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

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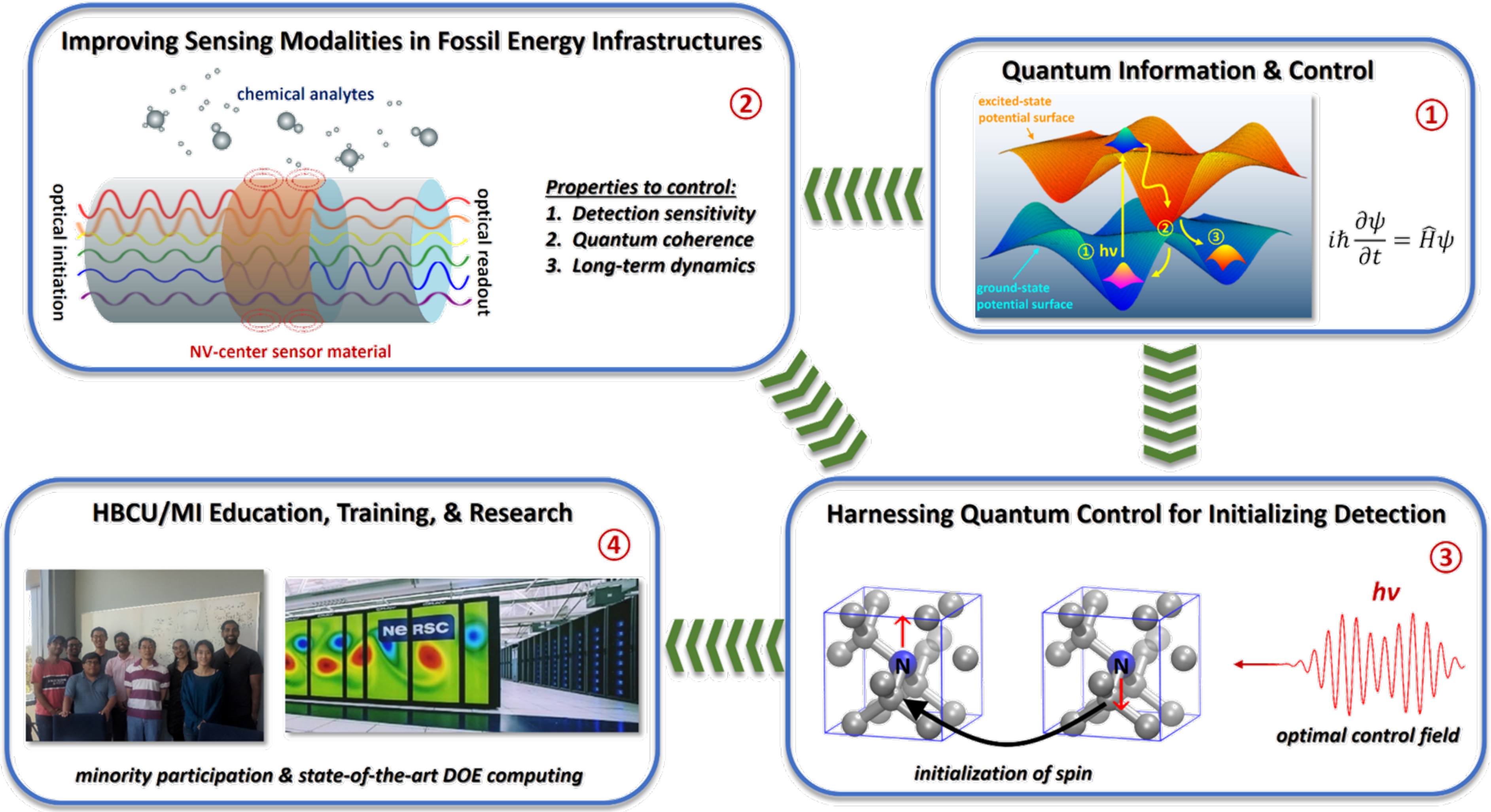
Outline

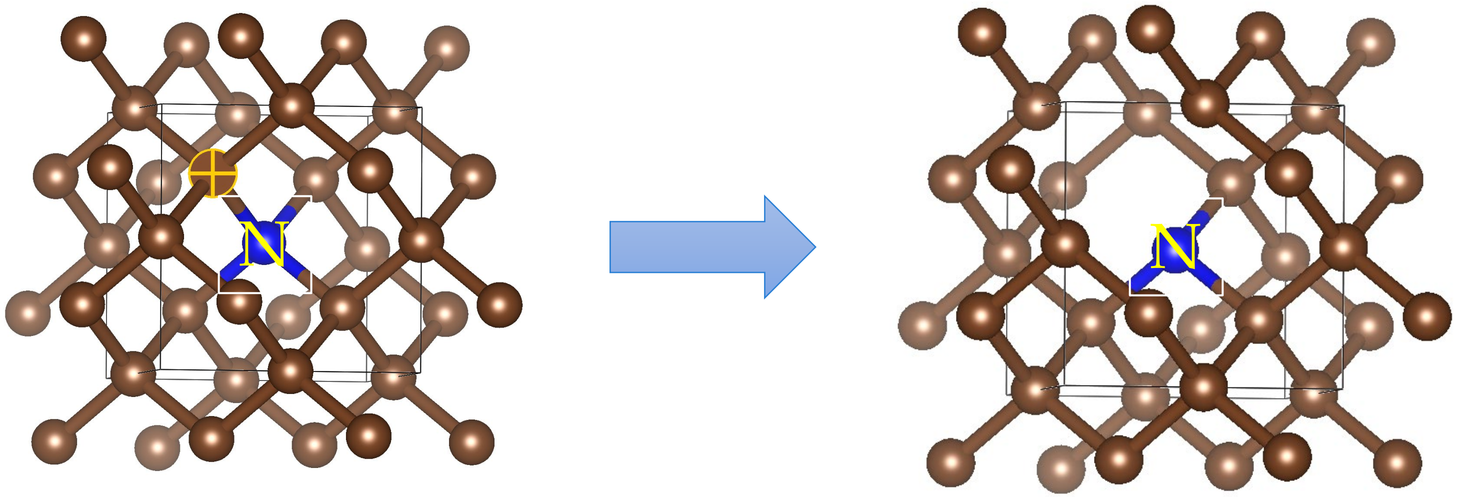
- General Project Objectives
- Large-scale quantum simulations for candidate materials
- Quantum information science for NV-center sensors
- Quantum optimal control frameworks
- Summary

General Project Objectives



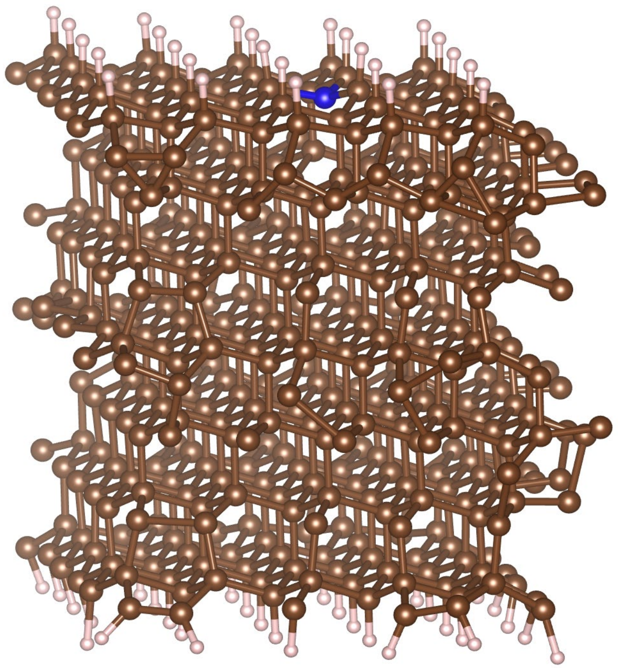
NV-Center Sensors

- Nitrogen-vacancy (NV) centers: structural point defects in diamonds
- Stable, localized electron spin can be used as sensor, controlled by electromagnetic pulses
- Coherence signals can persist at 700 – 1000 K, essential for harsh fossil energy environments

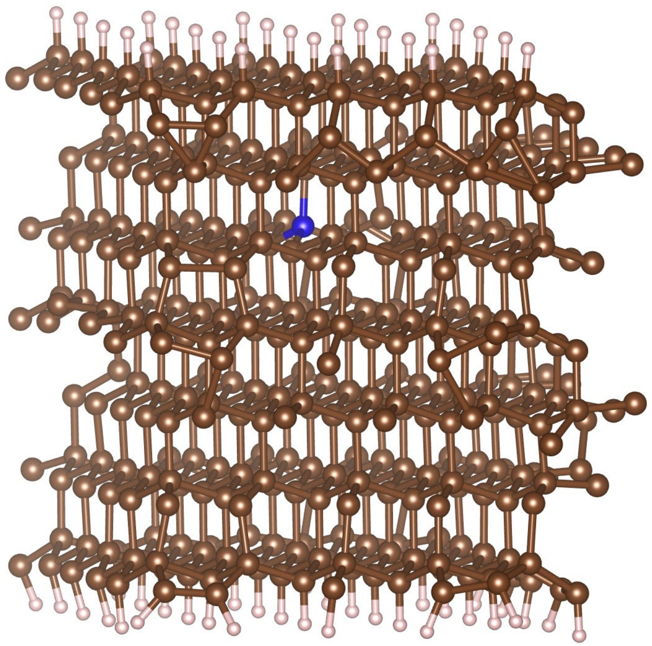


NV-Center Sensors

- NV centers near the surface have not been thoroughly explored
- Density functional theory (material simulation method) calculation:



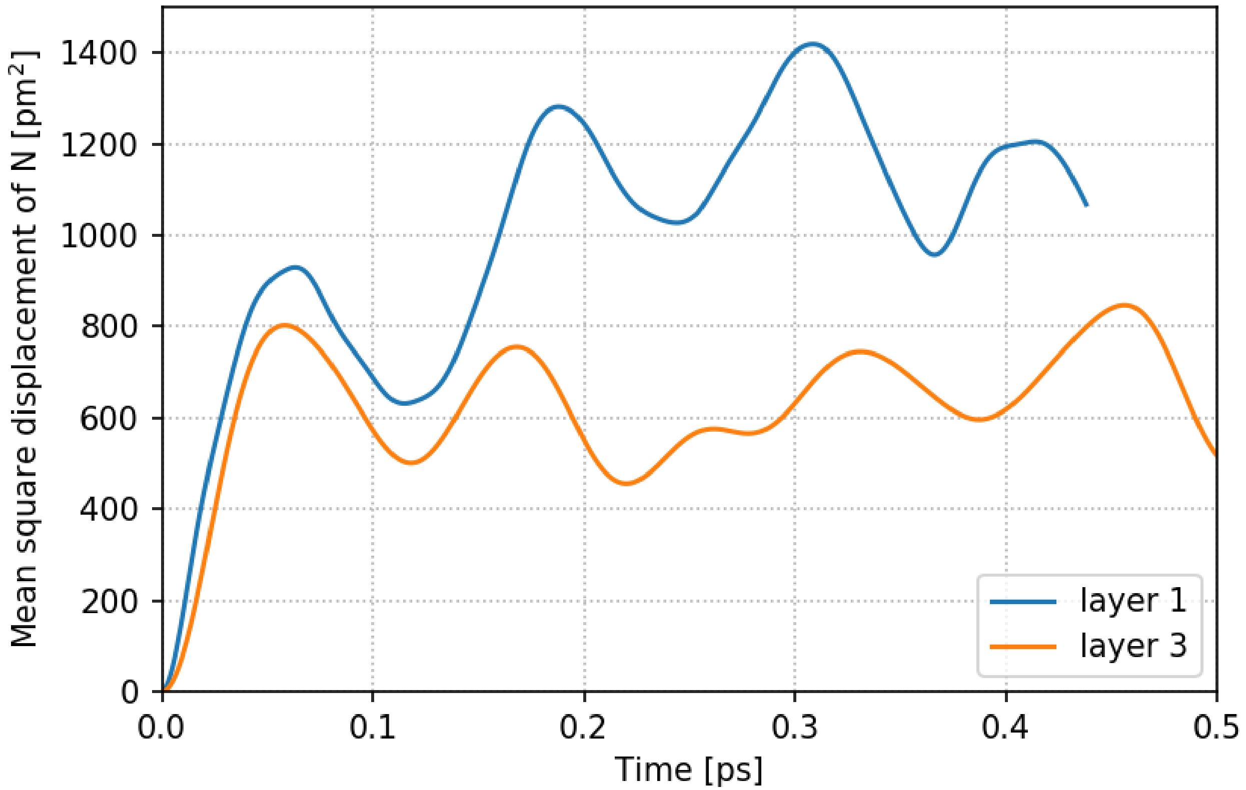
At Layer 1



At Layer 3

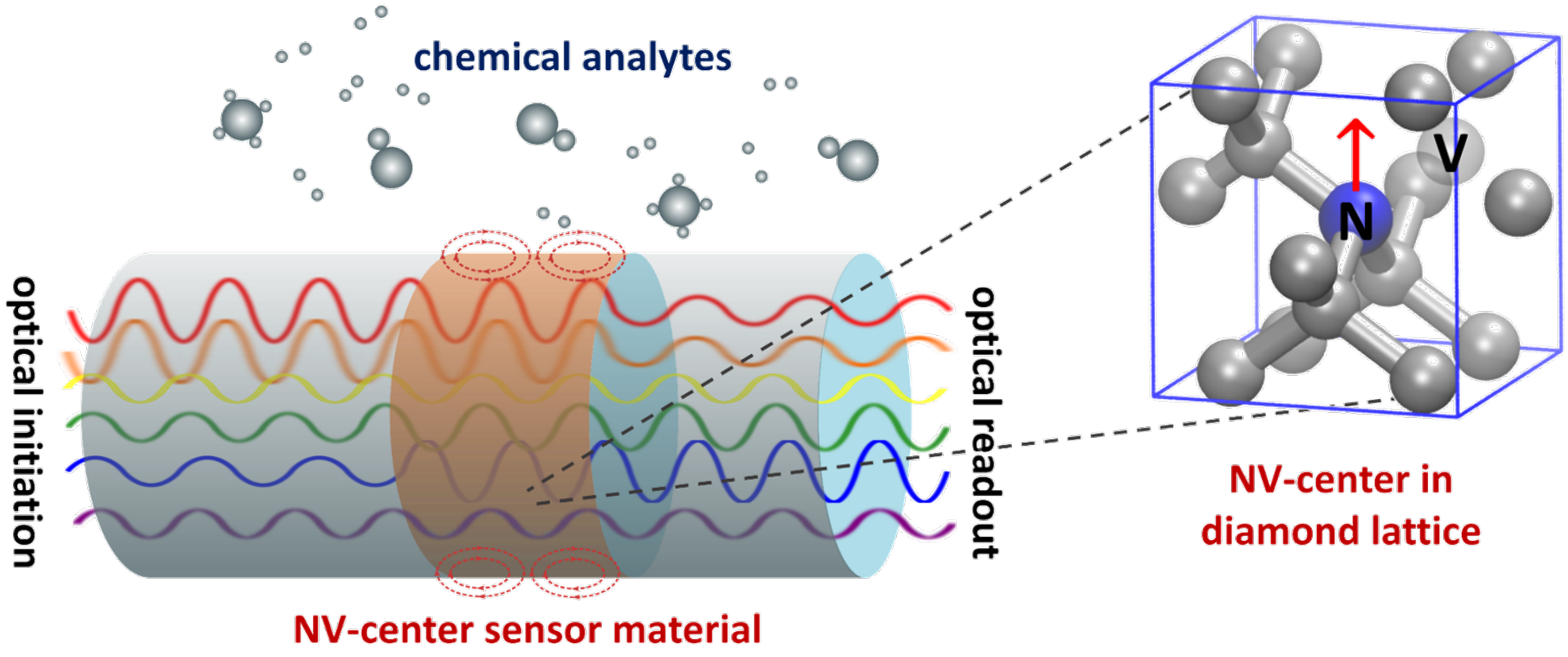
Large-Scale Quantum Simulations

- Mean square displacement of two locations, 1000 ℃



NV-Center Sensors

- NV-centers near surface can enable sensitive detection of chemical analytes in fossil energy infrastructures

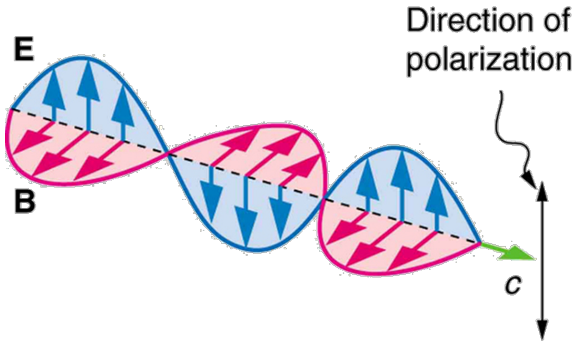


Excited-State QM for Dynamics

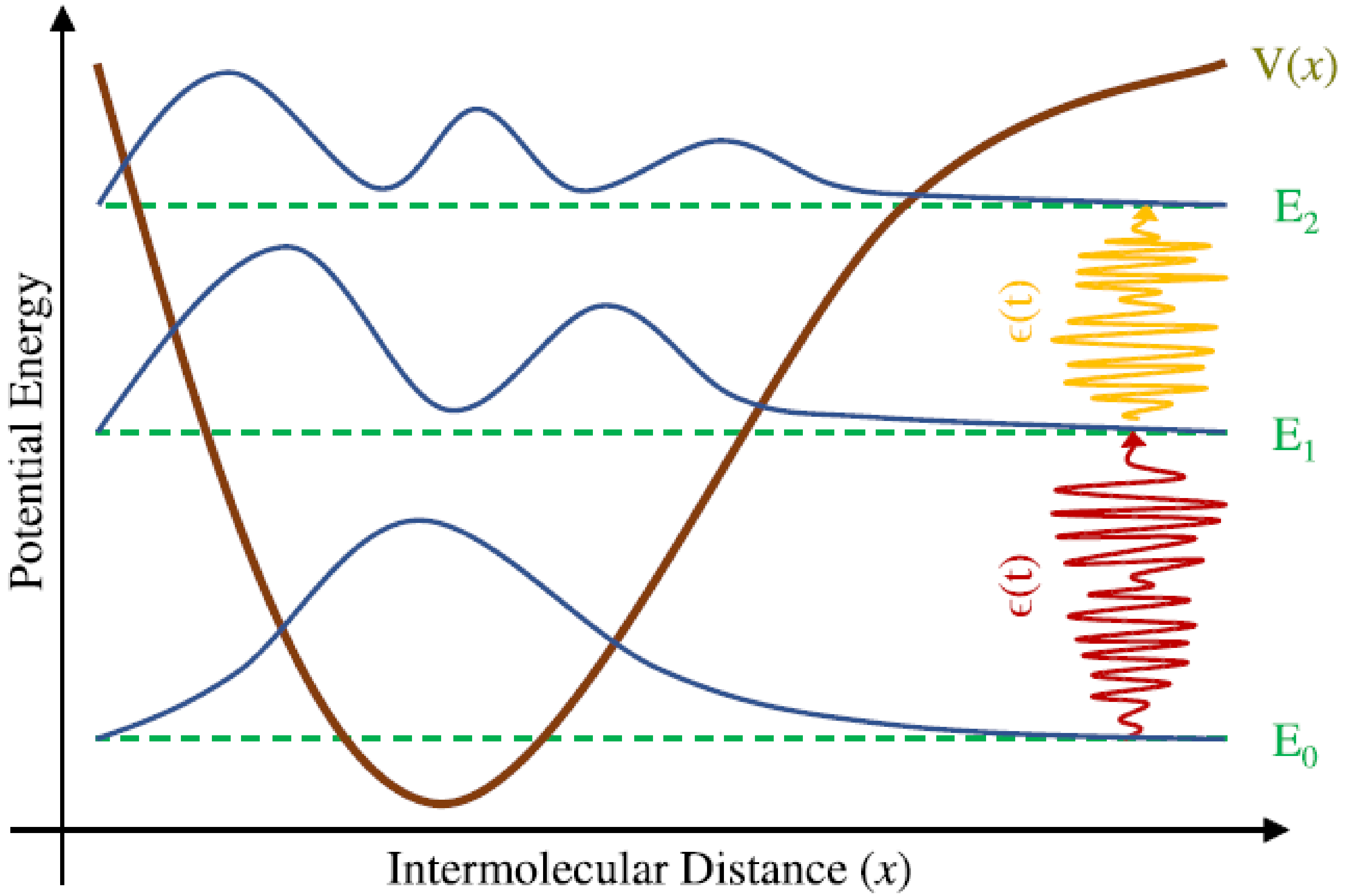
- (1) NV-center configurations down-selected with density functional theory

- (2) Excited-state quantum mechanics 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**) - spin
  - Electric pulse (**E**) - charge



Quantum Optimal Control (QOC) Problem



NIC-CAGE Algorithm

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

Computer Physics Communications 258 (2021) 107541

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

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

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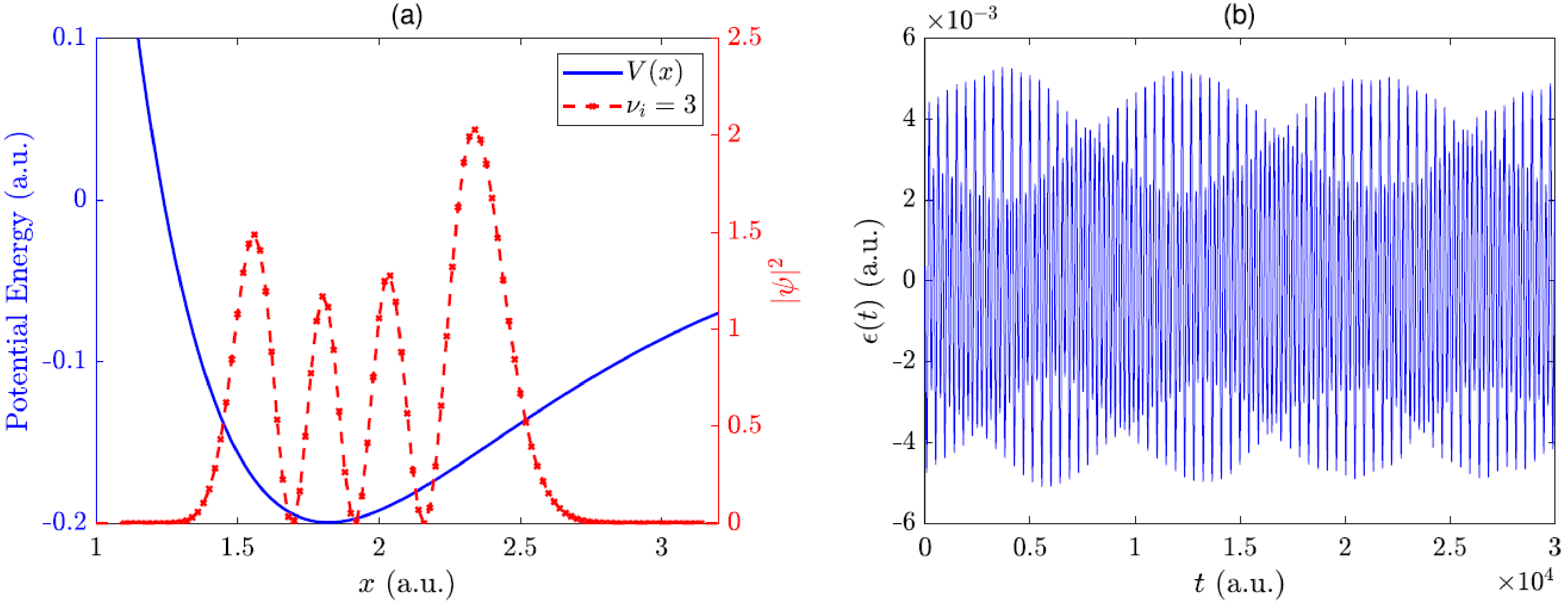
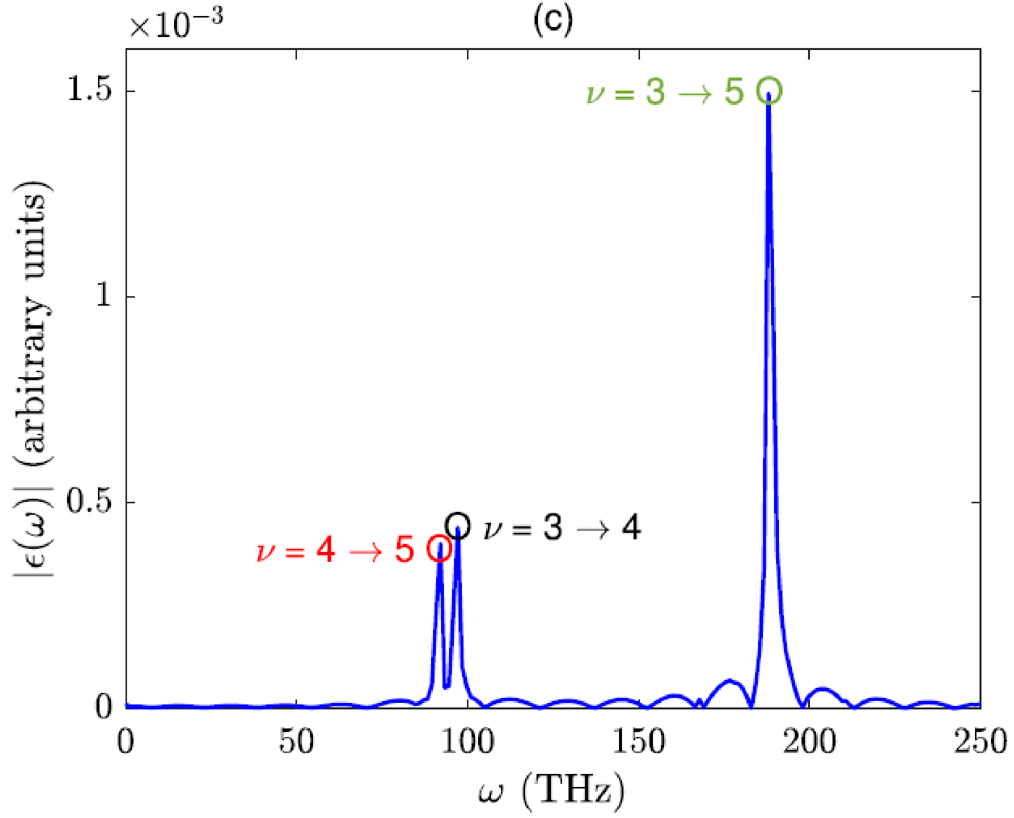
Results of NIC-CAGE

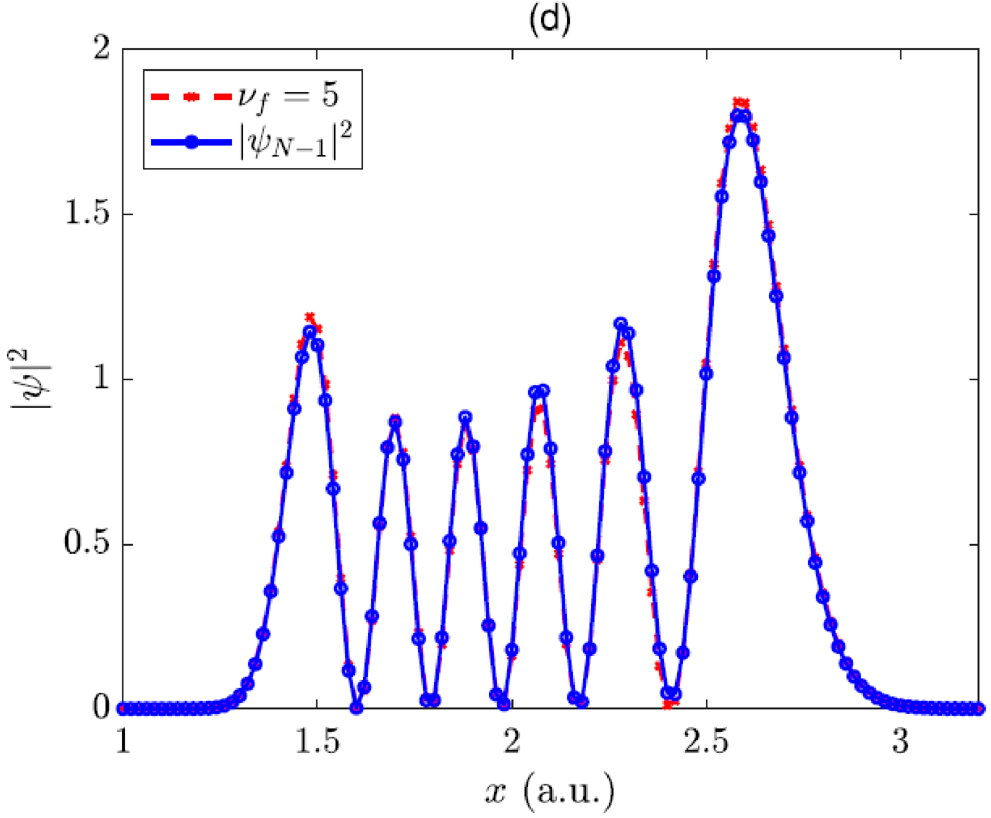
- Transition in vibrational system: 3 -> 5 excited state



Results of NIC-CAGE

- 3 resonance frequencies





QOC Problem for NV-centers

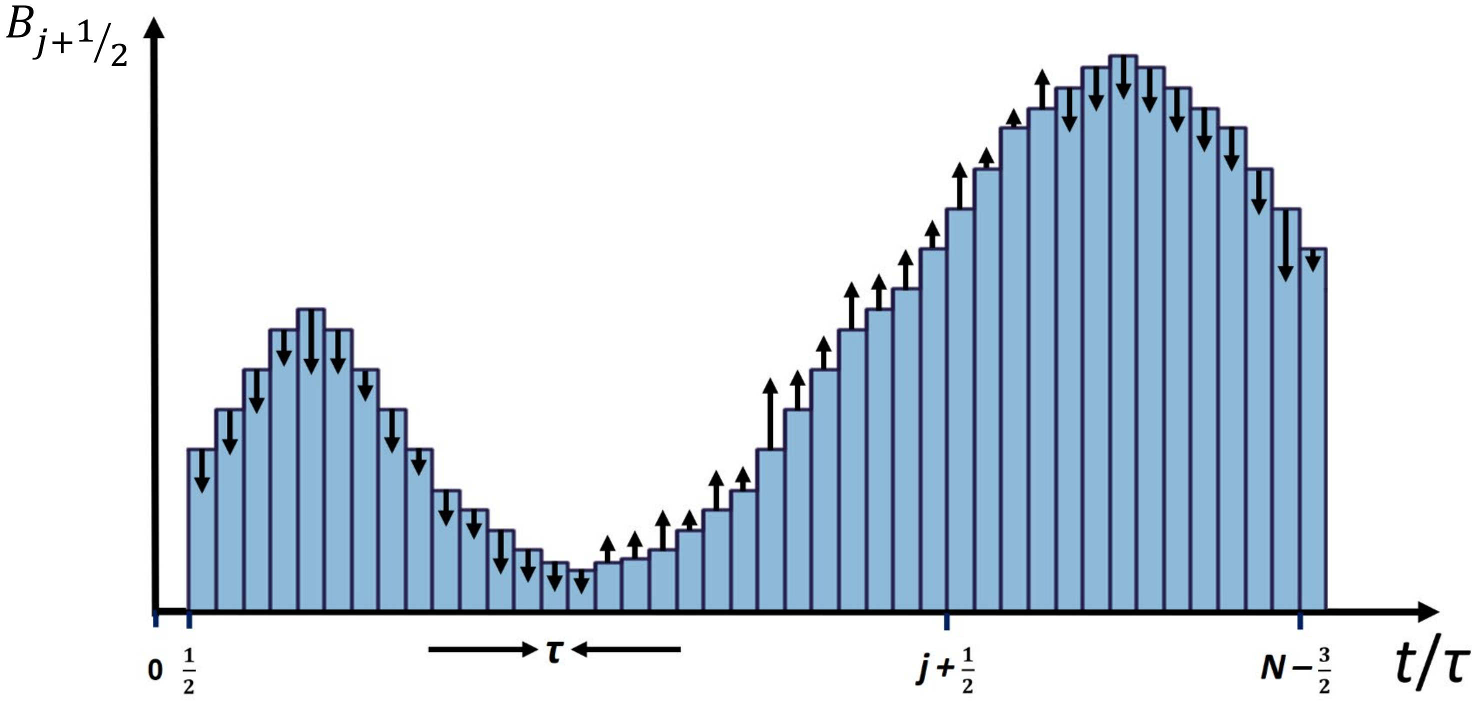
- NV-center sensors are controlled by external magnetic pulses

- Excited-state quantum mechanics is an initial value problem
- Challenge: How to construct magnetic pulses that enable desired behavior in NV center? Inverse problem in quantum mechanics

- Solution: Quantum optimal control (QOC) is the tool to solve for controlling pulses

Modified NIC-CAGE Algorithm

- Make an initial guess of the controlling pulses $B(t)$
- Iteratively optimize the pulse: $\boldsymbol{B}^{(l)} = \boldsymbol{B}^{(l-1)} + \gamma \frac{\mathrm{d}J}{\mathrm{d}\boldsymbol{B}^{(l-1)}}$



temporal shape of $B(t)$

vertical arrows = gradients indicating how amplitude changes to maximize transition probability

Modified NIC-CAGE Algorithm

$$\boldsymbol{B}^{(l)} = \boldsymbol{B}^{(l-1)} + \gamma \frac{\mathrm{d}J}{\mathrm{d}\boldsymbol{B}^{(l-1)}}$$

- J is the loss function, typically defined as probability of transition $P(|\psi_N\rangle) = |\langle\psi_{target}|\psi_N\rangle|^2$, may include regularization terms like square of pulse amplitude
- $\frac{\mathrm{d}J}{\mathrm{d}\boldsymbol{B}^{(l-1)}}$ (a functional of time) is evaluated with backpropagation as gradient evaluation in neural networks
- γ is the update rate, evaluated with bisection line-search
- l is the iteration

Symmetry-Assisted Hamiltonian Reduction

- Symmetry-assisted method: Reduce the size of Hamiltonian for multi-qubit systems
- Featured Article in *AVS Quantum Science*

Accelerating quantum optimal control of multi-qubit systems with symmetry-based Hamiltonian transformations

Cite as: AVS Quantum Sci. **5**, 043801 (2023); doi: 10.1116/5.0162455
Submitted: 14 June 2023 · Accepted: 5 September 2023 ·
Published Online: 3 October 2023

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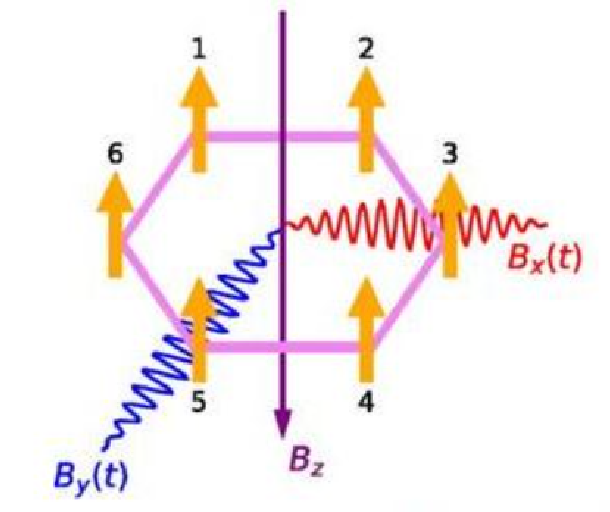
Symmetry-Assisted Hamiltonian Reduction

- Featured in *AVS Newsletter:* Beneath the AVS Surface November 2023

Accelerating Quantum Optimal Control of Multi-qubit Systems with Symmetry-based Hamiltonian Transformations



Authors: Xian Wang, Mahmut Sait Okyay, Anshuman Kumar, and Bryan M. Wong

Publication: *AVS Quantum Sci.*, 5, 043801 (2023)

READ ARTICLE

We present a novel, computationally efficient approach to accelerate quantum optimal control calculations of large multi-qubit systems used in a variety of quantum computing applications. By leveraging the intrinsic symmetry of finite groups, the Hilbert space can be decomposed and the Hamiltonians block diagonalized to enable extremely fast quantum optimal control calculations. Our approach reduces the Hamiltonian size of an n-qubit system from $2^n \times 2^n$ to $O(n \times n)$ or $O((2^n/n) \times (2^n/n))$ under S_n or D_n symmetry, respectively. Most importantly, this approach reduces the computational runtime of qubit optimal control calculations by orders of magnitude while maintaining the same accuracy as the conventional method. As prospective applications, we show that (1) symmetry-protected subspaces can be potential platforms for quantum error suppression and simulation of other quantum Hamiltonians and (2) Lie–Trotter–Suzuki decomposition approaches can generalize our method to a general variety of multi-qubit systems.

QOC Challenge in Multi-Qubit Systems

- Challenge: When there are multiple qubits, size of Hamiltonian $2^n \times 2^n$ increases exponentially by number of qubits n
- Static Hamiltonian

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

- Control Hamiltonian

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

- Solution: symmetry-assisted Hamiltonian reduction

Pauli matrices:

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

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

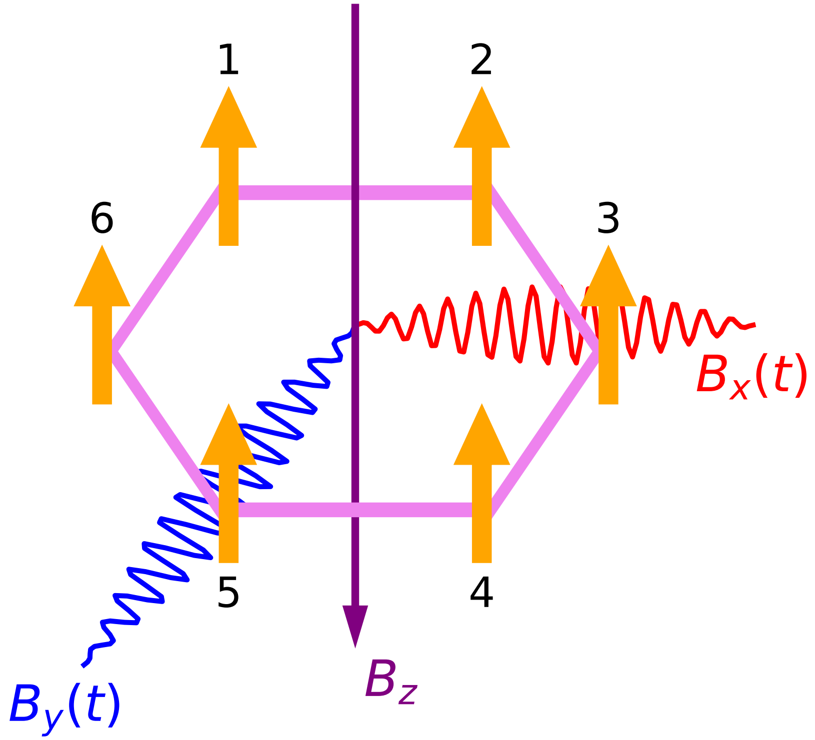
$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Symmetry-Assisted Hamiltonian Reduction

- Schrödinger equation

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

- 6-qubit system:



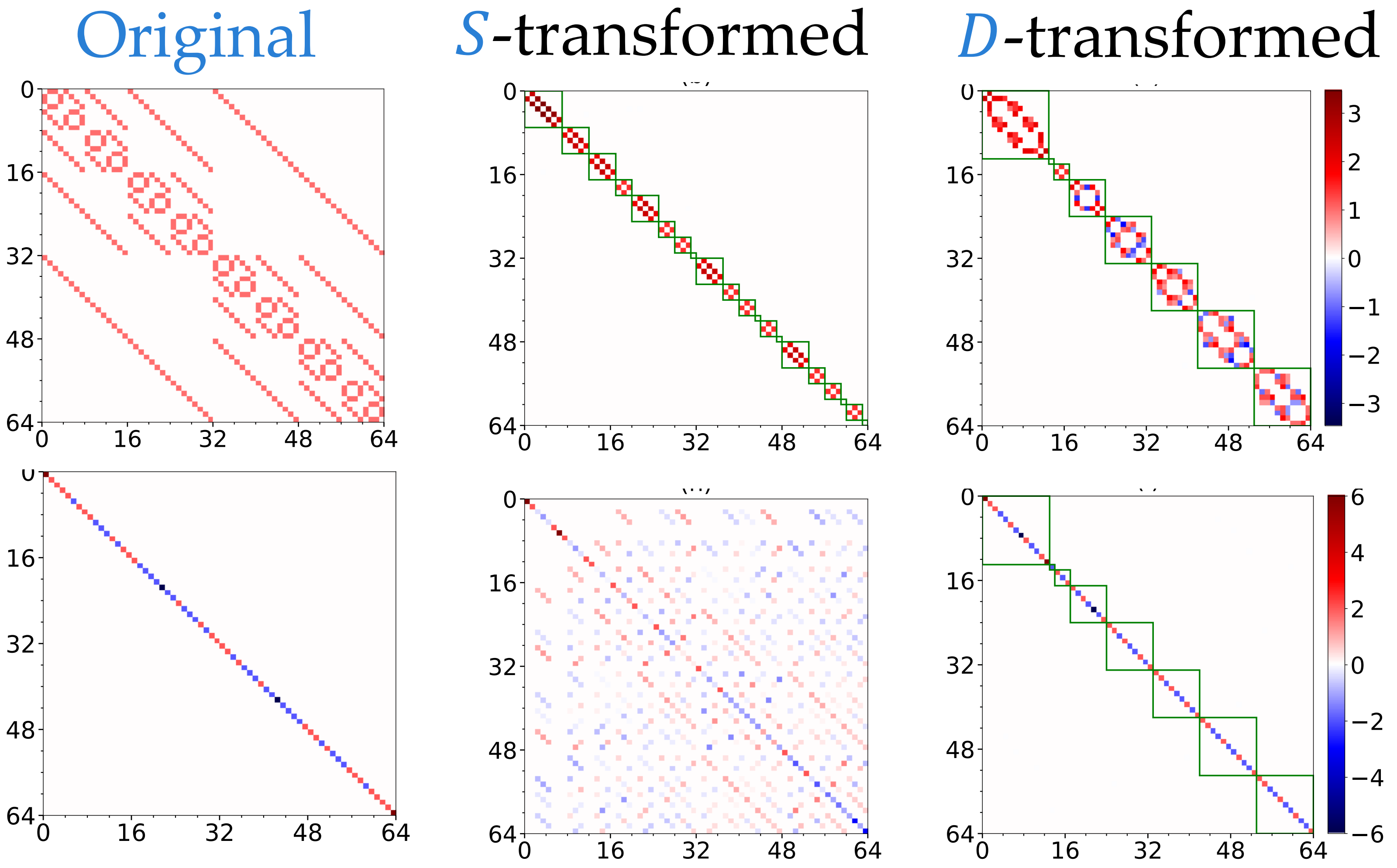
Symmetry-Assisted Hamiltonian Reduction

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

S symmetry

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

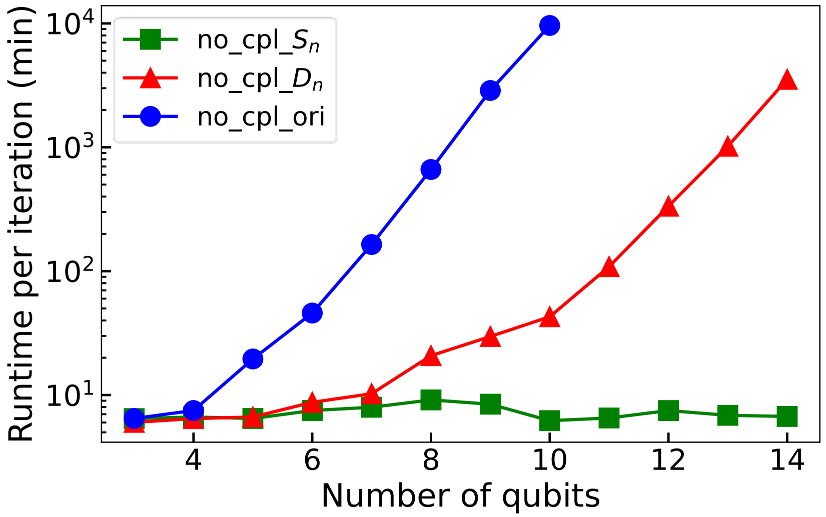
D symmetry

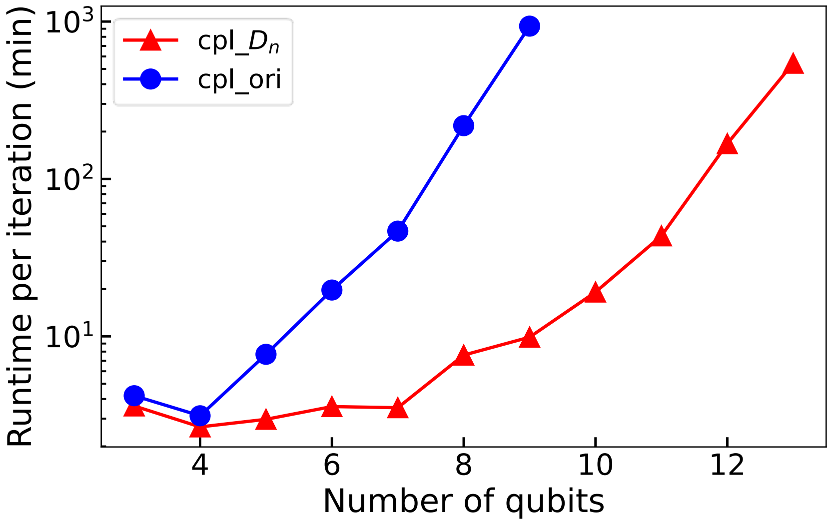


Results of Symmetry-Assisted Method

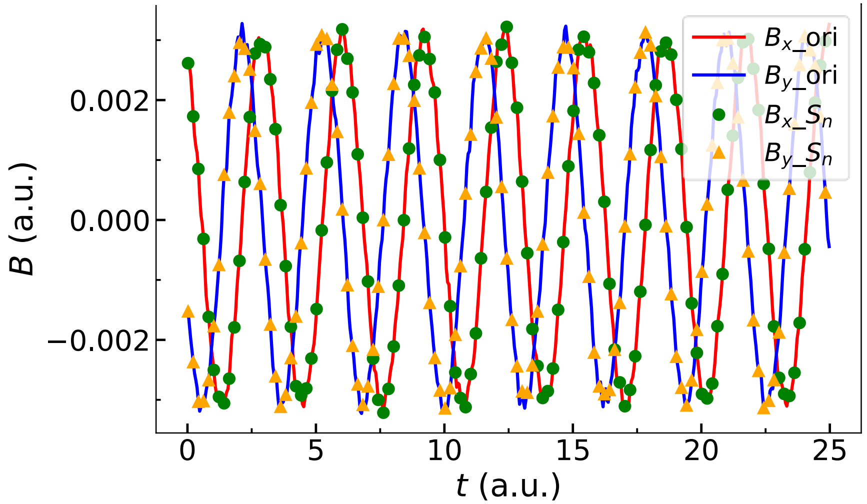
Non-coupled | Nearest-neighbor coupling

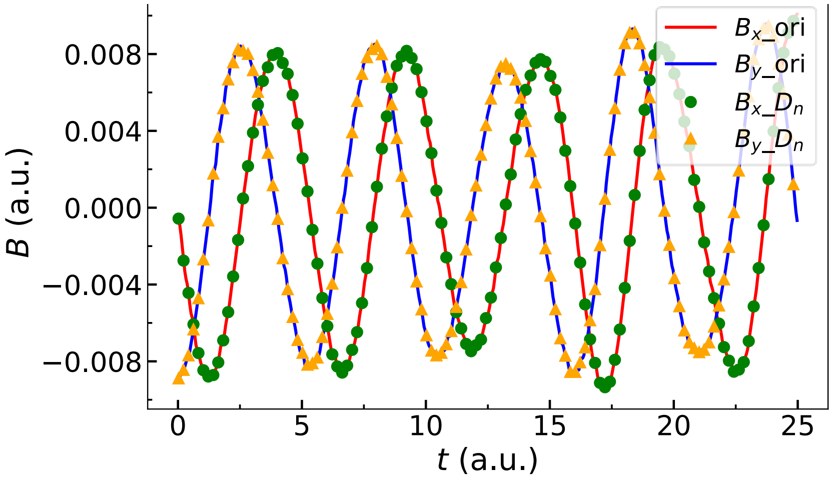
Runtime vs. number of qubits n





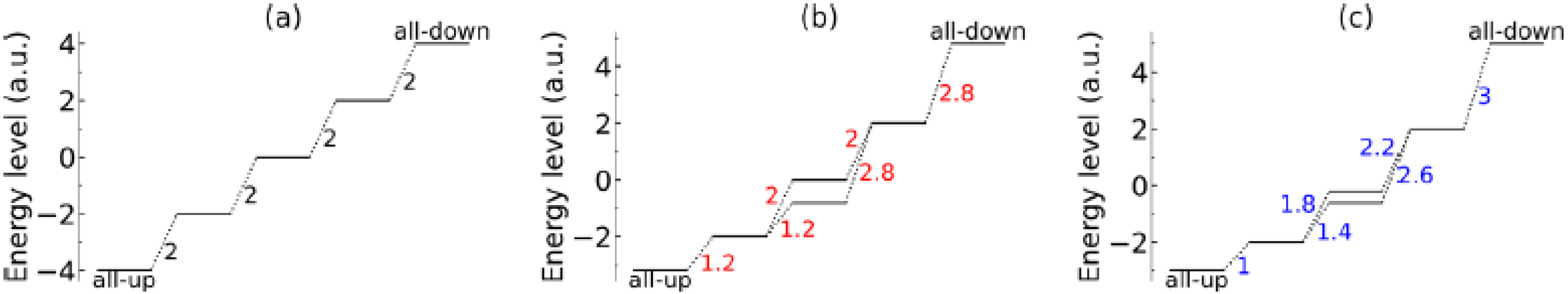
Optimized Controls





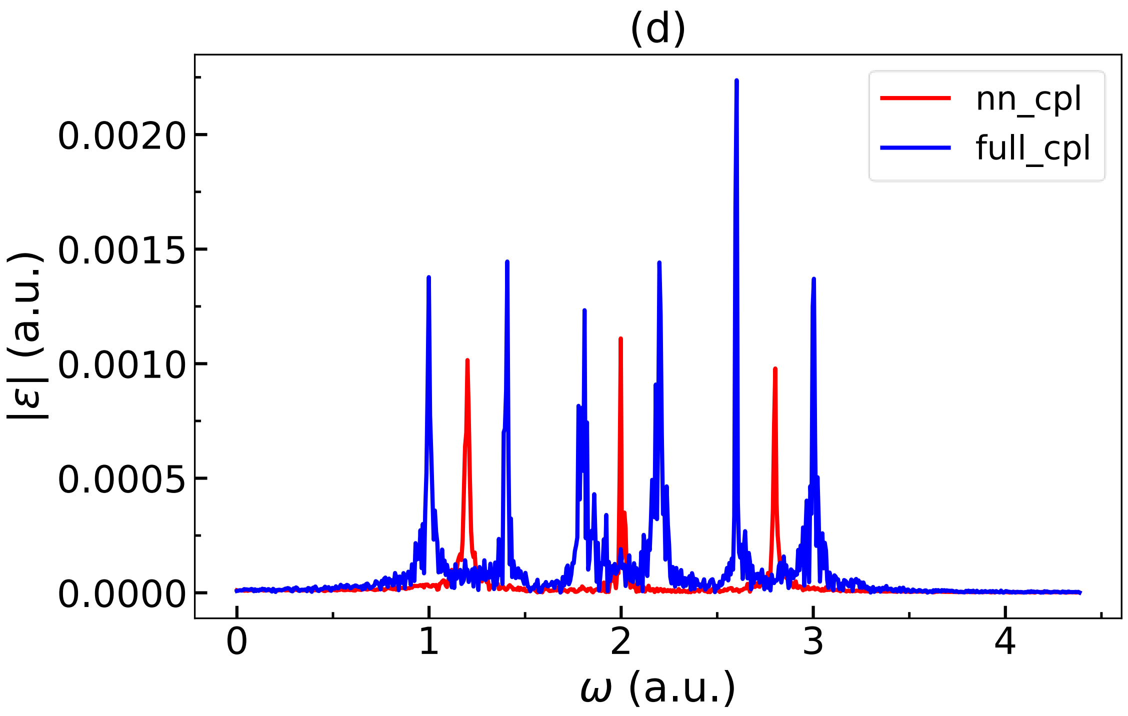
Results of Symmetry-Assisted Method

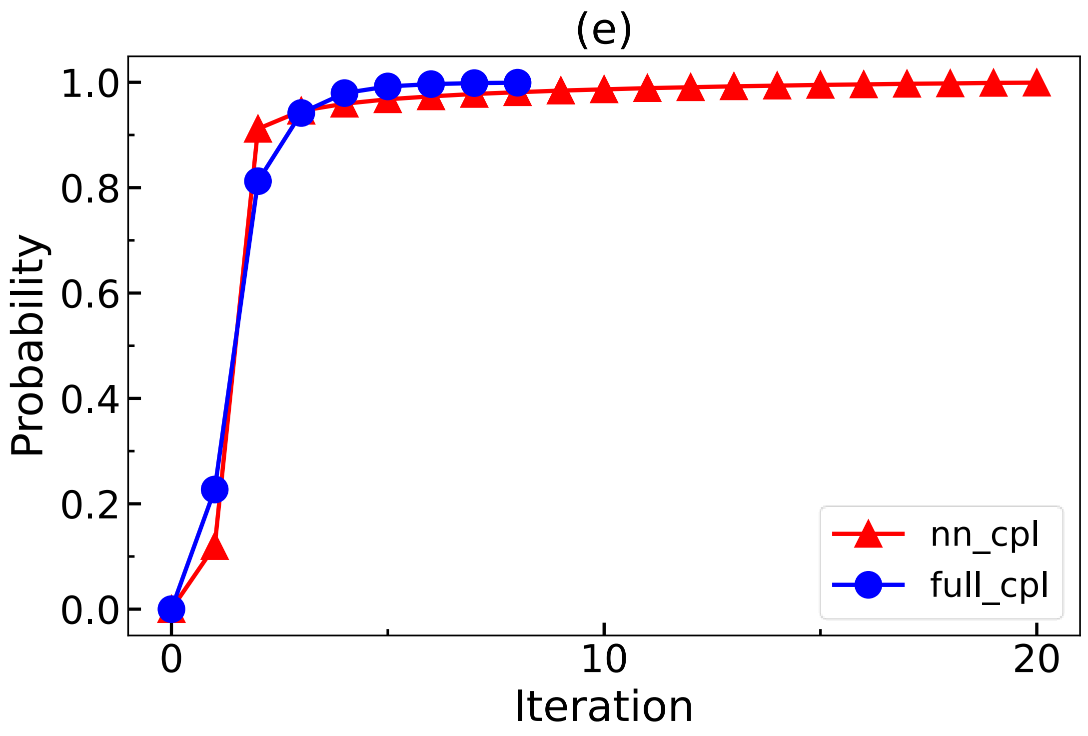
- Introduce coupling between further qubits to break degeneracy of energy differences
- 4 qubits:



No coupling | Nearest-neighbor coupling | Full coupling

Results of Symmetry-Assisted Method





Summary

- Predictive quantum simulations: Provide rational guidance for manufacturing quantum sensors for fossil energy infrastructures
- Modified NIC-CAGE: QOC algorithm for solving optimal controlling pulses, featuring analytical gradients

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

- Symmetry-assisted method: QOC algorithm for multi-qubit systems, featuring symmetry-based Hamiltonian reduction

- Wang, X., Okyay, M. S., Kumar, A., & Wong, B. M. (2023). *AVS Quantum Science*, 5(4). Featured Article, featured in *AVS Newsletter*

Acknowledgements

- Group website: http://bmwong-group.com
- E-mail: bryan.wong@ucr.edu
- Funded by U.S. Department of Energy, National Energy Technology Laboratory (Award Number DE-FE0031896)