Harnessing Quantum Information Science for Enhancing Sensors in Harsh Fossil Energy Environments

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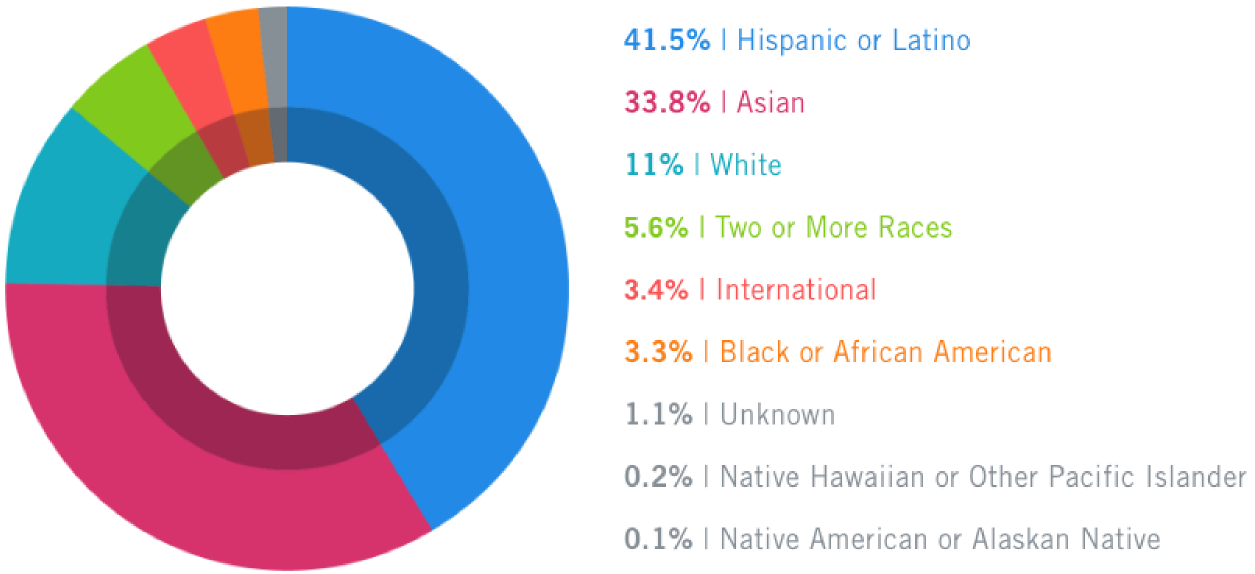
Outline

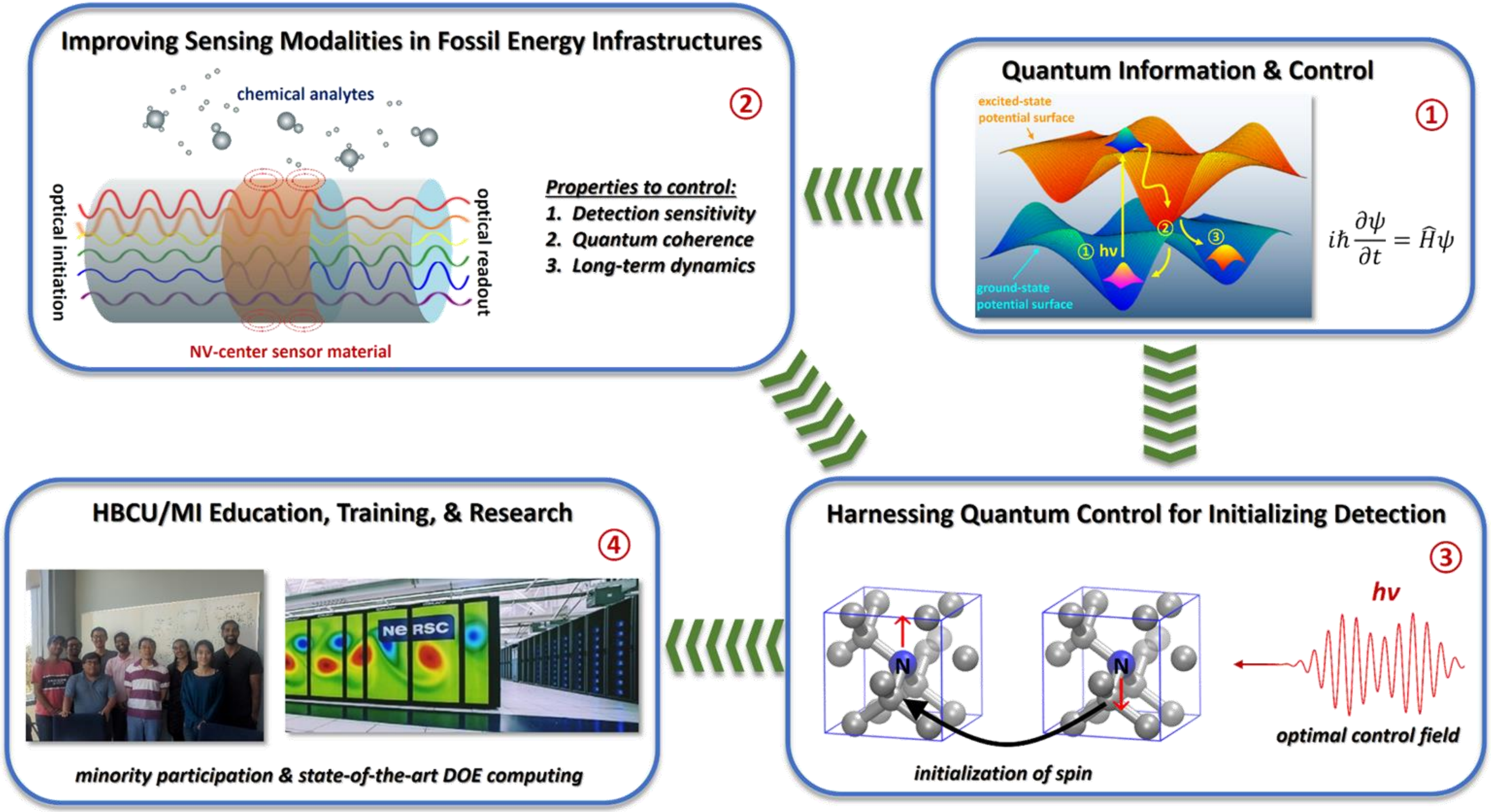
- Short introduction
- Why use quantum information science for sensors?
- Predictive quantum simulations for candidate materials
- Novel symmetry-based quantum optimal control framework
- Summary

UC Riverside (UCR)

- Official Hispanic Serving Institution
- Demographics:
- 57% first-generation students to attend college
- Designated as *"top-performing institution for African American & Latino/a students"* by The Education Trust – **1 of only 3 institutions in the nation**



General Project Objectives



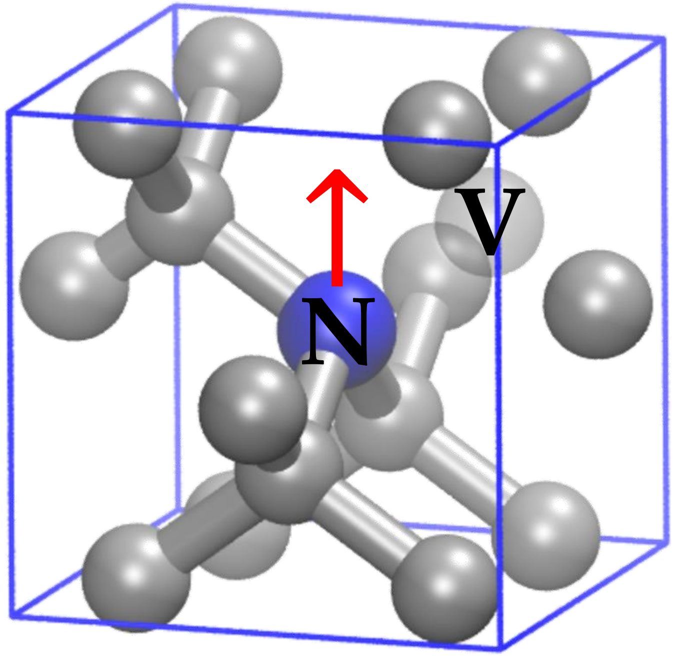
NV-Center Sensors

- Nitrogen-vacancy (NV) centers: structural point defects in bulk carbon

- Contain stable, localized electron spin that can be used as sensor

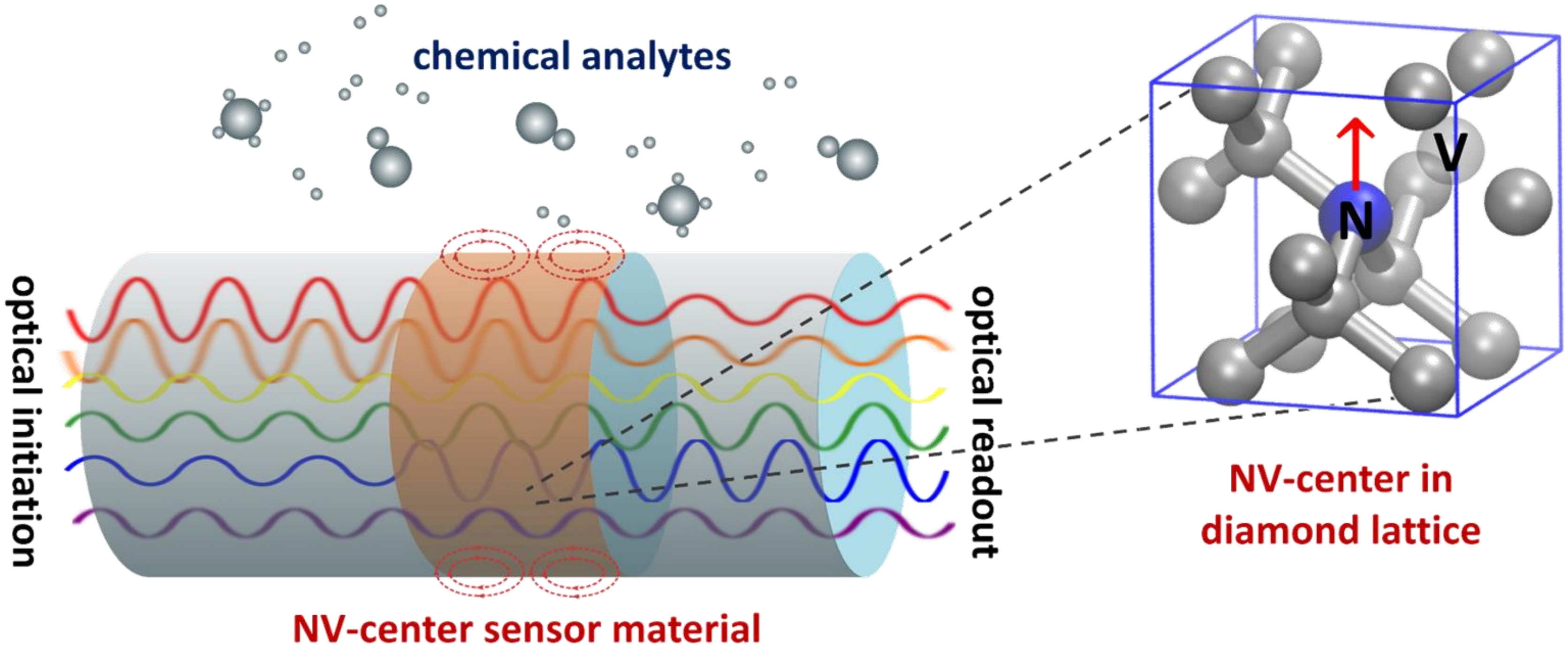
    - Coherence signals can persist at 700 – 1000 K (*essential for harsh fossil energy environments*)

    - Can be controlled with electromagnetic pulses



NV-Center Sensors (cont.)

- NV centers near the surface have not been thoroughly explored
  - Defects at surface can enable sensitive detection of chemical analytes in fossil energy infrastructures (discussed later)

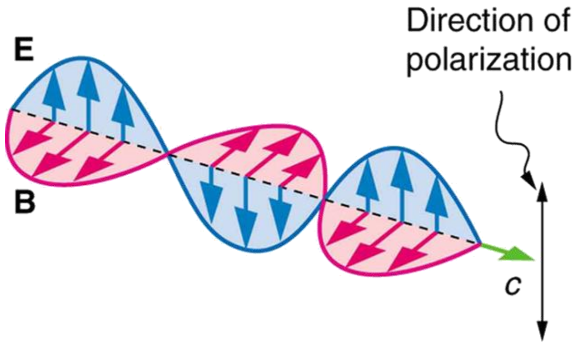


Excited-State QM for Dynamics

- (1) NV-center configurations down-selected with DFT

- (2) Excited-state QM will probe *real-time* interactions between NV centers & EM fields to understand sensor mechanisms

- Electromagnetic radiation (i.e., light) has two components
  - Magnetic pulse (**B**)
  - Electric pulse (**E**)



Optimal Control Fields

- Excited-state QM is an initial value problem
- Can we ask the inverse question: “Can we construct pulses that *enable desired behavior in NV center?”*

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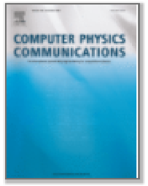


NIC-CAGE: An open-source software package for predicting optimal control fields in photo-excited chemical systems ☆, ☆☆

Akber Raza [a, 1], Chengkuan Hong [b, 1], Xian Wang [c], Anshuman Kumar [d], Christian R. Shelton [b], Bryan M. Wong [a, c, d, e, f]

NIC-CAGE: Novel Implementation of Constrained Calculations for Automated Generation of Excitations

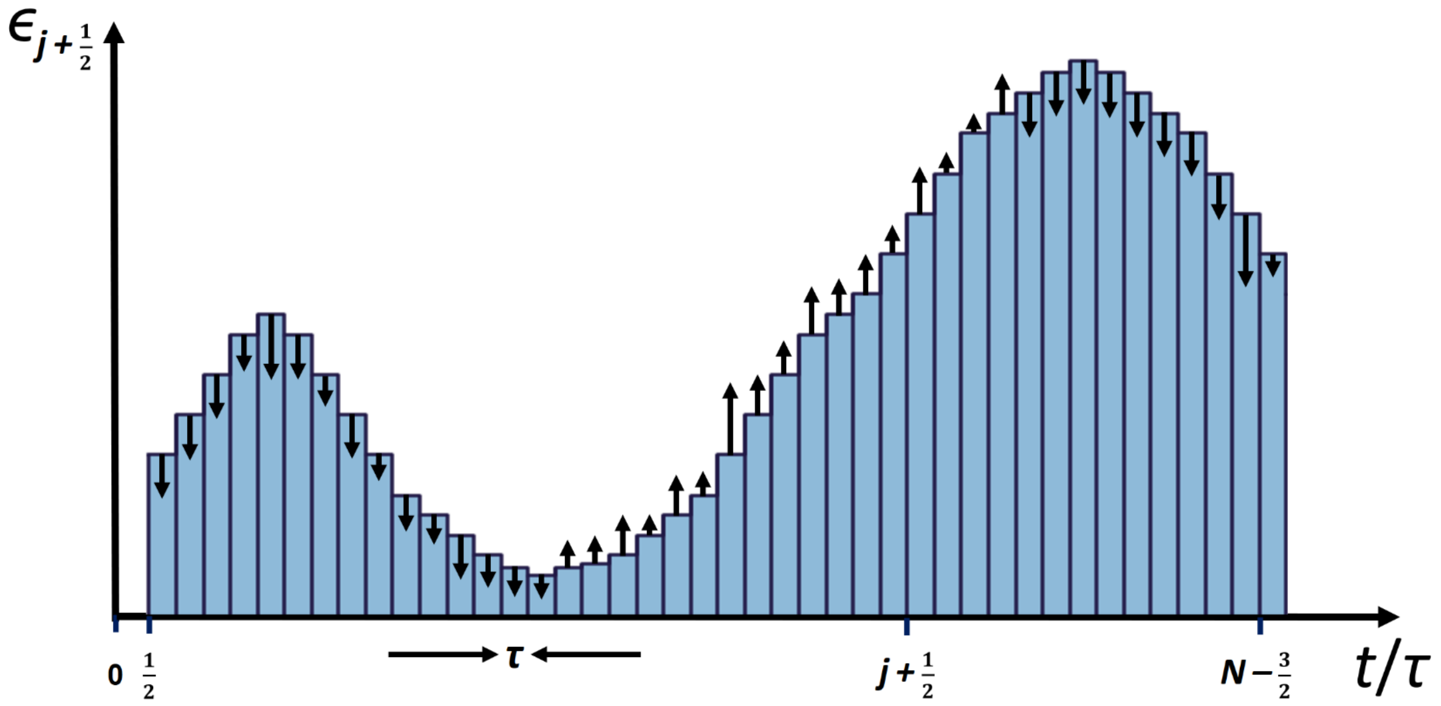
A. Raza. C. Hong, X. Wang, A. Kumar, C. R. Shelton, B. M. Wong, *Comput. Phys. Commun.* **258**, 107541 (2021)

Quantum Optimal Control

- Quantum optimal control (QOC) solves for optimized controlling pulses to evolve quantum system to target state
- Gate operation in quantum computing
- Challenge: size of Hamiltonian 2^n increases exponentially by number of qubits n
- Solution: accelerate QOC by transforming Hamiltonian using symmetry

Gradient-Based Program

- Calculates fields that enables transition to desired final state $|\psi_f\rangle$
- Uses scheme from GRAdient Pulse Engineering (GRAPE) algorithm



temporal shape of $B(t)$

<u>vertical arrows</u> = gradients indicating how amplitude changes to maximize transition probability

Dynamics of System

- Schrödinger equation

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = (H_0 + H_c(t))|\psi(t)\rangle$$

- Propagator

$$|\psi(T)\rangle = \exp\left(-i\int_0^T \big(H_0 + H_c(t)\big)\,\mathrm{d}t\right)|\psi(0)\rangle$$

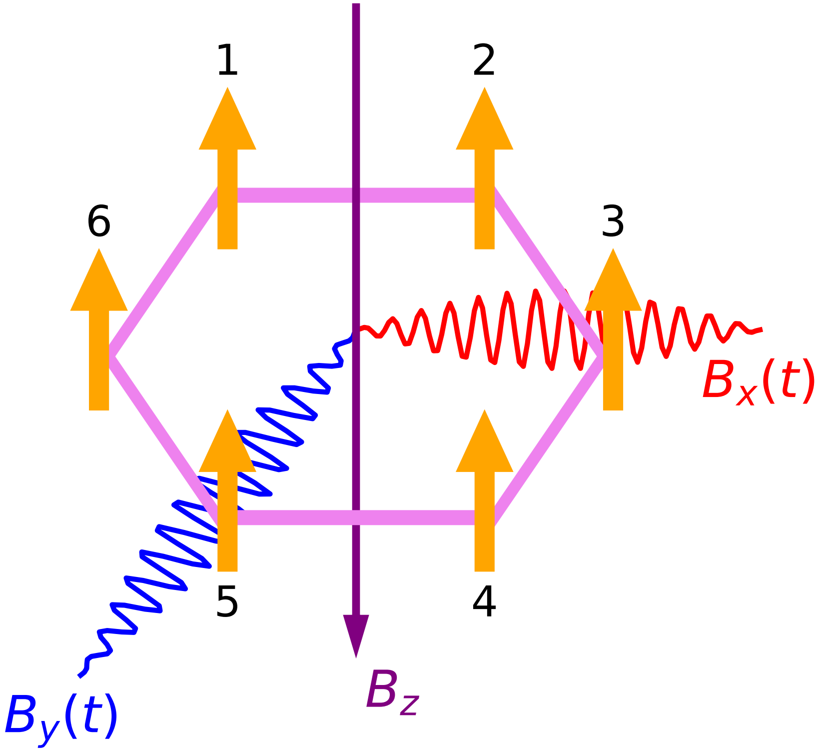
- Discretized propagator at the jth time step

$$|\psi_{j+1}\rangle = \exp\left(-i\tau\left(H_0 + H_c[(j+\frac{1}{2})\tau]\right)\right)|\psi_j\rangle$$

Dynamics of System

- Loss function in gradient-based method

$$P(|\psi_N\rangle) = \left|\langle\psi_f|\psi_N\rangle\right|^2$$



Pauli matrices:

$$\sigma_z = \begin{matrix} 1 & 0 \\ 0 & -1 \end{matrix}$$

$$\sigma_x = \begin{matrix} 0 & 1 \\ 1 & 0 \end{matrix}$$

$$\sigma_y = \begin{matrix} 0 & -i \\ i & 0 \end{matrix}$$

Symmetry of System

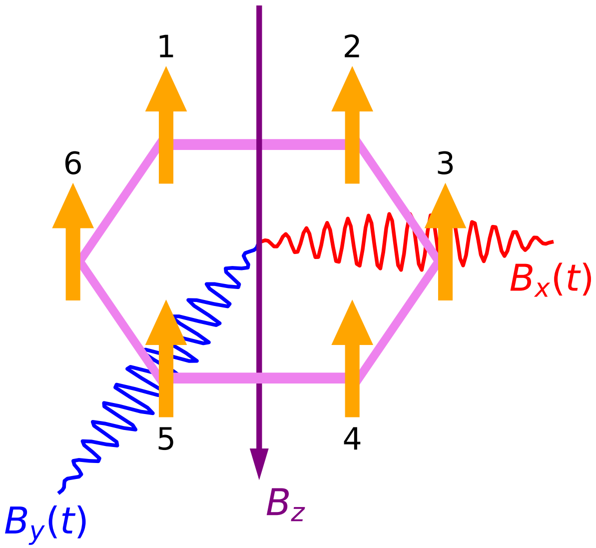
S_n permutation group

D_n dihedral group

- Static Hamiltonian

$$H_0 = B_z \cdot \frac{1}{2}\sum_{i=1}^{n} \sigma_z^{(i)} + c_{\text{cpl}} \cdot \frac{1}{4}\sum_{i=1}^{n} \sigma_z^{(i)} \sigma_z^{(i+1)}$$

S_n symmetry $\qquad$ D_n symmetry



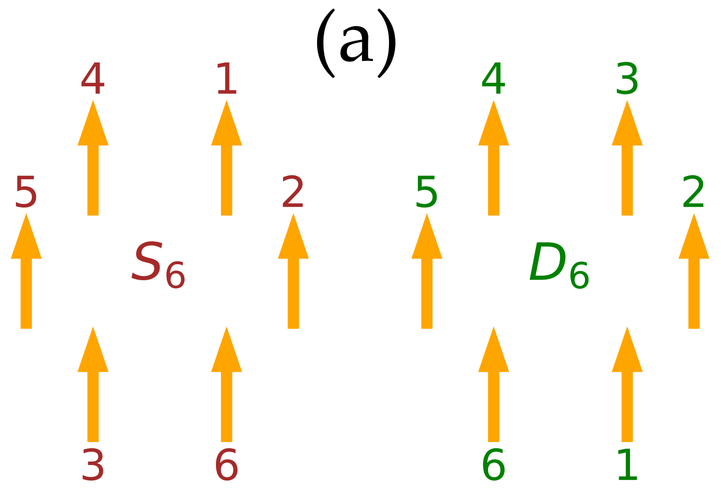
- Control Hamiltonian

$$H_c(t) = B_x(t) \cdot \frac{1}{2}\sum_{i=1}^{n} \sigma_x^{(i)} + B_y(t) \cdot \frac{1}{2}\sum_{i=1}^{n} \sigma_y^{(i)}$$

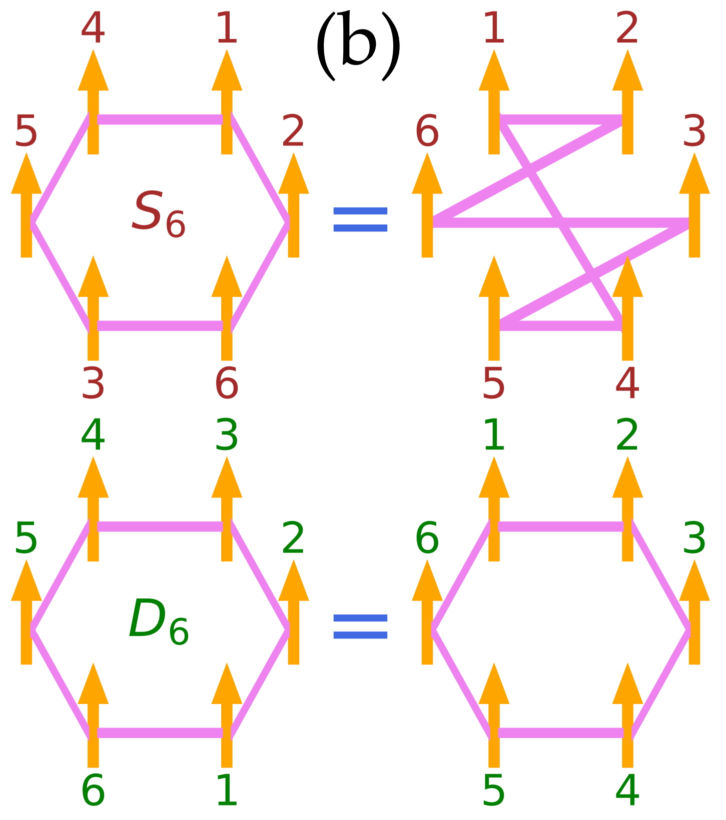
S_n symmetry $\qquad$ S_n symmetry

Symmetry of System

- (a) Configuration of qubits is not affected by any permutation of indices (S_6 action)



- (b) Nearest-neighbor coupling is generally affected by permutation (S_6 action), but not affected by rotation/reflection (D_6 action)

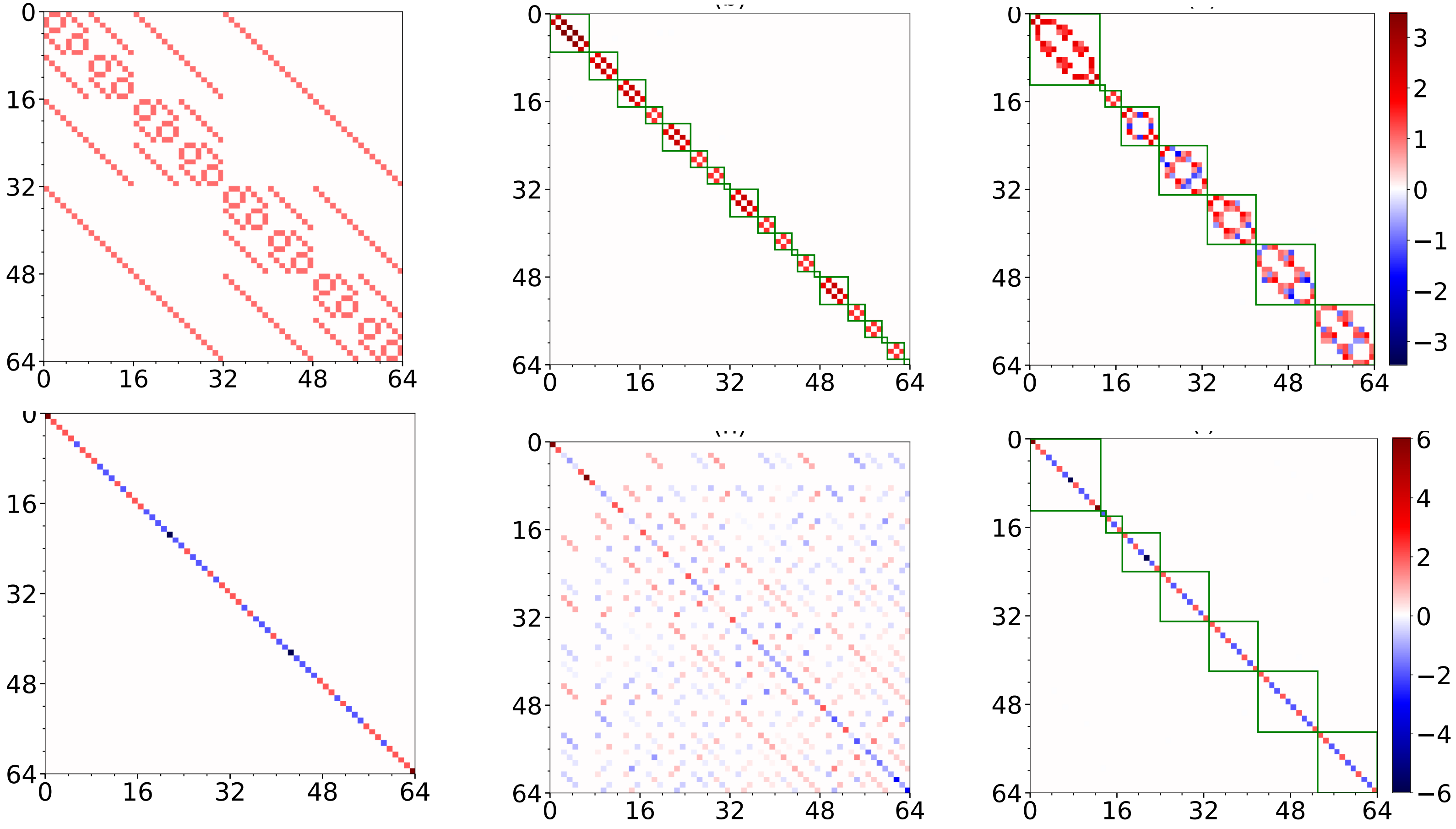


Symmetry-Based Hamiltonian Transformation

Original | S_6-transformed | D_6-transformed

$$\sum_{i=1}^{6} \sigma_x^{(i)}$$

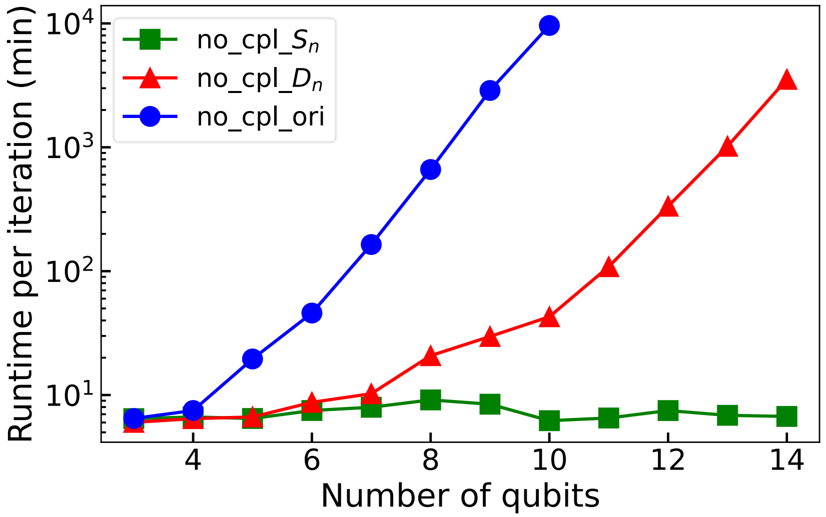
$$\sum_{i=1}^{6} \sigma_z^{(i)} \sigma_z^{(i+1)}$$

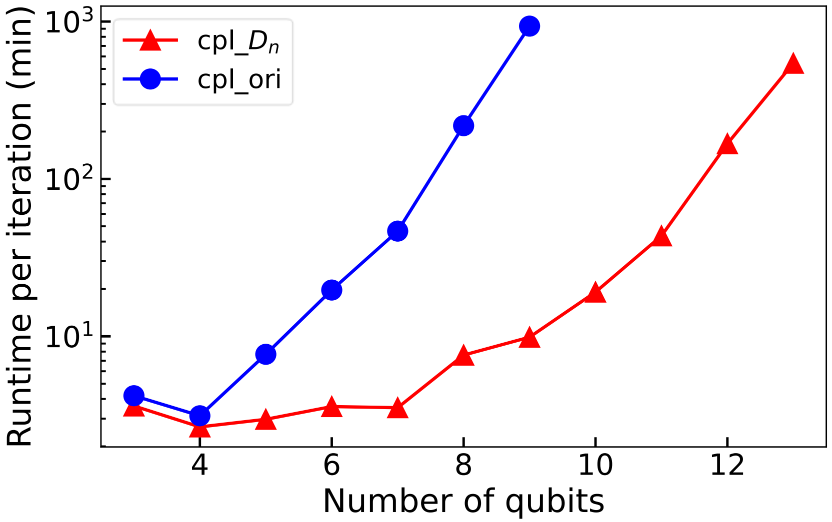


Comparison of Conventional and Symmetry-Based Method

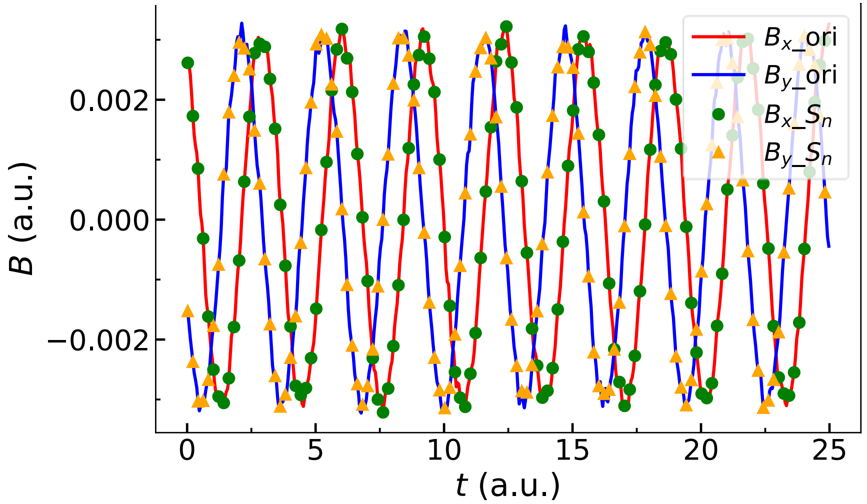
Non-coupled | Nearest-neighbor coupling

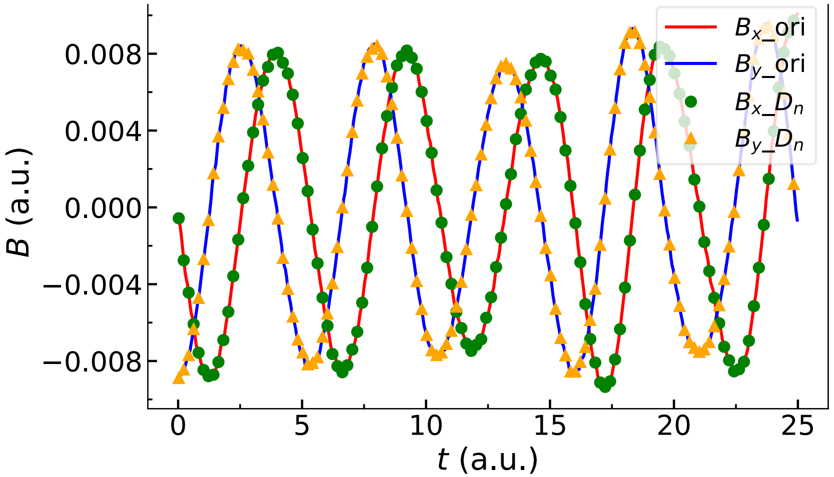
Runtime vs. # of qubits n





Optimized Controls

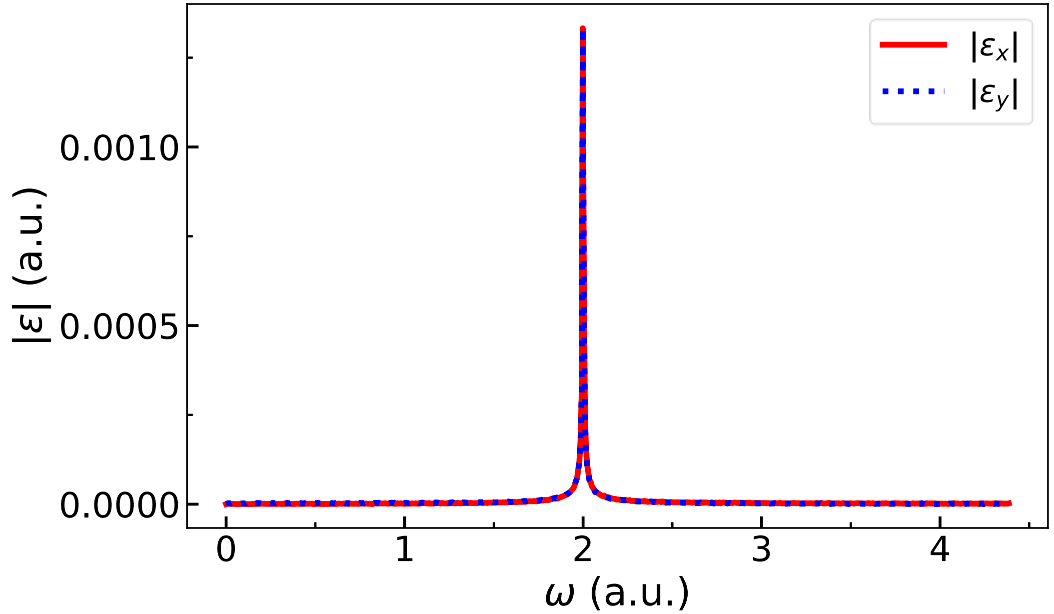




Symmetry-Protected Subspaces

- Symmetry-protected Subspaces: symmetry of system guarantees that transition is restricted within each subspace

- Only one resonance frequency in first subspace under S_n symmetry (no coupling)



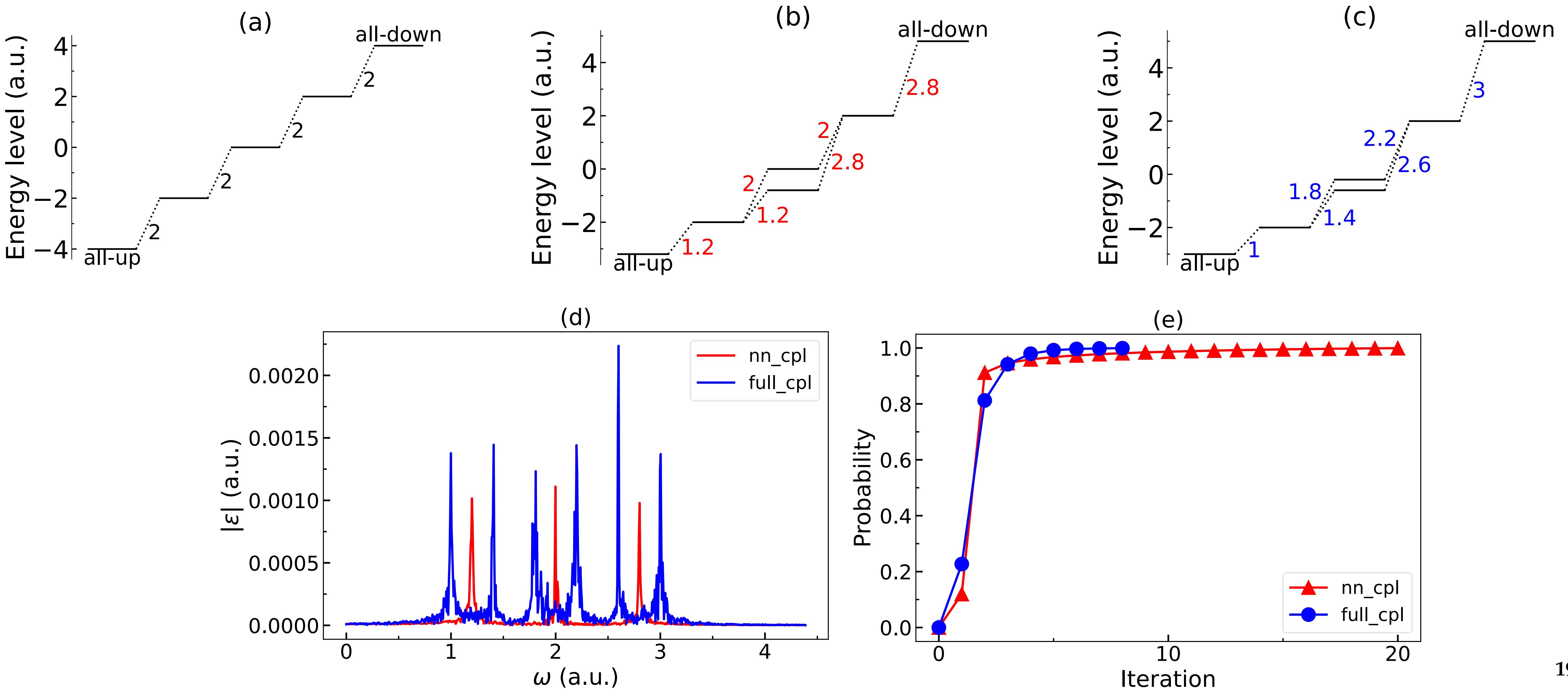
Symmetry-Protected Subspaces

- Three resonance frequencies in first subspace under D_n symmetry with nearest-neighbor coupling

- To enable more control in first subspace: introduce coupling between further qubits (preserves D_n symmetry)

$$H_0 = B_z \cdot \frac{1}{2}\sum_{i=1}^{n} \sigma_z^{(i)} + c_{\text{cpl}}^{(1)} \cdot \frac{1}{4}\sum_{i=1}^{n} \sigma_z^{(i)}\sigma_z^{(i+1)} + c_{\text{cpl}}^{(2)} \cdot \frac{1}{4}\sum_{i=1}^{n} \sigma_z^{(i)}\sigma_z^{(i+2)}$$
$$+ \cdots + c_{\text{cpl}}^{\left(\left\lfloor\frac{n}{2}\right\rfloor\right)} \cdot \frac{1}{4}\sum_{i=1}^{n} \sigma_z^{(i)}\sigma_z^{\left(i+\left\lfloor\frac{n}{2}\right\rfloor\right)}$$

Symmetry-Protected Subspaces



Lie-Trotter-Suzuki Decomposition

- Hamiltonian, symmetry is broken

$$H_0 + H_c(t) = \frac{1}{2}\sum_{i=1}^{n}\left(B_z \cdot \sigma_z^{(i)} + B_x^{(i)}(t)\cdot \sigma_x^{(i)} + B_y^{(i)}(t)\cdot \sigma_y^{(i)}\right)$$

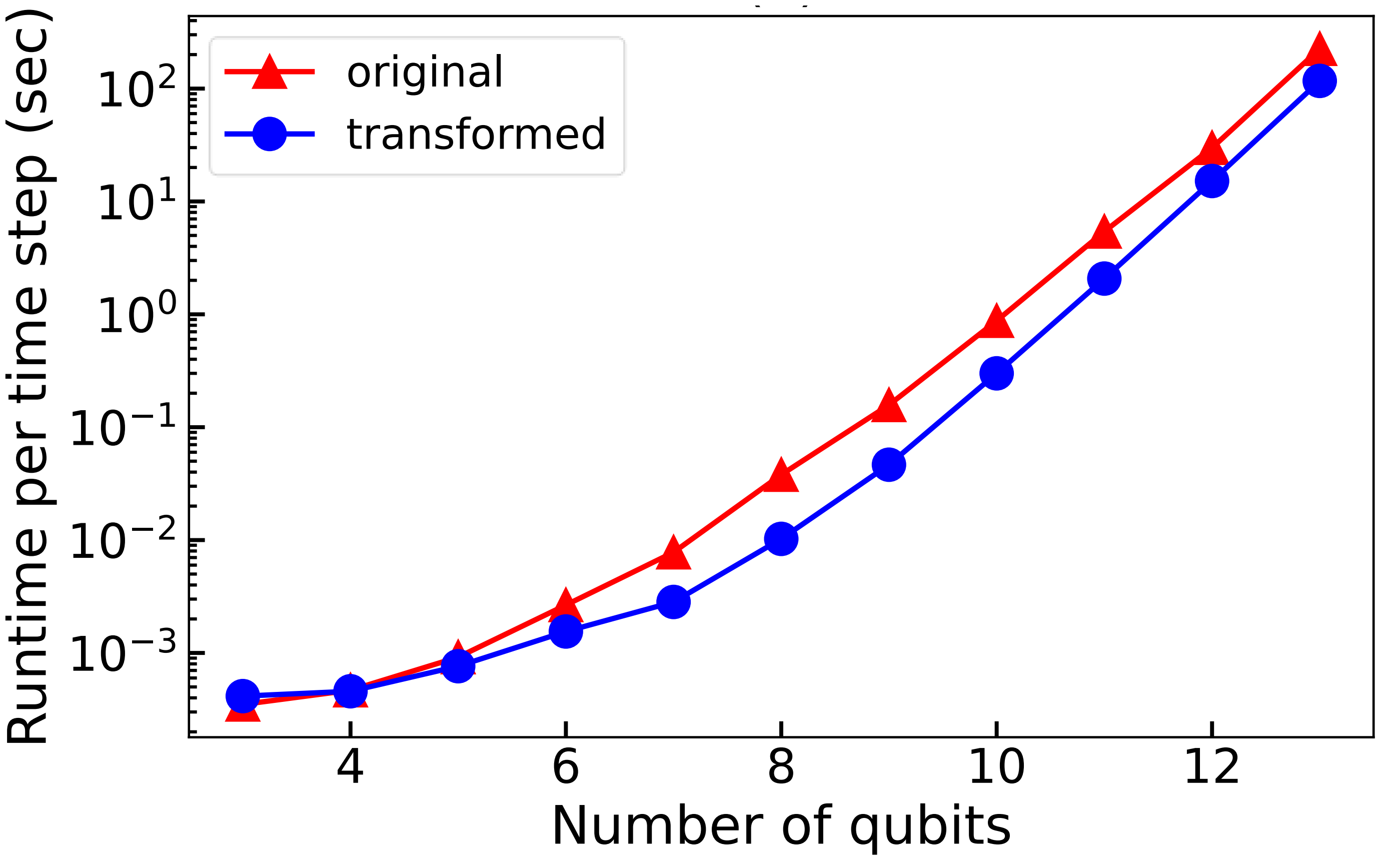
$$+c_{\text{cpl}} \cdot \frac{1}{4}\sum_{i=1}^{n} \sigma_z^{(i)}\sigma_z^{(i+1)}$$

- Propagator

$$U_j \approx \prod_{i=1}^{n}\left[\begin{array}{c} A_i \exp\left(-i\tau A_i^\dagger\left(H_0^{(i)} + H_c^{(i)}\left[(j+\frac{1}{2})\tau\right]\right)A_i\right)A_i^\dagger \\ A_D \exp\left(-i\frac{\tau}{n}A_D^\dagger H_{\text{cpl}} A_D\right)A_D^\dagger \end{array}\right]$$

Lie-Trotter-Suzuki Decomposition

- Time dependent terms reduce to n of 2×2 matrices from a $2^n \times 2^n$ matrix



Summary of QOC

- Transformed Hamiltonian based on symmetry
- Same output, but much faster
- More controllability by introducing further coupling
- Can be generalized to more systems with Lie-Trotter-Suzuki decomposition

Conclusion & Acknowledgements

- Predictive quantum simulations provide rational guidance for constructing quantum sensors for fossil energy infrastructures
- Quantum information science *almost perfect application of excited-state quantum calculations*

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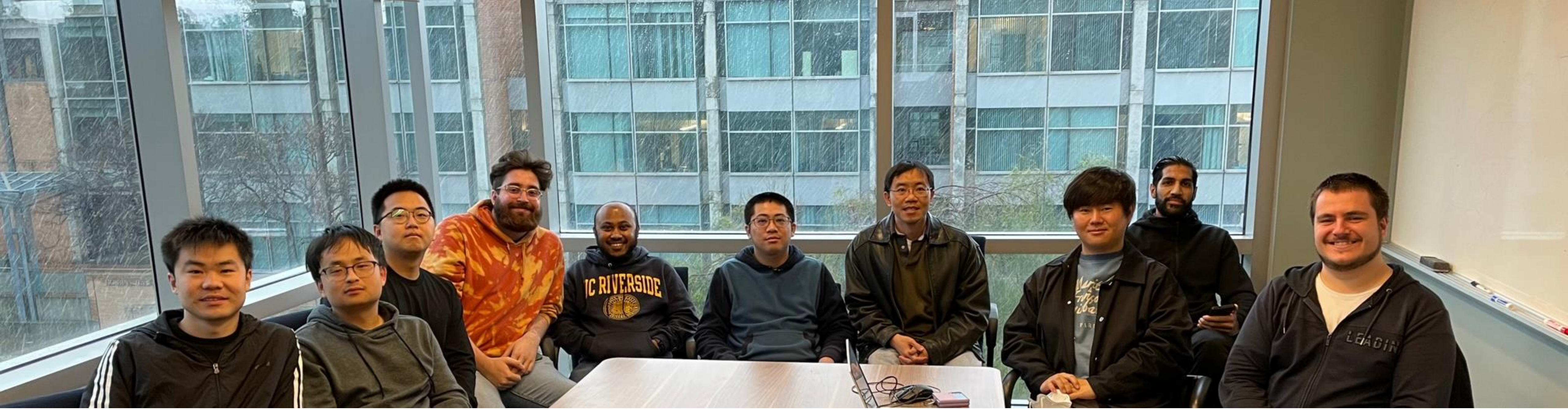

Thank you!