Overview of Quantum Chemistry

2024 SIAM Quantum Intersections Convening

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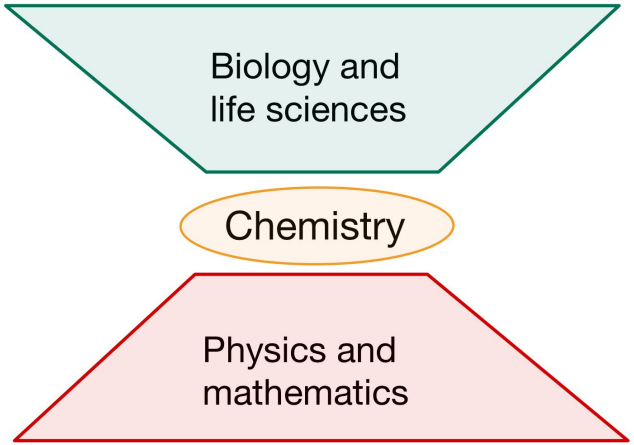
Amazon Visiting Academic

Overview

1. Welcome
2. Quantum chemistry
3. Warning on simulation: ground states vs propagation
4. Statistical boundaries between quantum and classical
5. Density functional theory

Quantum chemistry



- Chemistry is…
- Physical chemistry is…
- Computational chemistry is…
  - Molecular dynamics (informed by quantum)…
- Quantum chemistry is…
  - Electronic structure
  - Strong/weak correlation, molecular orbitals

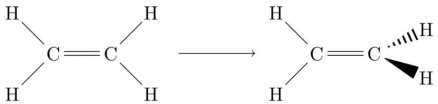
Quantum chemistry

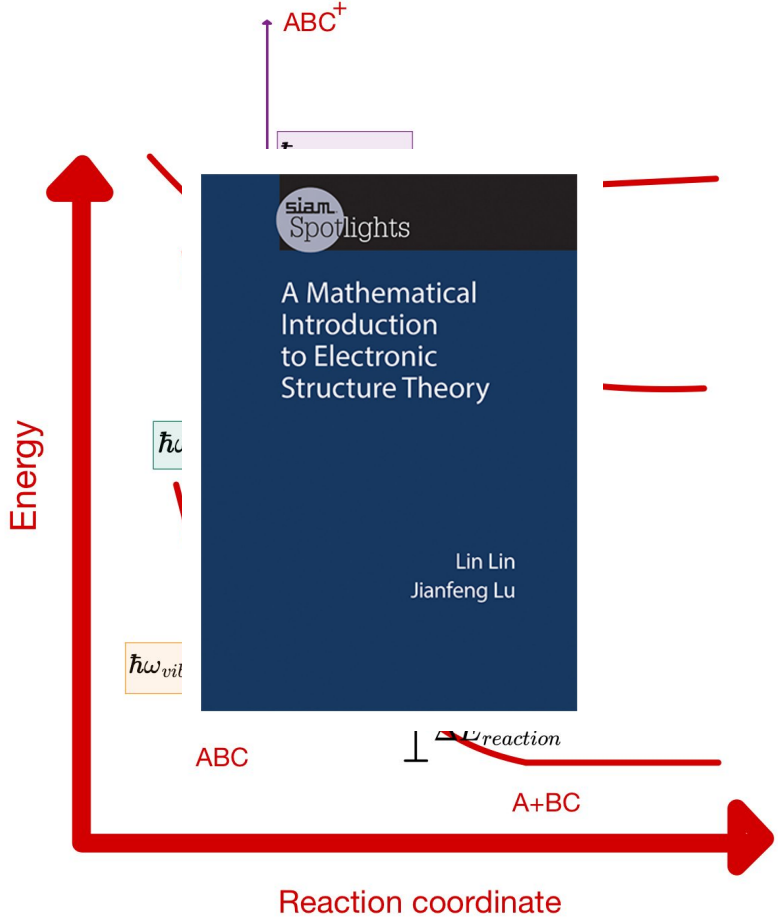
Molecules → Computations → Physical Quantities

Input	Task	Output
$\hat{H} \mapsto [H_{ij}]$	$H\psi_g = E_g\psi_g$	$E_g(R)$
$\hat{\psi} \mapsto [\psi_k]$	$H_t\psi_t = i\partial_t\psi_t$	$\psi = \psi(t, \psi_0)$

Examples

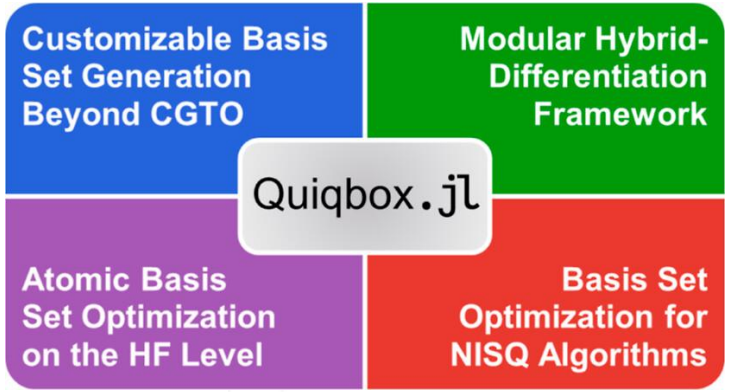
- Proton affinity
  H+Cl→ HCl
- Barrier heights

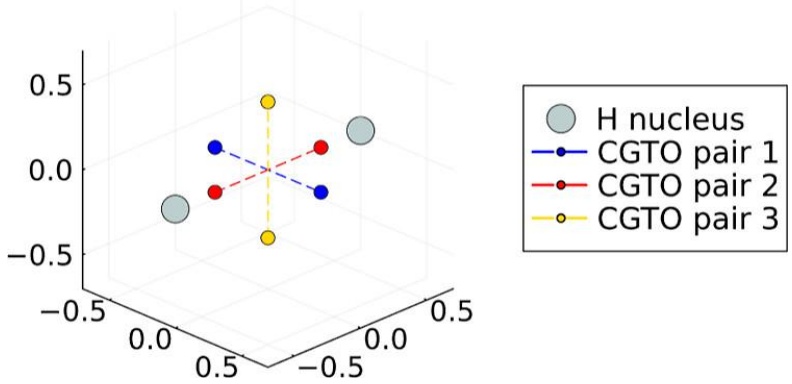




Discretization in Quantum Chemistry

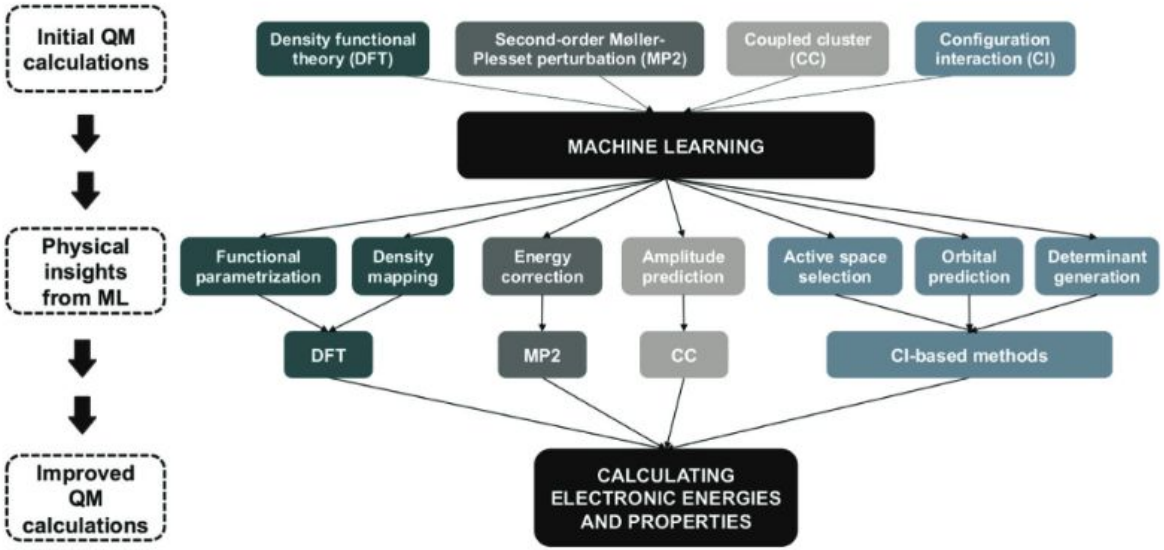
- In order perform computations, need to project onto finite basis
  - Gaussian orbitals
  - Planes waves
  - Orthogonal polynomials
- Challenges
  - Capture correlations
  - Treating coalescence cusp conditions
  - Convergence in complete basis limit
  - Optimization of basis set parameters





Wang & Whitfield Basis set generation and optimization in NISQ era with Quiqbox.jl. *J Chem. Theory Comp.* (2023)

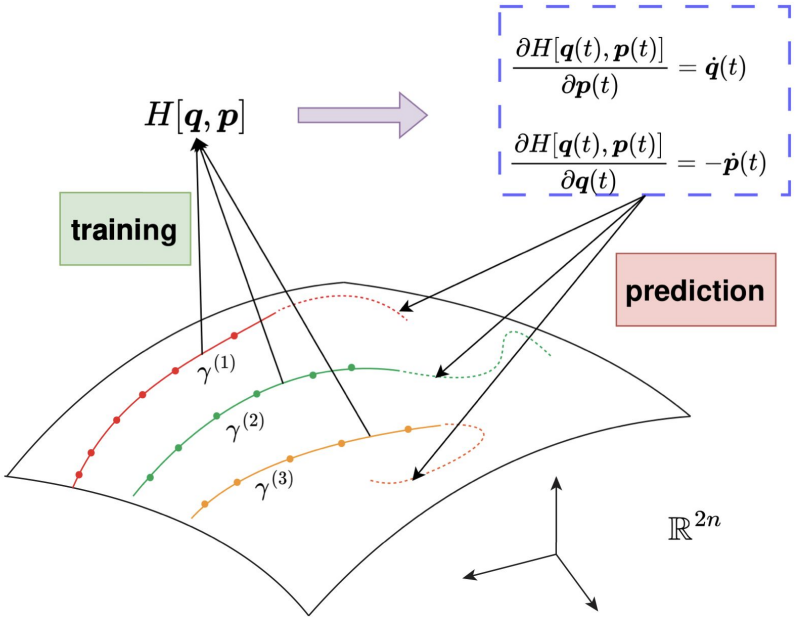
Active research in quantum chemistry: machine learning



- Models only as good as data “Garbage in, garbage out…”
- Density functional theory is de facto standard for training data

Aldossary et al. "In silico chemical experiments in the Age of AI: From quantum chemistry to machine learning and back." *Advanced Materials* (2024)

Active research in quantum chemistry: machine learning



- Models only as good as data “Garbage in, garbage out…”
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- *Time-dependence*

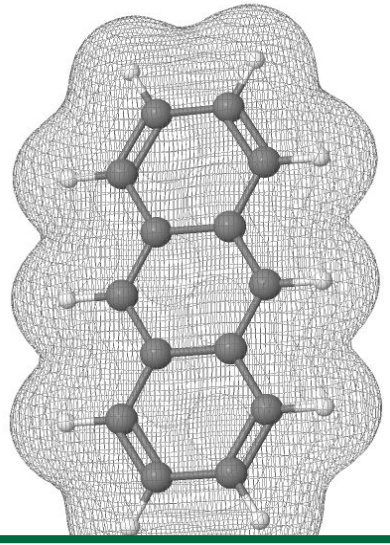
Yang, Whitfield “Machine-learning Kohn-Sham potential from dynamics in time-dependent Kohn-Sham systems” Mach. Learn.: Sci. Technol. (2023)

Current state of the art: density functional theory

Theoretical basis for DFT

- The probability density corresponds (usually uniquely) to the V_{ext} and E_0
- Intuition behind correspondence
  - $E_0 = \langle\psi|(T + W_{int})|\psi\rangle + \int n(x)V_{ext}(x)dx$
  - T and W_{int} are always the same, only V_{ext} changes
- Universal functional

  $F[n] = \min_{\psi\to n(r)}\langle\psi|(T + W_{int})|\psi\rangle$
- It is theoretically impossible to obtain this functional [Schuch, Verstraete 2009]

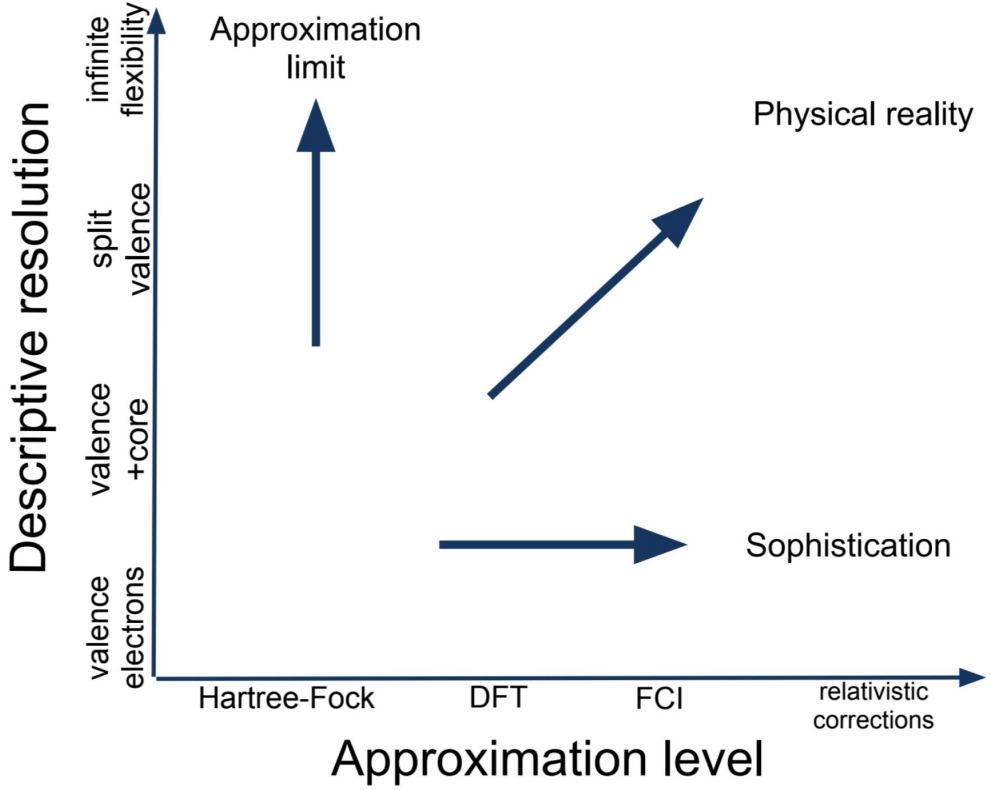


3N coordinates → 3 coordinates

The single electron **probability** density replaces the wave function

Key considerations

- Resolution vs volume
  - Input as molecule
  - Input as numerical data
- Accuracy
  - Discretization error
  - Approximation error
  - Physically relevant
- Resource constraints
  - Energy
  - Time



Future of research in quantum chemistry
Broad area: quantum technology

A Practical Introduction to Quantum Computing

May 01, 2024 | By Casey Dowdle and James Whitfield

Quantum technology

- Communication
- Computation
- Sensing

Quantum simulation

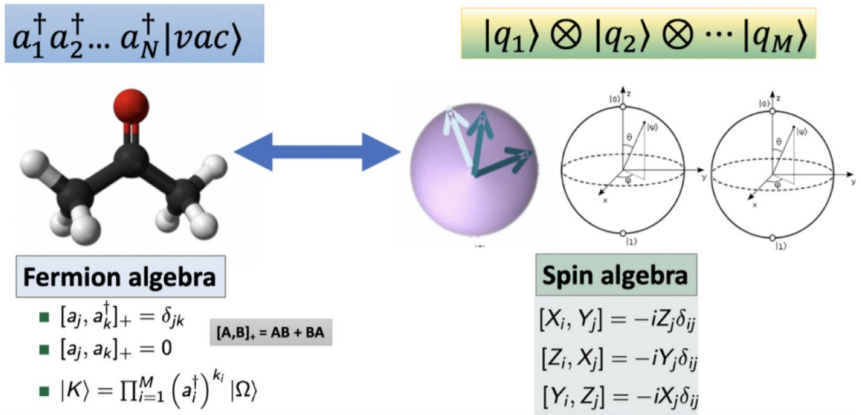
- Experimental realizations
- Mostly with minimal basis sets

Quantum programming

- Amazon Braket

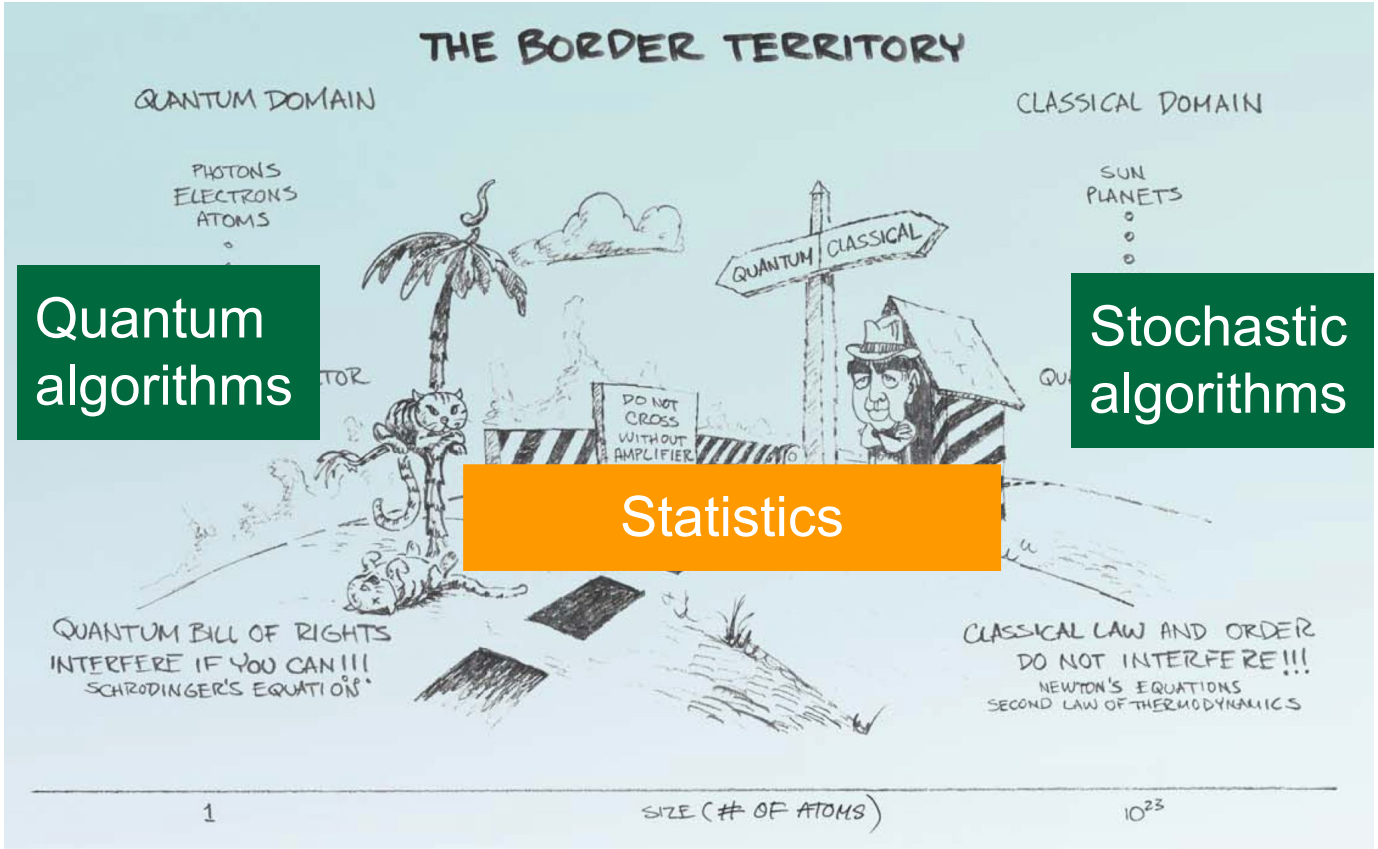
Quantum chemistry and quantum computing

- NISQ efforts center around optimization (VQE)
- Current simulation sizes limited by hardware
- Encoding fermions as qubits for simulation



Fundamental question

Image from Zurek (2003)
arXiv:quant-ph/0306072



Quantum algorithms

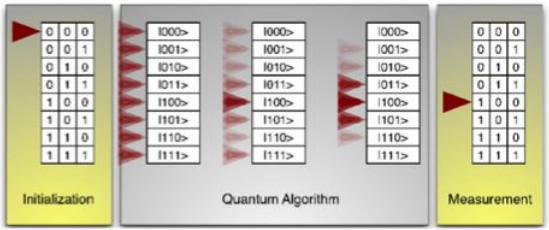
Stochastic algorithms

Statistics

Quantum primacy

Alternate protocols

- FourierSampling
- BosonSampling
- IQP
- Random circuit sampling



Article

Quantum supremacy using a programmable

arXiv > quant-ph > arXiv:2406.02501

Quantum Physics

[Submitted on 4 Jun 2024 (v1), last revised 21 Jun 2024 (this version, v3)]

The computational power of random quantum circuits in arbitrary geometries

Matthew DeCross, Reza Haghshenas, Minzhao Liu, Enrico Rinaldi, Johnnie Gray, Yuri Alexeev, Charles H. Ba

QUANTINUUM

Quantum supremacy

- Relies on statistical arguments
- Requires implementing randomly selected $U_{circuit}$
- Sample from $\rho = \mathcal{E}_{circuit}[\rho(i)]$ with $\mathcal{E}_{circuit} \approx U_{circuit}(\bullet)U^{\dagger}_{circuit}$

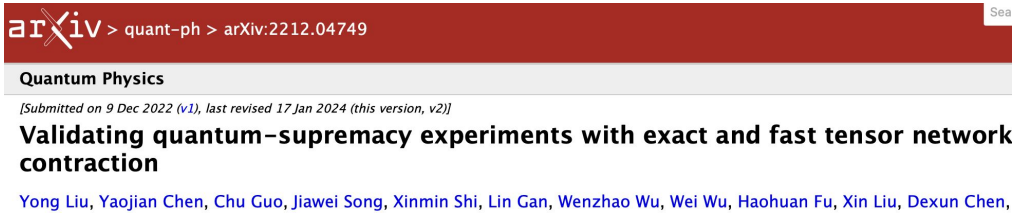
Quantum primacy

Quantum primacy relies on benchmarks

- ***Statistical spoofing***

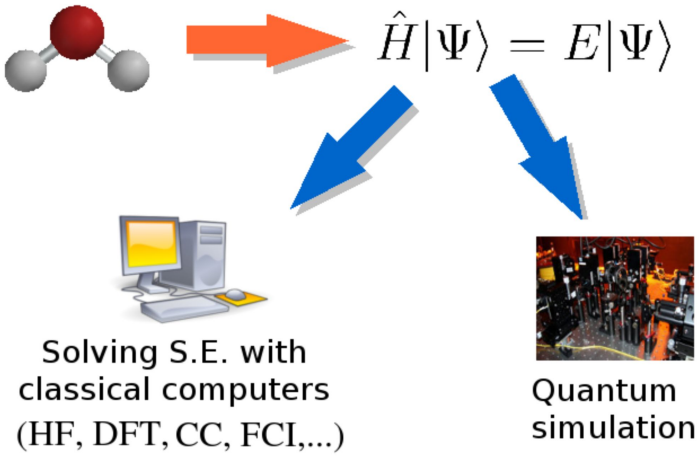
Tensor network simulations

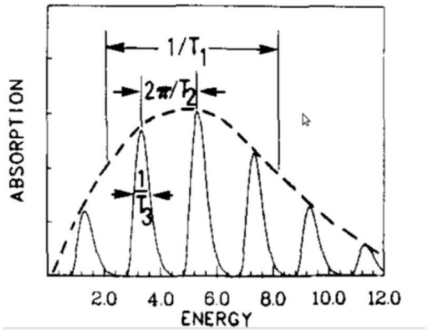
- ***Mimicking quantum computers***

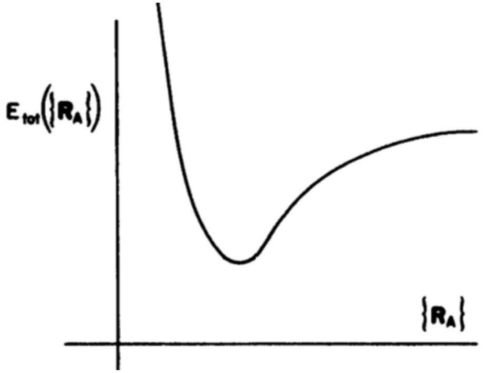


Fundamentally: **What is the difference between quantum and probability theory?**

Quantum simulation







Dynamics vs Ground states

Given ψ_i and H,
compute $\psi_t = \exp(-iHt/\hbar)$

Quantum dynamics is quantum computation

Given H, find Ψ_0 where
$\langle H \rangle_{\Psi_0} \leq min_\psi \langle H \rangle_\psi$

Quantum optimization is still optimization problem

Key takeaways

1. Quantum chemistry on quantum computers is here (but irrelevant so far)
2. Ground states ***is not*** propagation
3. Density functional theory as baseline
4. Better quantum data means machine learning models
5. Quantum chemistry is where quantum physics connects to the central science

Thank you

$\langle\Psi|W\rangle + \langle G|\Psi\rangle$ Whitfield Group

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Outlook

Quantum advances

- Hardware advances
- Quantum error correction (QEC)
- Quantum simulation as QEC

Classical advances

- Exascale computing
- Machine learning
- Solvable chemical instances

Discussion questions

- What solutions to electronic structure do we formally have?
  - What makes quantum chemistry difficult for computers?
- How can quantum computers show advantage in practice?
  - Quantum algorithms for high-throughput?
- Can we formulate quantum chemistry as a quantum primacy challenge?

Appendix

How mathematics is involved and needed

- Optimization theory
- Group theory
- Linear algebra
- Coding theory
- Differential equations
- Geometry
- Probability/statistics

- Parameterized ansatz for quantum chemistry
- Point group symmetries, angular momentum, spin
- Linear combinations of molecular orbitals
- Quantum compression and error correction
- Model solutions e.g. hydrogen atom solution
- Potential energy surfaces, ansatz manifolds
- Distinction between quantum and probability

How to best foster partnerships and collaborations to drive progress

Technical

Quantum intermediate representation (https://github.com/qir-alliance)
OpenQASM (https://openqasm.com/intro.html)

https://github.com/amazon-braket

Theoretical

Defining and solving “standard” quantum chemistry
Well-wrought techniques from applied mathematics
Statistics and quantum-classical divide
Spoofing quantum computers

Thank you

SIAM Quantum Intersections Convening
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