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

Prof. Bryan M. Wong & Xian Wang

Department of Physics & Astronomy

Materials Science & Engineering Program

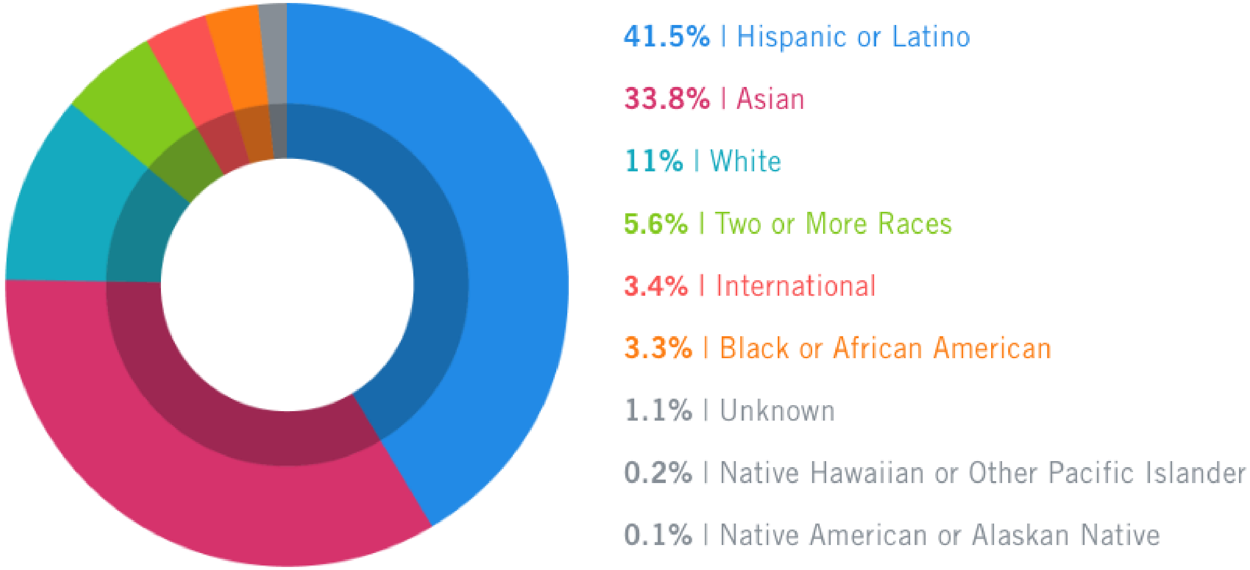
University of California, Riverside

Outline

- Short introduction
- Why use quantum information science for sensors?
- Predictive quantum simulations for candidate materials
- Preliminary work with quantum control calculations

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

Improving Sensing Modalities in Fossil Energy Infrastructures

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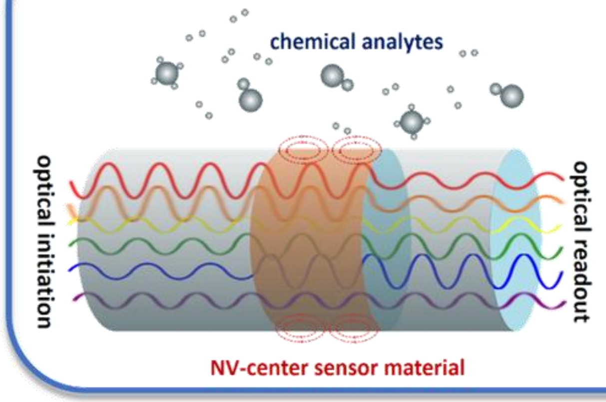

Properties to control:

1. ***Detection sensitivity***
2. ***Quantum coherence***
3. ***Long-term dynamics***

Quantum Information & Control

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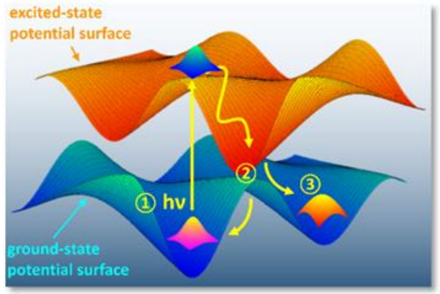

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$$

Harnessing Quantum Control for Initializing Detection

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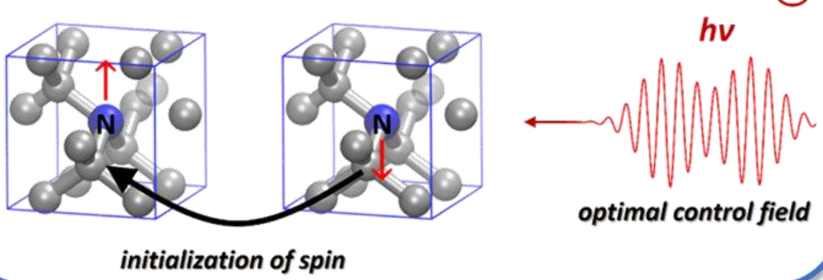

HBCU/MI Education, Training, & Research

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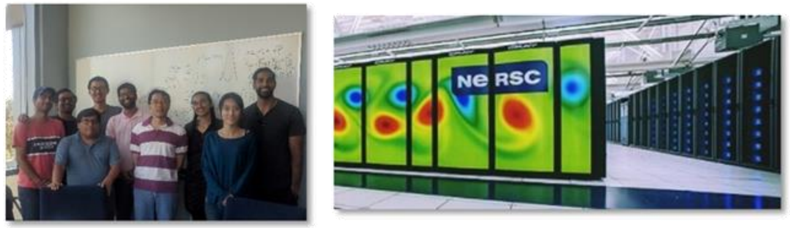


minority participation & state-of-the-art DOE computing

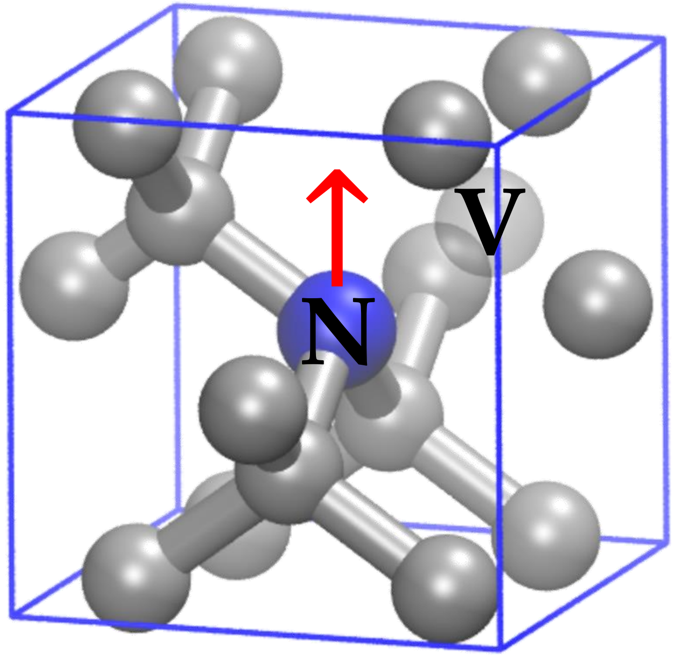
NV-Center Sensors

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

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

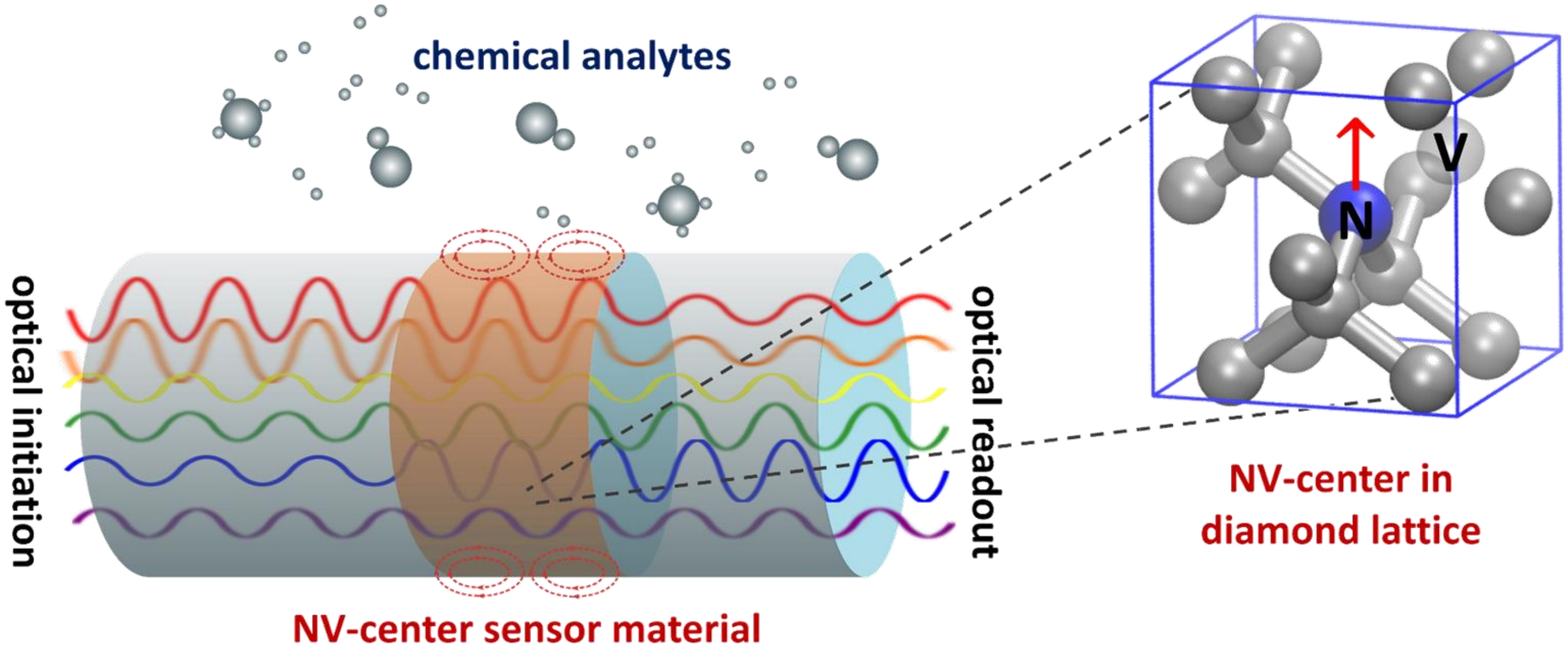
  - Coherence signals can persist at 700 – 1000 K (*essential for harsh fossil energy environments*)

  - Can be controlled with electromagnetic fields



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)

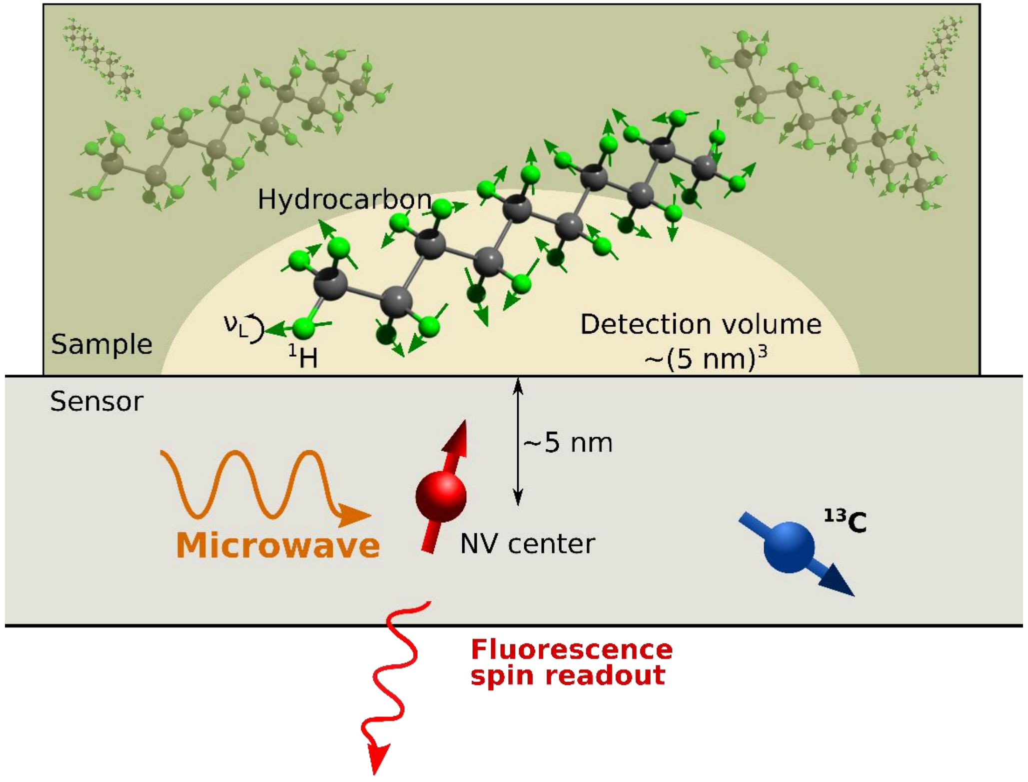


Near-Surface NV-Centers

- Current resolution of NV-center sensors ~(5 nm)^3 (size of large protein)

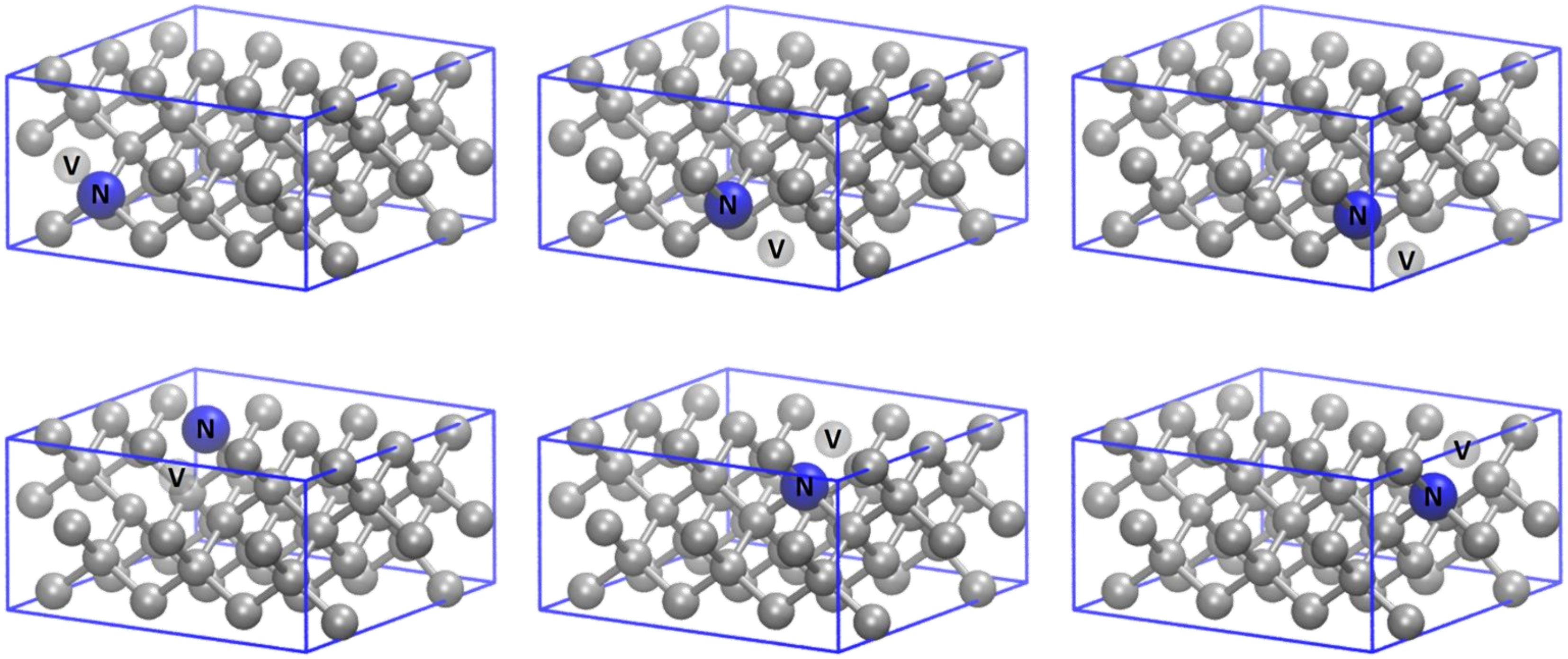
- Dipolar magnetic field $B_{\text{dip}} = \frac{\mu\mu_0}{4\pi}\frac{\sqrt{3\cos^2\theta+1}}{r^3}$

  - Since $B_{\text{dip}} \sim \frac{1}{r^3}$, sensitivity can be increased 3 orders of magnitude by reducing distance of NV center from surface by factor of 10



Initial NV-Center Configurations

- Use DFT to down-select initial NV-center configurations

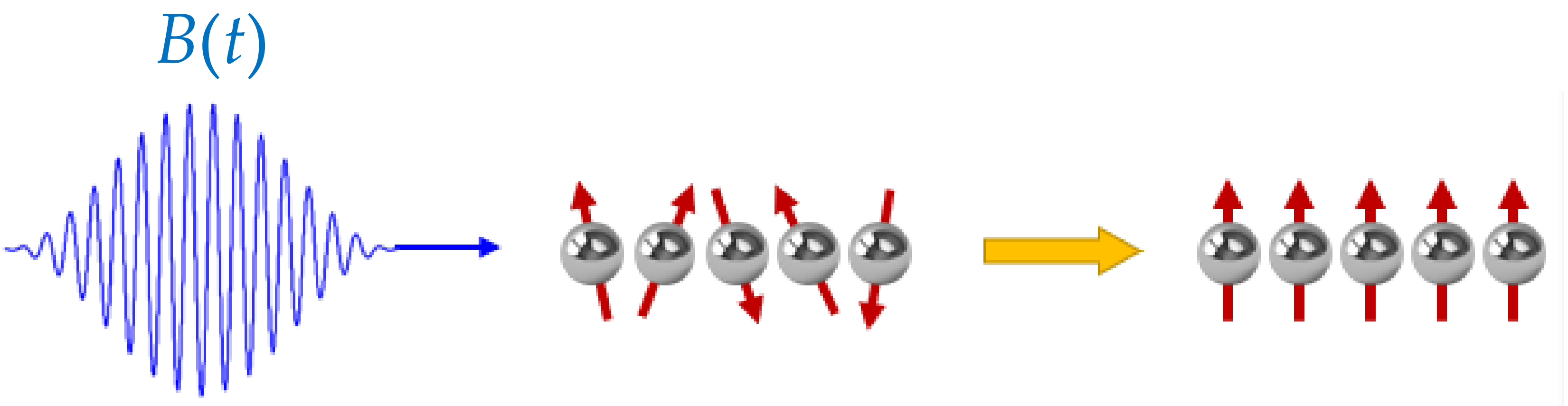


examples of NV-center configurations near top surface of lattice

- Carry out ab initio MD at various temperatures to test their stability

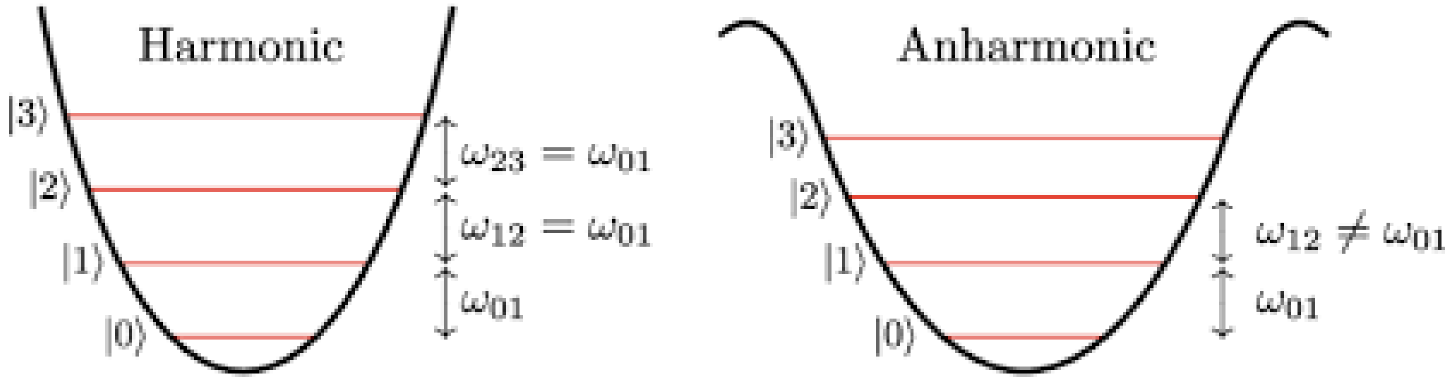
Purpose of Project

- Efficient manipulation of large qubit systems with external magnetic fields
- Quantum gate operation
- Quantum computing

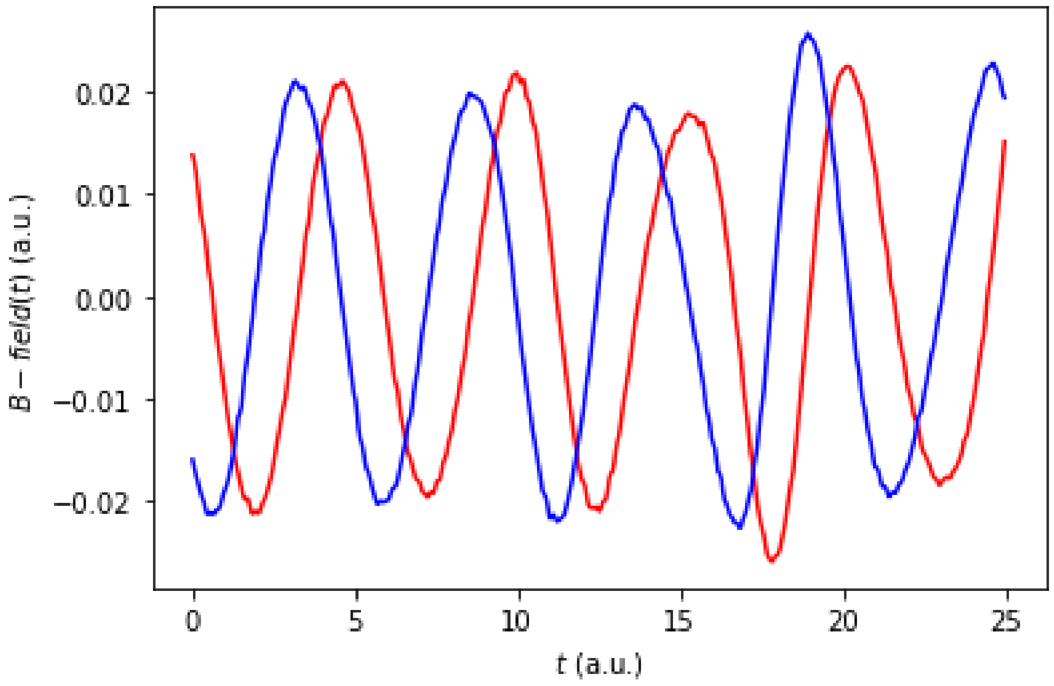


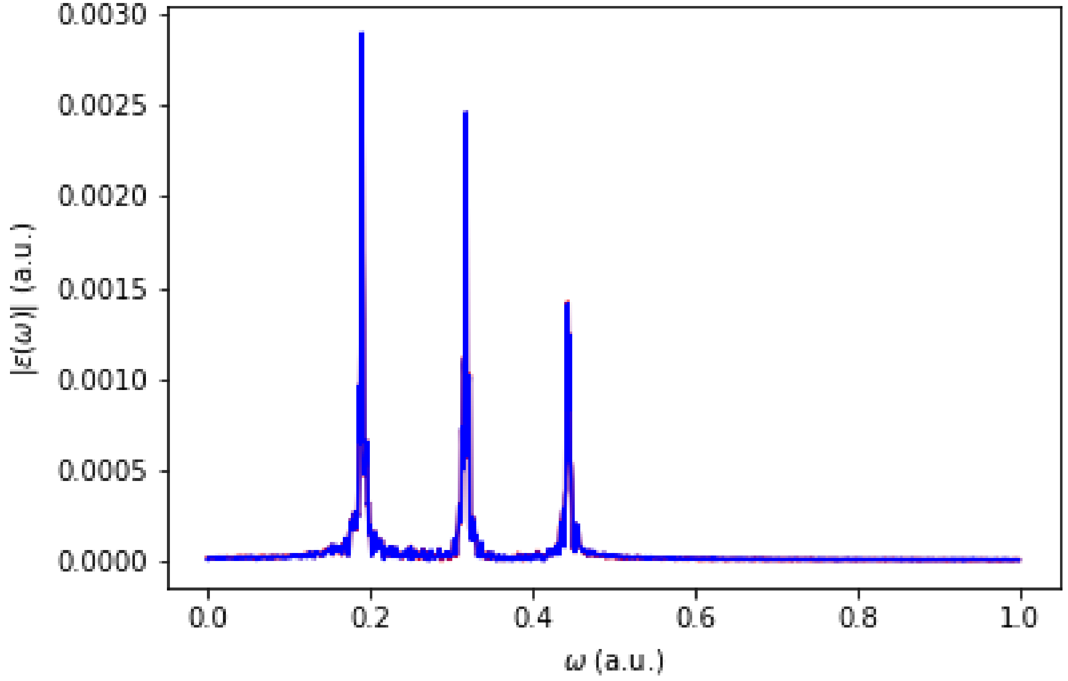
Hamiltonian of Multi-Qubit System

- $H = H_0 + H_c$
- $H_0 = -\left(\sum_i \sigma_z^i\right) \cdot B_z + c_{\text{coupling}}\left(\sum_i \sigma_z^i \sigma_z^{i+1}\right)$
- $H_c = \left(\sum_i \sigma_x^i\right) \cdot B_x(t) + \left(\sum_i \sigma_y^i\right) \cdot B_y(t)$



Optimal B-fields and Power Spectrum



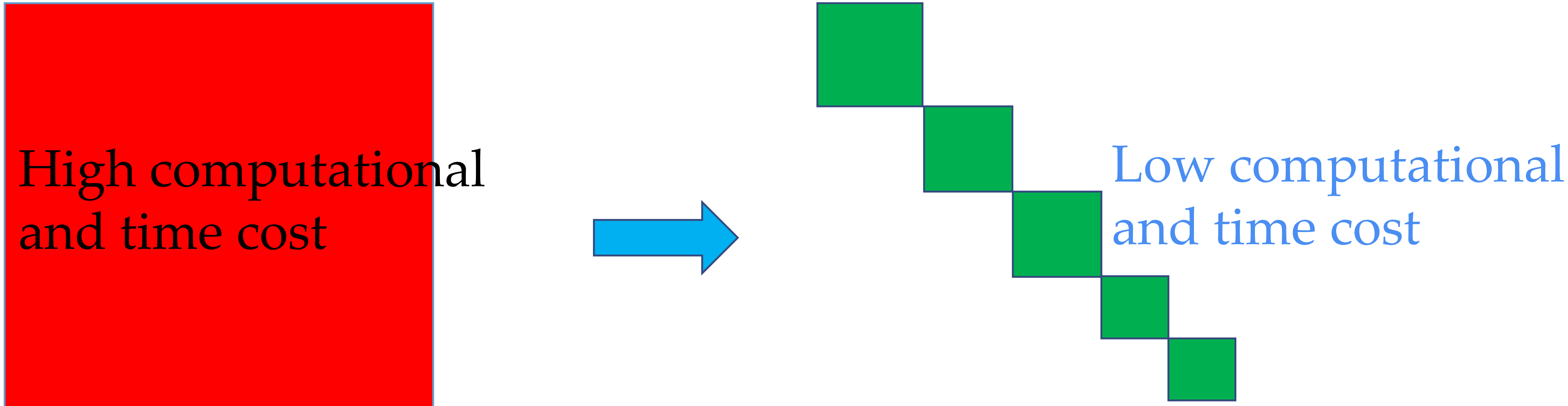


$B(t)$ vs. t

$\varepsilon(\omega)$ vs. ω

Symmetry-based Hamiltonian Decomposition

- Size of Hamiltonian increases as 2^n
- Decompose Hamiltonian matrix with symmetry of finite groups
- Developed for with-coupling and no-coupling cases



Symmetry-based Hamiltonian Decomposition

- $H_0 = -\left(\sum_i \sigma_z^i\right) \cdot B_z + c_{\text{coupling}}\left(\sum_i \sigma_z^i \sigma_z^{i+1}\right)$
- $H_c = \left(\sum_i \sigma_x^i\right) \cdot B_x(t) + \left(\sum_i \sigma_y^i\right) \cdot B_y(t)$
- $\sum_i \sigma_z^i,\ \sum_i \sigma_x^i,\ \sum_i \sigma_y^i$ has S_n (permutation group) symmetry
- $\sum_i \sigma_z^i \sigma_z^{i+1}$ has D_n (dihedral group) symmetry

- Size of Hamiltonian decreases from 2^n to $O(n)$ or $O(2^n/n)$

Symmetry-based Hamiltonian Decomposition

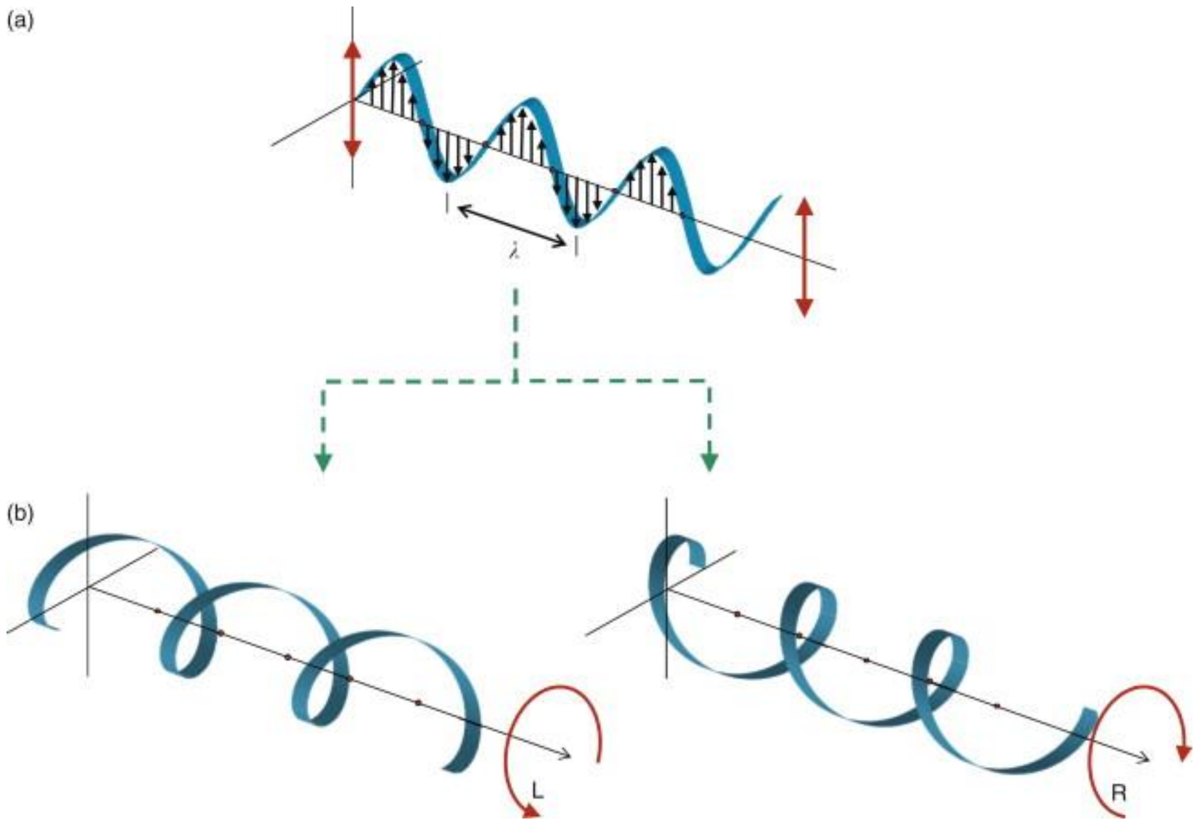
Number of qubits n	**Size of Hamiltonian**		
	Original 2^n	S_n decomposition $O(n)$	D_n decomposition $O(2^n/n)$
3	8	4	4
4	16	5	6
5	32	6	8
6	64	7	13
7	128	8	18
8	256	9	30
9	512	10	46
10	1024	11	78
11	2048	12	126
12	4096	13	224
13	8192	14	380
14	16384	15	687

Linear Unitary Operator

- Exponential propagator
- $\exp\left[i\tau H\left(t+\frac{\tau}{2}\right)\right]\psi(t+\tau)=\psi(t)$
- Linear unitary propagator from NIC-CAGE: Novel Implementation of Constrained Calculations for Automated Generation of Excitations
- $[\mathrm{I}+\frac{i\tau}{2}H(t+\frac{\tau}{2})]\psi(t+\tau)=[\mathrm{I}-\frac{i\tau}{2}H(t+\frac{\tau}{2})]\psi(t)$
- Analytical form of the gradient $\frac{\mathrm{d}P}{\mathrm{d}B}$ for back-propagation

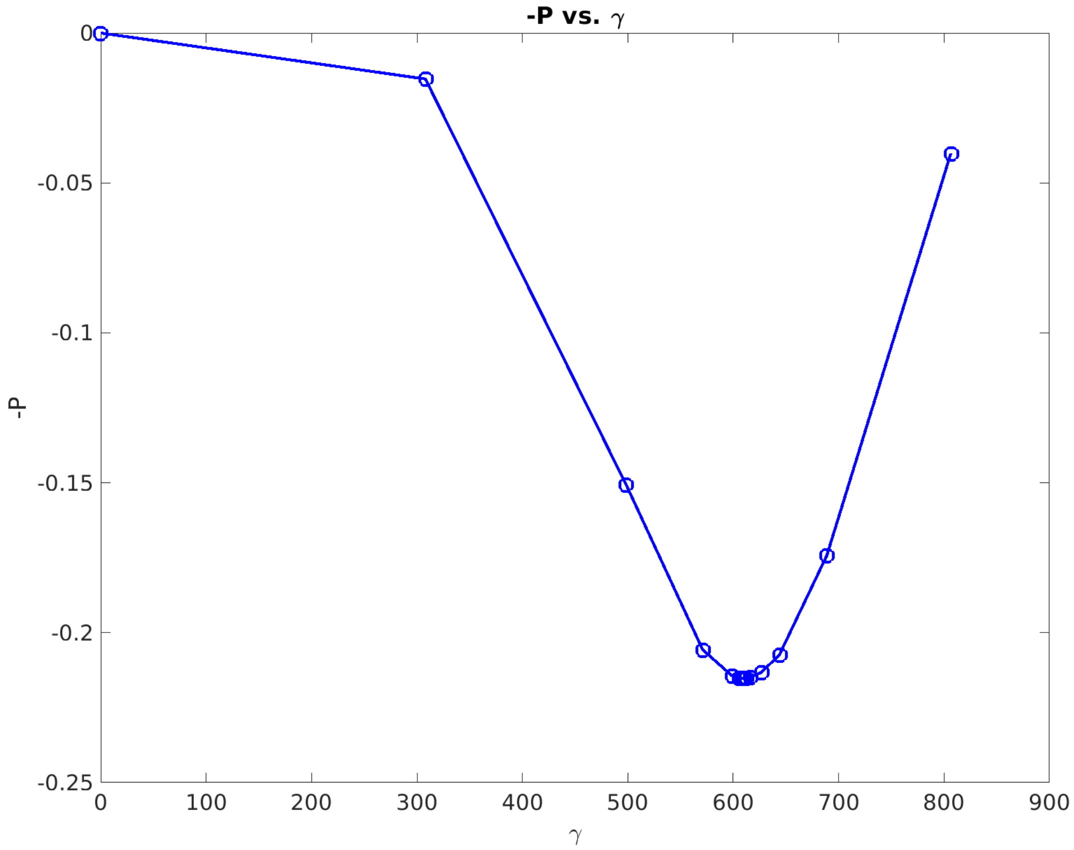
Technical Improvements

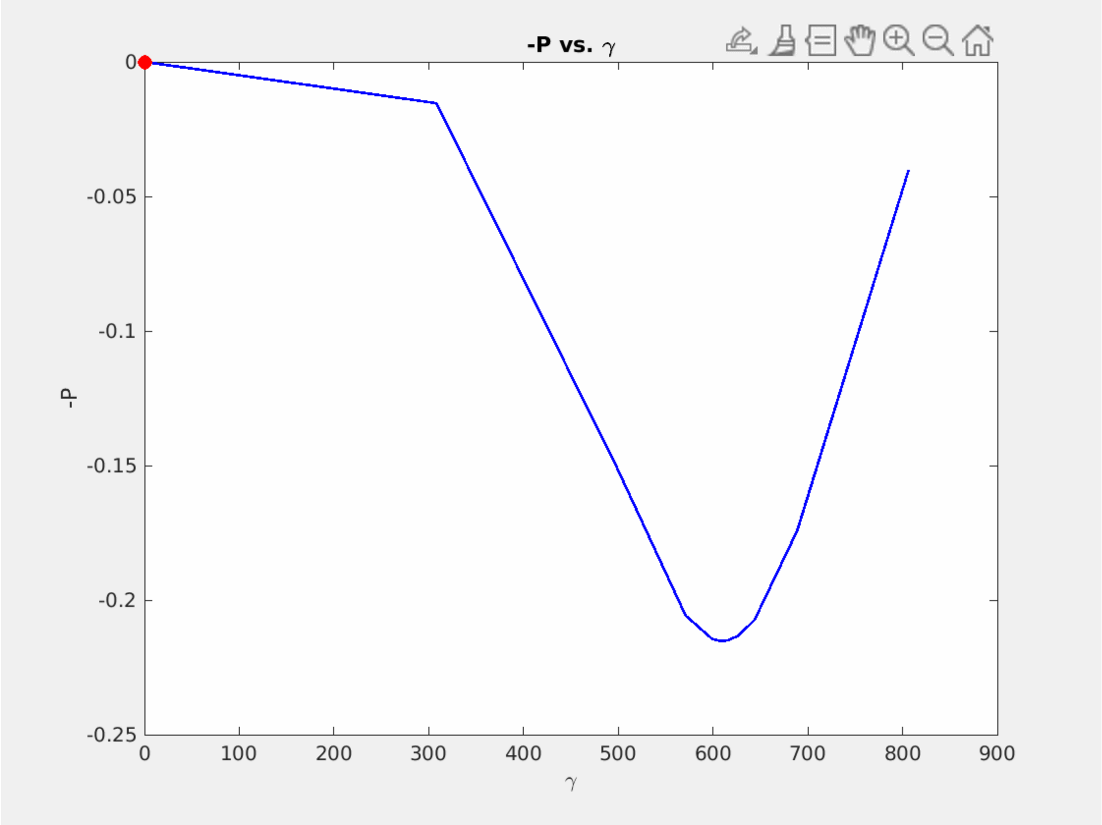
- B-fields in x- and y- direction, polarization



Technical Improvements

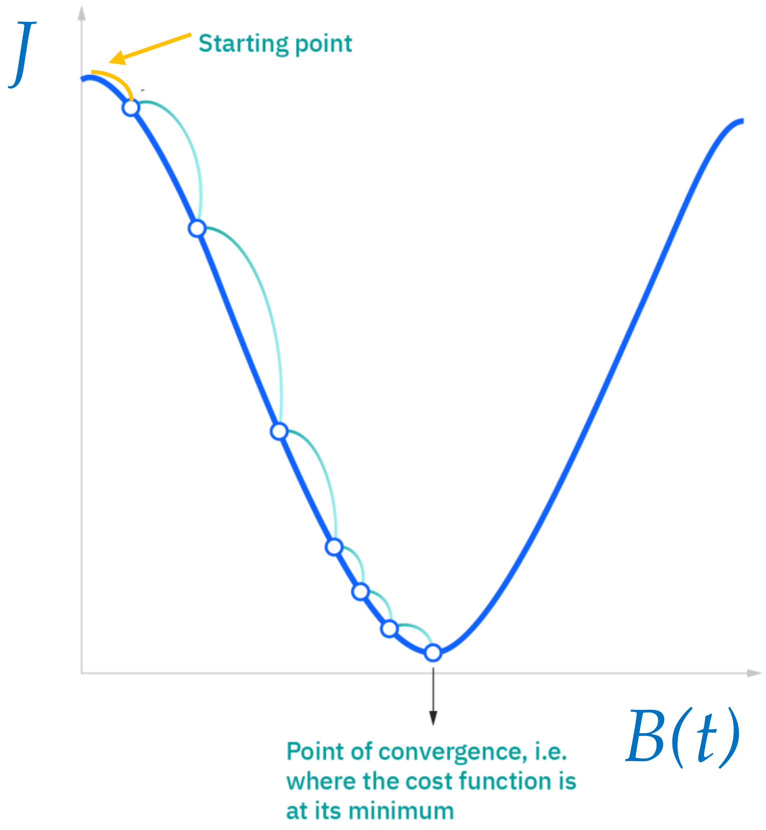
- Golden section search, more robust & faster





Technical Improvements

- Heuristic amplified gradient



Conclusion & Acknowledgements

- Predictive quantum simulations provide rational guidance for constructing quantum sensors for fossil energy infrastructures
- Quantum information science *almost perfect application for sensors & interaction with external fields*

Web: http://bmwong-group.com

E-mail: bryan.wong@ucr.edu

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