



Quantum Simulation

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

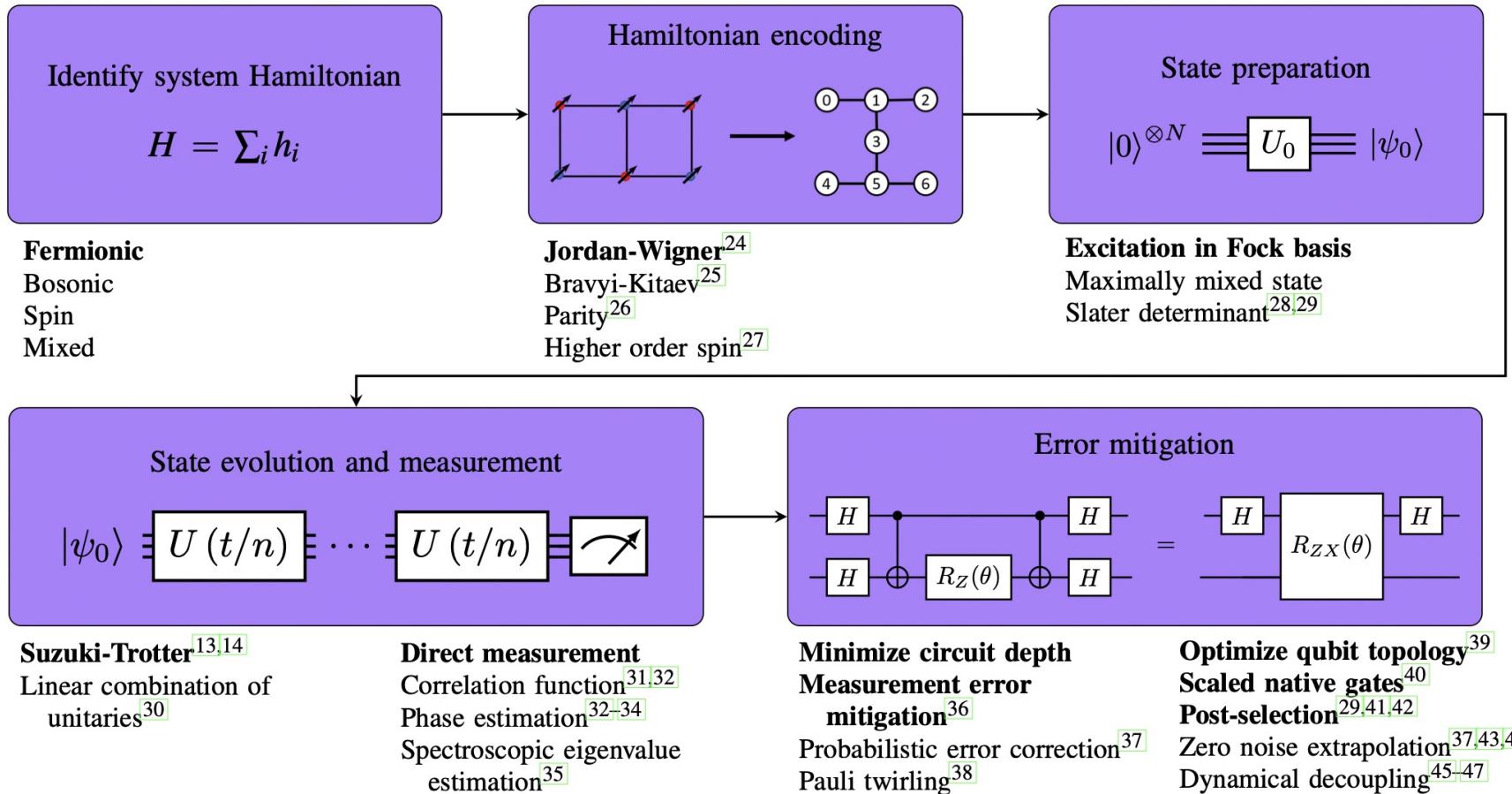
# Quantum Simulation

“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

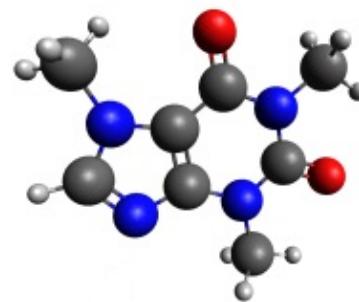
# Potential Applications

# Pipeline

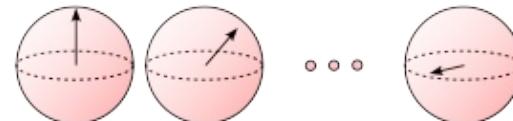


# Translating Matter into Qubits

Molecules



Qubits



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

Jarrod R. McClean

# Hydrogen Gas Hamiltonian

- 1.05 II

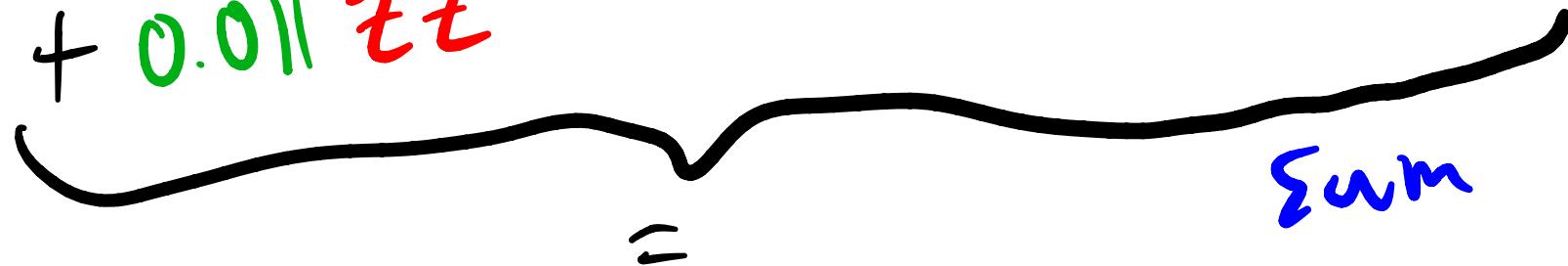
$H_2$

+ 0.397 IZ

+ 0.181 XX

- 0.392 ZI

+ 0.011 ZZ



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

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

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

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

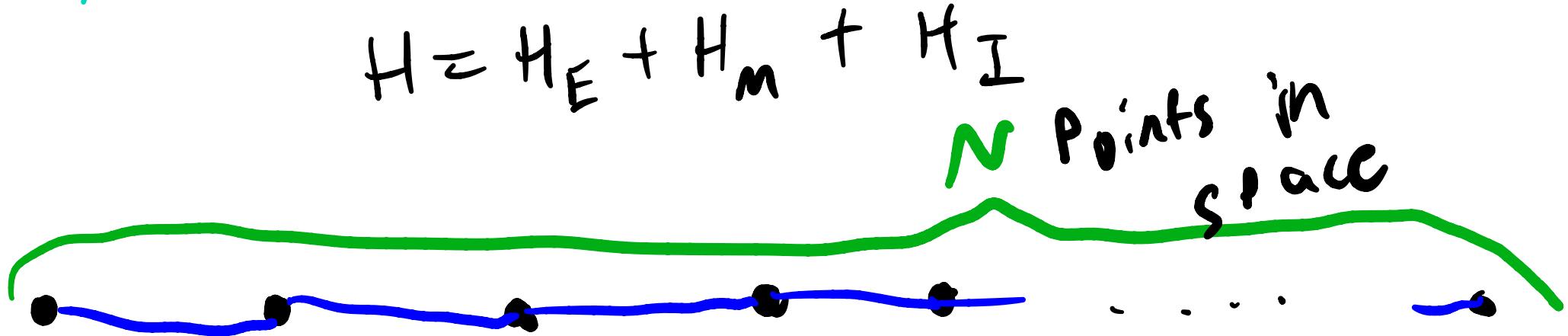
| spatial  
+ | time

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

$$2 \rightarrow 16$$

in Ham.

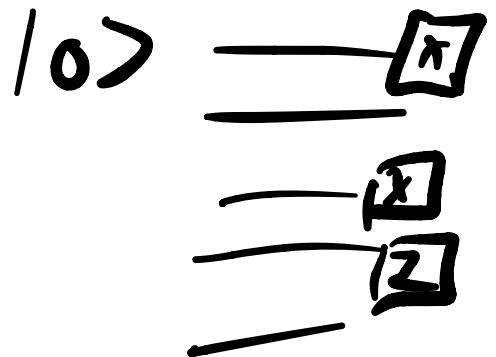
$$\text{XXIIIYY} \quad 6 \rightarrow 4096$$

!!  
()

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

Particles  
in universe

Luckily

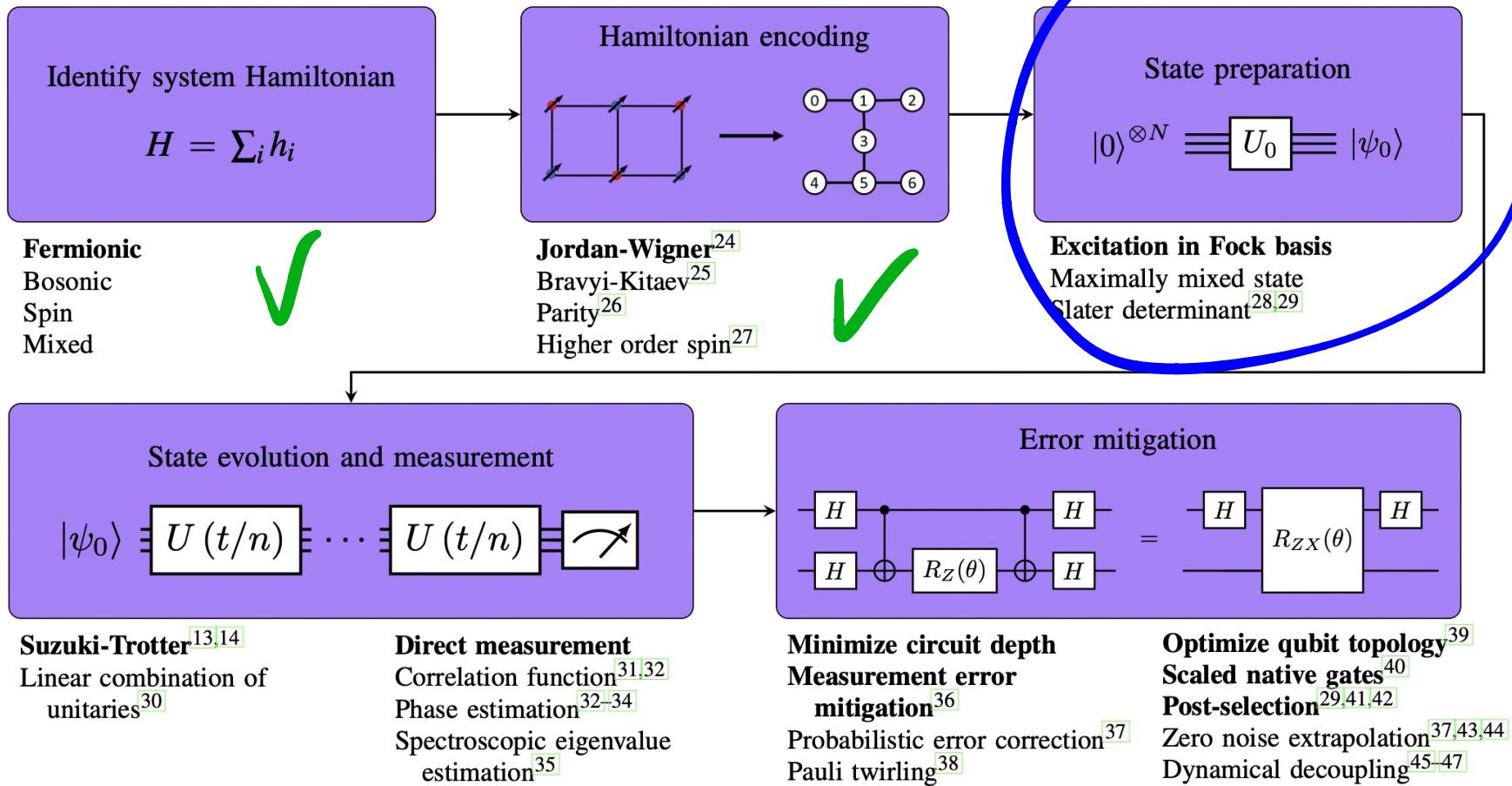


$$N \sim N_{\text{qubits}}!$$

Quantum Computers have Polynomial  
complexity b/w points and Qubits  
(at least for Schrödinger model)

# Preparing the state

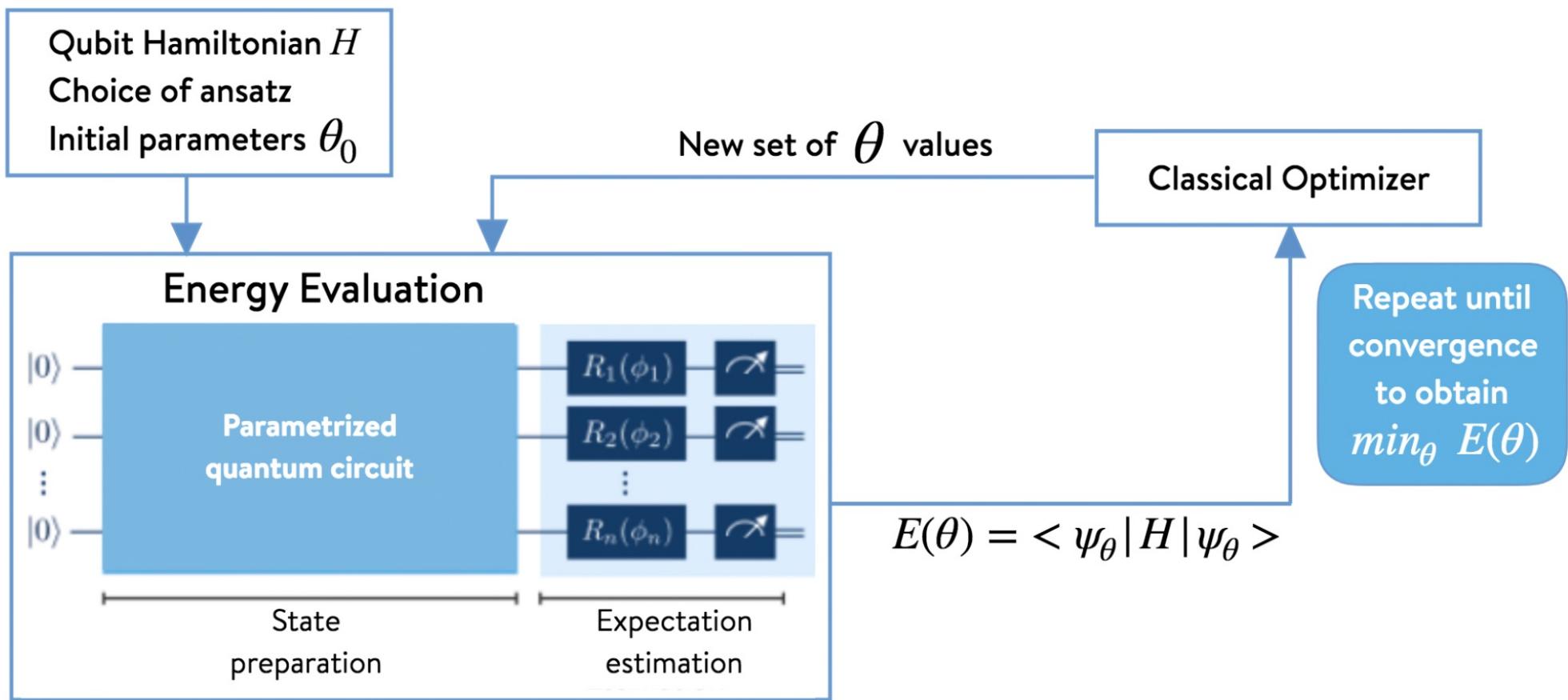
Diverging...





Burning

# VQE - The Noisy State Preparation



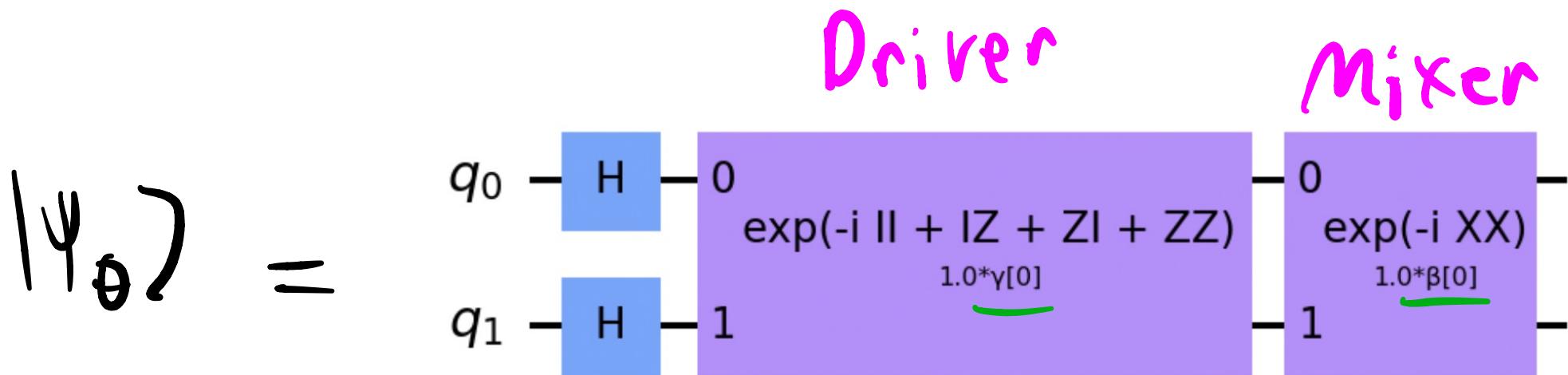
ansatz =  $|\Psi_\theta\rangle$  = state prep.

# Example QAOA

Ansatze for  $H_2$

$H =$

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



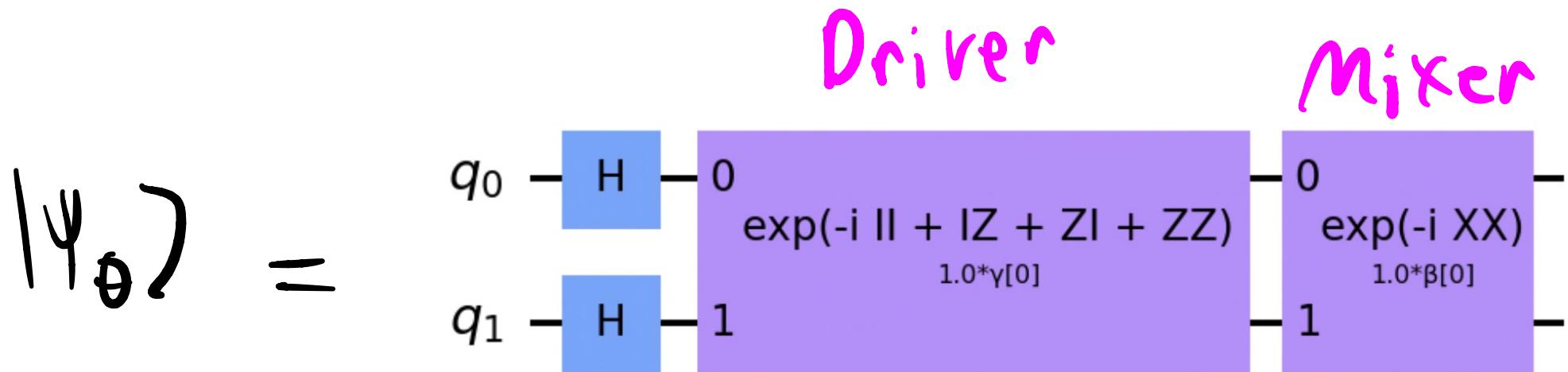
$e^{iH_{\text{Hamiltonian}}} = U_{\text{unitary}}$

$$\text{eval} = \langle \Psi_0 | H | \Psi_0 \rangle$$

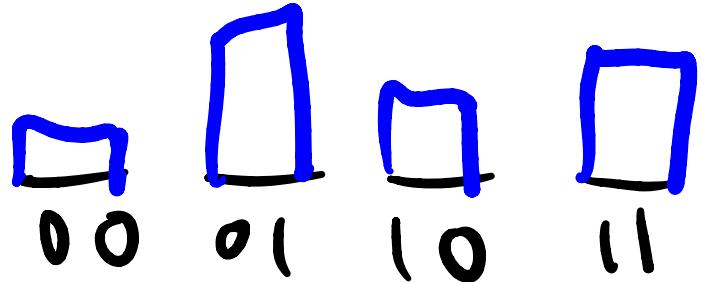
Parameters

$$\vec{\theta} = [\gamma \ \beta]$$

Noisy!



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



$$\sim |\Psi_0\rangle = \begin{bmatrix} 0.375 \\ 0.6 \\ 0.375 \\ 0.6 \end{bmatrix}$$