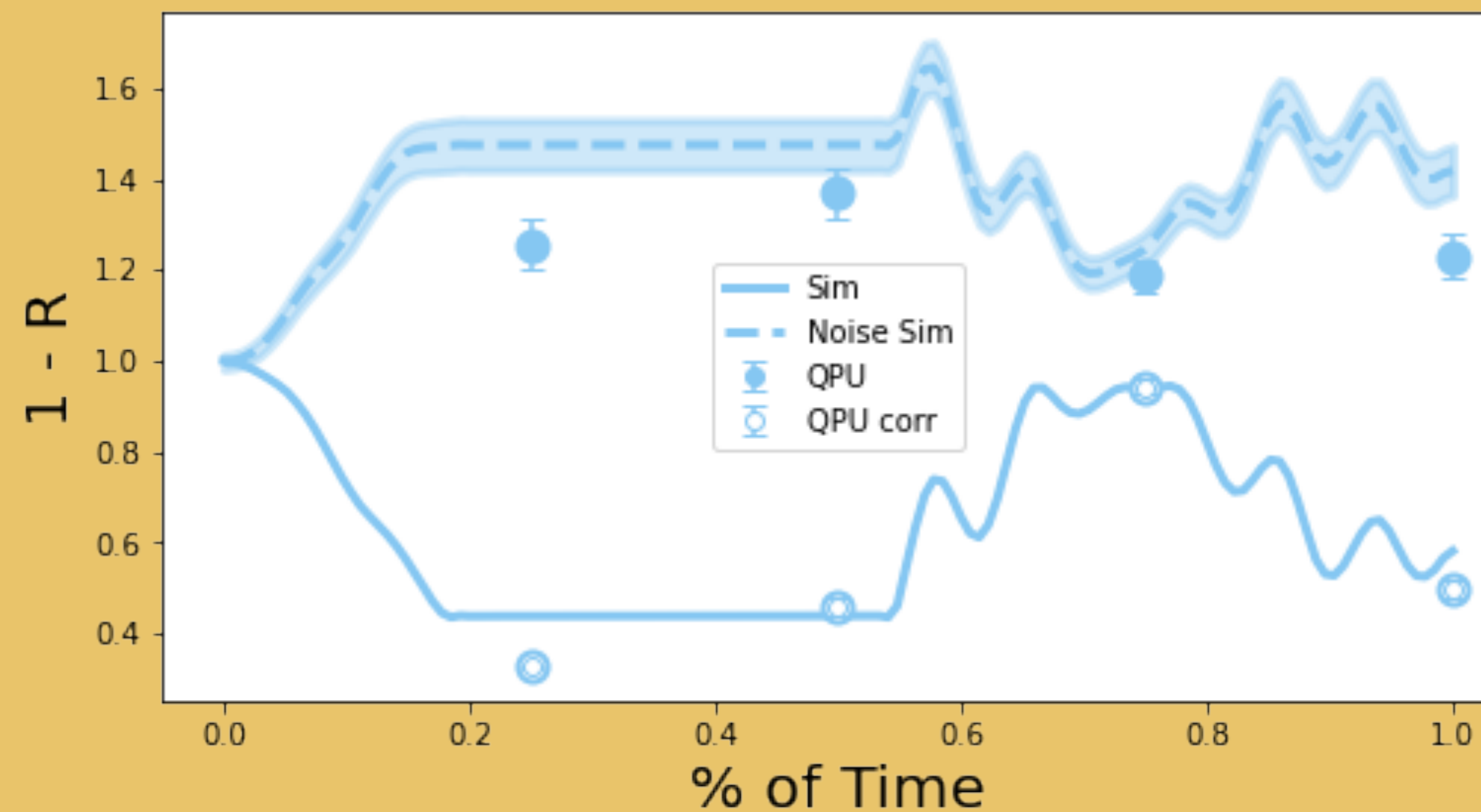
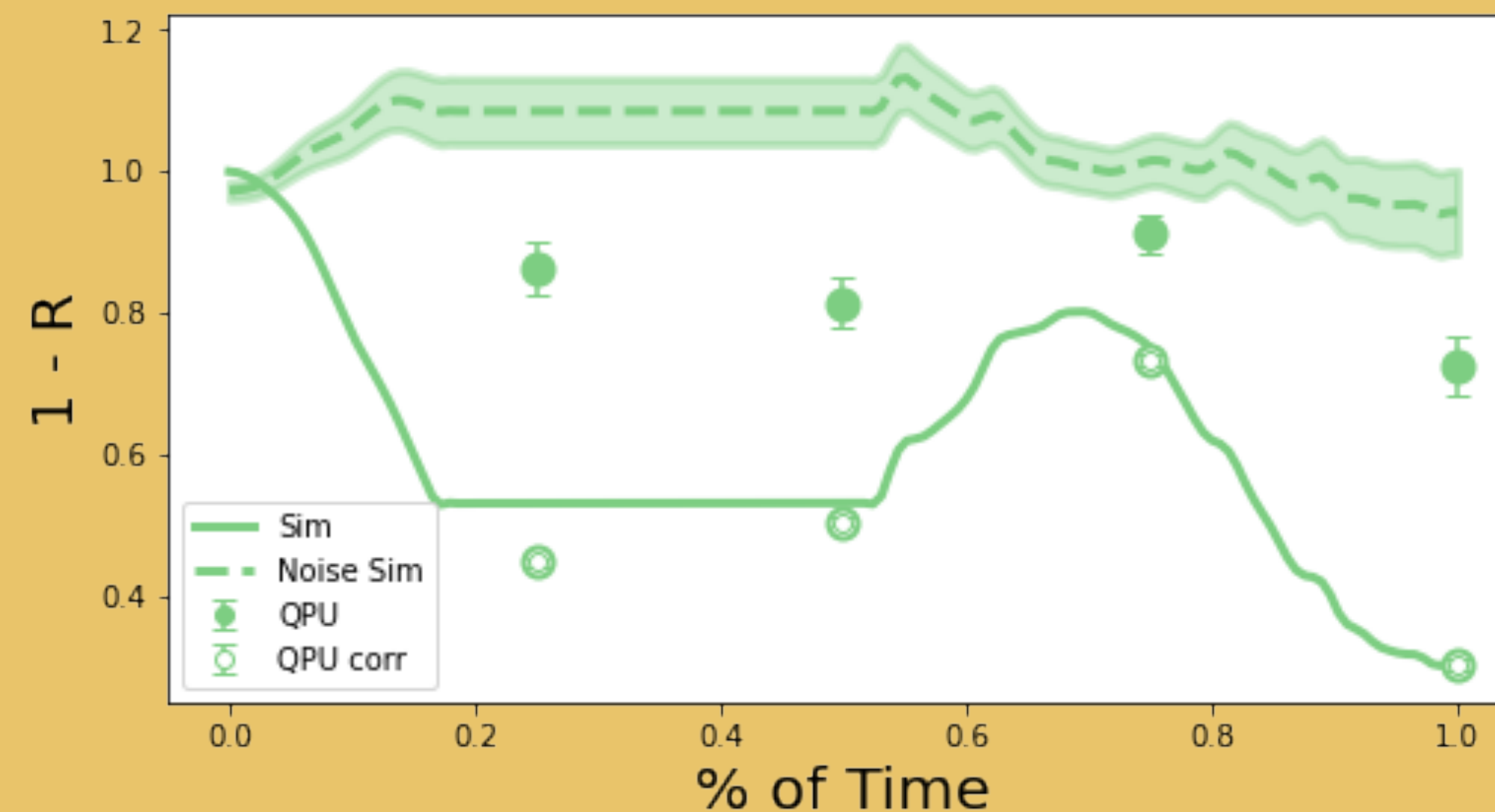
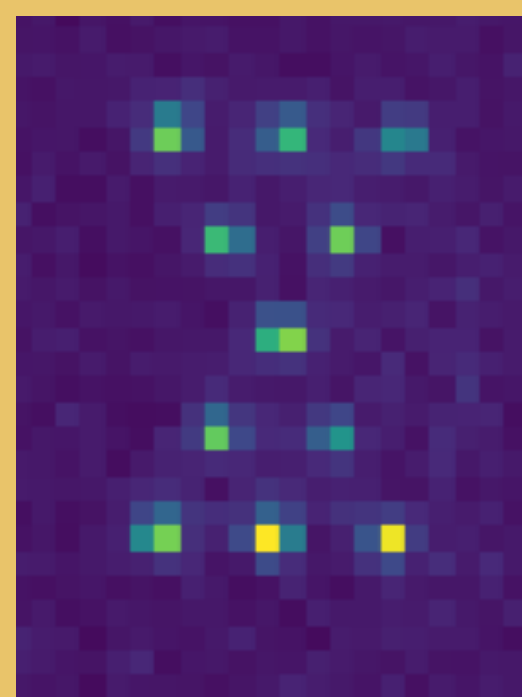
CREATE A TRANSFER MATRIX WITH BINOMIAL PROBABILITIES

$$P_{i \rightarrow j}$$

N=6

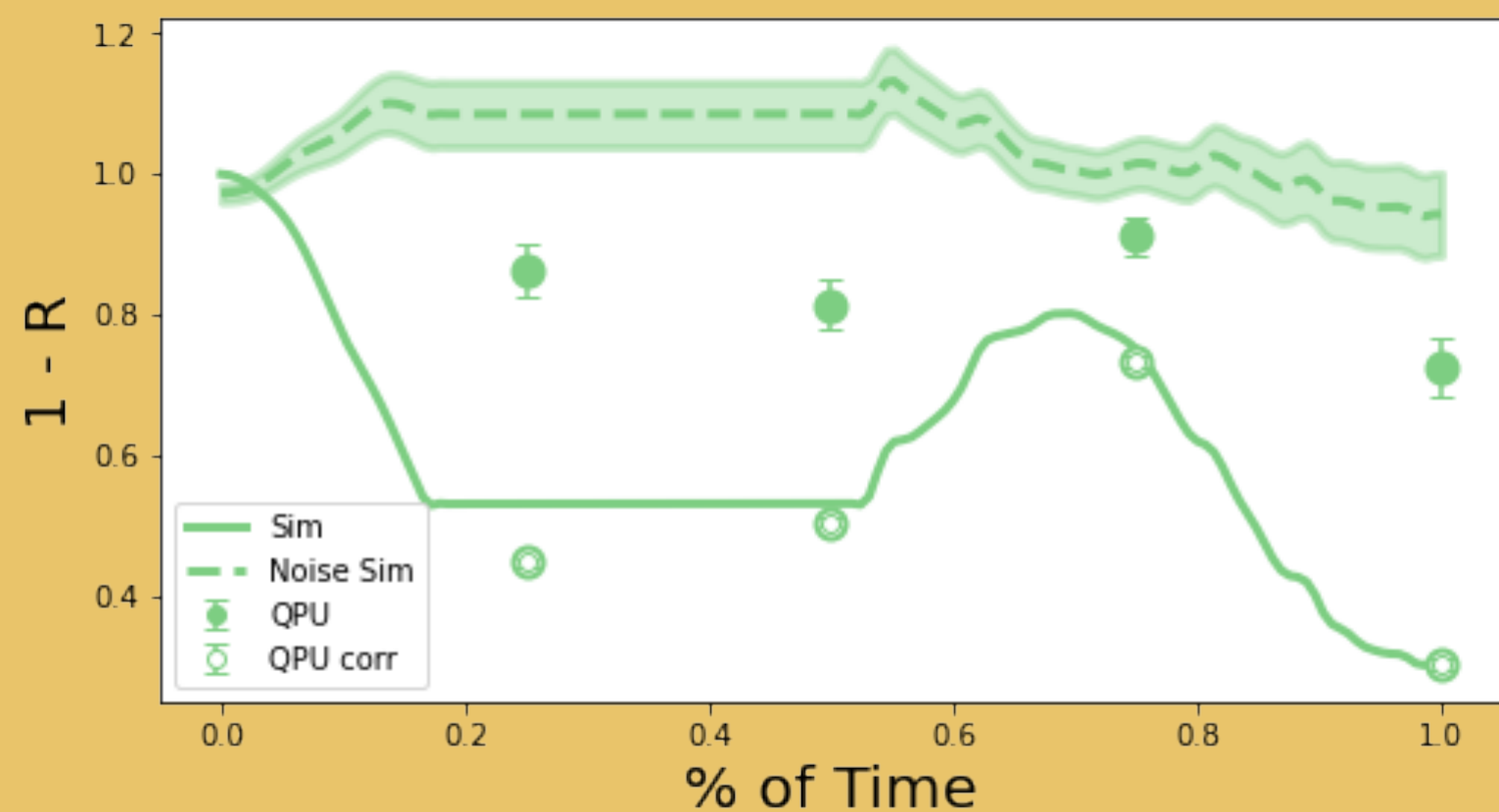


N=11

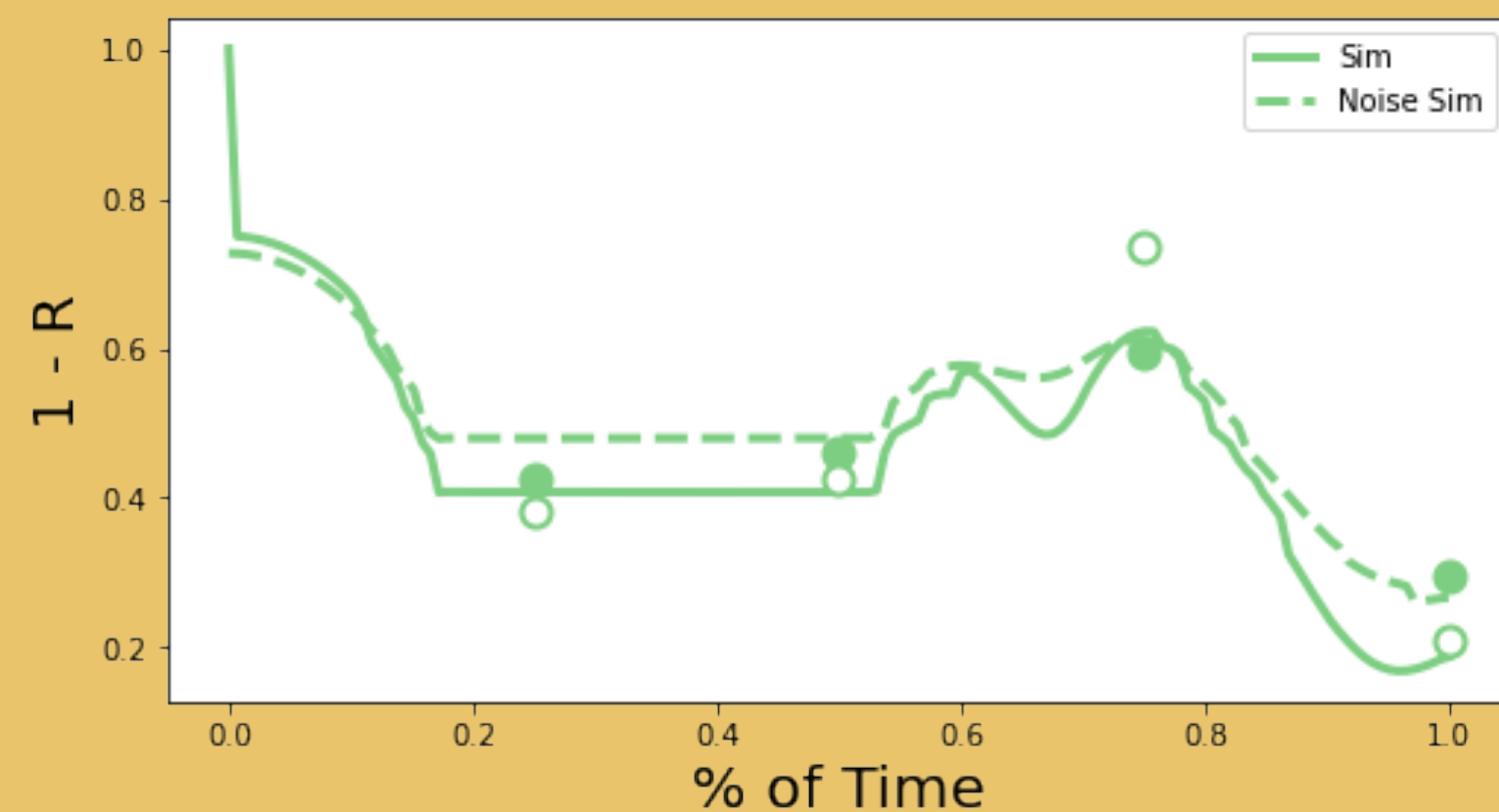


# BENCHMARK Another way: discard bitstrings

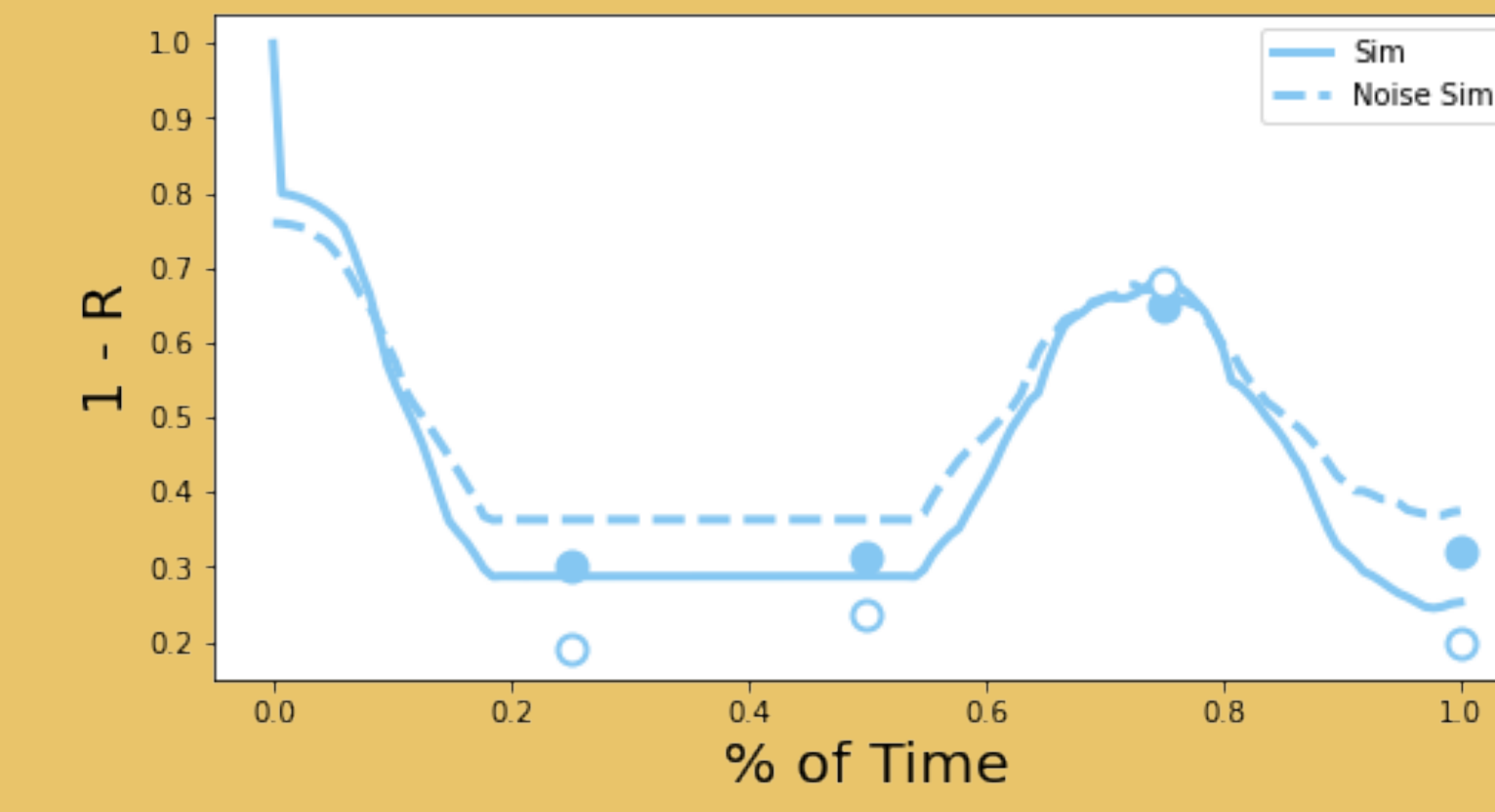
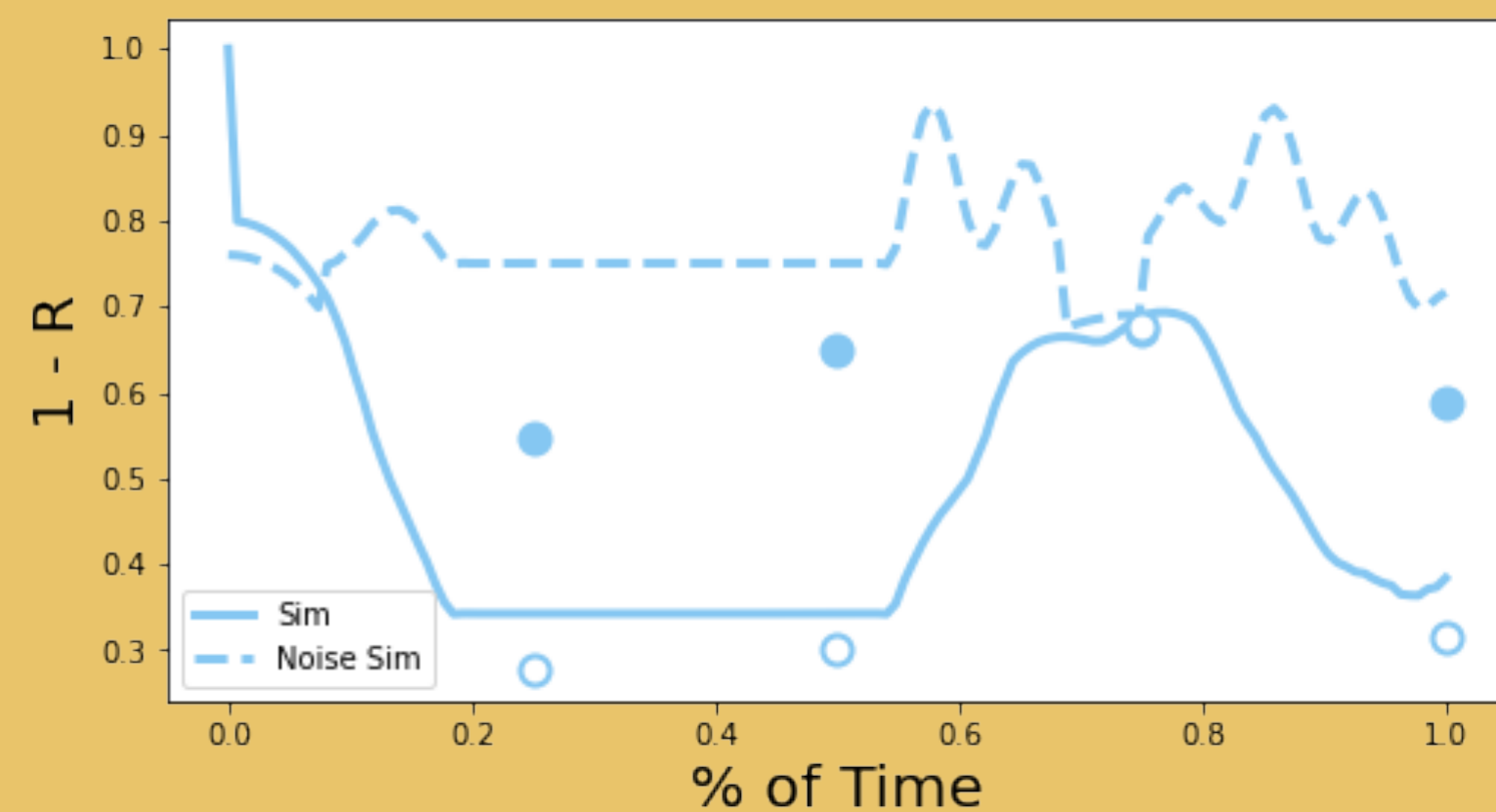
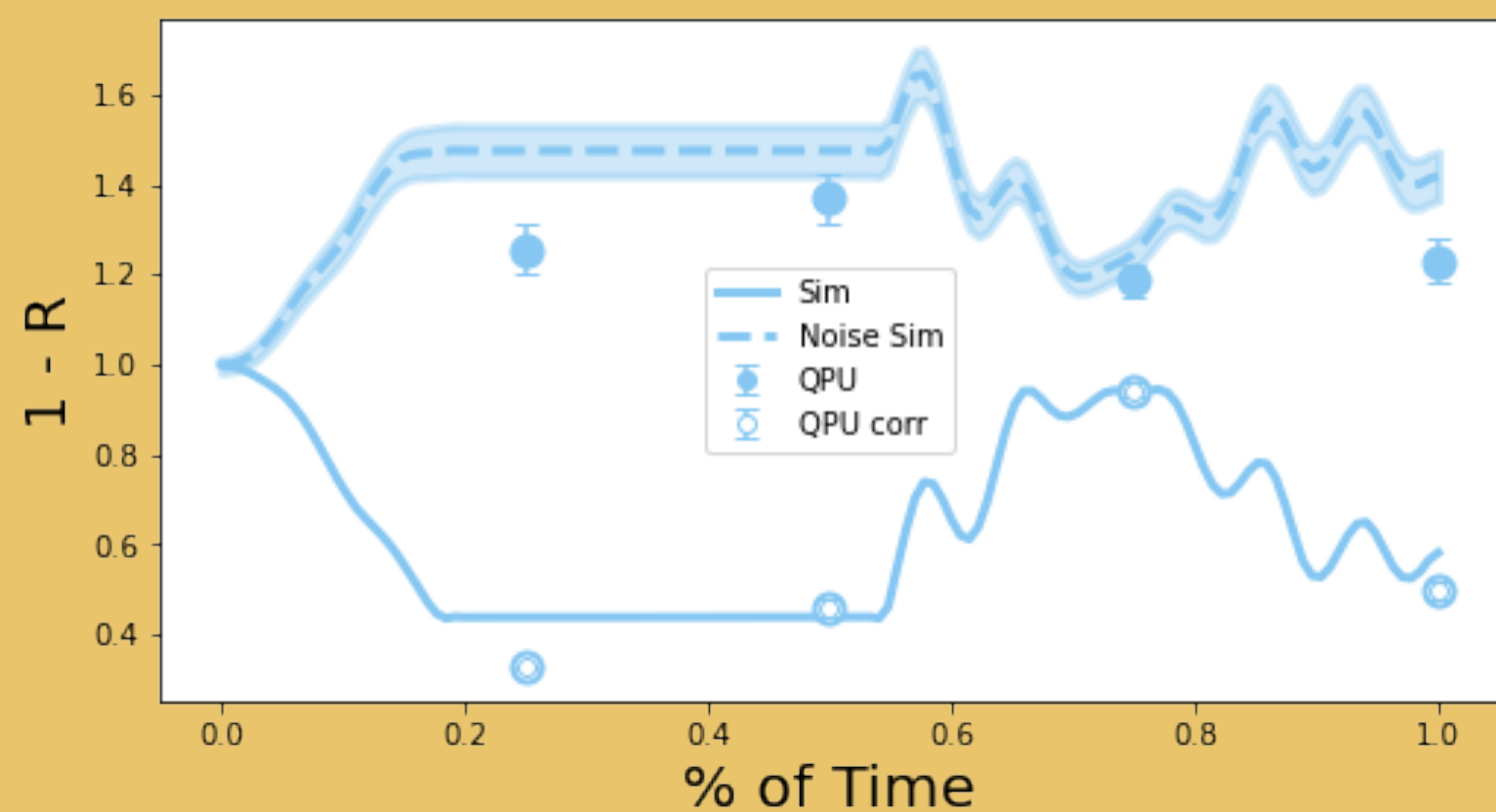
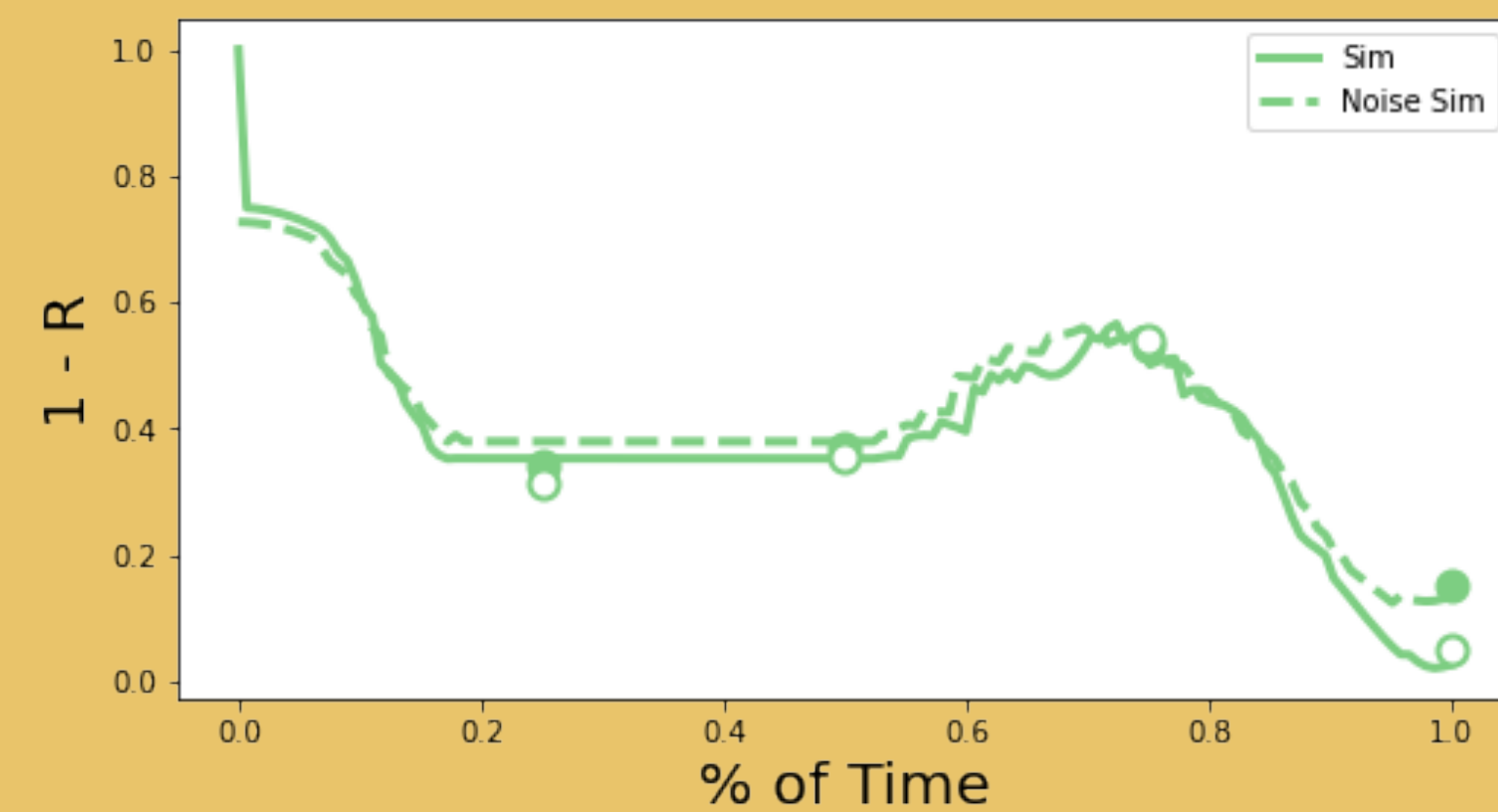
ORIGINAL DATA



DISCARD 20%



DISCARD 50%

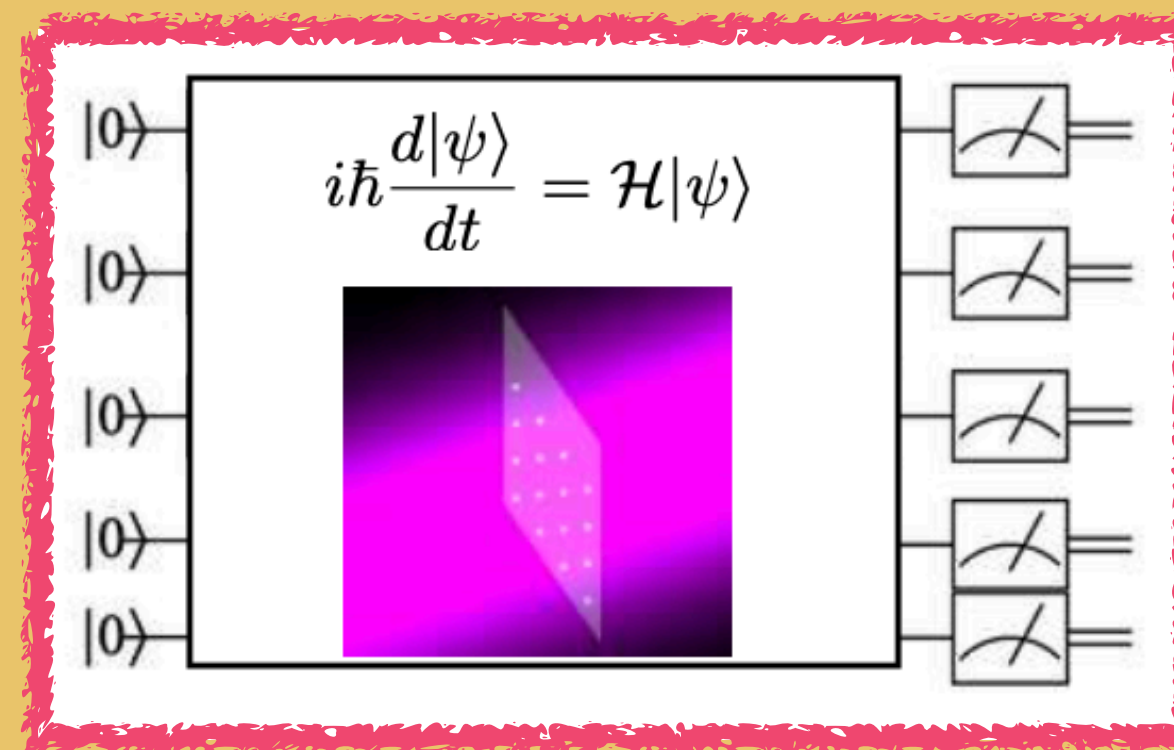


# Bayesian Optimization to optimize QAOA

[L Heneriet et al, Quantum (2020)]

Parameters

$(\theta_1, \theta_2, \dots)$



Output

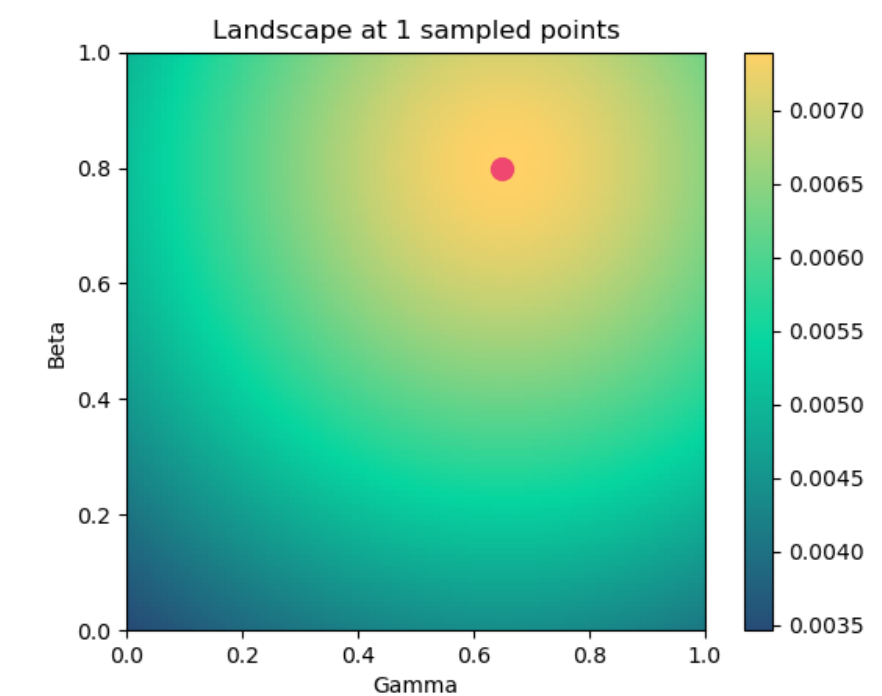
$E(\theta_1, \theta_2, \dots)$

Acquisition Function

$$\mathbb{E}I(\vec{\theta}) = \sigma[\theta^* \Phi(\theta^*) + \phi(\theta^*)]$$

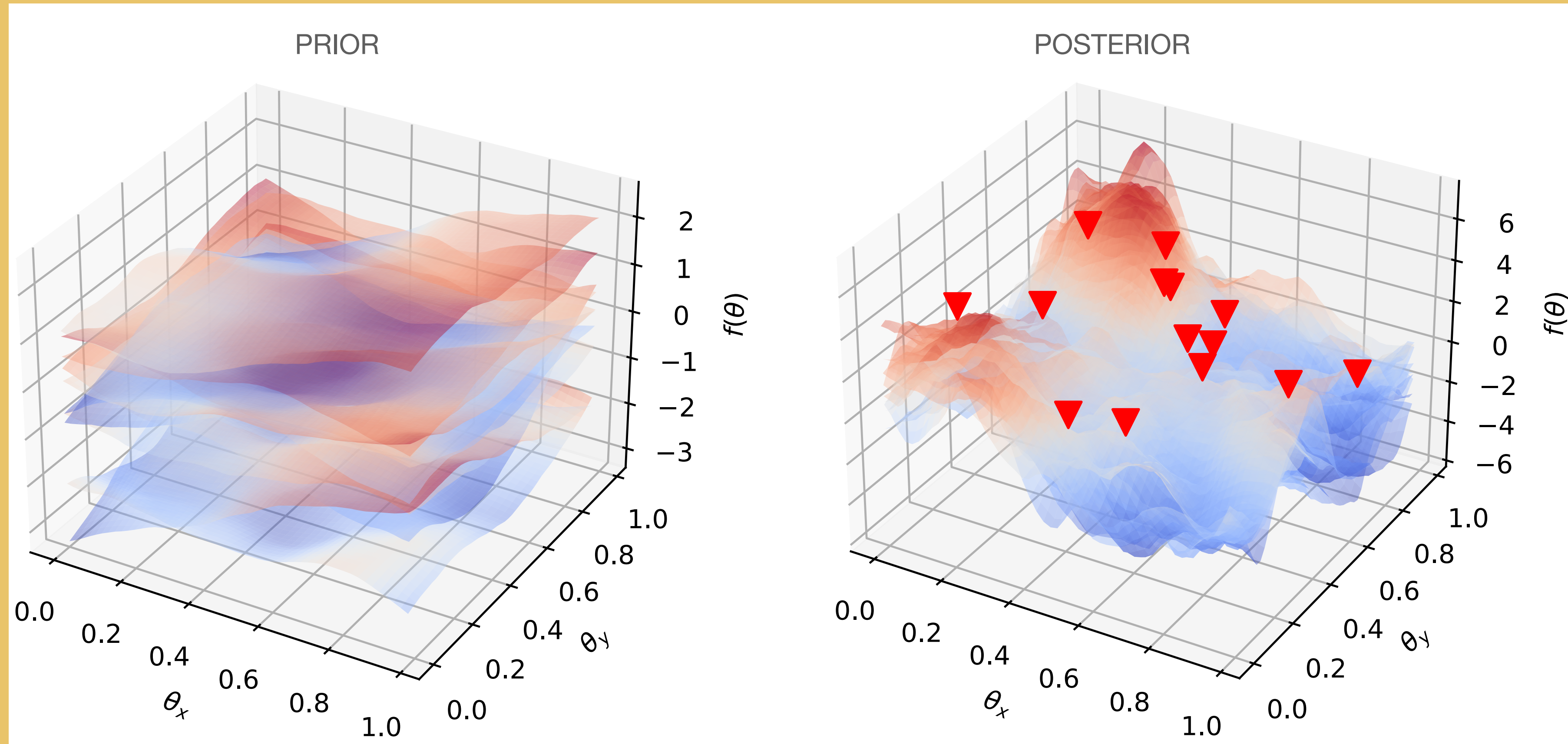
$$\vec{\theta} = \max_{\vec{\theta}} \mathbb{E}I(\vec{\theta})$$

Gaussian Process





# What is a Gaussian Process



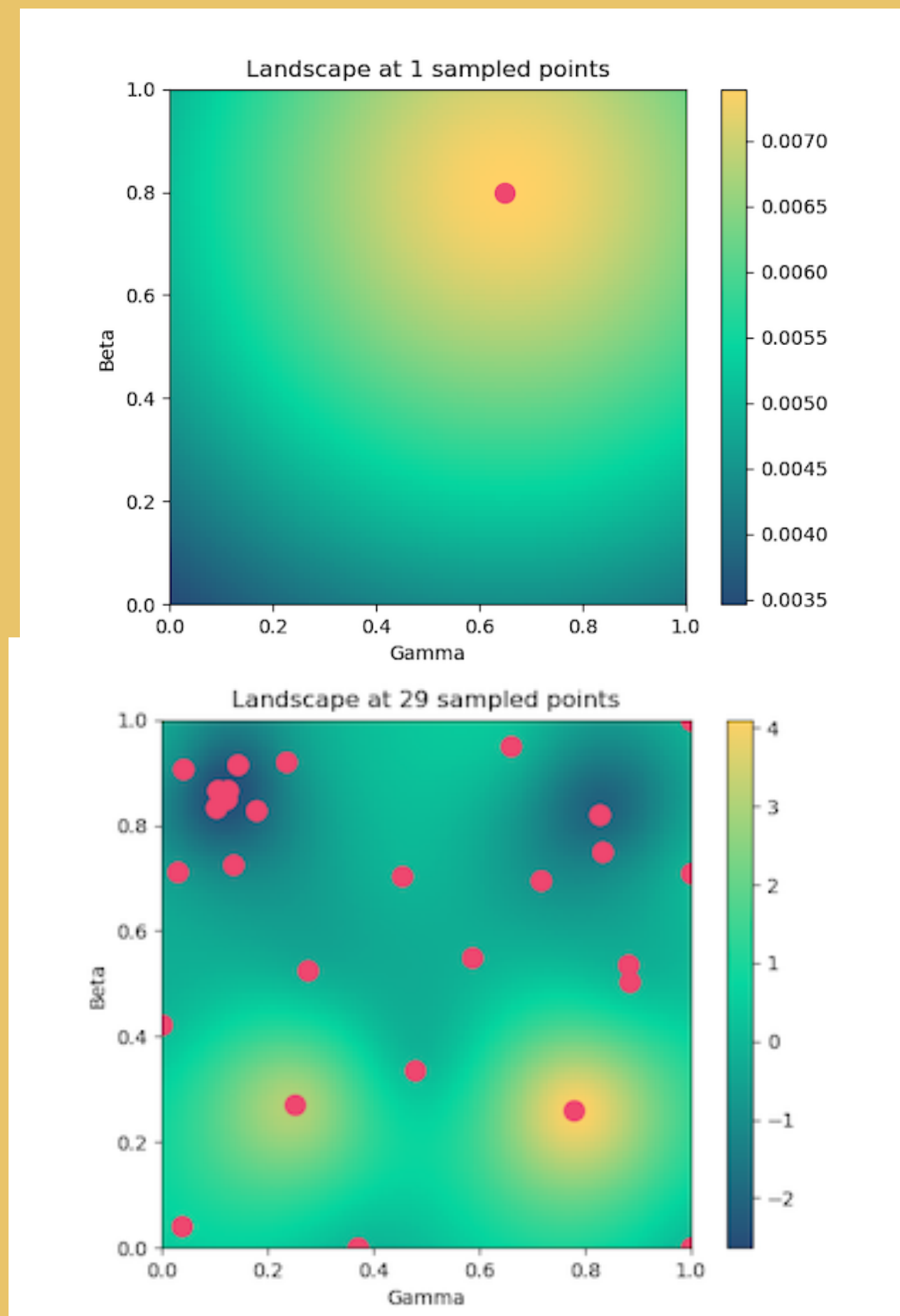
Kernel

$$k(\theta_i, \theta_j) \propto \sigma^2 e^{-\frac{\sqrt{3} \|\theta_i - \theta_j\|}{\ell}} + \sigma_N^2$$

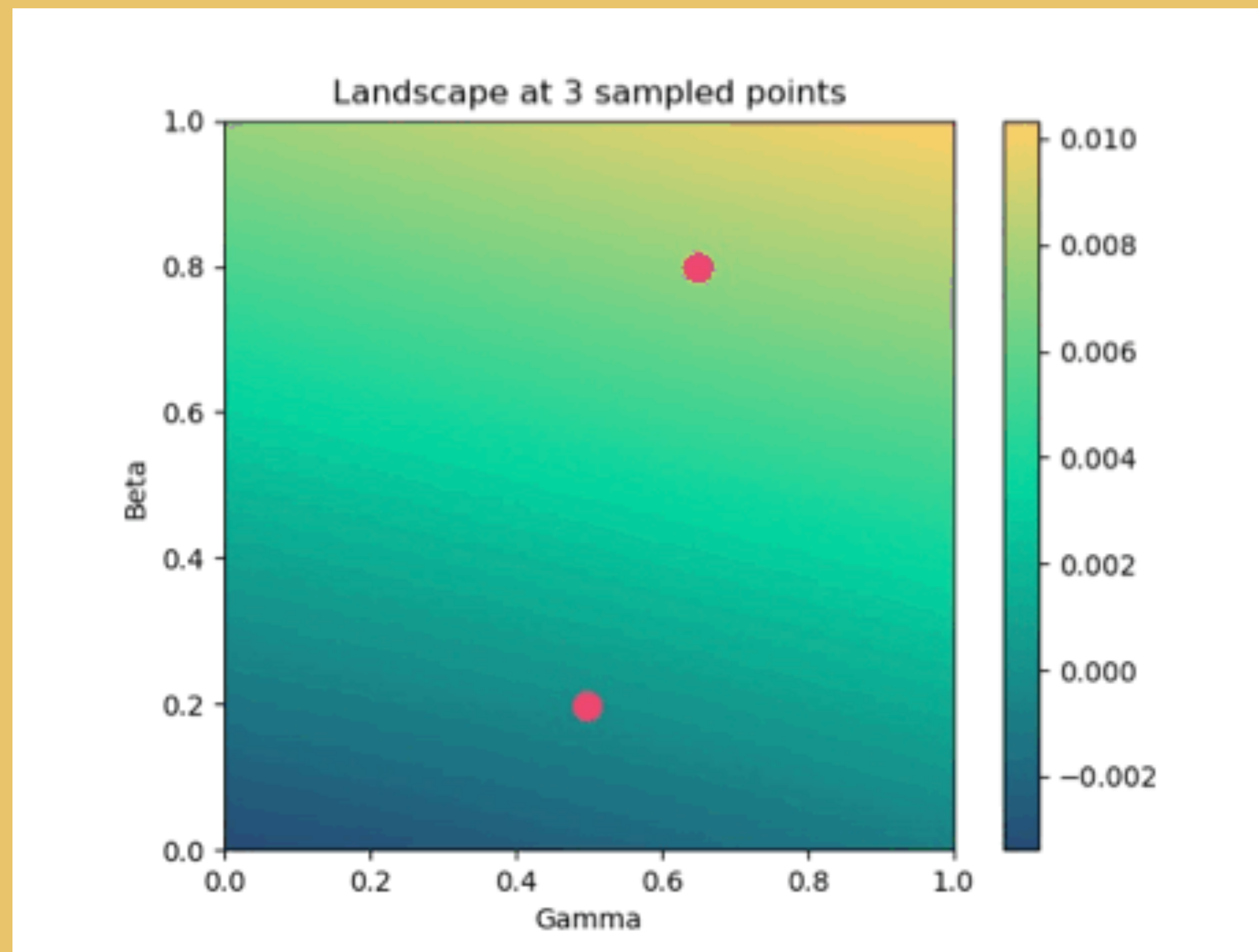
Hyperparameters  
Selected with optimization

# What is a Gaussian Process

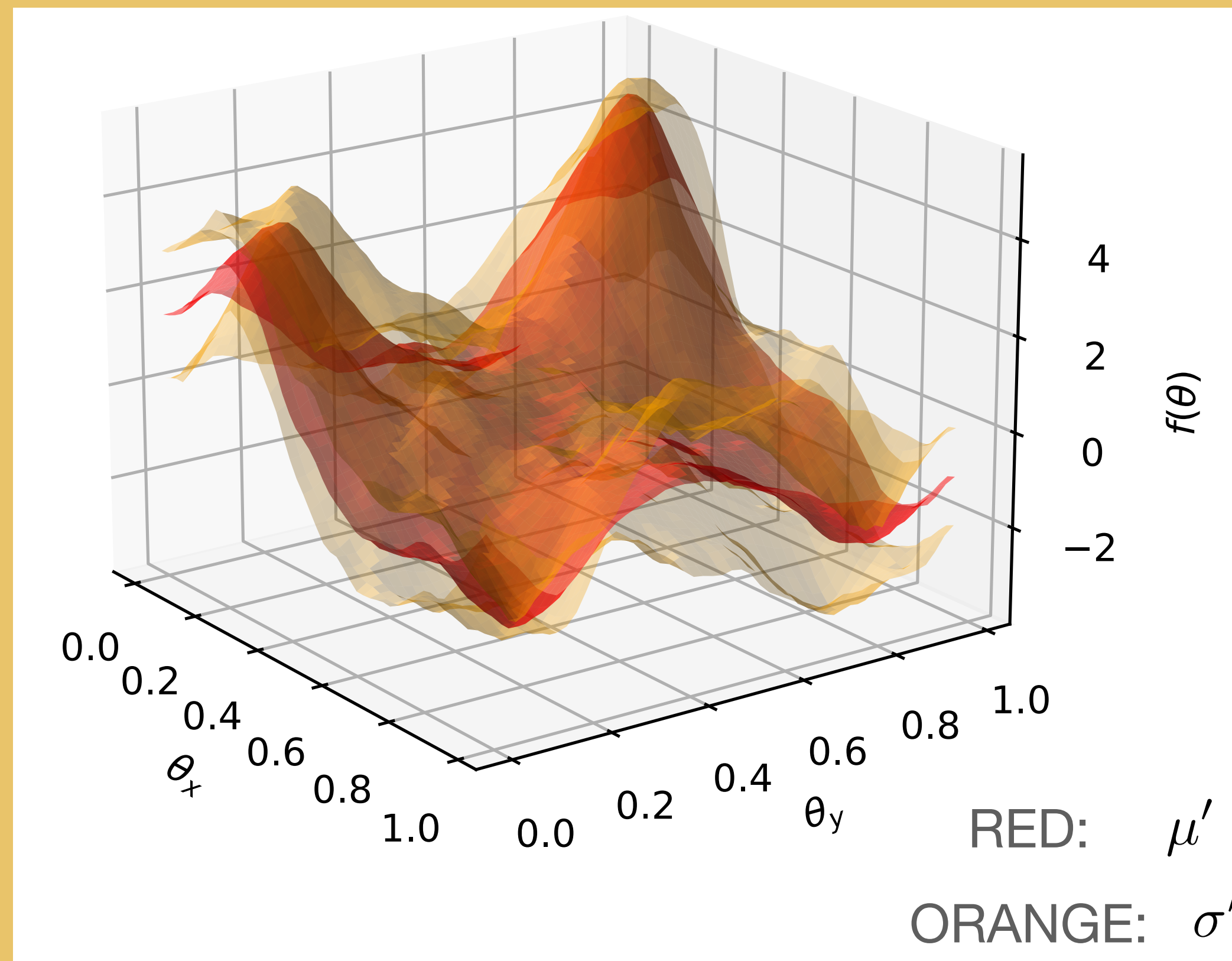
After sampling  
1 point



After sampling  
30 points



# What is an Acquisition Function



$$\text{EI}(\theta) = \Phi(z)(\theta_{BEST} - \mu') + \phi(z)\sigma'$$

CURRENT BEST

p

POSTERIOR  
MEAN

POSTERIOR  
VARIANCE

AT EACH BAYESIAN OPT STEP:

$$\vec{\theta} = \max_{\vec{\theta}} \text{EI}(\vec{\theta})$$