



Quan tum Simulation

- Motivation
- Pipeline
- Matter \rightarrow Hamiltonian
- Awful Scaling
- Demo of my research!

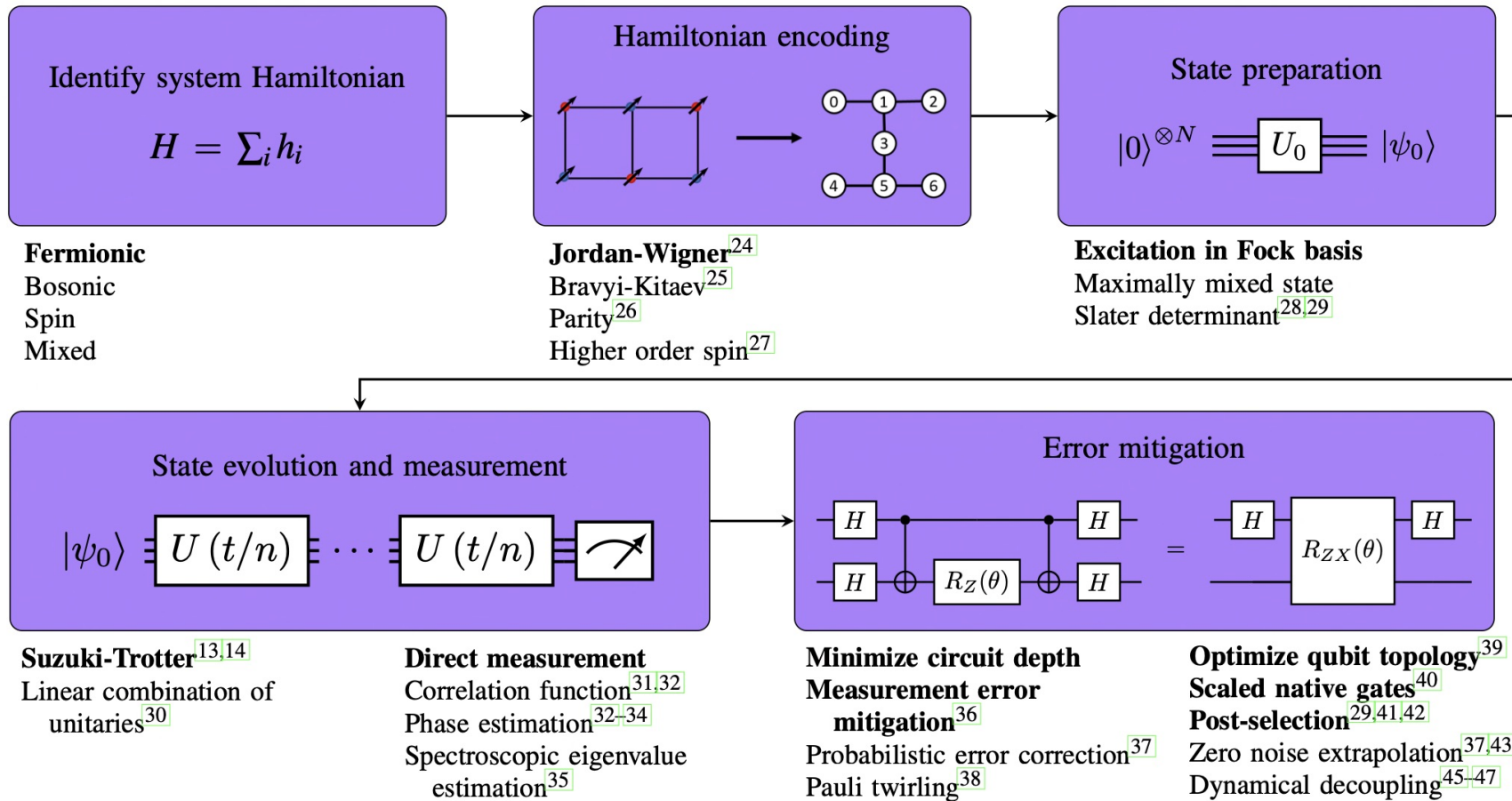
Quantum Simulation

“The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.”

— Dirac

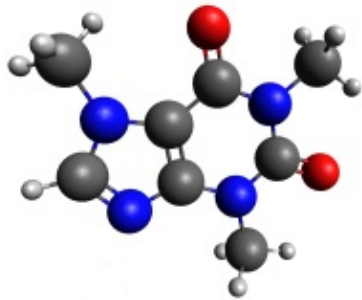
Potential Applications

Pipeline

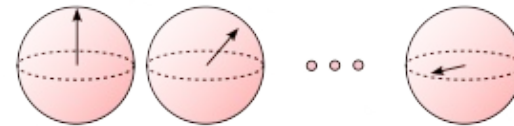


Translating Matter into Qubits

Molecules



Qubits



$$H|\Psi\rangle = E|\Psi\rangle$$

Jarrod R. McClean

Hydrogen Gas

Hamiltonian

$$-1.05 \text{ II}$$

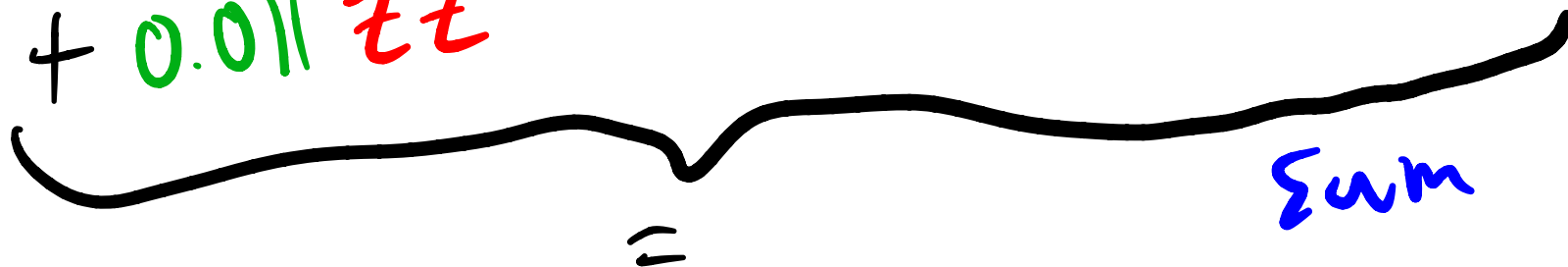
$$\text{H}_2$$

$$+ 0.397 \text{ IZ}$$

$$+ 0.181 \text{ XX}$$

$$- 0.397 \text{ ZI}$$

$$+ 0.011 \text{ ZZ}$$



-1.06365335002909	0	0	0.180931199784232
0	-1.83696799120298	0.180931199784232	0
0	0.180931199784232	-0.245218291830263	0
0.180931199784232	0	0	-1.06365335002909

Want to Know Eigenvalues

$$H = \begin{bmatrix} -1.06365335002909 & 0 & 0 & 0.180931199784232 \\ 0 & -1.83696799120298 & 0.180931199784232 & 0 \\ 0 & 0.180931199784232 & -0.245218291830263 & 0 \\ 0.180931199784232 & 0 & 0 & -1.06365335002909 \end{bmatrix}$$

Hamiltonian \rightarrow Energy Function

Eigenvalues \rightarrow Energy

lowest Eigenvalue \rightarrow Groundstate

Math

Physics

Horrible Scaling

Schwinger
model

$$H_E = \frac{g^2 a}{2} \sum_{i=1}^{N-1} \left(\sum_{j<i} \frac{Z_j + (-1)^j}{2} + \frac{\theta}{2\pi} \right)^2$$

QED

1 spatial

+ 1 time

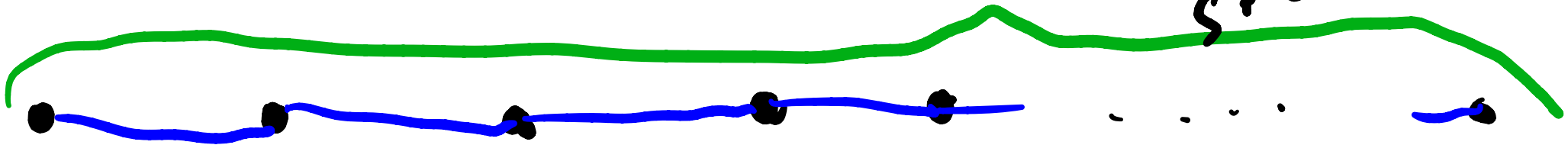
$$H_M = \frac{m}{2} \sum_{i=1}^N (-1)^i Z_i$$

Toy
Model

$$H_I = \frac{1}{4a} \sum_{i=1}^{N-1} X_i X_{i+1} + Y_i Y_{i+1}$$

$$H = H_E + H_M + H_I$$

N Points in
space



Hilbert Space is a BIG Place

$$N \rightarrow 2^N \cdot 2^N = 2^{2N}$$

Numbers
in Ham.

$$2 \rightarrow 16$$

⋮

XXIIYY

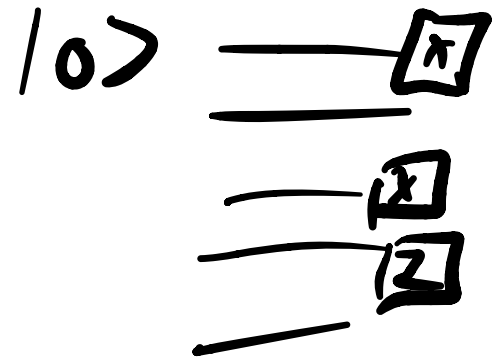
$$6 \rightarrow 4096$$

||
)

$$134 \rightarrow 4.7 \times 10^{80} > 3.28 \times 10^{80}$$

Particles
in universe

Luckily

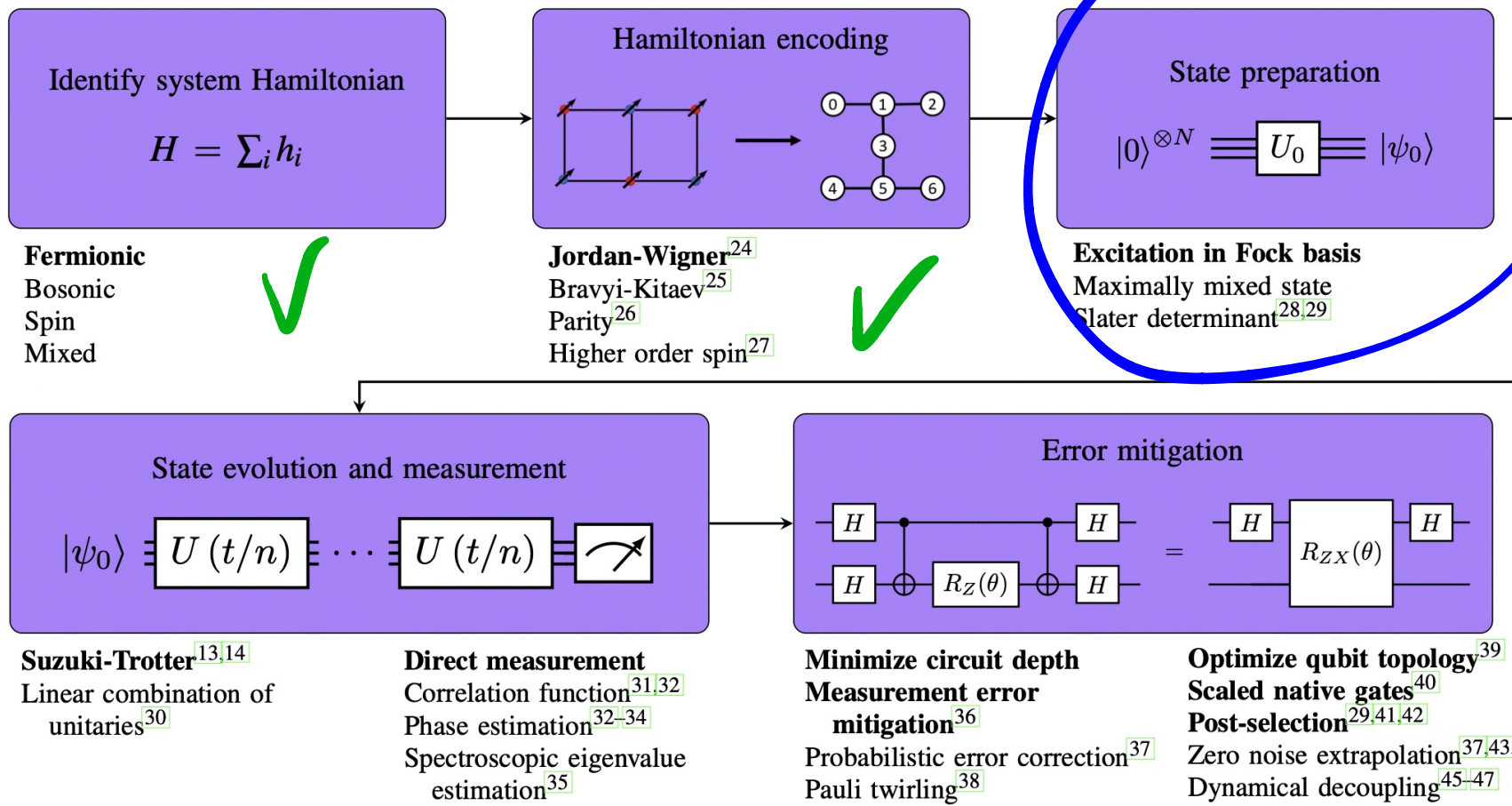


$N \sim N$ qubits!

Quantum Computers have Polynomial
complexity btwn points and Qubits
(at least for Schwinger model)

Prepping the state

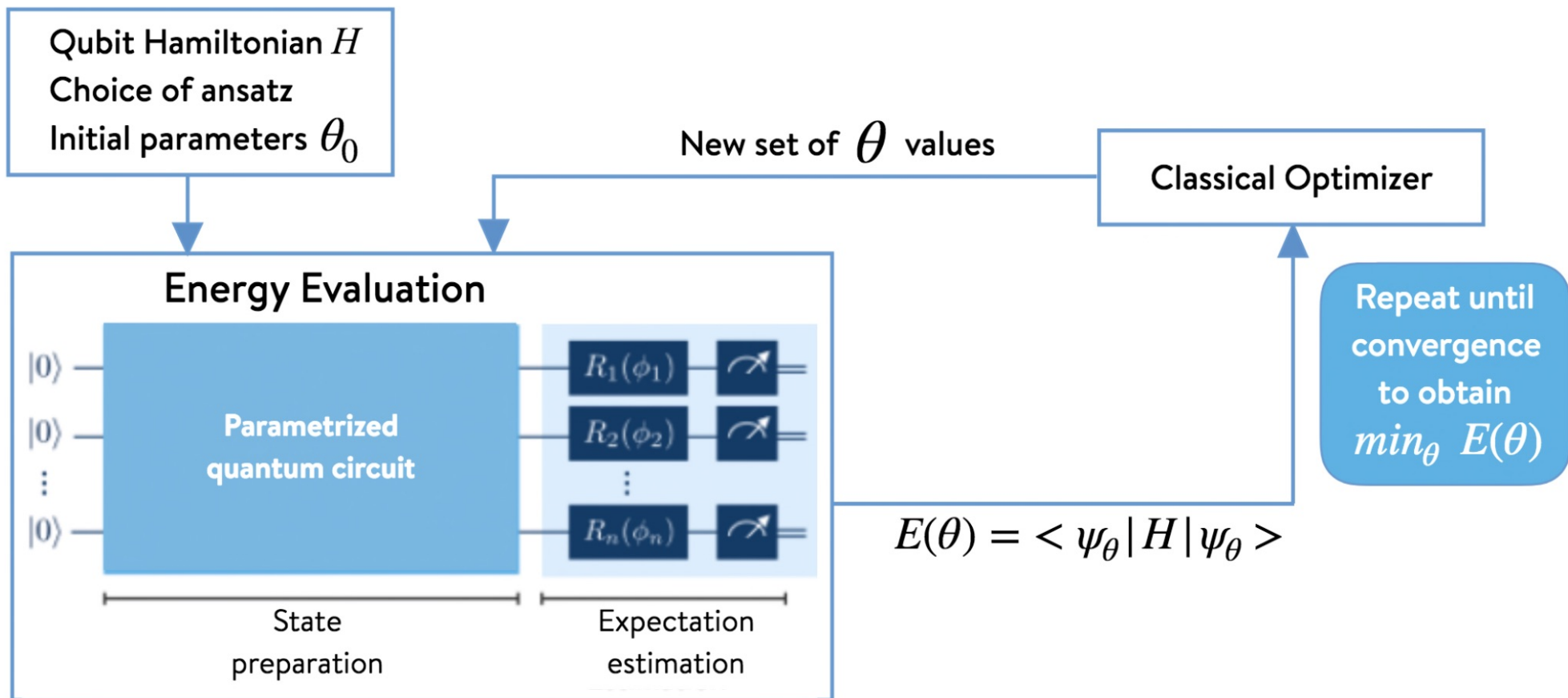
Diverging...





Burning

VQE - The Noisy State Preparation



ansatz = $|\psi_\theta\rangle$ = state prep.

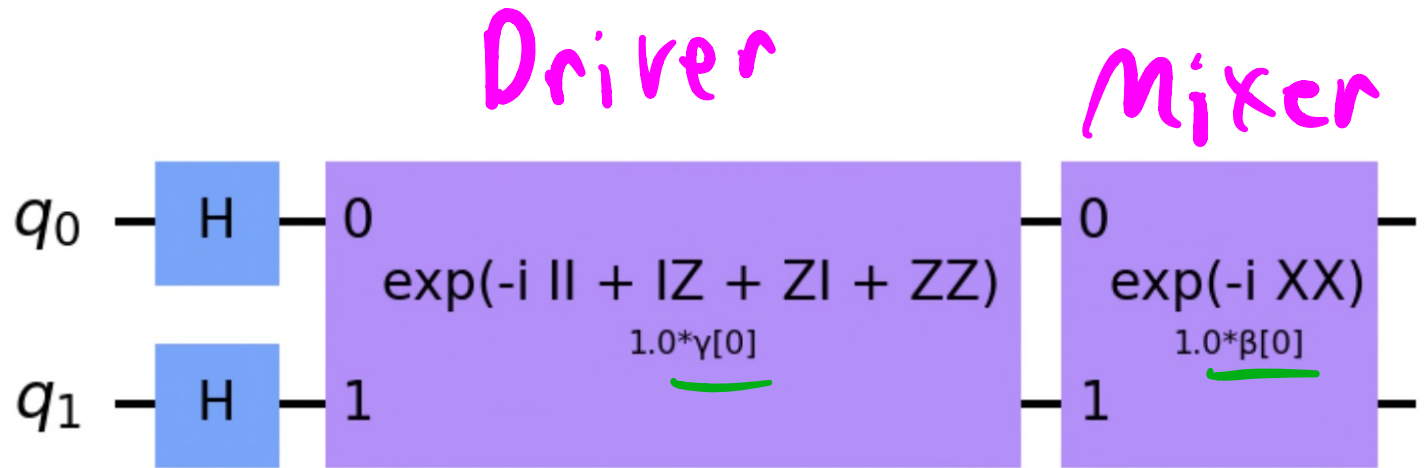
Example QAOA

$H =$

Ansatz for H_2

$$\begin{bmatrix} -1.06365335002909 & 0 & 0 & 0.180931199784232 \\ 0 & -1.83696799120298 & 0.180931199784232 & 0 \\ 0 & 0.180931199784232 & -0.245218291830263 & 0 \\ 0.180931199784232 & 0 & 0 & -1.06365335002909 \end{bmatrix}$$

$|\psi_\theta\rangle =$



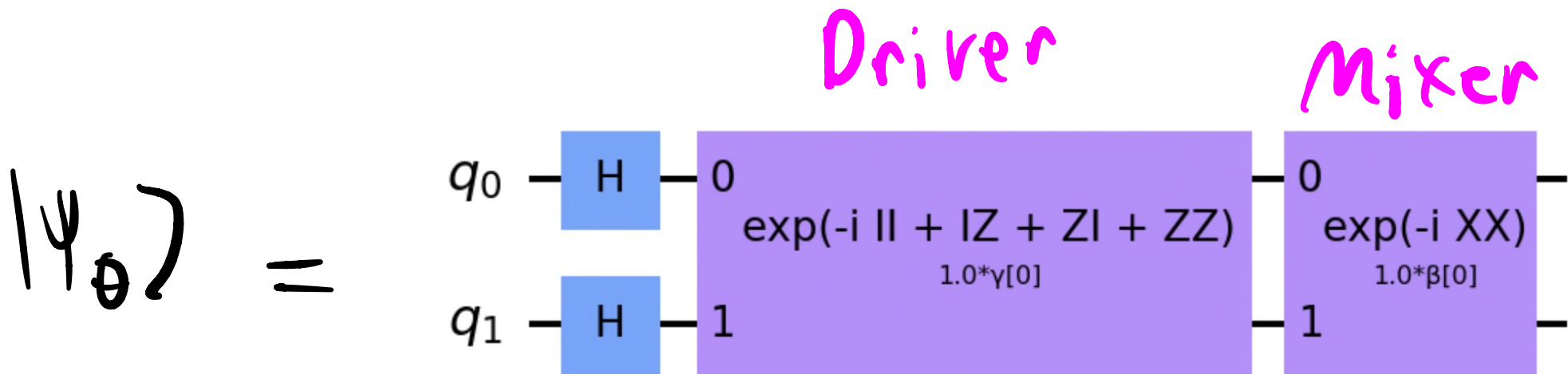
$e^{iH_{\text{Hamiltonian}}} = U_{\text{unitary}}$

$\text{eval} = \langle \psi_0 | H | \psi_0 \rangle$

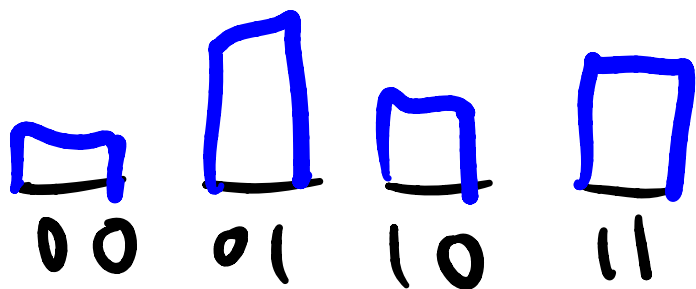
Parameters

$\vec{\theta} = \begin{bmatrix} \gamma \\ \beta \end{bmatrix}$

Noisy!



You measure this circuit a bunch of times, getting some distribution that is the wave function



$$\sim |\psi_0\rangle = \begin{bmatrix} 0.375 \\ 0.6 \\ 0.375 \\ 0.6 \end{bmatrix}$$