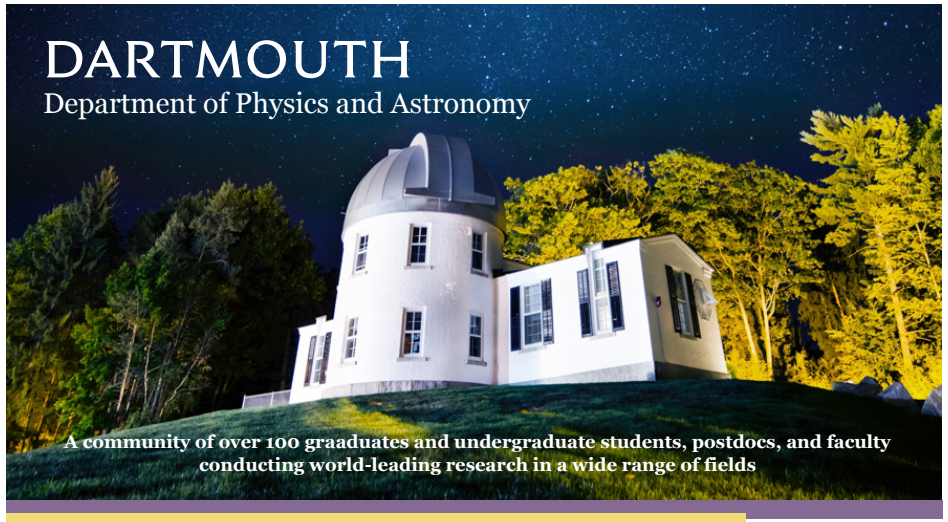
Quantum chemistry on quantum computers

James Daniel Whitfield
Department of Physics and Astronomy
Dartmouth College



PhD Program in Physics and Astronomy

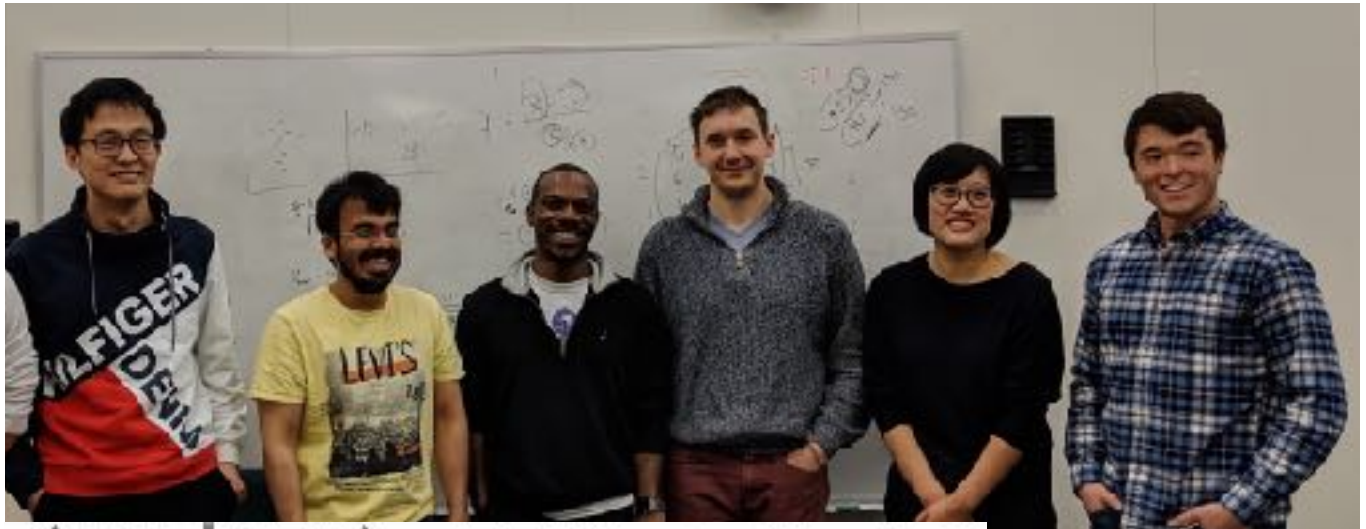
Major research efforts include:
astrophysics; gravitation and cosmology; quantum information and condensed matter; physics of plasmas, fluids, and beams; and space physics.

Apply Here:
app.applyyourself.com/?id=dart-grad

Learn more at:
physics.dartmouth.edu/graduate

Contact:
James.W.Labelle@dartmouth.edu

Deadline: January 15, 2019



⟨Ψ|W⟩ Whitfield
⟨Ψ|G⟩ Group

Quantum Information Science at Dartmouth

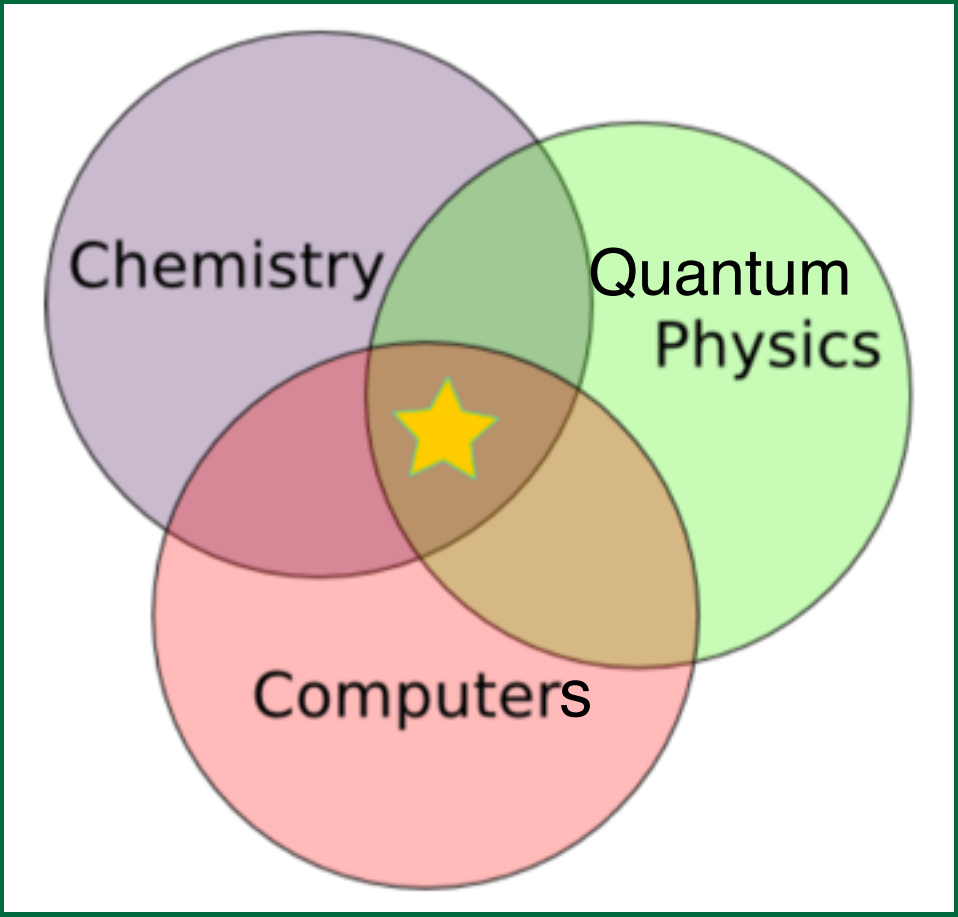
Course overview

Lecture 1: QCQC (slides)
Lecture 2: Technical introduction (board)
Lecture 3: Quantum for simulation (slides/board)

Objectives

1. Understand how quantum mechanics intersects chemistry
2. Connect quantum computation to quantum chemistry
3. Background knowledge to get start in the literature

Part 1:
Quantum, chemistry, computers



Goals of chemistry:
Identification of the substances of which matter is composed; their properties and the ways in which they interact, combine, and change; and the use of these processes to form new substances.

Goals of quantum:
To graduate from mechanics to engineers

Schrödinger Equation

$H\psi_n = E_n\psi_n$	Solving an eigensystem
$-iH\psi = \frac{\partial\psi}{\partial t}$	Propagating a partial differential equation

Goals of computers:
One who computes, reckons.

First use of word was in 1600's

Quantum **chemistry computers**

Goals of computational chemistry:

1. *A priori;* screening
2. *Post facto;* explanation
3. *In silico;* safety and feasibility

DFT

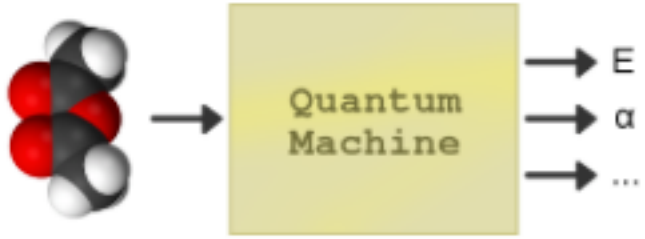
CC, DMRG, CI, etc.

Programming is cheaper than experiments

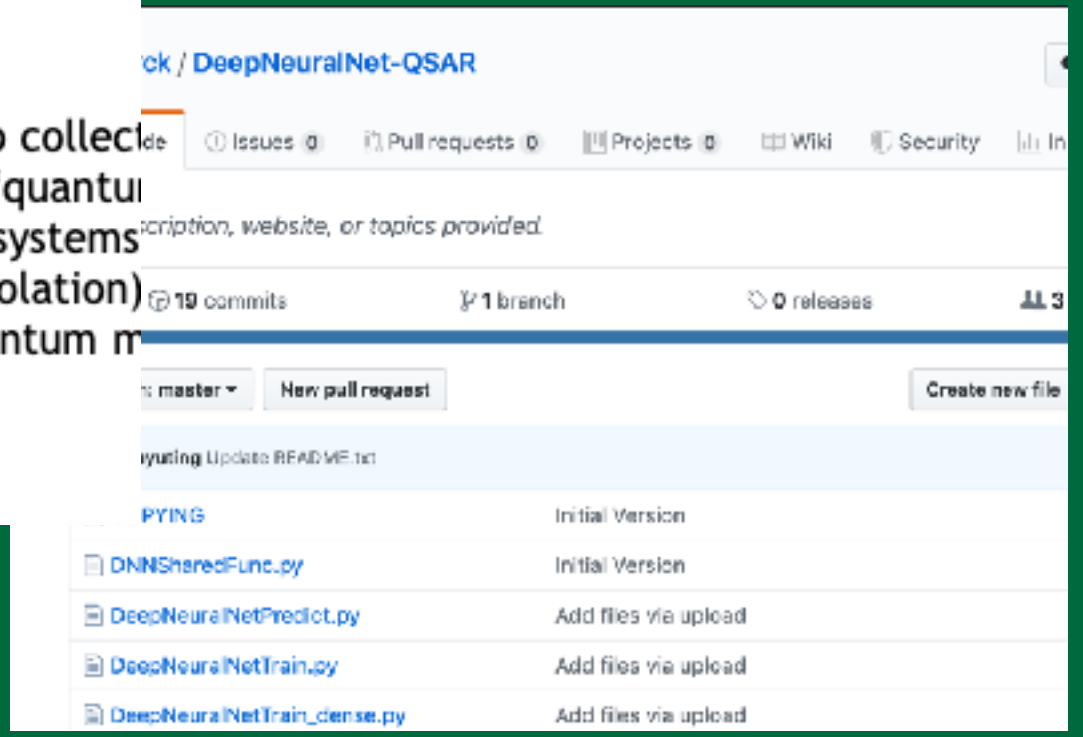
Quantum **chemistry computers**

QUANTUM-MACHINE.ORG

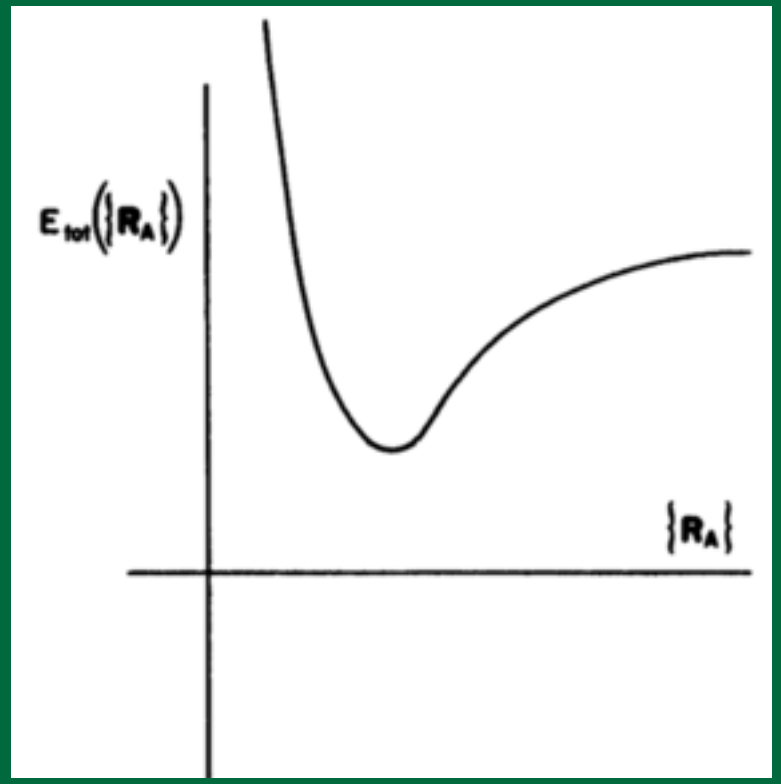
Home | Datasets | Publications | Software



This website aims to collect
development of a "quantu
quantum-chemical systems
induction (or interpolation)
illustration of a quantum m
the left.



Quantum **chemistry computers**



Born-Oppenheimer approximation

$$\mathbf{F} = -\nabla E_{tot}(\mathbf{R}_A) = m\ddot{\mathbf{R}}_A$$

Classical equations of motion

Nuclear dynamics

Vibration

Rotation

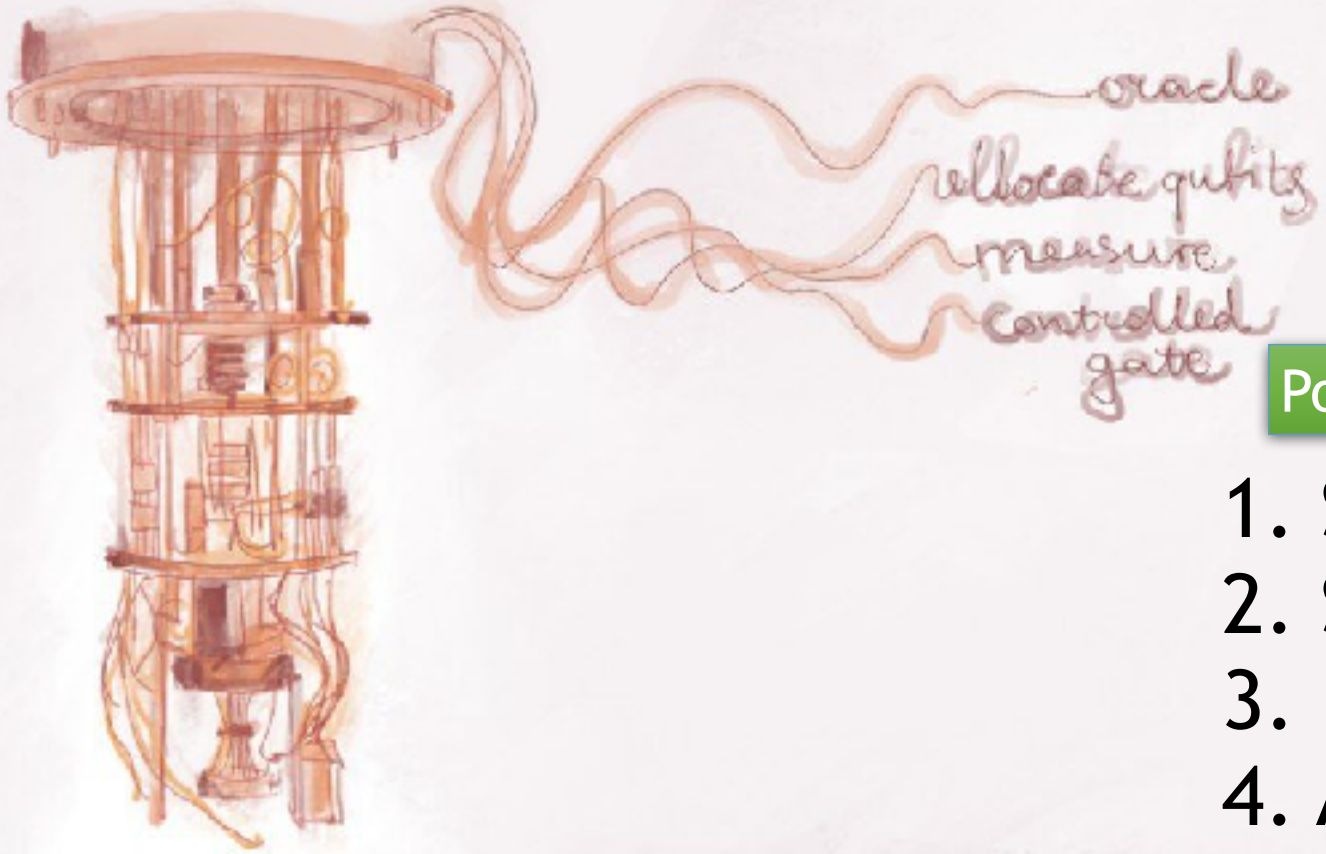
Bonding

Quantum **chemistry computers**

Atomic units

Quantity	**Atomic Units**	**SI units**
Reduced Planck's constant	1 $\hbar$	1.055×10^{-36} J s
Mass of electron	1 m_e	9.109×10^{-31} kg
Proton charge	1 e	1.602×10^{-19} C
Bohr radius	1 a_0	5.292×10^{-11} m
Hartree Energy	1 E_h	4.360×10^{-18} J

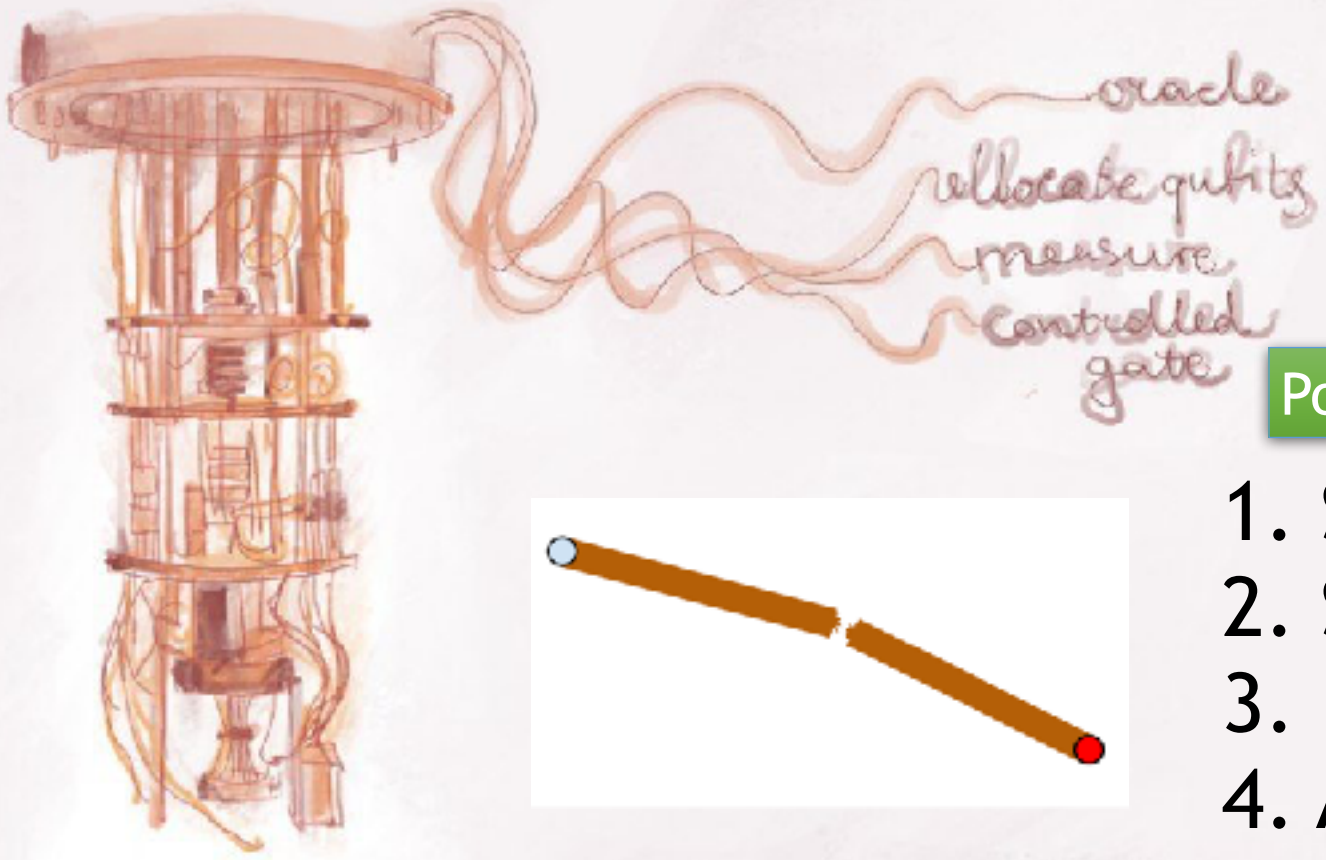
Quantum chemistry **computers**



Power of quantum computers

1. Superposition
2. Size of Hilbert space
3. Entanglement
4. All of the above

Quantum chemistry **computers**



Power of quantum computers

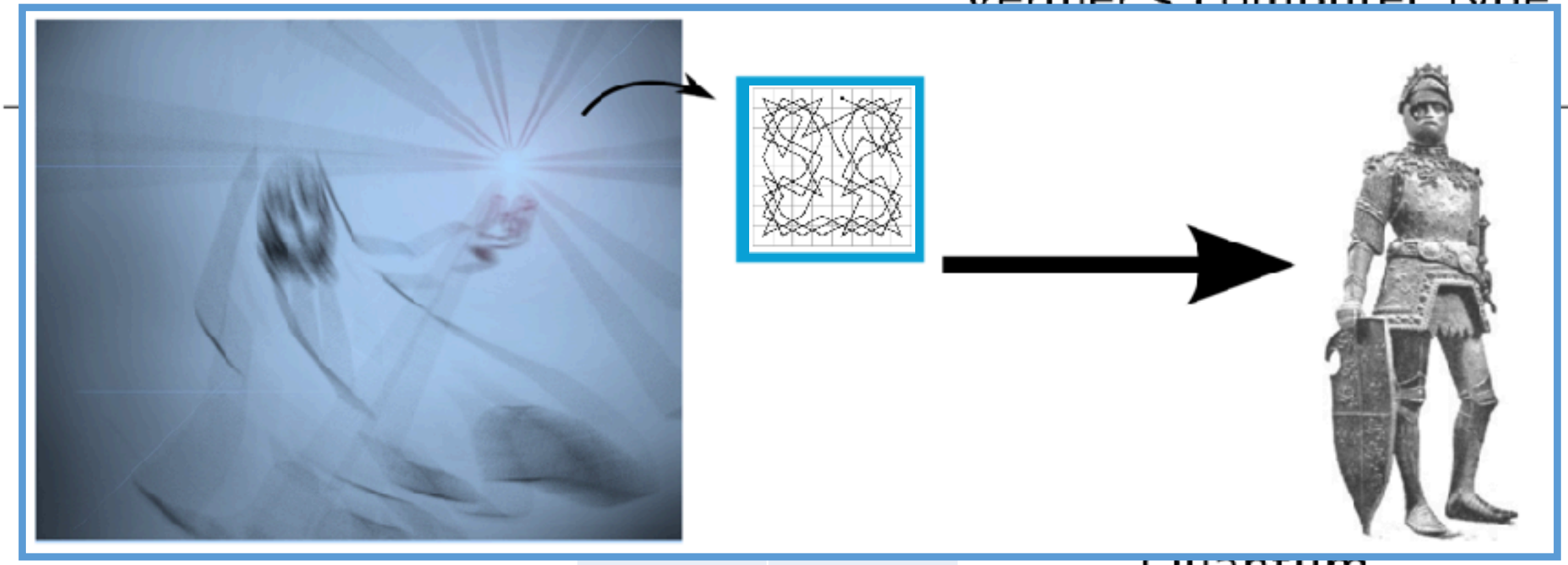
1. Superposition
2. Size of Hilbert space
3. Entanglement
4. All of the above

See Ozols

Quantum chemistry **computers**

Complexity Class	Abbreviations		Verifier's computer type taking only poly. time
Non-deterministic Polynomial Time	NP	P	Deterministic
Merlin-Arthur	MA	BPP	Probabilistic
Quantum Merlin-Arthur	QMA	BQP	Quantum

Quantum chemistry **computers**



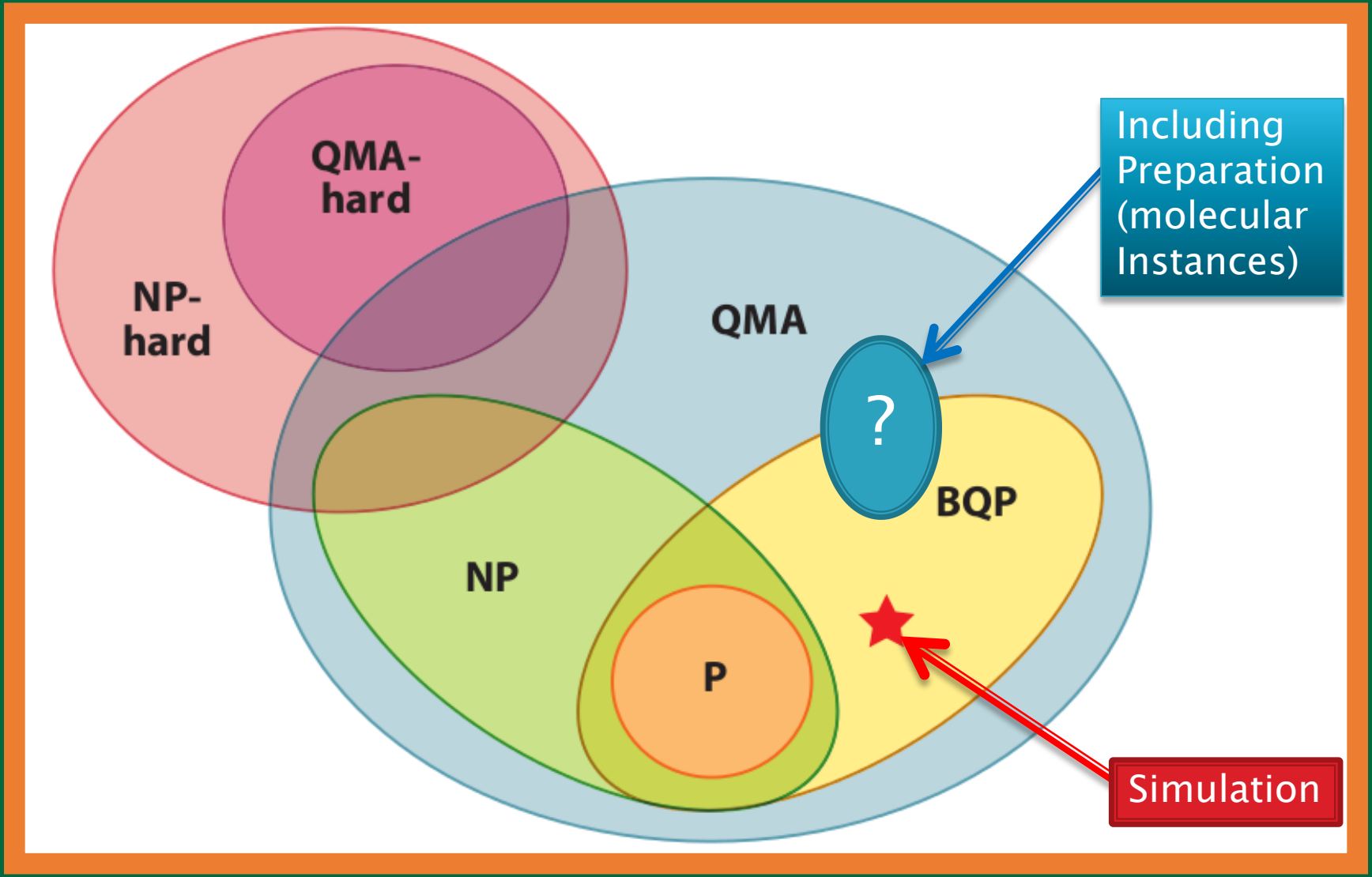
Quantum chemistry **computers**

	Polynomial time	Non-deterministic
Basic Classes	P	NP
Probabilistic version	BPP	MA
Quantum version	BQP	QMA

Computational complexity classes

- **P** (easy) polynomial time
  - "What is Alan Turing's number?"
- **NP** (easy to check) non-deterministic polynomial time
  - "Who has phone number 202-520-7847?"

Quantum chemistry **computers**



Quantum chemistry **computers**

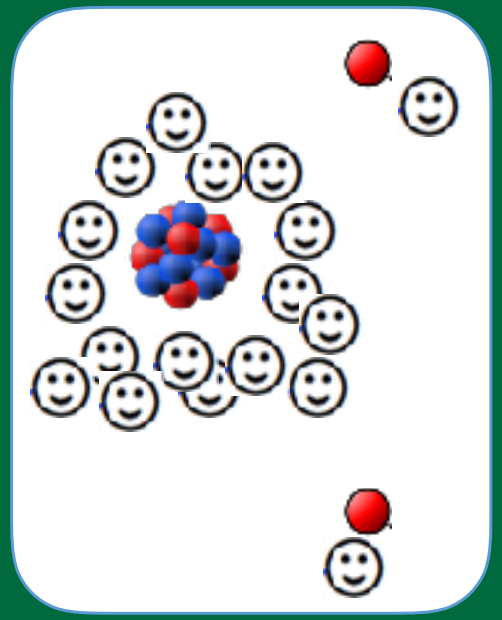
Computational Problem: k-LOCAL-SPIN HAMILTONIAN. Given k-spin-local Hamiltonian acting on N spins,

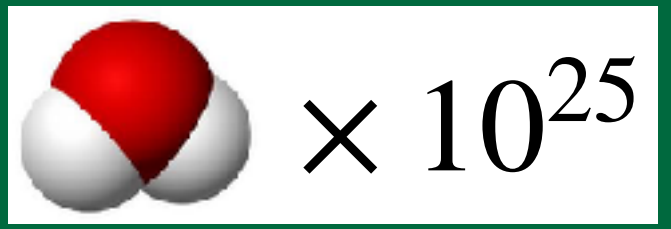
$$H_{kQMA} = -\sum_{\substack{D=(d_1,\ldots,d_k)\\ C=(c_1,\ldots,c_k)}}^{m} J_{C,D}\, \sigma_{c_1}^{d_1} \otimes \sigma_{c_2}^{d_2} \otimes \cdots \sigma_{c_k}^{d_k} \qquad (9)$$

where $d_i \in \{x, y, z, 0\}$, c_i labels a spin, there are m =poly(N) terms, and $|J_{C,D}| \leq 1$, decide if the ground state energy is less that $E_0 - \delta$ or if the ground state energy is greater than $E_0 + \delta$ with $\delta < 1/\text{poly}(N)$ promised that is is not between $E_0 \pm \delta$.

QMA-hard for k>1

Quantum chemistry computers





Quantum chemistry computers

Quantum Mechanics of Many-Electron Systems.

By P. A. M. Dirac, St. John's College, Cambridge.

Proceeding of the Royal Society of London A. vol. 33, page 714 (1929)

various electrons and atomic nuclei. The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It there-

fore becomes desirable that approximate practical methods of applying quantum

Quantum chemistry computers

Formal statement of quantum chemistry problem

Consider $H = \hat{T}(x) + \hat{W}(x, x') + \hat{V}_{ext}(x)$, decide if the lowest energy in the anti-symmetric subspace of N particles is $E_0 < E_T - \delta$ or $E_0 > E_T + \delta$. Here V_{ext}, N, E_T, and δ are inputs and outputs are either $\{ABOVE, BELOW\}$.

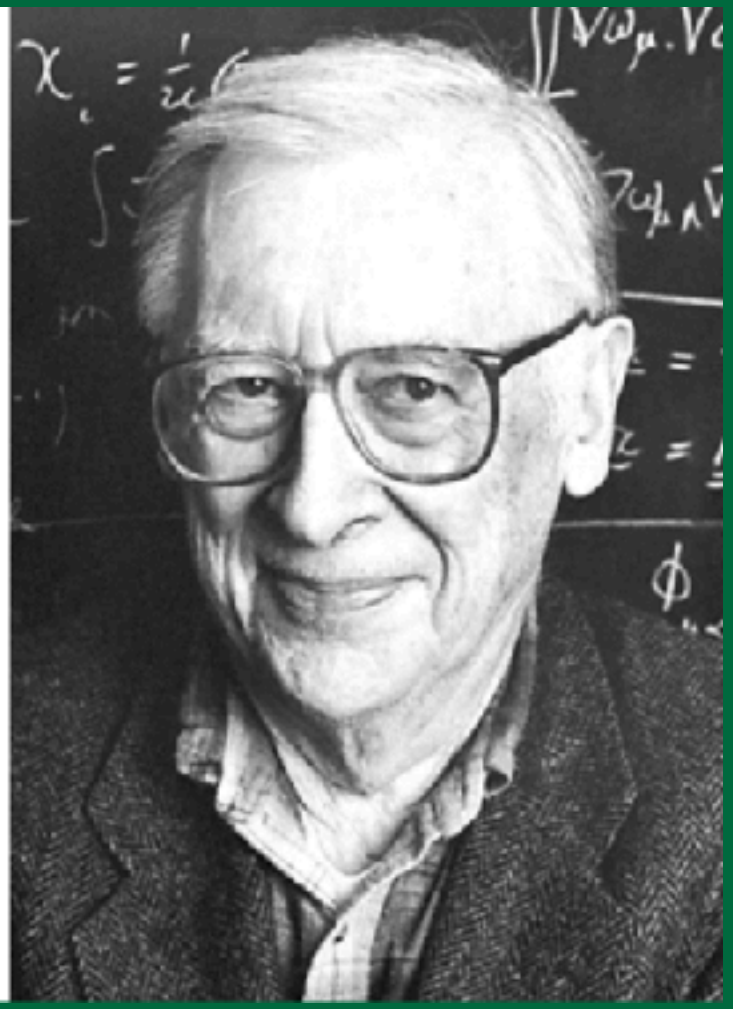
Quantum chemistry computers

1998 Nobel Prize Lecture

A model chemistry is an approximate but well-defined mathematical procedure of simulation applied to chemistry

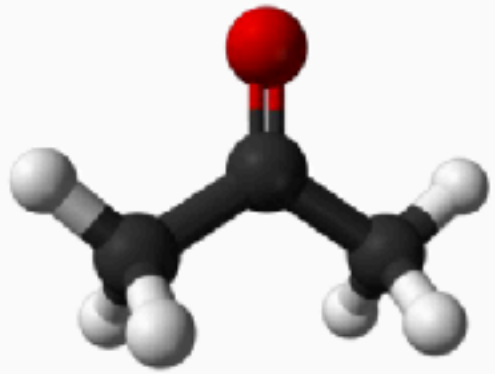
Stages of a model chemistry

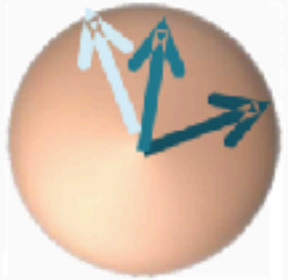
- Target accuracy
- Formulation
- Implementation
- Verification
- Prediction



John Pople

Quantum chemistry computers





quantum system

quantum system
(quantum information)

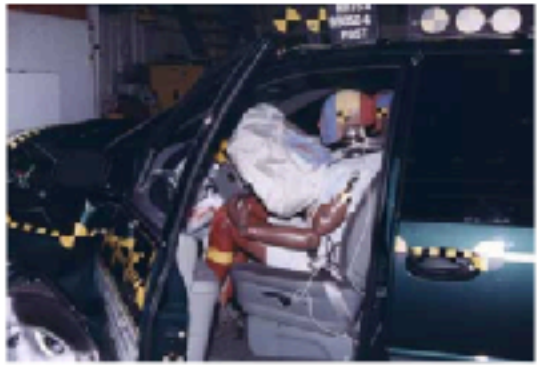
R. P. Feynman, *Int. J. Theor. Phys.* (1982)

Quantum chemistry computers

Stages of simulation

Initialization

Propagation



Measurement

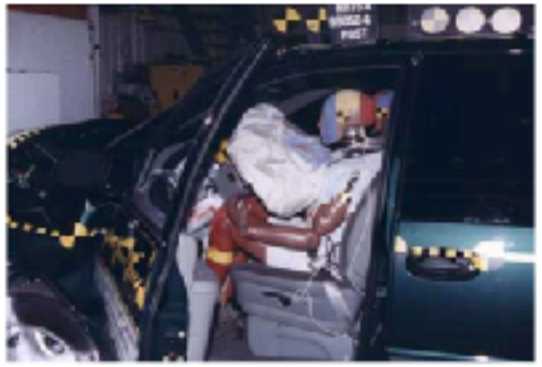
Quantum chemistry computers

Stages of simulation

Initialization

Propagation

Measurement



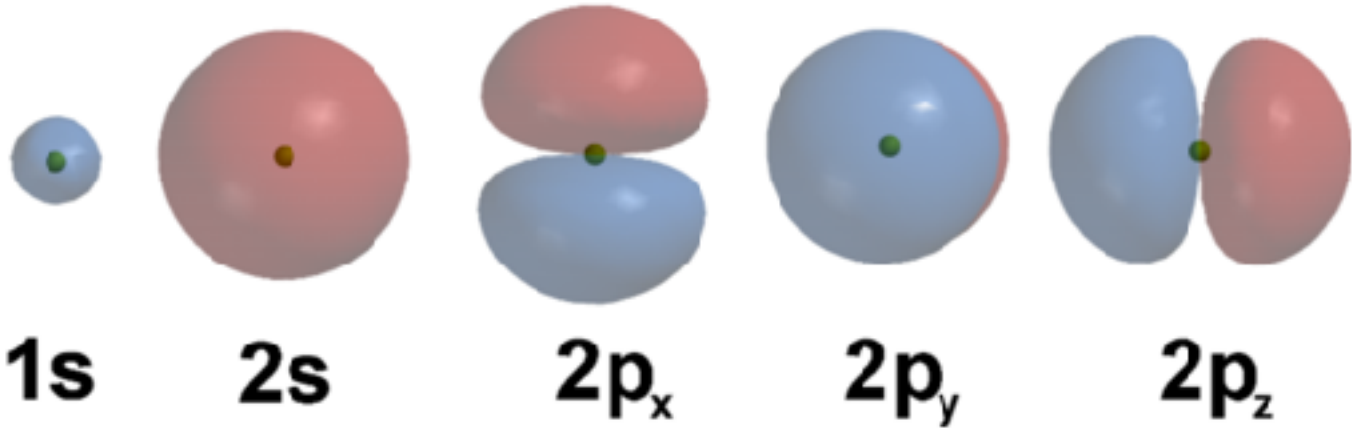
Tomorrow

Quantum chemistry computers

Outline

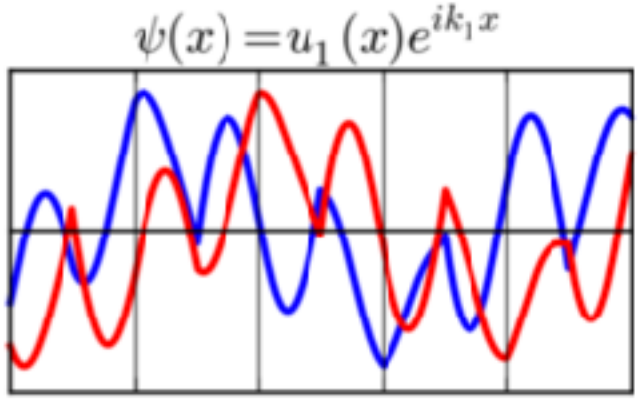
1. Formal Electronic Structure problem
    1. Subspace of interest: one-body
    2. Subspace of interest: N-body
2. Variants on Electronic Structure problem
    1. Variants
    2. Connected problems
3. Qubit Hamiltonians
    1. Qubit/fermion algebras
    2. Jordan-Wigner example

Examples of orbitals

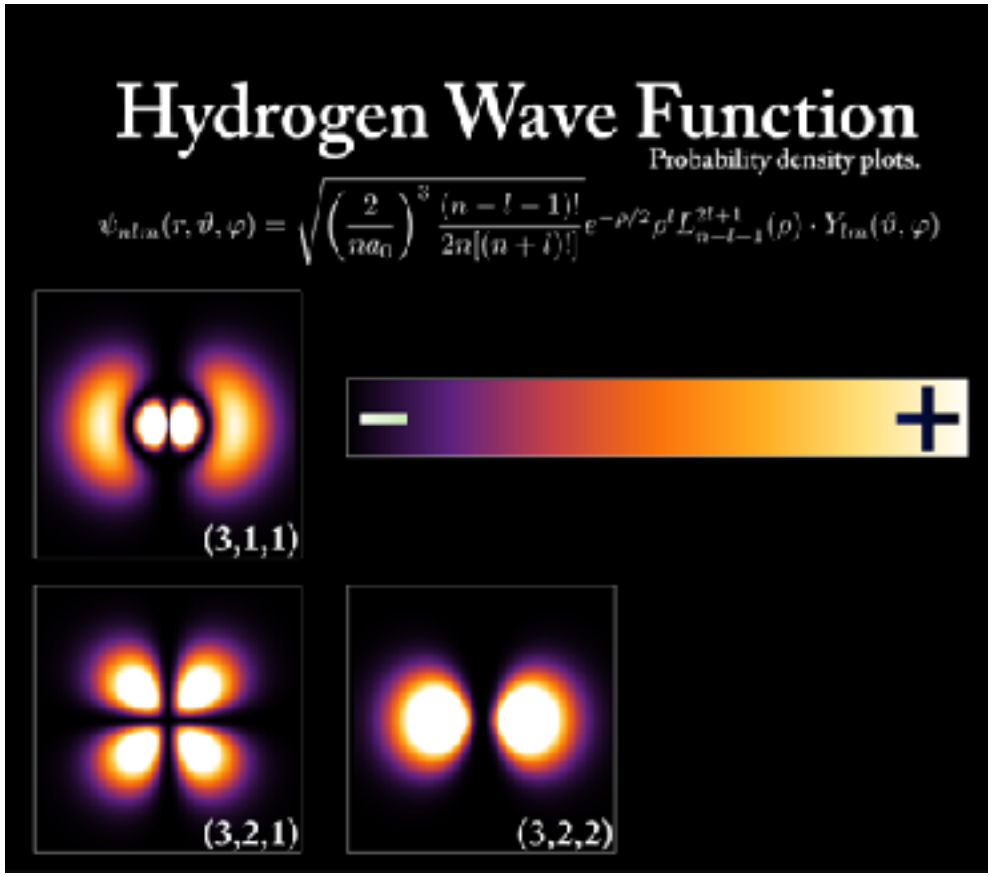


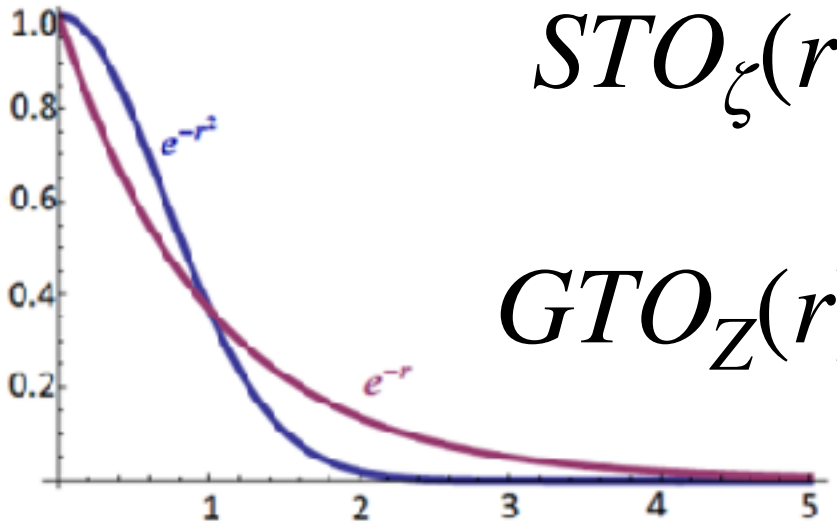
falstad.com

See 1D tutorial QM



Orbitals





$$STO_\zeta(r) = \mathcal{N} e^{-\zeta r}$$

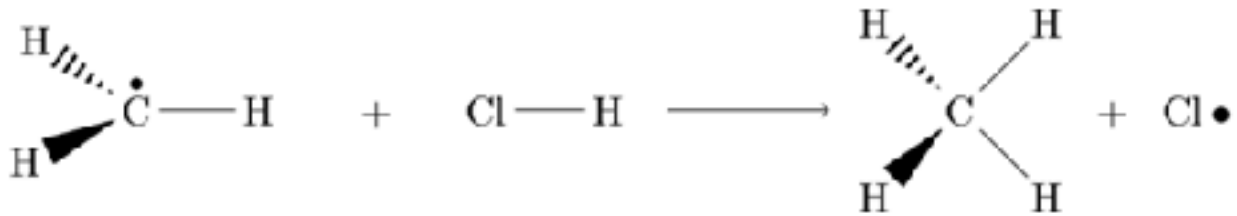
$$GTO_Z(r) = \mathcal{N} e^{-Zr^2}$$

$$\psi_{L=0,m_l=0}(r) = poly(r)e^{-Zr}$$

$$\psi_{STO-3G}(r) = \sum_{j=1}^{3} d_j GTO_{\alpha_j}(r)$$

Computational chemistry problem instances

- Radical stabilization energy



- Barrier heights

- Proton affinity

  $H + Cl \rightarrow HCl$

Atomic units (derived from Gaussian units)

Quantity	**Atomic Units**	**SI units**
Reduced Planck's constant	1 $\hbar$	1.055×10^{-36} J s
Mass of electron	1 m_e	9.109×10^{-31}kg
Proton charge	1 e	1.602×10^{-19} C
Bohr radius	1 a_0	5.292×10^{-11} m
Hartree Energy	1 E_h	4.360×10^{-18} J