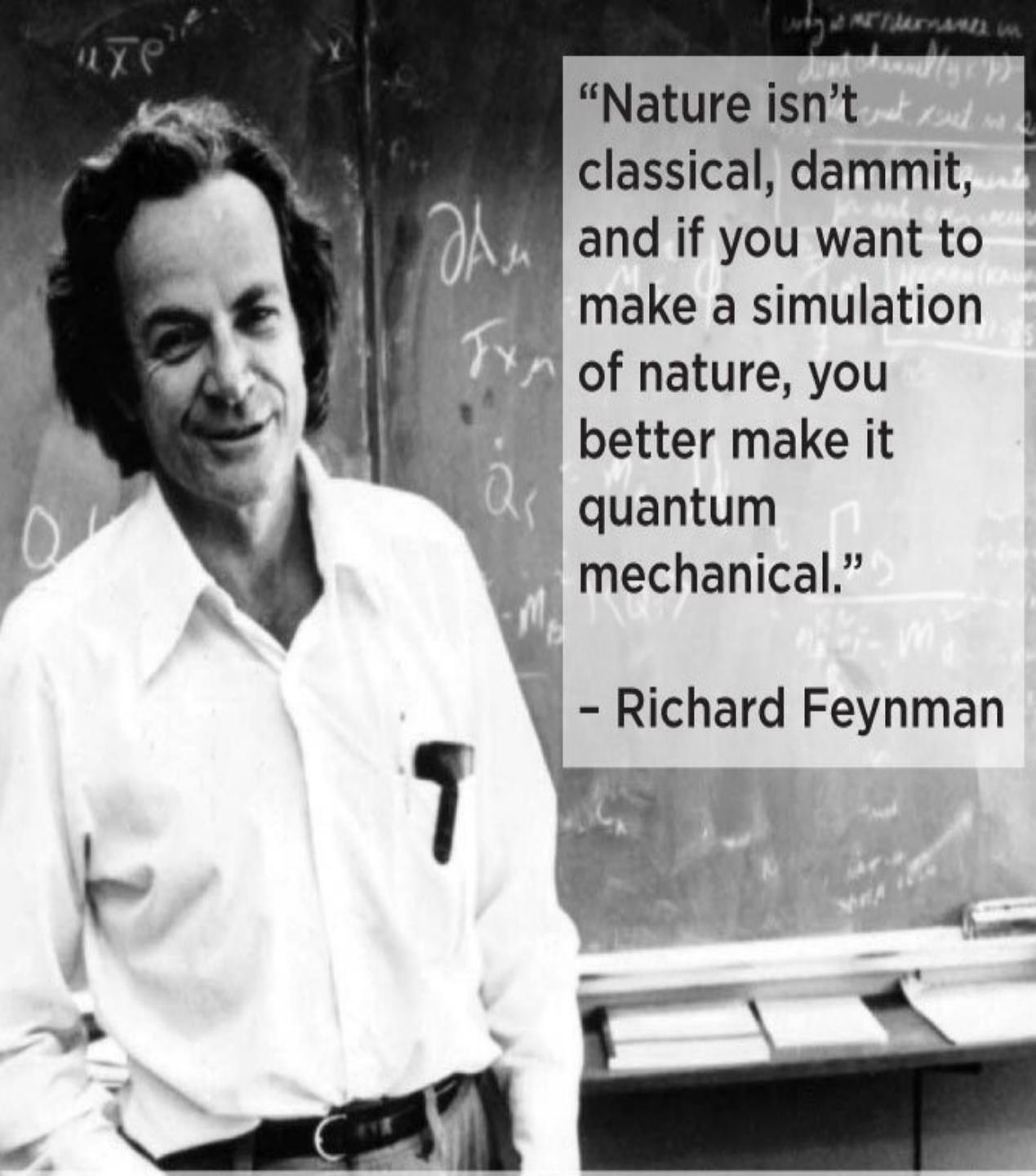


Efficient Hamiltonian Encoding And Gate Simulations

Manqoba Hlatshwayo
mbn6916@wmich.edu

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“Nature isn’t classical, dammit, and if you want to make a simulation of nature, you better make it quantum mechanical.”

- Richard Feynman

Realizing Feynman’s dream of quantum simulation requires

Minimizing Errors:

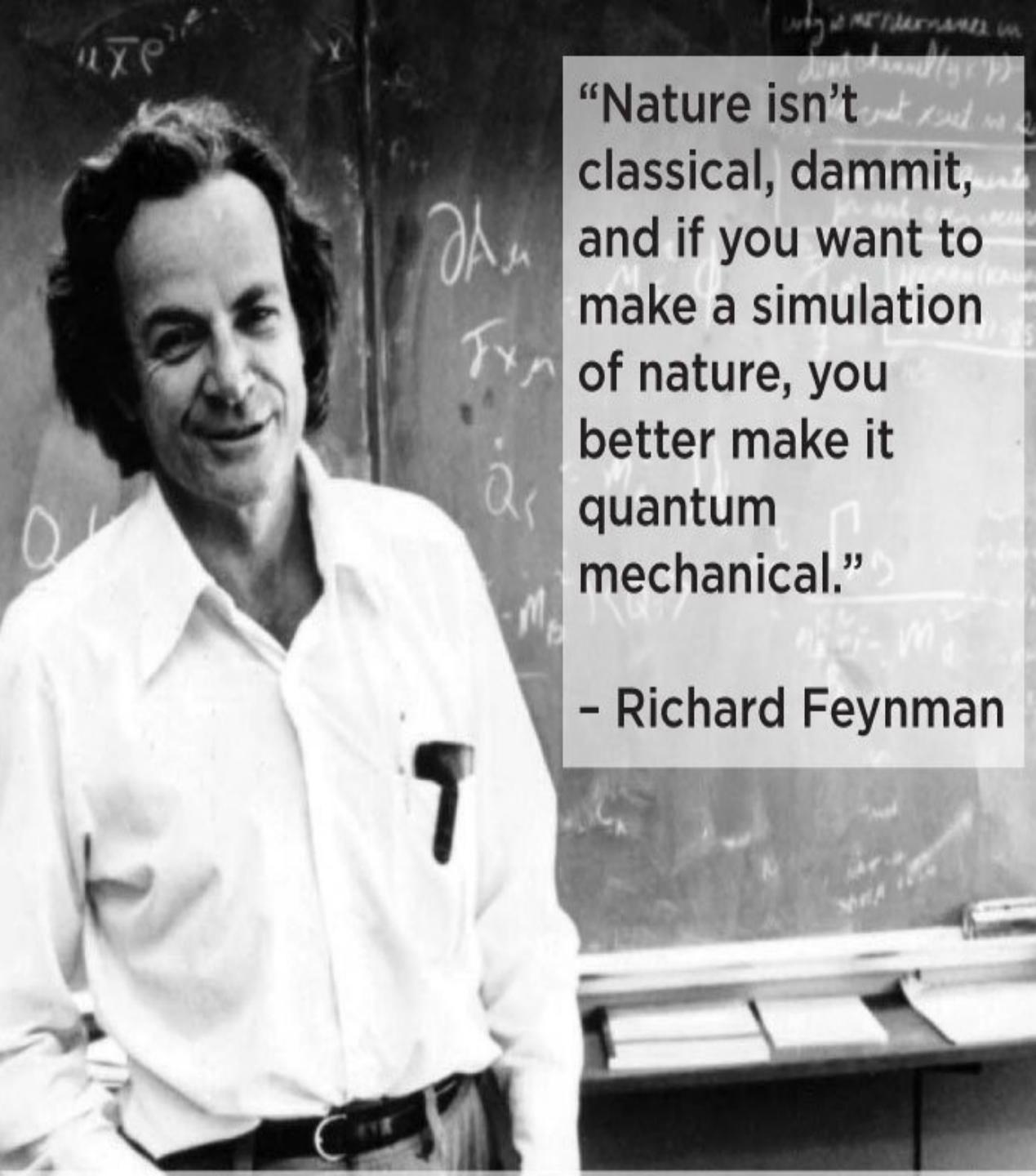
- Better hardware
- High-fidelity gates
- Error mitigation / correction

Optimizing efficiency:

- Better encoding schemes
- Better quantum algorithms

Experimental accuracy:

- Better theoretical models
- Predict new phenomena



“Nature isn’t classical, dammit, and if you want to make a simulation of nature, you better make it quantum mechanical.”

- Richard Feynman

My research contributes to the highlighted subsections

Minimizing Errors:

- Better hardware
- **High-fidelity gates**
- Error mitigation / correction

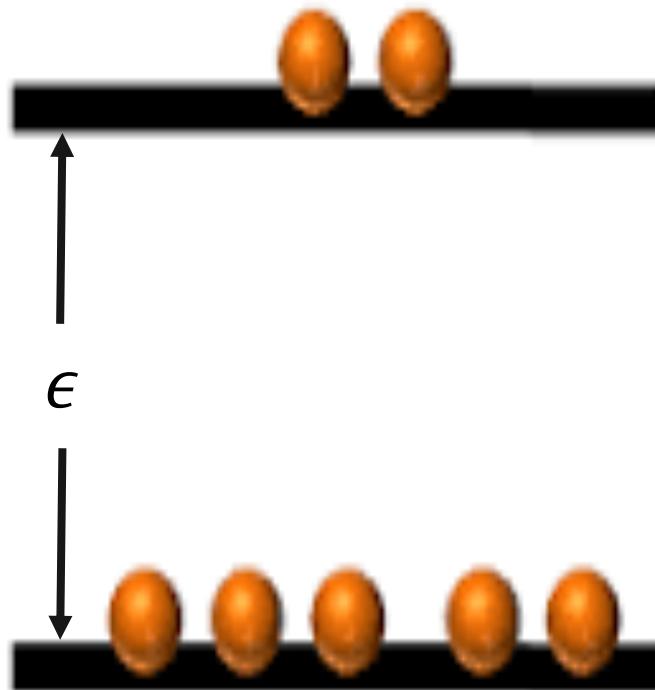
Optimizing efficiency:

- **Better encoding schemes**
- Better quantum algorithms

Experimental accuracy:

- **Better theoretical models**
- Predict new phenomena

The Lipkin Hamiltonian is a good toy model for proof concept quantum simulations for fermionic many-body dynamics

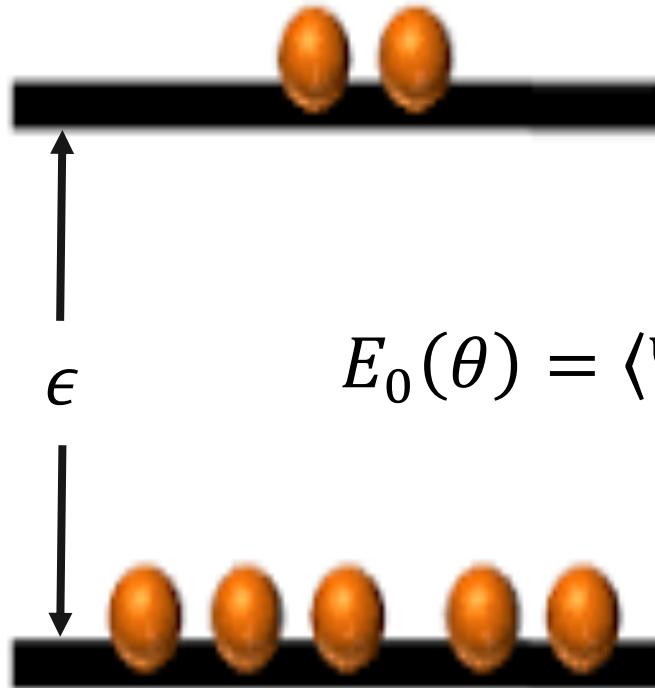


Hamiltonian encoding schemes

- 1) Fock space occupied/empty $H_F(2^{2N} \times 2^{2N})$
- 2) Individual spin up/down $H_I(2^N \times 2^N)$
- 3) Total J spin $|J, M\rangle$ for (w=0) $H_J(N \times N)$

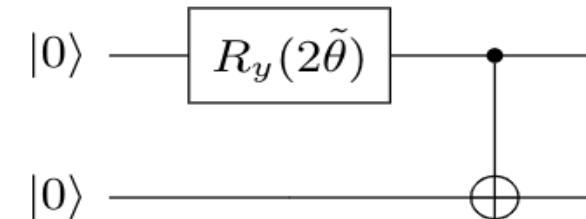
$$\frac{H}{\epsilon} = J_0 - \frac{V}{2\epsilon}(J_+^2 + J_-^2) - \frac{W}{2\epsilon}(J_+J_- + J_-J_+)$$

An efficient encoding of the Lipkin Hamiltonian by exploiting its symmetries and employing the Gray code: example N=2



$$E_0(\theta) = \langle \Psi(\theta) | H | \Psi(\theta) \rangle$$

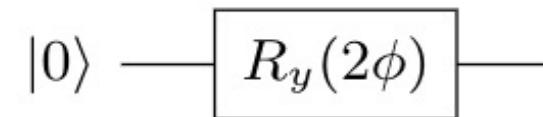
$$H_I = \frac{1}{2}(ZI + IZ) - \frac{\nu}{2}(XX + YY)$$



M. Cervia et al. Phys. Rev. C **104**, 024305 (2021)

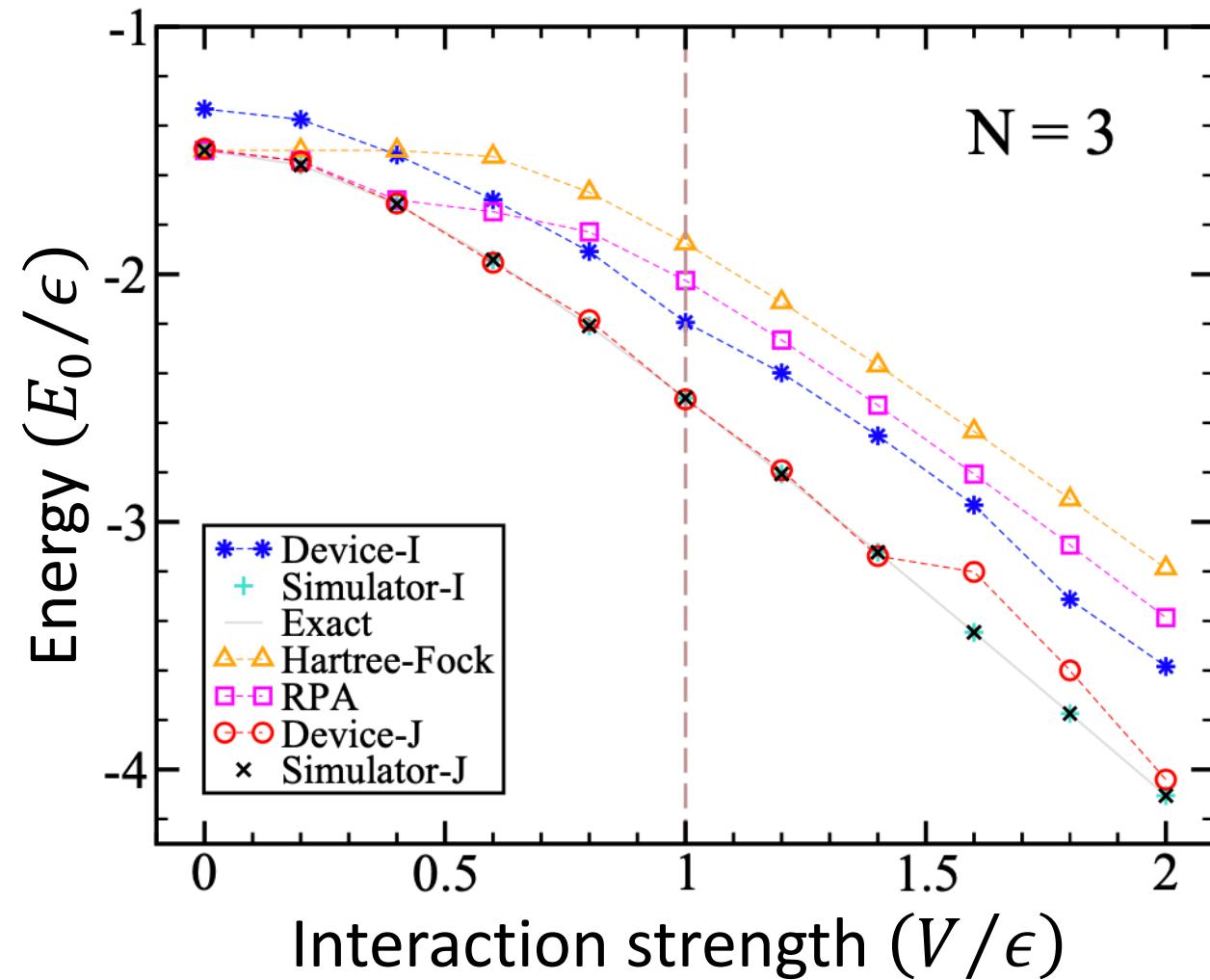
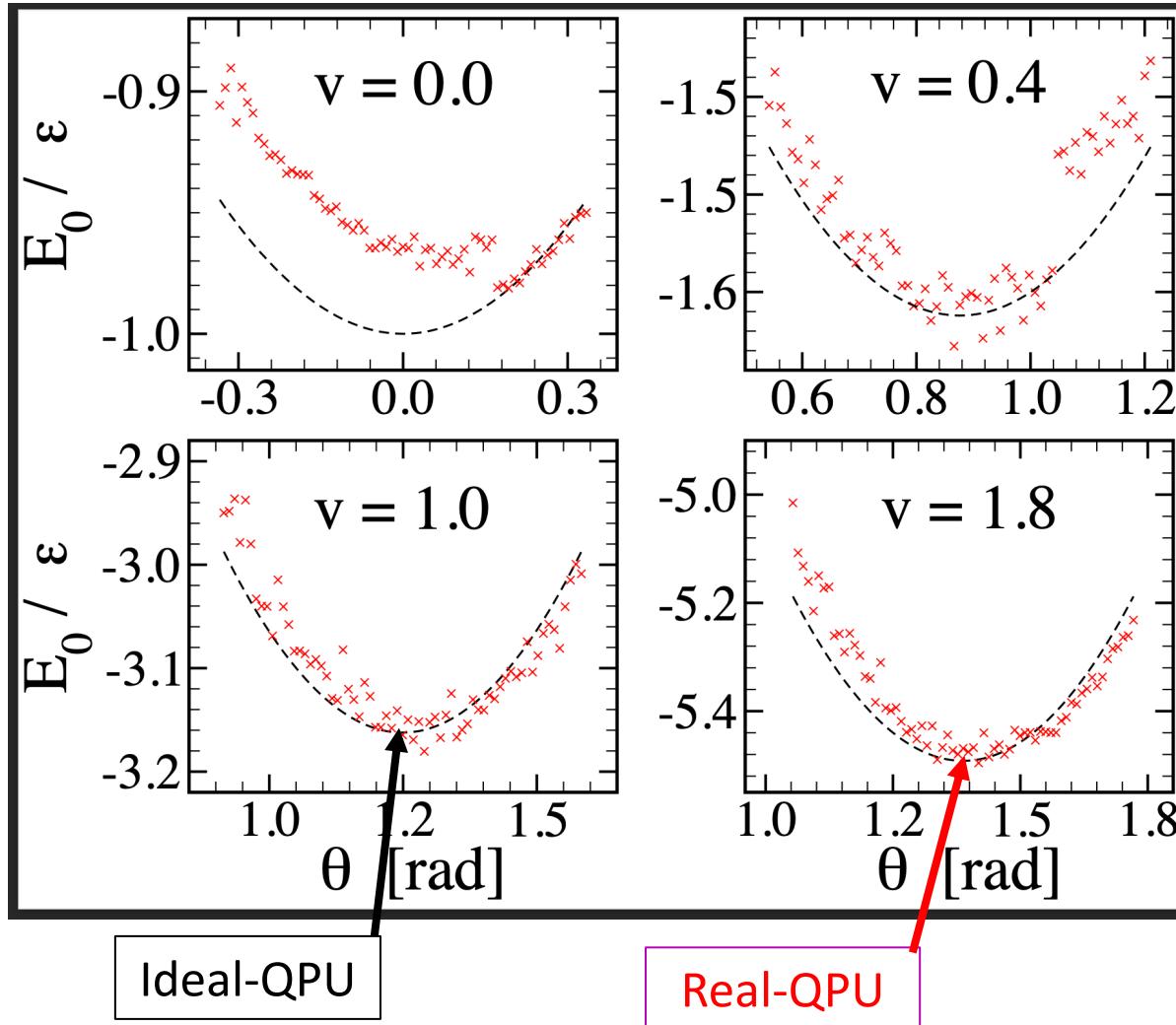
$$\frac{H}{\epsilon} = J_0 - \frac{V}{2\epsilon}(J_+^2 + J_-^2) - \frac{W}{2\epsilon}(J_+J_- + J_-J_+)$$

$$H_J = -Z - \nu X$$



M.Q. Hlatshwayo, D. Lacroix, E. Litvinova et al. Phys. Rev. C **106**, 024319 (2022)

Ground state energy results of using the variational quantum eigensolver (VQE) on a noisy IBM QPU closely agree with exact solution.



How to simulate the excited states of the Lipkin model using the quantum equation of motion (qEOM)

Solve for $H|n\rangle = E|n\rangle$ given $|0\rangle$

Define excitation $O^\dagger_n|0\rangle = |n\rangle$, $O_n|0\rangle = 0$

configuration complexity

$$E_{n0} = (E_n - E_0) = \frac{\langle 0 | [O_n, [H, O^\dagger_n]] | 0 \rangle}{\langle 0 | [O_n, O^\dagger_n] | 0 \rangle}$$

g.s and $\langle . \rangle$
estimated by
VQE on a QPU

$$O^\dagger_n(\alpha) = \sum_{\alpha, \mu_\alpha} \left[X_{\mu_\alpha}^\alpha(n) K_{\mu_\alpha}^\alpha - Y_{\mu_\alpha}^\alpha(n) (K_{\mu_\alpha}^\alpha)^\dagger \right]$$

$$K_{\mu_1}^1 = a_p^\dagger a_h \text{ (RPA)} \quad \text{and} \quad K_{\mu_2}^2 = a_{p1}^\dagger a_{p2}^\dagger a_{h2} a_{h1} \text{ (SRPA)}$$

Solving the equation of motion leads to a generalized eigenvalue equation to be solved on classical computers

$$E_{n0} = \frac{\langle 0 | [O_n, [H, O_n^\dagger]] | 0 \rangle}{\langle 0 | [O_n, O_n^\dagger] | 0 \rangle}, \quad \delta E_{n0} = 0 \quad \xrightarrow{\text{variation with respect to the coefficients of } O_n^\dagger}$$

$$\hat{O}_n^\dagger = \sum_{\alpha} \sum_{\mu_\alpha} [X_{\mu_\alpha}^\alpha(n) \hat{K}_{\mu_\alpha}^\alpha - Y_{\mu_\alpha}^\alpha(n) (\hat{K}_{\mu_\alpha}^\alpha)^\dagger]$$

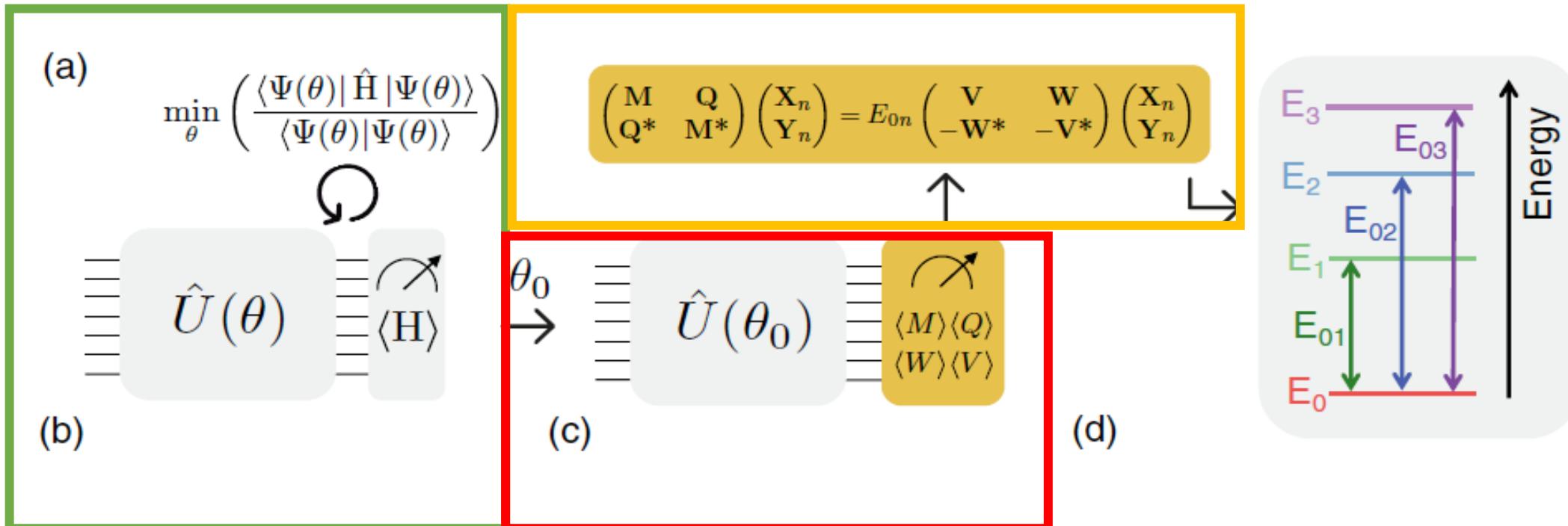
$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B}^* & \mathcal{A}^* \end{pmatrix} \begin{pmatrix} X^n \\ Y^n \end{pmatrix} = E_{n0} \begin{pmatrix} \mathcal{C} & \mathcal{D} \\ -\mathcal{D}^* & -\mathcal{C}^* \end{pmatrix} \begin{pmatrix} X^n \\ Y^n \end{pmatrix}$$

$$\begin{aligned} \mathcal{A}_{\mu_\alpha \nu_\beta} &= \langle [(\hat{K}_{\mu_\alpha}^\alpha)^\dagger, [\hat{H}, \hat{K}_{\nu_\beta}^\beta]] \rangle, \\ \mathcal{B}_{\mu_\alpha \nu_\beta} &= -\langle [(\hat{K}_{\mu_\alpha}^\alpha)^\dagger, [\hat{H}, (\hat{K}_{\nu_\beta}^\beta)^\dagger]] \rangle, \\ \mathcal{C}_{\mu_\alpha \nu_\beta} &= \langle [(\hat{K}_{\mu_\alpha}^\alpha)^\dagger, \hat{K}_{\nu_\beta}^\beta] \rangle, \\ \mathcal{D}_{\mu_\alpha \nu_\beta} &= -\langle [(\hat{K}_{\mu_\alpha}^\alpha)^\dagger, (\hat{K}_{\nu_\beta}^\beta)^\dagger] \rangle. \end{aligned}$$

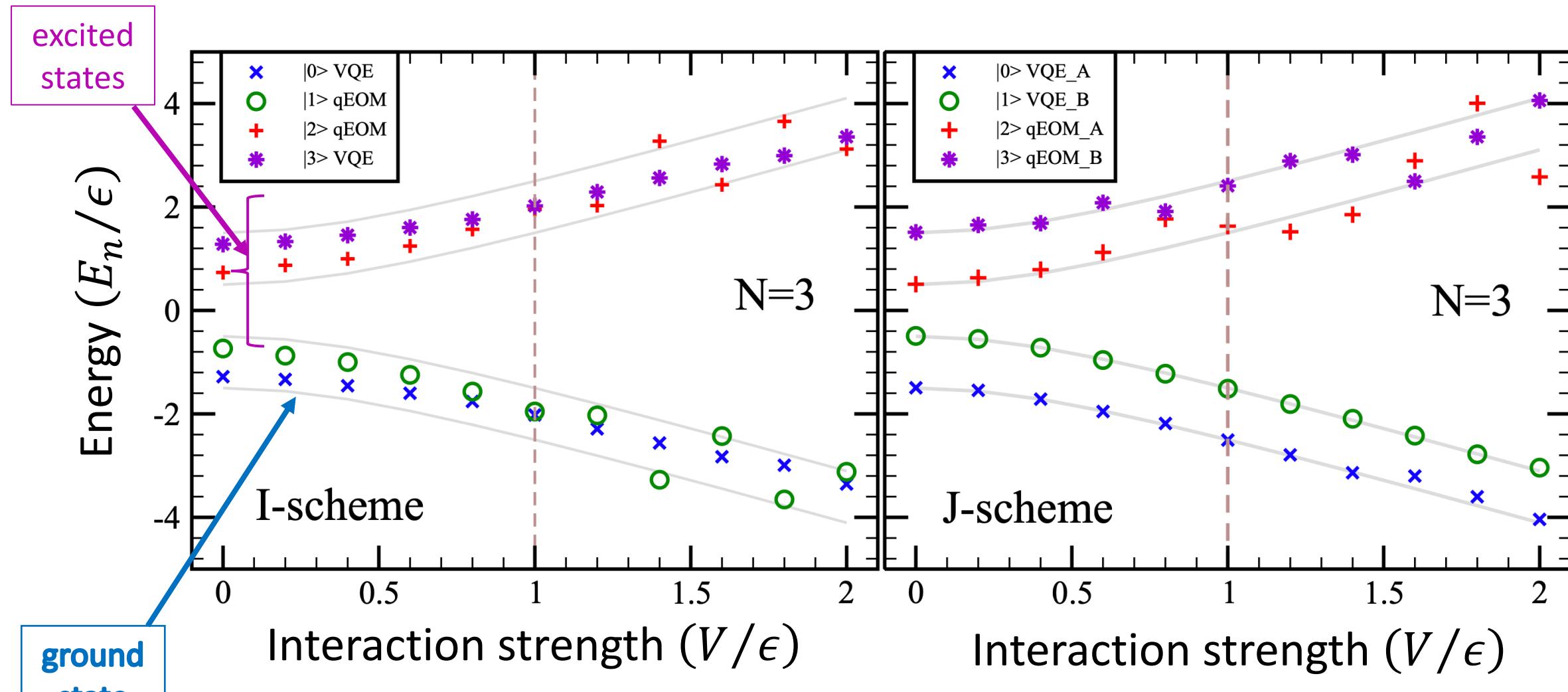
$\langle . \rangle$ measured on a QPU

Overview of the quantum equation of motion (qEOM)

1. Use VQE to find ground state $|0\rangle$
2. Use QPU to find matrix expectation values $\langle \cdot \rangle$
3. Use CPU to solve for the GEE for excitation energies E_{0n}



Results of Lipkin Hamiltonian's excited states energy found using qEOM for N=3 particles on a noisy IBM-QPU



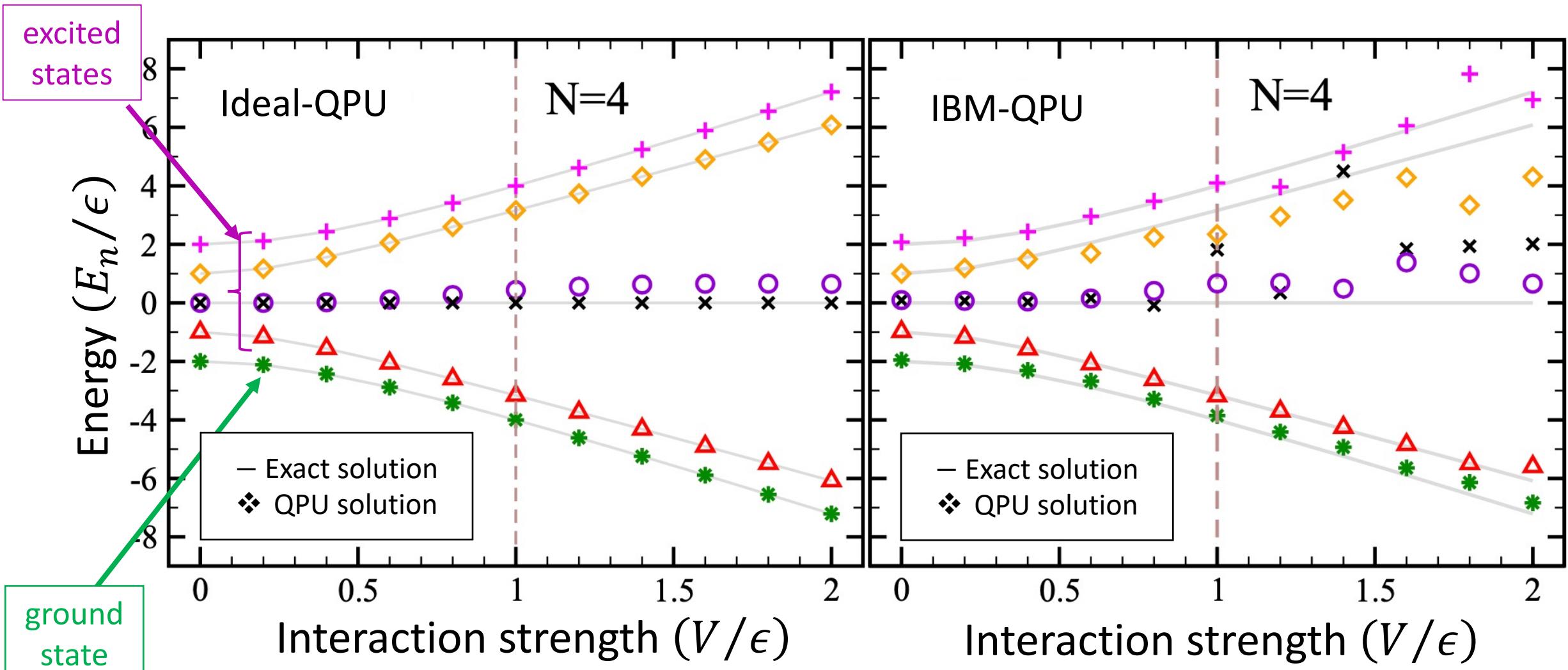
Do we get a better theoretical model by including higher configuration complexity (α) terms in the excitation operator?

$$O^\dagger_n(\alpha) = \sum_{\alpha, \mu_\alpha} [X_{\mu_\alpha}^\alpha(n) K_{\mu_\alpha}^\alpha - Y_{\mu_\alpha}^\alpha(n) (K_{\mu_\alpha}^\alpha)^\dagger]$$

$$K_{\mu_1}^1 = a_p^\dagger a_h \quad (\alpha = 1, RPA)$$

$$K_{\mu_2}^2 = a_{p1}^\dagger a_{p2}^\dagger a_{h2} a_{h1} \quad (\alpha = 2, SRPA)$$

Yes, SRPA shows more accurate results than RPA on an ideal QPU but has significant deviations on a noisy QPU for $V/\epsilon > 1$



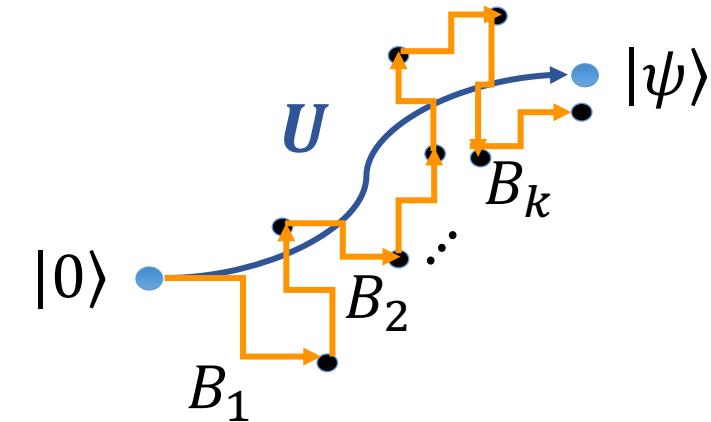
In the near-term quantum computers, we can build custom gates for the problem of interest



$$U \approx B_k \cdots B_2 B_1$$



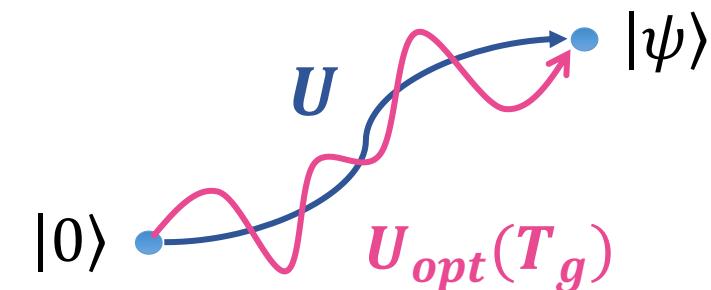
Buildup of noise, error



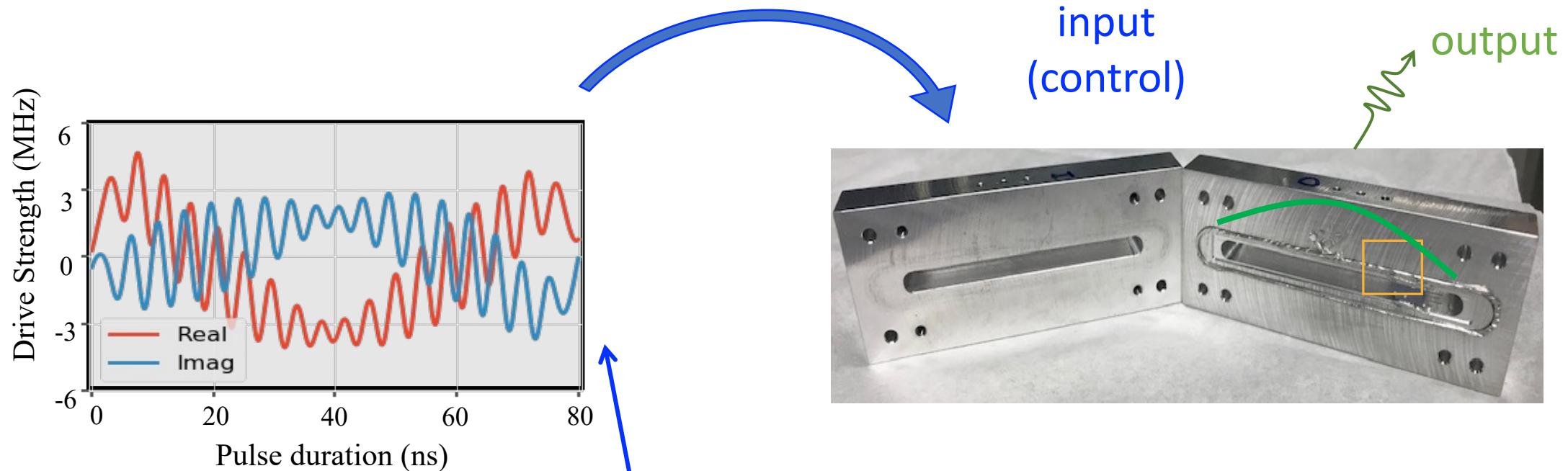
$$U \approx U_{opt}(T_g)$$



Single gate,
noise resilient



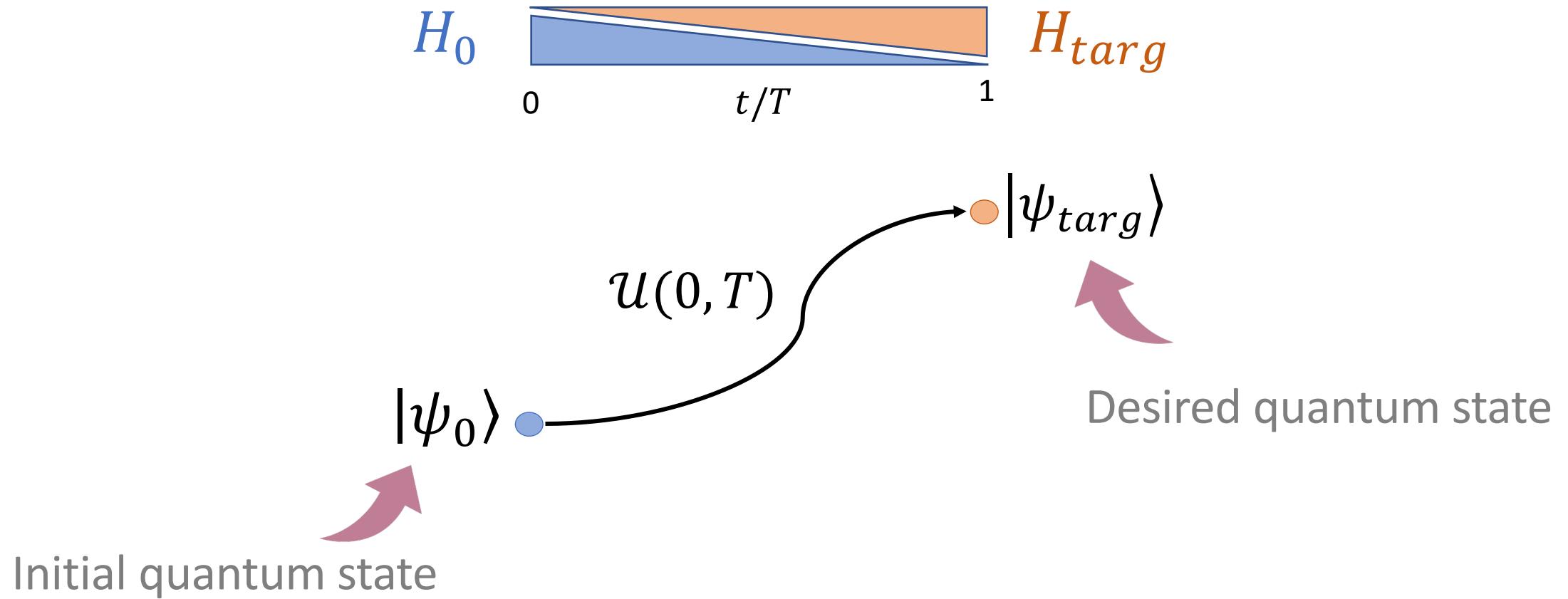
'Basic' quantum gates are realized with optimization techniques, hinging on a realistic model of the physical quantum device



Goal: find control pulses that optimizes the fidelity

$$F = |\text{tr}(U_{targ}^\dagger U_{opt})| / \dim(H)$$

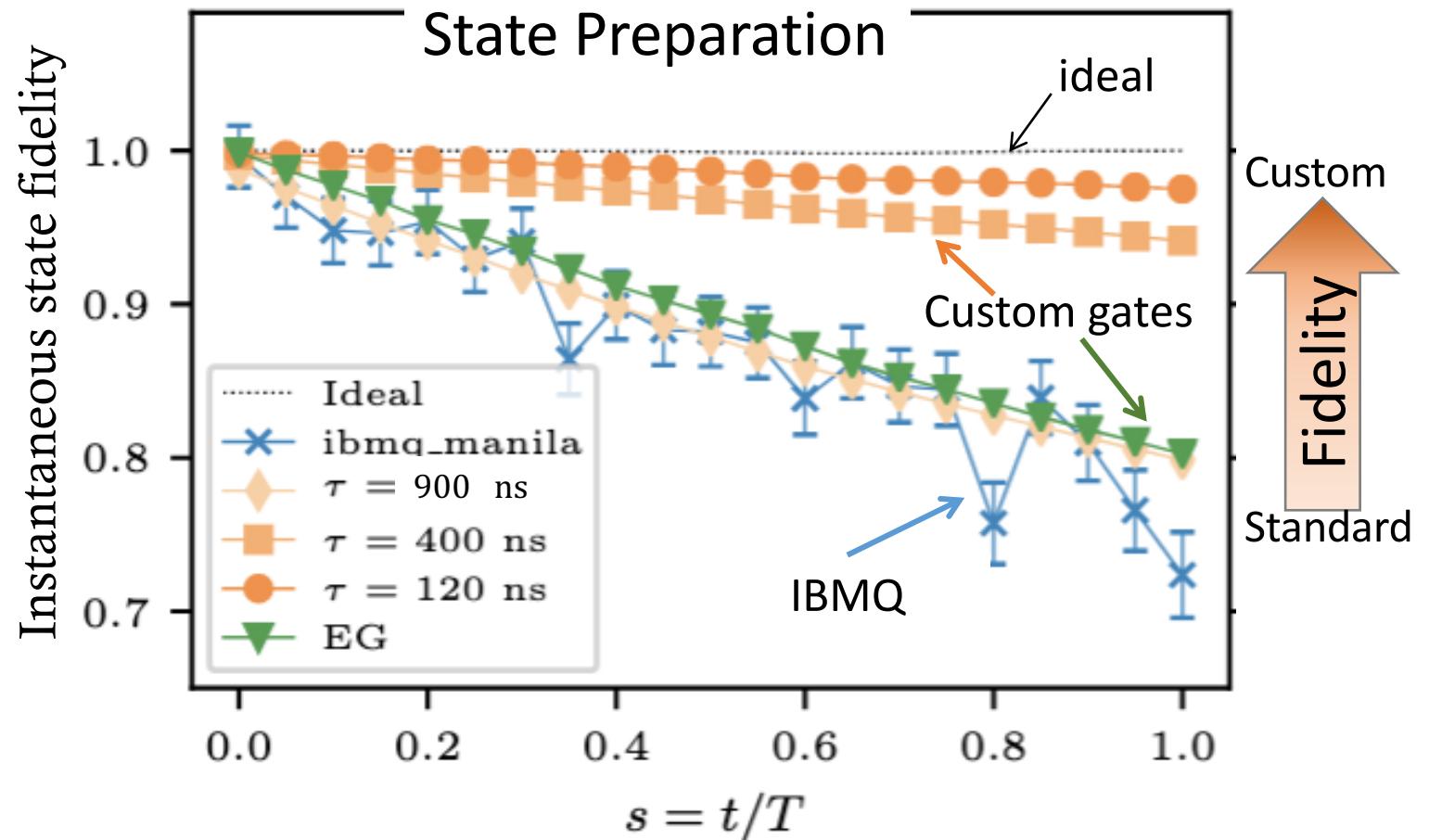
To simulate scattering we need state preparation approach, e.g., using adiabatic evolution



Custom gates enable major performance improvements for state preparation, and broader class of problems

Any long sequence
of arbitrary operations

Can be realized on IBMQ
using pulse control



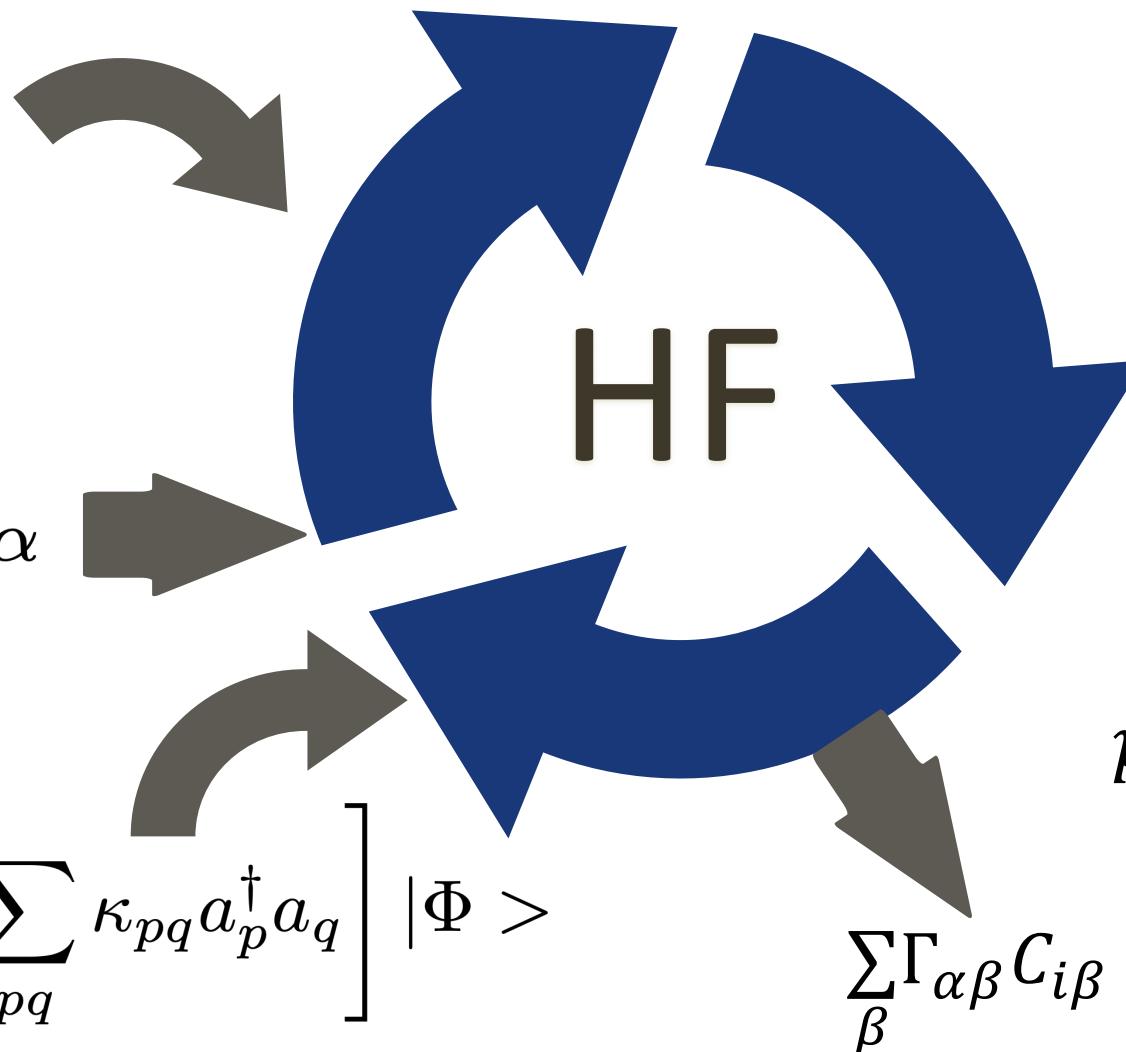
Self-consistent reference states are a critical starting point for computing various many-body phenomena

$$\psi_i = \sum_{\alpha=1} C_{i\alpha} \phi_{\alpha}$$

$$\psi_i = \sum_{\alpha=1} [e^{\kappa}]_{i\alpha} \phi_{\alpha}$$

Thouless Theorem

$$|\Psi\rangle = e^{\hat{K}} |\Phi\rangle = \exp \left[\sum_{pq} \kappa_{pq} a_p^\dagger a_q \right] |\Phi\rangle$$



Parameters $\{x\}$

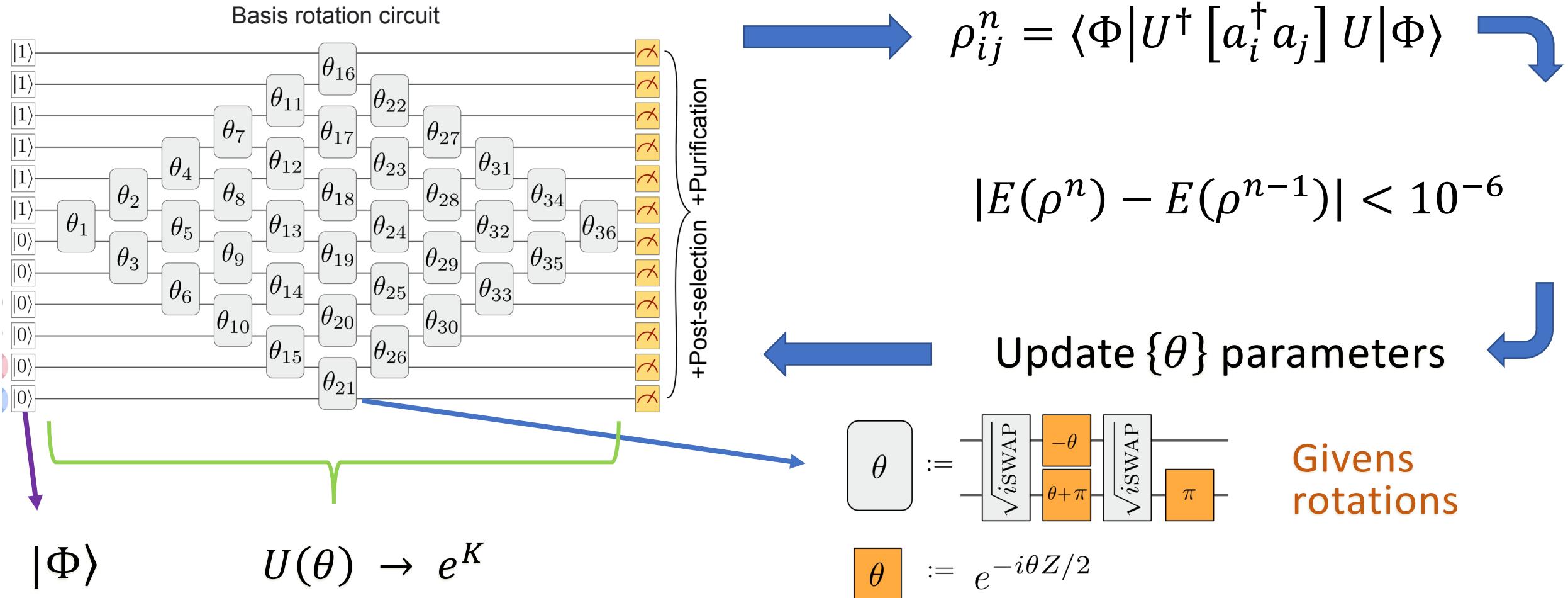
$$p_1 = N \times N$$

$$p_2 = \frac{N \times (N - 1)}{2}$$

$$p_3 = A \times (N - A)$$

$$\sum_{\beta} \Gamma_{\alpha\beta} C_{i\beta} = \epsilon_i C_{i\alpha}$$

Employing the variational quantum eigensolver to perform Hartree-Fock basis rotation on a quantum computer



Preliminary results of the quantum Hartree-Fock algorithm for simulating the Negele model with A=3 particles on a real QPU

$$V(x) = \sum_{i=1,2} \frac{v_i}{\sigma_i \sqrt{\pi}} e^{-\frac{x^2}{\sigma_i^2}}$$



Properties:

- 1D simple nuclear model
- contains main features of many-body problem
- has a numerical exact solution
- has tunable coupling strength

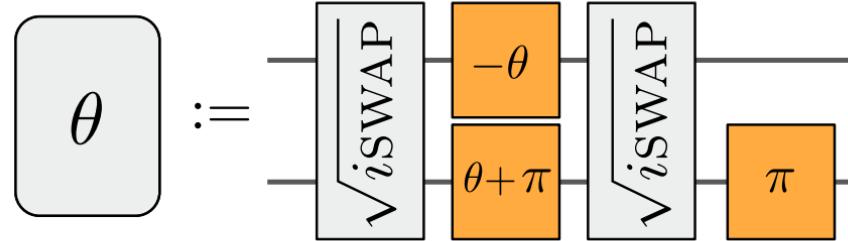
TABLE I: HF ground-state energy of Negele model with $A = 3$ particles.

	Methods	N -States		Errors (%)	
		81	6	exact	approx
Classical	HF Eqns.	-1.0494	-1.0112	3.64	
	Opt. $C = e^\kappa$		-1.0009	4.56	1.02
Quantum	Ideal QPU	-1.0105	3.71	0.07	
	Real QPU	-0.9253	11.77	8.49	

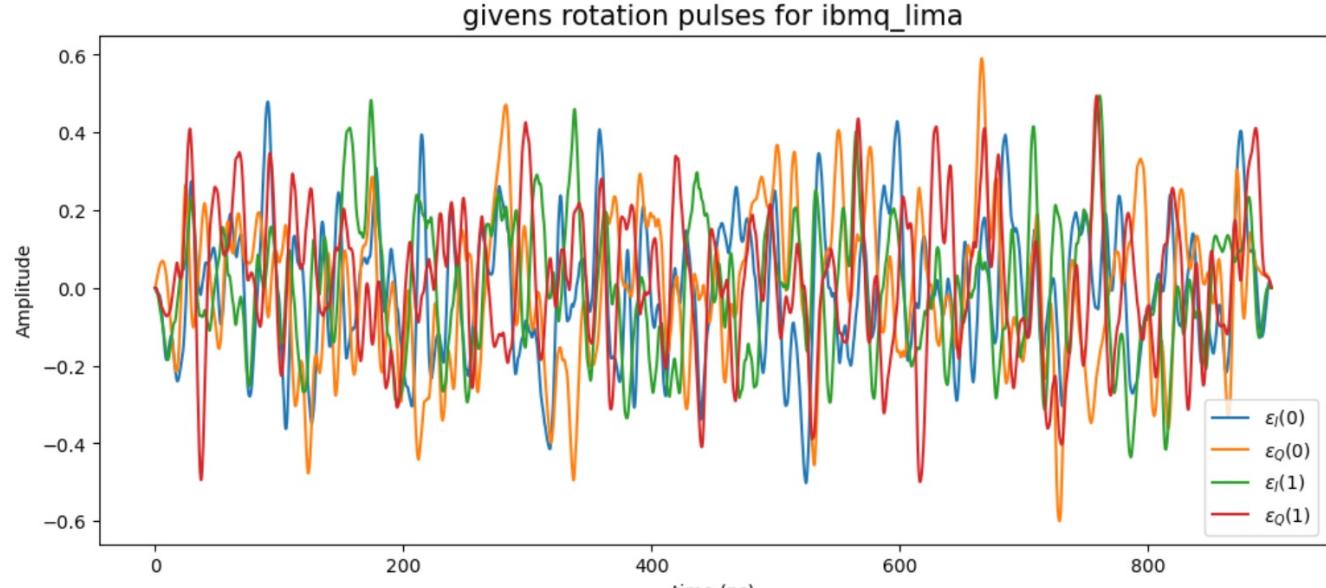
ibmq_nairobi (7 qubits)

M.Q. Hlatshwayo, K.A. Wendt et al. In preparation.

A more efficient and less noisy method is to replace the Givens rotation gates with optimal control pulses

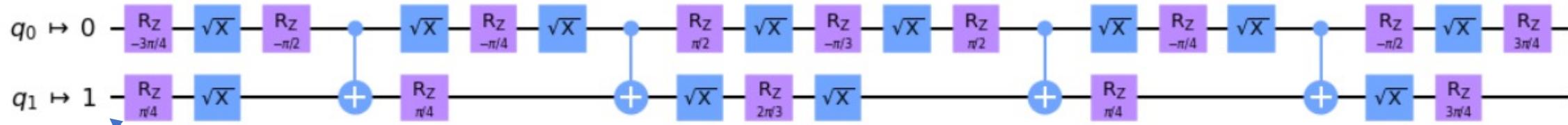


$$\theta := e^{-i\theta Z/2}$$



M.Q. Hlatshwayo, K.A. Wendt et al. In preparation.

Global Phase: 2π



Compiled into 30 native device gates for the `ibmq_lima`

Summary of talk

1. To realize Feynman's dream of simulation nature, progress is needed in minimizing errors from quantum devices, optimizing efficiency of quantum algorithms, and improvements on the theoretical models for many-body physics.
2. Efficient Hamiltonian encoding of the Lipkin model by exploiting its symmetries and employing the Gray code for minimal qubit usage and shallow circuit depths.
3. Promising results of quantum simulation of the ground state energy (using VQE) and excited states energies (using qEOM) of the Lipkin model for small systems on noisy QPUs. Extension to larger systems and closed shell nuclear is underway.
4. Higher configuration complexity (within the EOM framework leads to more accurate results as expected. Efficient encoding scheme requires
5. Custom gates leads to higher fidelities for state preparation via adiabatic process
6. Perform Hartree-Fock basis rotation via Given rotations on a quantum computer. And how to improve the gate fidelity by using optimal control-pulse theory.

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Experiments

We appreciate cloud access of IBM quantum computers to run simulations for parts of this work. The views expressed are those of the authors, and do not reflect the official policy or position of IBM.

Collaborators:

Elena Litvinova, Western Michigan University (dissertation advisor)

Denis Lacroix, University of Paris-Saclay (dissertation committee)

Kyle Wendt, Lawrence Livermore National Lab (dissertation committee)

Sofia Quaglioni, Lawrence Livermore National Laboratory

Yinu Zhang, Western Michigan University

Ryan LaRose, EPFL Computational Quantum Science Lab

Herlik Wibowo, York University

Coello Tono Perez, Oak Ridge National Laboratory

Ngiyabonga
Merci
Thank You

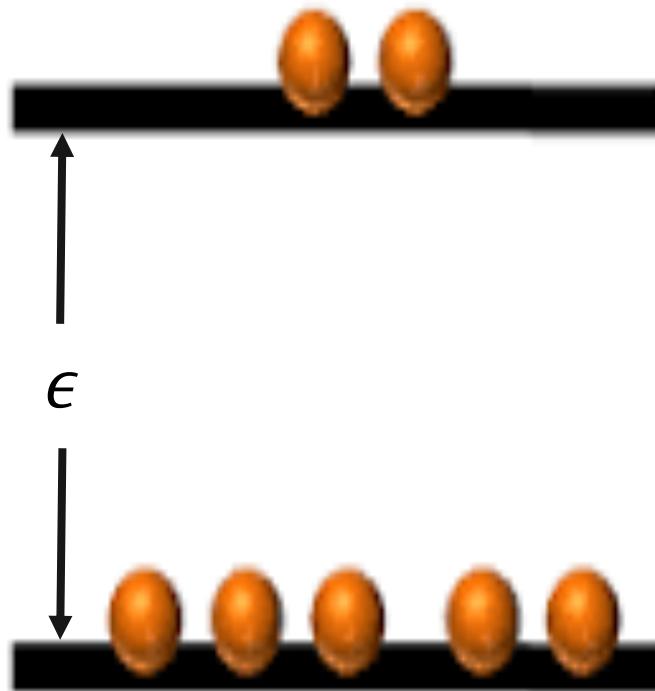


Email: mbn6916@wmich.edu



Extra Slides for Q&A

An efficient encoding of the Lipkin Hamiltonian by exploiting its symmetries and employing the Gray code



$$\frac{H}{\epsilon} = J_0 - \frac{V}{2\epsilon}(J_+^2 + J_-^2) - \frac{W}{2\epsilon}(J_+J_- + J_-J_+)$$

M.Q. Hlatshwayo et al. Phys. Rev. C **106**, 024319 (2022)

O. Di Matteo et al. Phys. Rev. A **103**, 042405 (2021)

$$J_{\pm}^2 |J, M\rangle \propto |J, M \pm 2\rangle$$

$$\bar{H}_J^{(N)} = \begin{pmatrix} \bar{H}_A & 0 \\ 0 & \bar{H}_B \end{pmatrix}$$

$$\begin{aligned} |J, -J\rangle &\equiv |0\rangle \rightarrow |\text{bin}(0)\rangle, \\ |J, -J + 2\rangle &\equiv |1\rangle \rightarrow |\text{bin}(1)\rangle, \end{aligned}$$

$$2^q = \frac{N}{2} + 1$$

$$\begin{aligned} &\vdots \\ |J, J - 2\rangle &\equiv |d - 2\rangle \rightarrow |\text{bin}(d - 2)\rangle, \\ |J, J\rangle &\equiv |d - 1\rangle \rightarrow |\text{bin}(d - 1)\rangle, \end{aligned}$$

$$q = \lfloor \log_2(\frac{N}{2} + 1) \rfloor$$

$|\text{bin}(k)\rangle$

Standard binary (SB)

$$H_J(2^q \times 2^q)$$

Gray code (GC)

$$H_J(N \times N)$$

The GC uses less gates than
SB with lower circuit depth

Basis rotation of Hartree-Fock via Given rotations

$$U(e^\kappa) = \exp \left[\sum_{pq} \kappa_{pq} a_p^\dagger a_q \right]$$

$$U(e^\kappa)U(e^{\kappa'}) = U(e^\kappa e^{\kappa'})$$

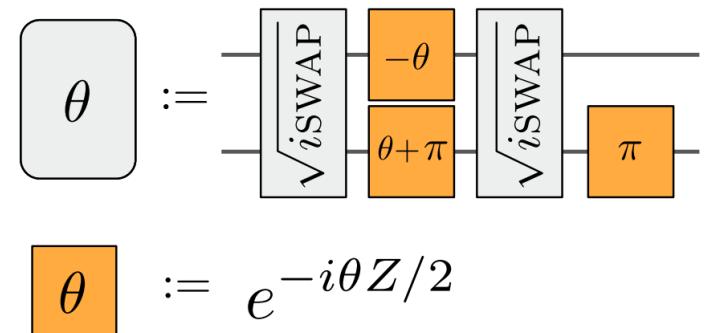
Thouless
Theorem

$$G_k(\theta, p, q) = \begin{pmatrix} 1 & \dots & 0 & \dots & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \dots & \cos(\theta) & \dots & -\sin(\theta) & \dots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \dots & \sin(\theta) & \dots & \cos(\theta) & \dots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \dots & 0 & \dots & 0 & \dots & 1 \end{pmatrix}$$

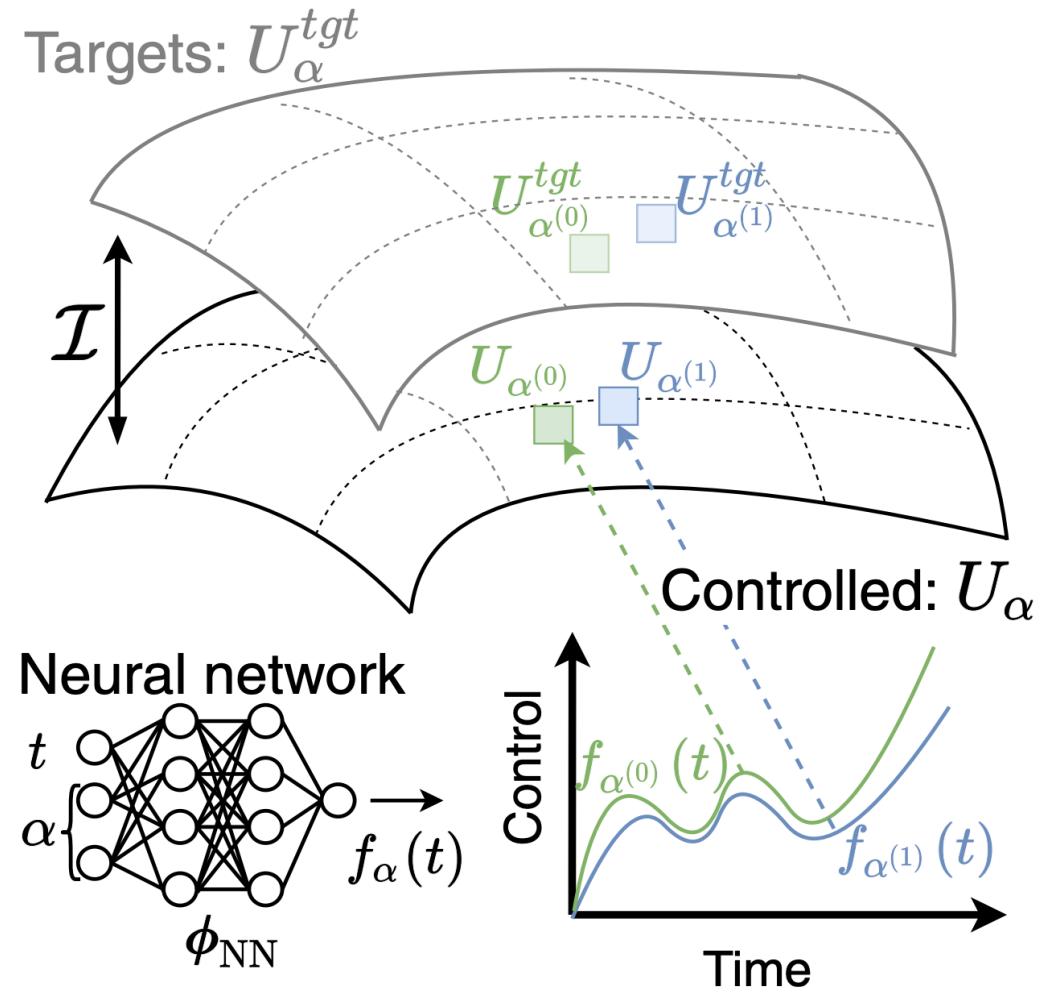
QR - decomposition via Givens rotation

$$A = QR \quad Q = G_1^T G_1^T \dots G_{k-1}^T G_k^T \quad R = G_k G_{k-1} \dots G_2 G_1 A$$

$$|\Psi\rangle = U(Q)U(R)|\Phi\rangle = U(Q) \prod_{p=1}^k e^{i\omega_p n_p} |\Phi\rangle = e^{i\Omega} U(Q)|\Phi\rangle$$



The final step is to train a neural network to find optimal control pulses for an arbitrary Givens rotation gate

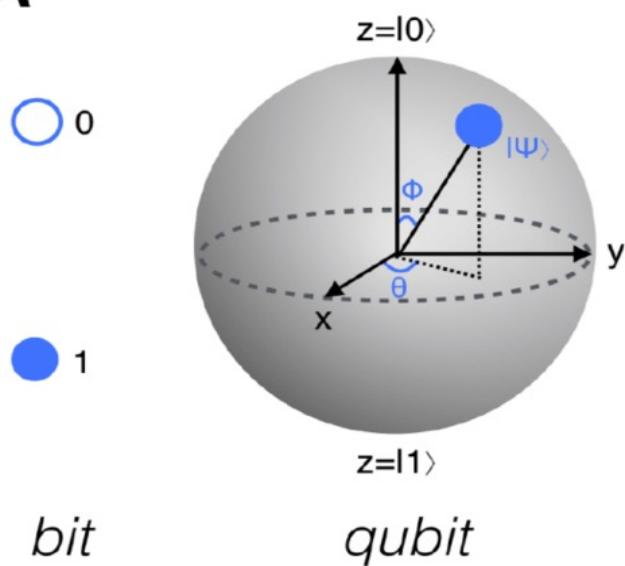


$$\mathcal{I} = \int \left[1 - \frac{1}{\dim[H(\alpha, t)]} |\text{Tr}[U_\alpha^\dagger U_\alpha^{tgt}]|^2 \right] d\alpha$$

- Assume smooth transition $U^{tgt}(\alpha + \delta\theta) \rightarrow H(\alpha + \delta\theta, t)$.
- Avoid unwanted intermediate excitations to higher states.
- Account for all physics constraints from nuclear model.

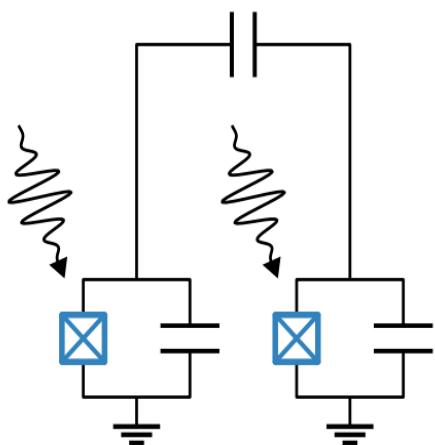
How a superconducting quantum computer works

A

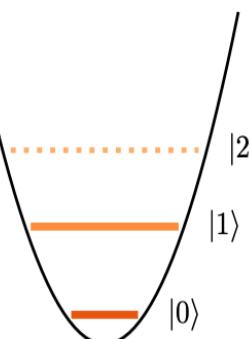


bit

a)

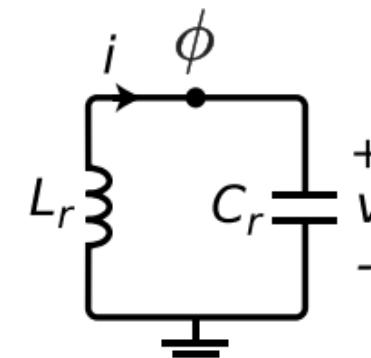


b)

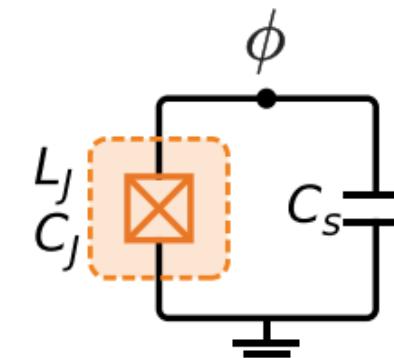


B

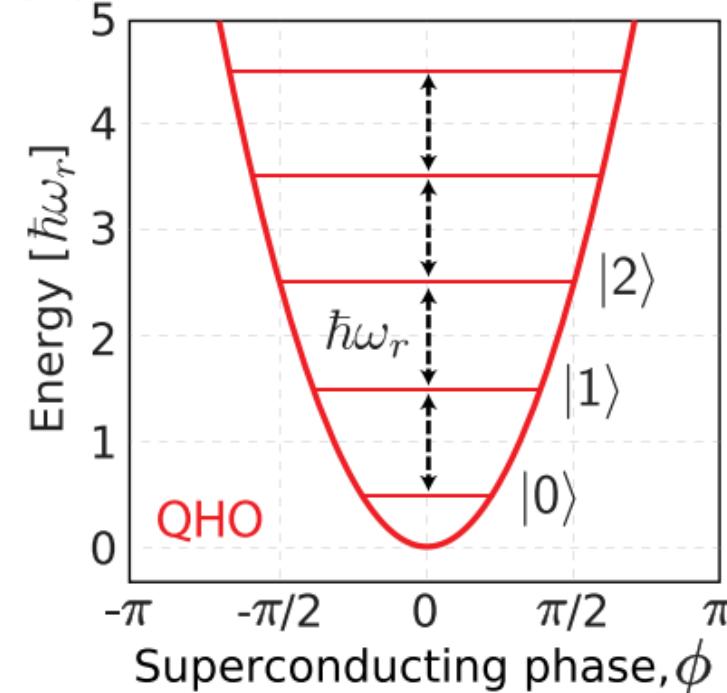
(a)



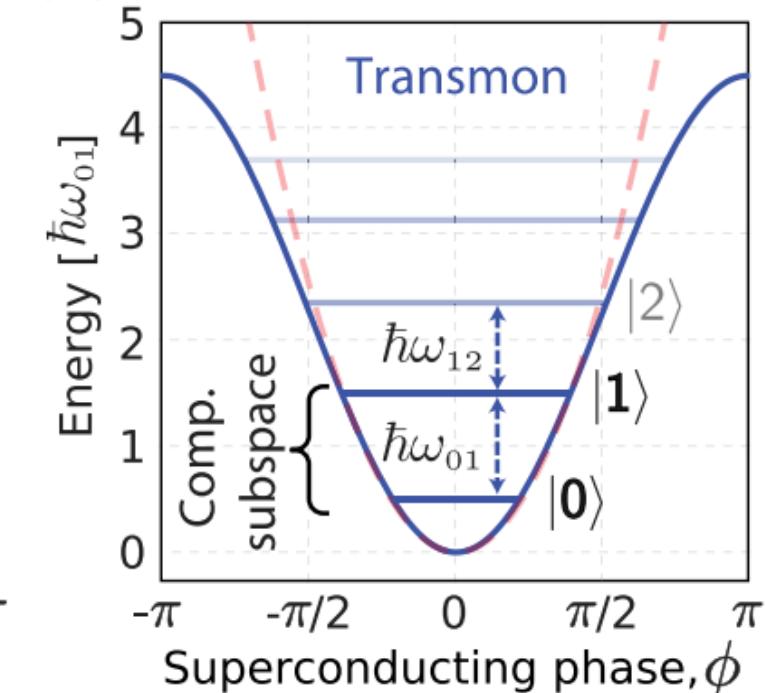
(c)



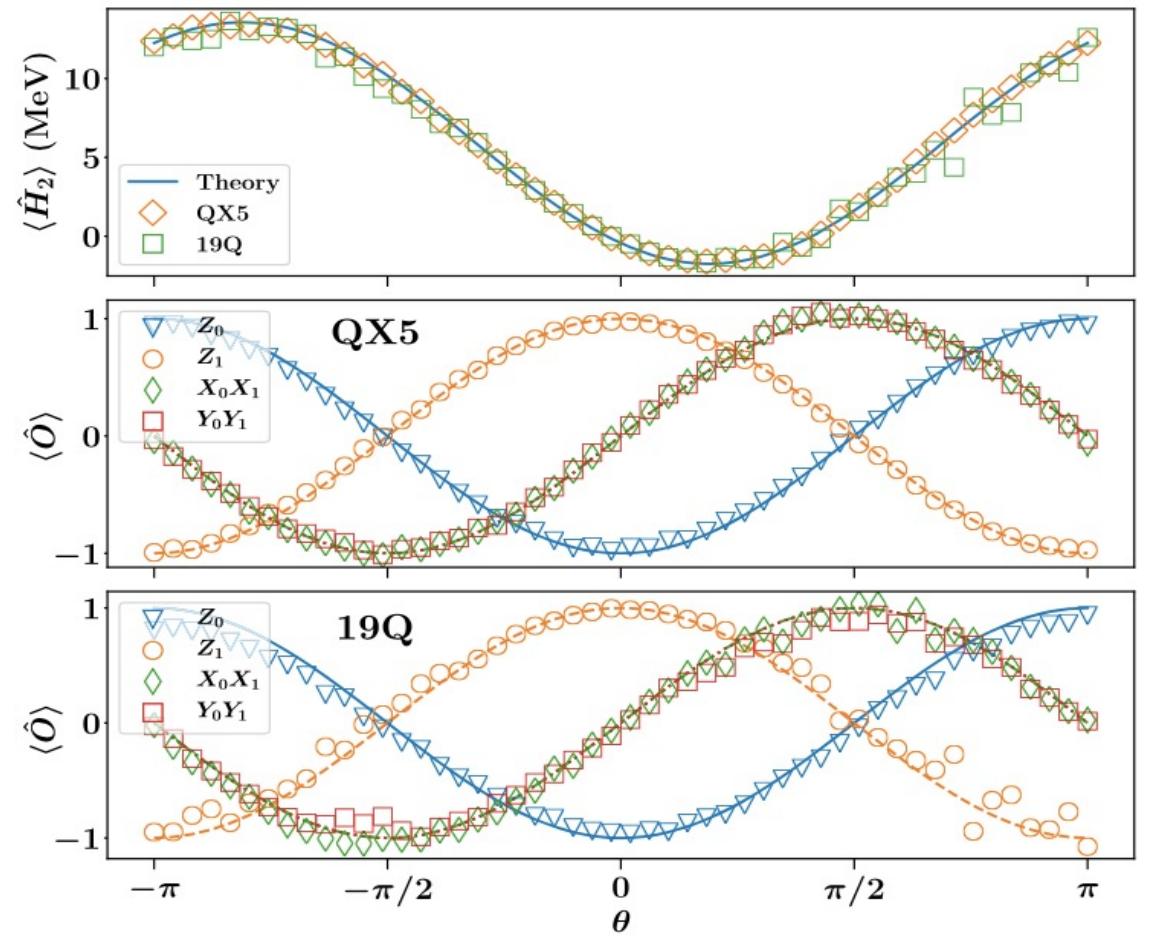
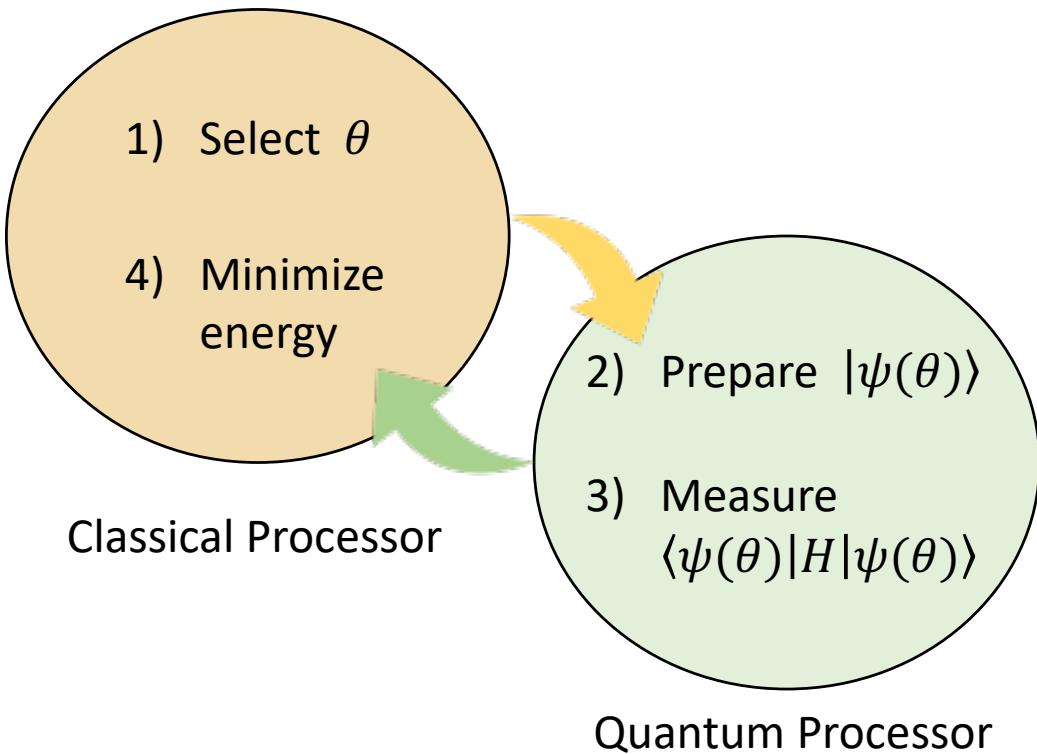
(b)



(d)

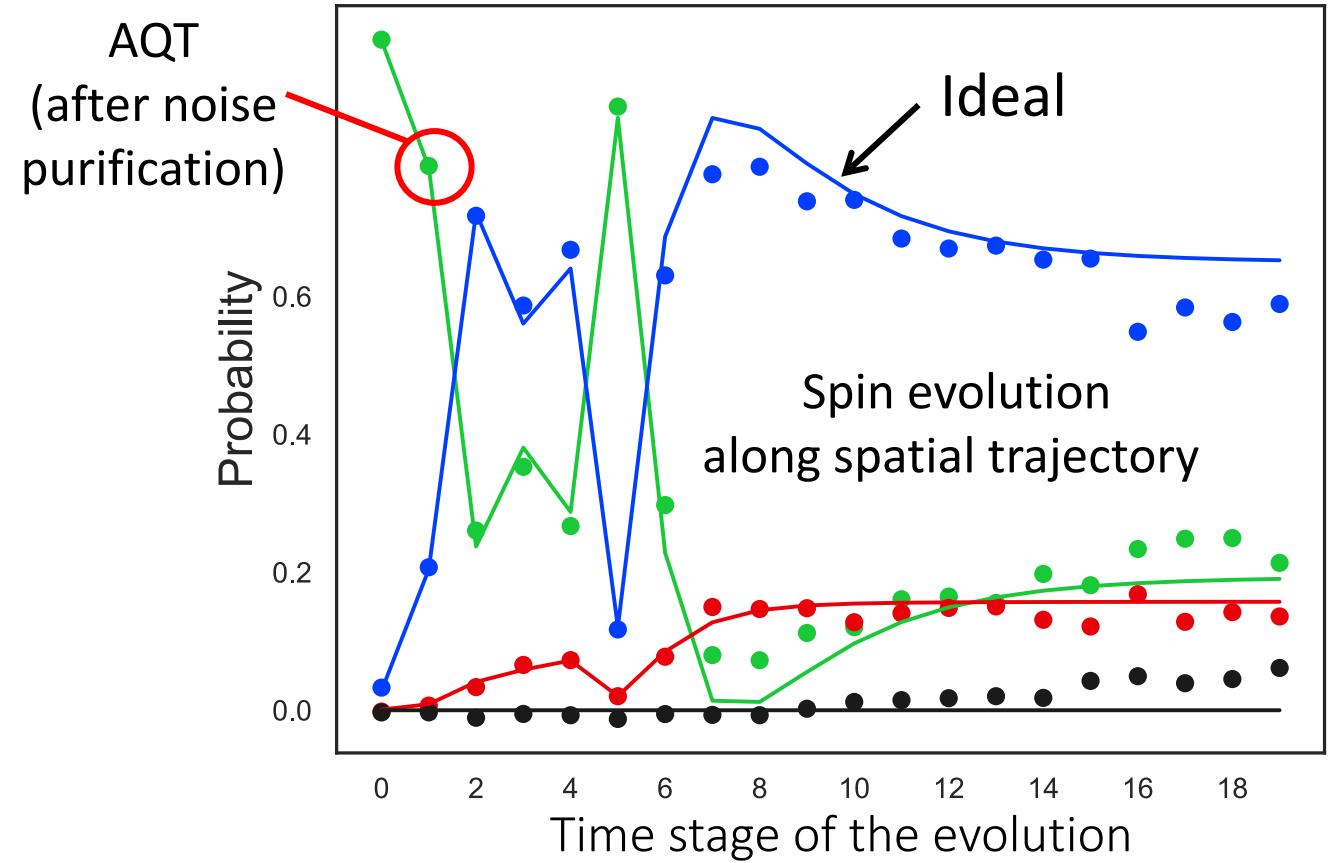
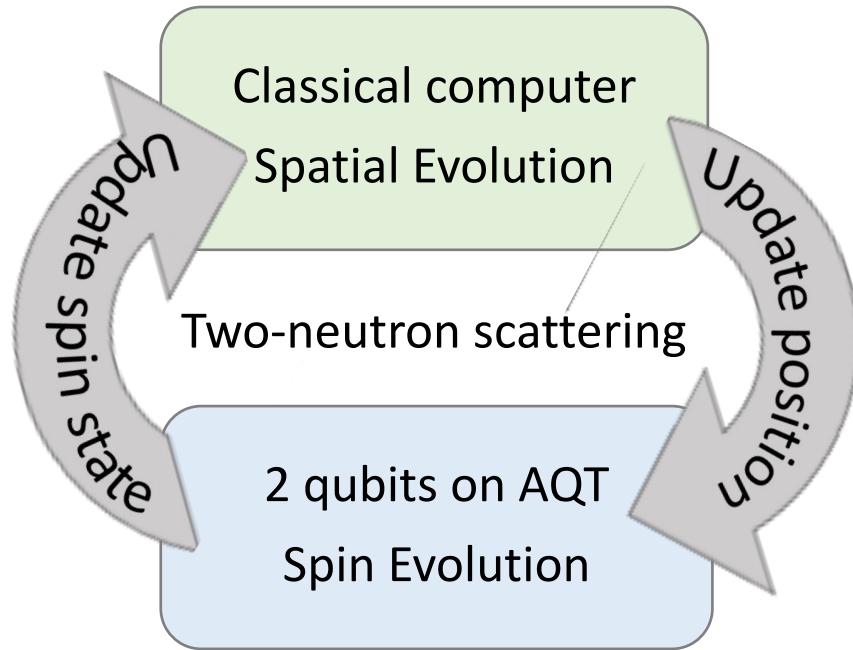


The variational quantum eigensolver is noise resilient hybrid classical-quantum algorithm

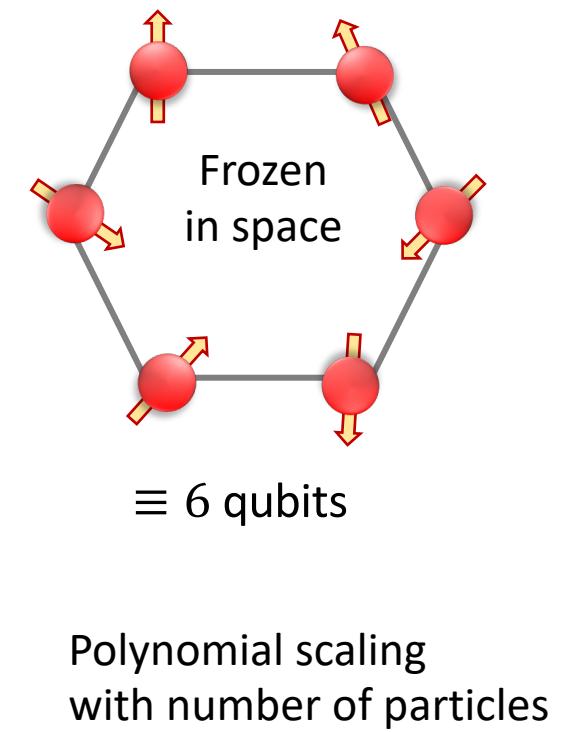
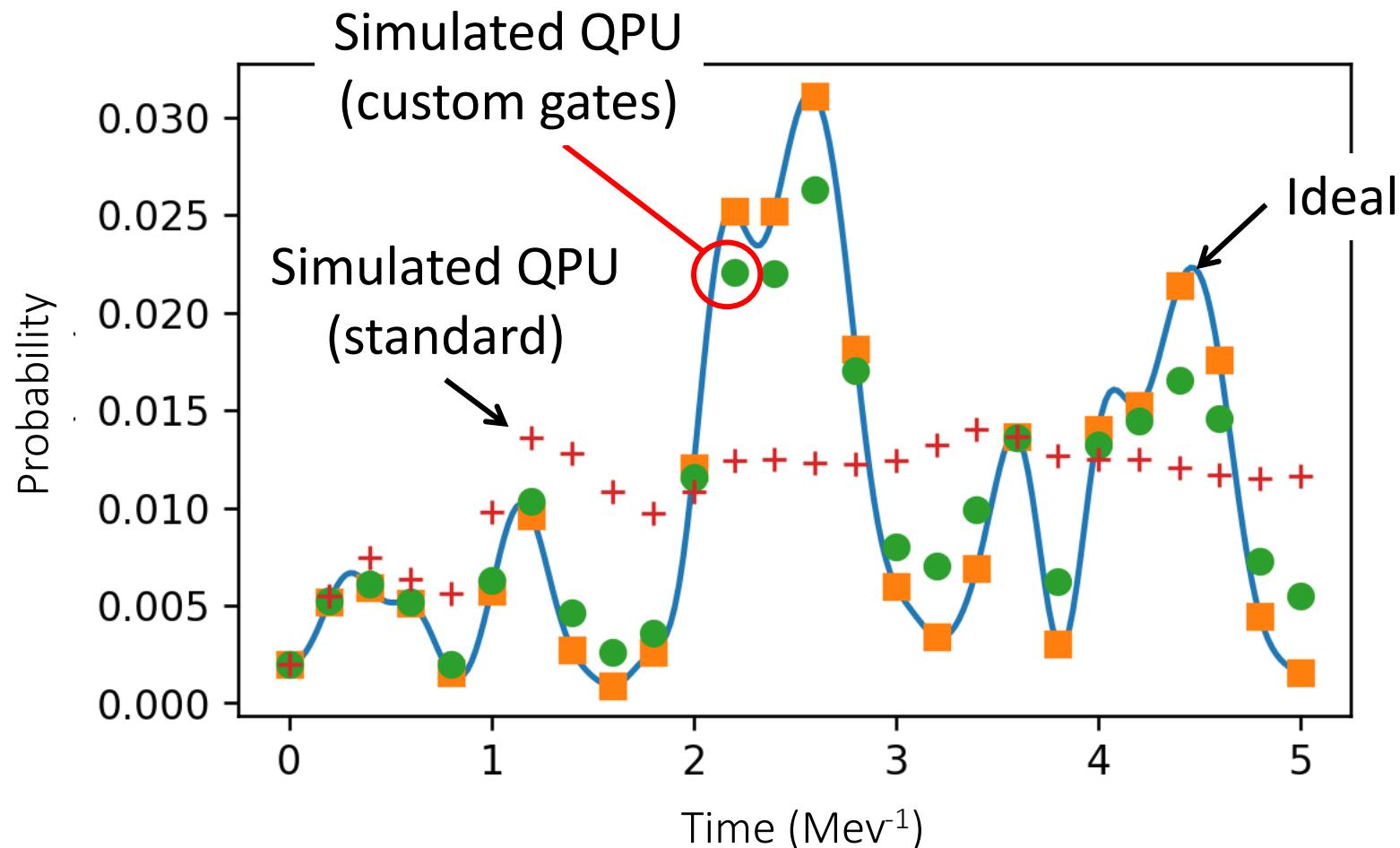


quantum simulation of the
binding energy of deuteron

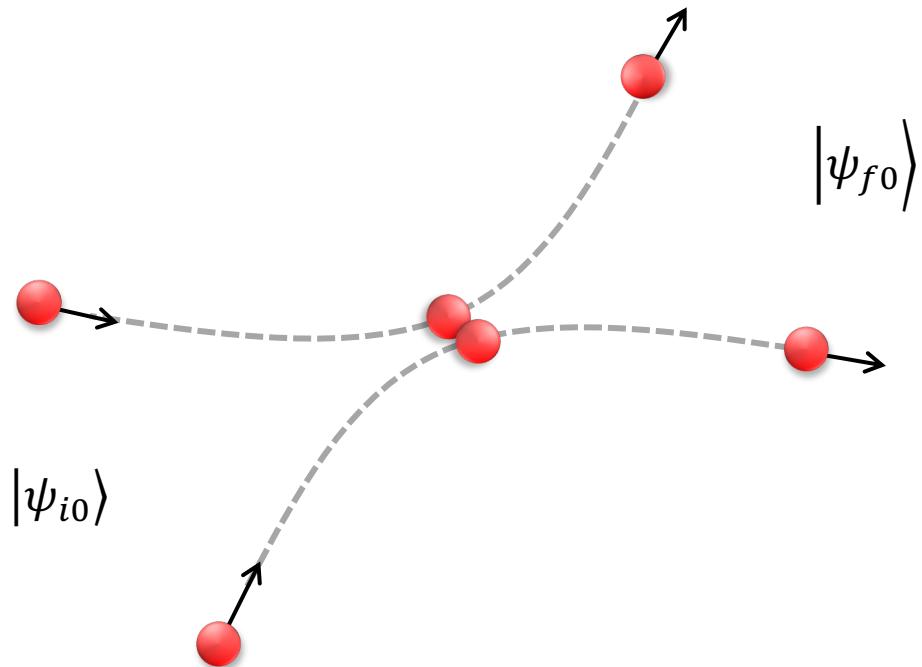
Demonstrated hybrid quantum-classical simulation of nuclear scattering on the Advanced Quantum Testbed



With custom gates, designed noise-resilient algorithm
for quantum simulation of multi-nucleon spin dynamics



Quantum computing offers a natural framework for simulating time-dependent scattering theory



$$P = |S_{fi}|^2 = |\langle \psi_f(0) | \psi_i(0) \rangle|^2 \\ \approx |\langle \psi_{f0}(t) | e^{-2iHt} | \psi_{i0}(-t) \rangle|^2$$

$U(2t)$

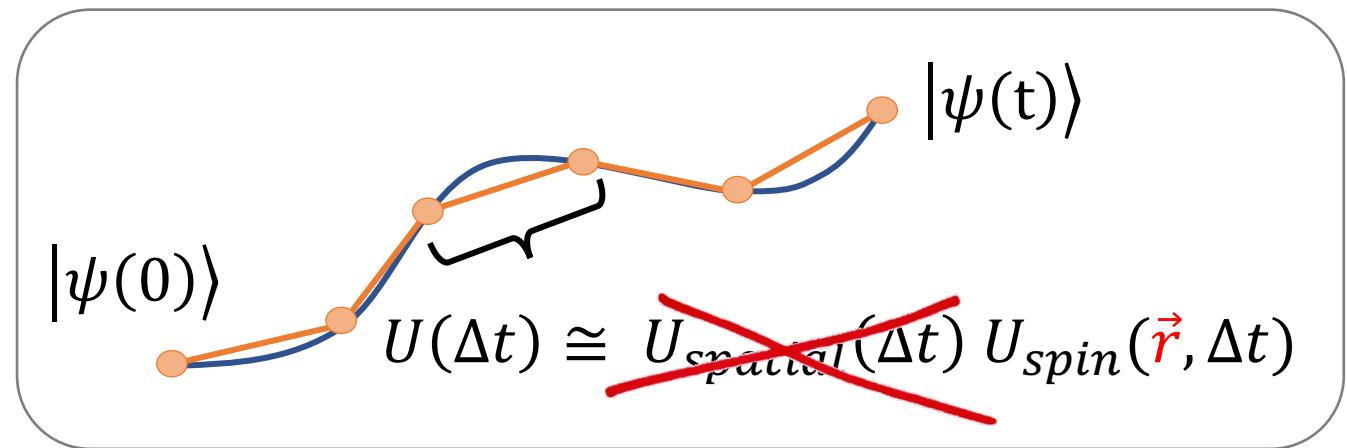
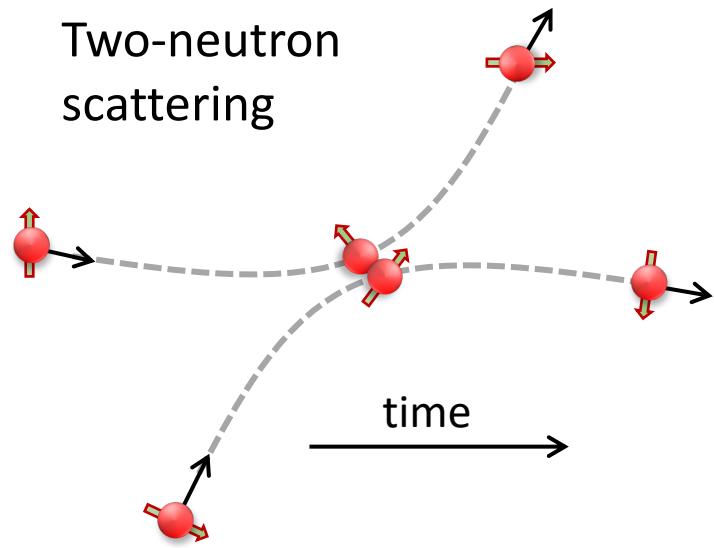
Real-time evolution

State preparation

Application of unitary transformations (= gates)



Our target problem: evolution of two interacting neutrons frozen in space



Nuclear \leftrightarrow quantum register map:

$$|\bullet\bullet\rangle \leftrightarrow |00\rangle$$

$$\left| \frac{\bullet\bullet + \bullet\bullet}{\sqrt{2}} \right\rangle \leftrightarrow |01\rangle$$

$$|\bullet\bullet\rangle \leftrightarrow |10\rangle$$

$$\left| \frac{\bullet\bullet - \bullet\bullet}{\sqrt{2}} \right\rangle \leftrightarrow |11\rangle$$

With minimal number of custom gates, we demonstrated >99% fidelity, significant increase in quantum simulation time

