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# Quantum Simulation: Solving Schrödinger Equation on a Quantum Computer

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# Quantum Simulation: Solving Schrödinger Equation on a Quantum Computer

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## Alan Aspuru-Guzik

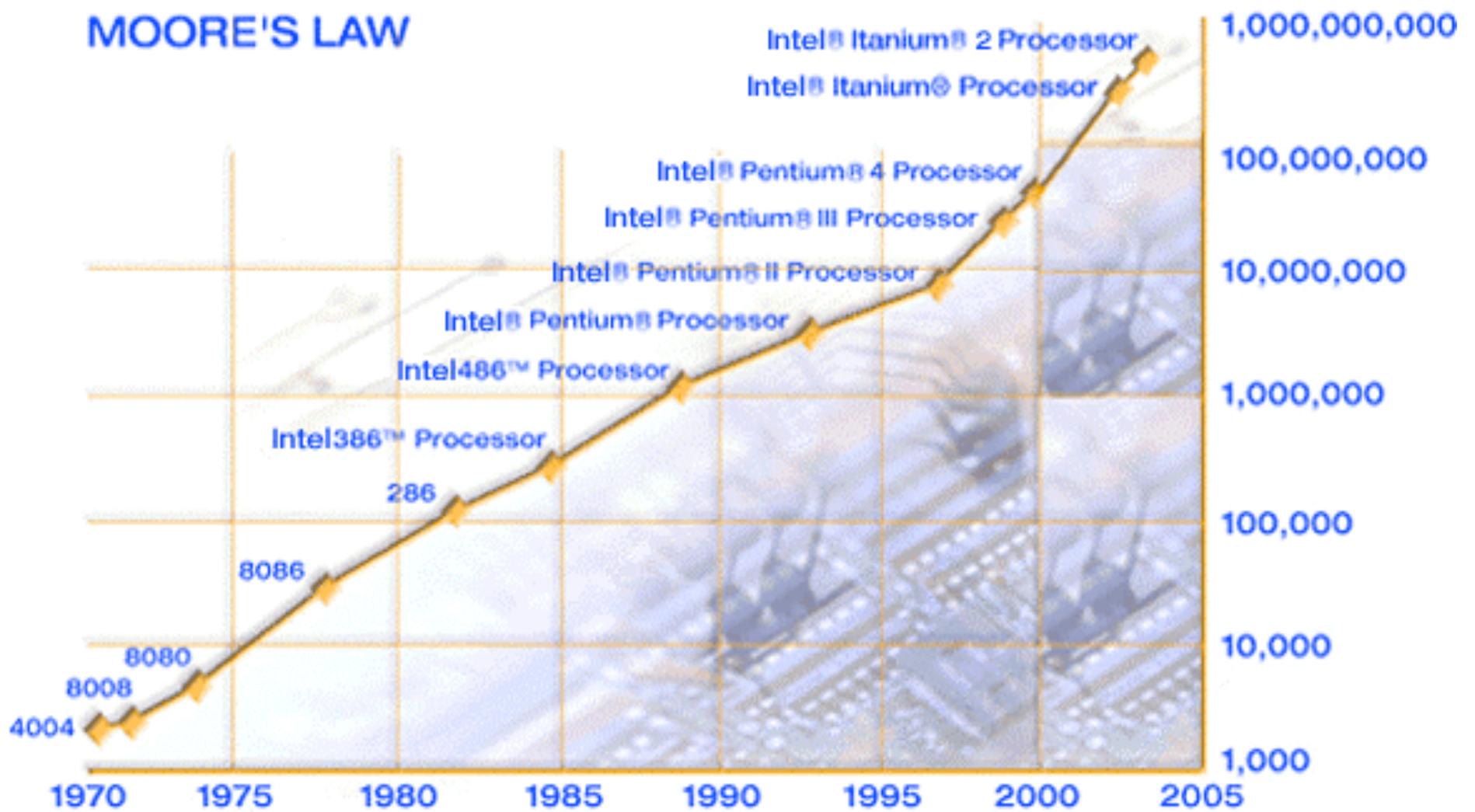Department of Chemistry and Chemical Biology, Harvard

# Why Quantum Computing?

Come forth into the light of things,
let nature be your teacher
--W. Wordsworth

o Why not? If nature is quantum mechanical

o Rolf  Landauer: Information is physical

o Quantum computation, quantum communication,
quantum teleportation, superdense coding, quantum
cryptography, etc.

# Bit vs. Qubit

## Classical Bit

- State 0 or 1

- Measurements doesn't change the state

- Deterministic result

- Can make a copy of bit

## Qubit

- State |0> , |1> or Superposition

- Measurements change the system

- Probability results

- Can not clone the qubit

# Power of Quantum Computing

- Quantum parallelism: superposition principle

$$|\phi\rangle = \sum_{i=0}^{2^n-1} c_i |i\rangle \qquad A|\phi\rangle = \sum_{i=0}^{2^n-1} c_i A|i\rangle$$

- Quantum entanglement: nonlocal correlation

$$|\psi\rangle = \sum_{k_1,k_2} c_{k_1,k_2} |k_1\rangle |k_2\rangle$$

$$|\beta_{00}\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

Bell state:

# Shor's Algorithm

## Finding Prime Factors

$$
\begin{array}{c}
1807082088687 \\
4048059516561 \\
6440590556627 \\
8102516769401 \\
3491701270214 \\
5005666254024 \\
4048387341127 \\
5908123033717 \\
8188796656318 \\
2013214880557
\end{array}
=
\begin{array}{c}
3968599945959 \\
7454290161126 \\
1628837860675 \\
7644911281006 \\
4832555157243
\end{array}
\times
\begin{array}{c}
4553449864673 \\
5972188403686 \\
8972744088643 \\
5630126320506 \\
9600999044599
\end{array}
$$



Shor '94

The difficulty of factorization underpins the security of many common methods of encryption

# Quantum Simulation

❑ Problems of simulating quantum systems on a classical computer

➢ Exponential complexity growth of quantum systems.

➢ The Schrödinger equation, which in most cases is too complicated to be exactly solvable.

➢ As the Hilbert space increases exponentially with the increase of the size of the system, numerical methods like Configuration Interaction (CI) are too expensive.

# Continue

❑ 1982, Feynman: The exponential complexity of quantum systems might be put to good use to simulate dynamics of another quantum system.

❑ Seth Lloyd: the conjecture is correct, it is possible to build universal quantum simulators. For a fairly general class of quantum systems, especially discrete systems, it is possible to achieve an exponential speedup.

Richard P. Feynman, Simulating physics with computers. Inter. J. Theo. Phys., **1982**, *21*, 467-488.

Seth Lloyd, Universal Quantum Simulators. Science, **1996**, *273*, 1073-1078.

# Solving Schrödinger Equation

- The Schrödinger equation

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

- The solution

$$\psi(r,t) = \sum_n A_n u_n(r)\exp(-iE_n t)$$

- The energy spectrum

$$P(t) = \langle \psi(r,0) | \psi(r,t) \rangle = \sum_n |A_n|^2 \exp(-iE_n t)$$

$$P(E) = \sum_n |A_n|^2 \delta(E - E_n)$$

# Quantum Phase Estimation

- To estimate a number $\omega \in [0,1)$ given unitary operator $U$ with eigenvector $|\psi\rangle$, eigenvalue $e^{2\pi i\omega}$

- Prepare two qubit registers: index register and target register

- Perform the controlled-$U^{2^j}$ on the target register

- Inverse QFT on the first register, then make a measurement.

# Quantum Algorithm to Obtain Eigenenergy through Phase Estimation

❑ Construct two registers: The index register and the target register, an approximate eigenvector.

$$\left|\Psi_0\right\rangle = \left|0\right\rangle\left|V_a\right\rangle \xrightarrow{\;\;H\;\;} \left|\Psi_1\right\rangle = \frac{1}{\sqrt{M}} \sum_{j=0}^{M-1} \left|j\right\rangle\left|V_a\right\rangle$$

$$\xrightarrow{\;\;Control-U\;\;} \left|\Psi_2\right\rangle = \frac{1}{\sqrt{M}} \sum_{j=0}^{M-1} \left|j\right\rangle U^j\left|V_a\right\rangle$$

$$U = \exp\left(iHt\right) \qquad \left|V_a\right\rangle = \sum_k c_k\left|\phi_k\right\rangle$$

$$\left| \Psi_2 \right\rangle = \frac{1}{\sqrt{M}} \sum_{j=0}^{M-1} \left| j \right\rangle (U)^j \sum_k c_k \left| \phi_k \right\rangle = \frac{1}{\sqrt{M}} \sum_k c_k \sum_{j=0}^{M-1} \left| j \right\rangle (\lambda_k)^j \left| \phi_k \right\rangle$$

$$= \frac{1}{\sqrt{M}} \sum_k \sum_{j=0}^{M-1} c_k e^{i 2\pi \omega_k j} \left| j \right\rangle \left| \phi_k \right\rangle$$

$$\xrightarrow{QFT^{-1}, Meas.} \left| \Psi_3 \right\rangle = \left| \omega_k \right\rangle \left| \phi_k \right\rangle$$

$$\lambda_k = e^{i 2\pi \omega_k} \qquad c_k = \left\langle V_a \middle| \phi_k \right\rangle \qquad p = \left| c_k \right|^2$$

$$U \left| \Psi \right\rangle = e^{iHt} \left| \Psi \right\rangle = e^{i 2\pi \omega_k} \left| \Psi \right\rangle; \qquad E = 2\pi \omega_k / t$$

# Basis Set Method

❑ HF wave function: one determinant

❑ Mapping the Fock space of the FCI wave function to the Hilbert space of the qubits.

  – Direct mapping: each qubit represents the fermionic occupation state of an atomic orbital. Occupied or not.
  – Compact mapping: only a subspace of Fock space with fixed electrons is mapped onto the qubits.
  – Compact (spin) mapping

Alan Aspuru-Guzik, et. al   Science , **2005**, *309*, 1704-1707.

# Problems of Using HF Wave Function as Initial Guess

❑Excited states have different leading configurations

❑For some complicated curves, several states have to be considered simultaneously in order to obtain an accurate description.

❑The success probability is small at regions far from the equilibrium geometry and avoided crossing.

# General CI Scheme

❑ FCI is too expensive even on a quantum computer for moderate size molecules.

❑ For most chemical problems, the information of ground state and a few low-lying excited states is sufficient.

❑ MCSCF provides good initial guess wave functions, which can be evolved efficiently to the CI wave function.

❑ The success probability can be increased dramatically at critical regions by using appropriate MCSCF wave function as initial guess.

# MCSCF Wave Function

❑ MCSCF wave function

$$\Psi_{MCSCF} = \sum_K A_K \Phi_K \qquad \Phi_K = A\prod_{i \subset K} \phi_i$$

$$\phi_i = \sum_\mu \chi_\mu C_{\mu i}$$

❑ Averaged MCSCF wave function

$$E_n = \frac{\langle \Psi_n |H| \Psi_n \rangle}{\langle \Psi_n | \Psi_n \rangle} \qquad E = \sum_i w_i E_i$$

# Implement CI Based on MCSCF Wave Function

❑ Mapping the Fock space of the averaged MCSCF wave function to the Hilbert space of the qubits.

❑ More compact mapping, consider the symmetry of the molecule, states belong to different irreducible representation do not interact.

❑ Using the MCSCF wave function as the initial guess, for either the ground or excited state.

❑ Probability of getting the corresponding CI wave function is $\left| \left\langle \Psi^i \middle| \Psi^i_{MCSCF} \right\rangle \right|^2$

# Application to Water Molecule

- Ground state:

$$(1a_1)^2(2a_1)^2(1b_2)^2(3a_1)^2(1b_1)^2$$

- cc-pVDZ basis set, singlet state, C2$v$ symmetry.

- MCSCF method: freeze first two $a1$ orbitals, active space, 152 CSFs:

$$3a_1 - 6a_1 \quad \text{orbitals, } 1b_1 \text{ and } 1b_2 - 2b_2 \text{ orbitals}$$

- MRCI using the same active space, but the single and double excitations to the external space, 13872 CSFs.

# Results

| Digits(qubits) | Energy (MCSCF) | Energy (HF) |
|---|---|---|
| 2 | $-83 \pm 2.07 \times 10^1$ | $-83 \pm 2.07 \times 10^1$ |
| 8 | $-83.6386 \pm 5.04 \times 10^{-1}$ | $-83.6386 \pm 5.04 \times 10^{-1}$ |
| 16 | $-83.4486 \pm 1.28 \times 10^{-3}$ | $-83.4435 \pm 1.27 \times 10^{-3}$ |
| 24 | $-83.44919786 \pm 4.95 \times 10^{-6}$ | $-83.44318182 \pm 4.95 \times 10^{-6}$ |

TABLE I: Results for the first singlet excited state of the water molecule using the phase estimation algorithm. The MCSCF and HF wave function are used as initial guesses. The FCI energy is -83.464130 a.u., the exact energy for using MCSCF wave function is -83.449186 a.u. and for using HF wave function is -83.443206 a.u.
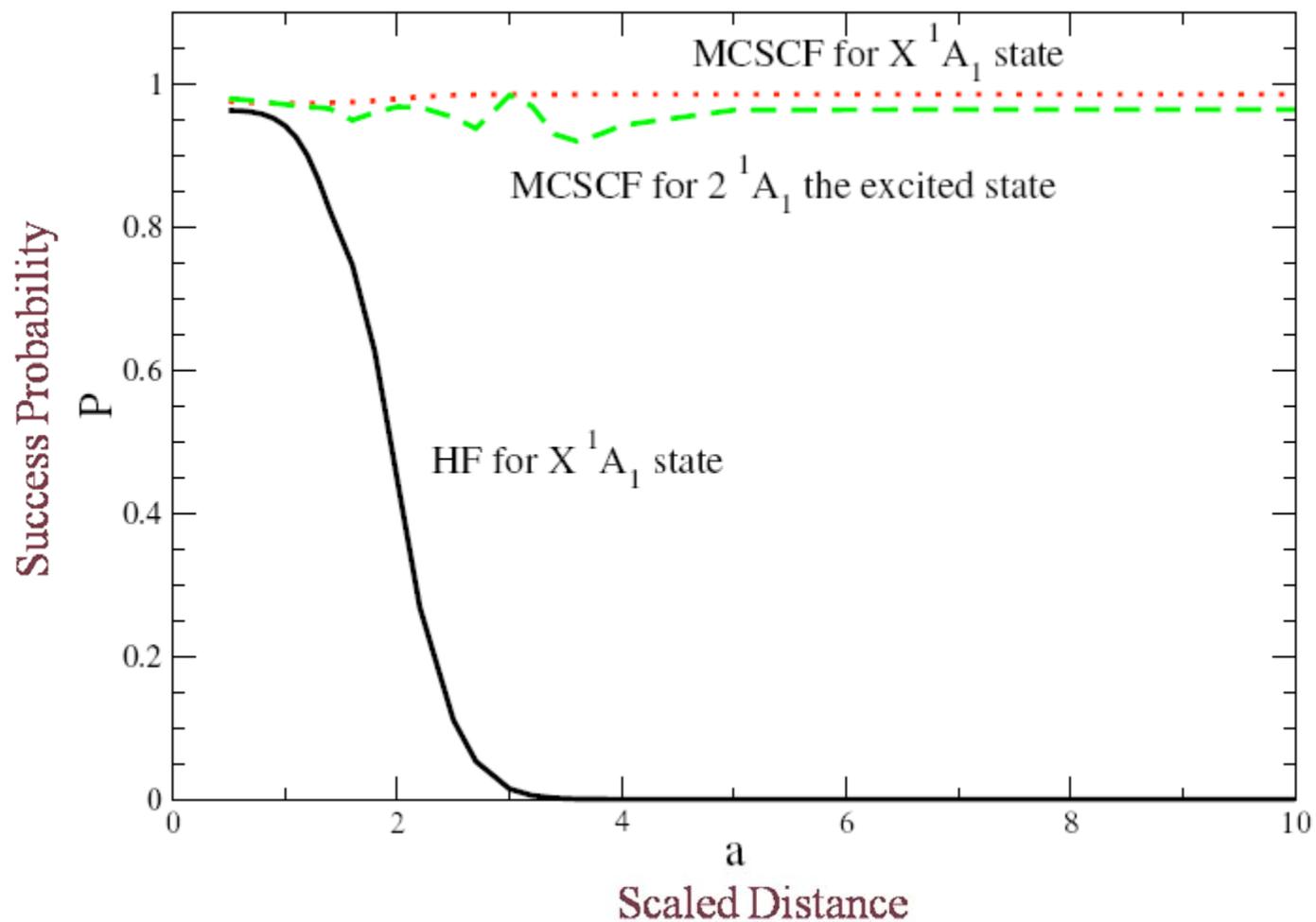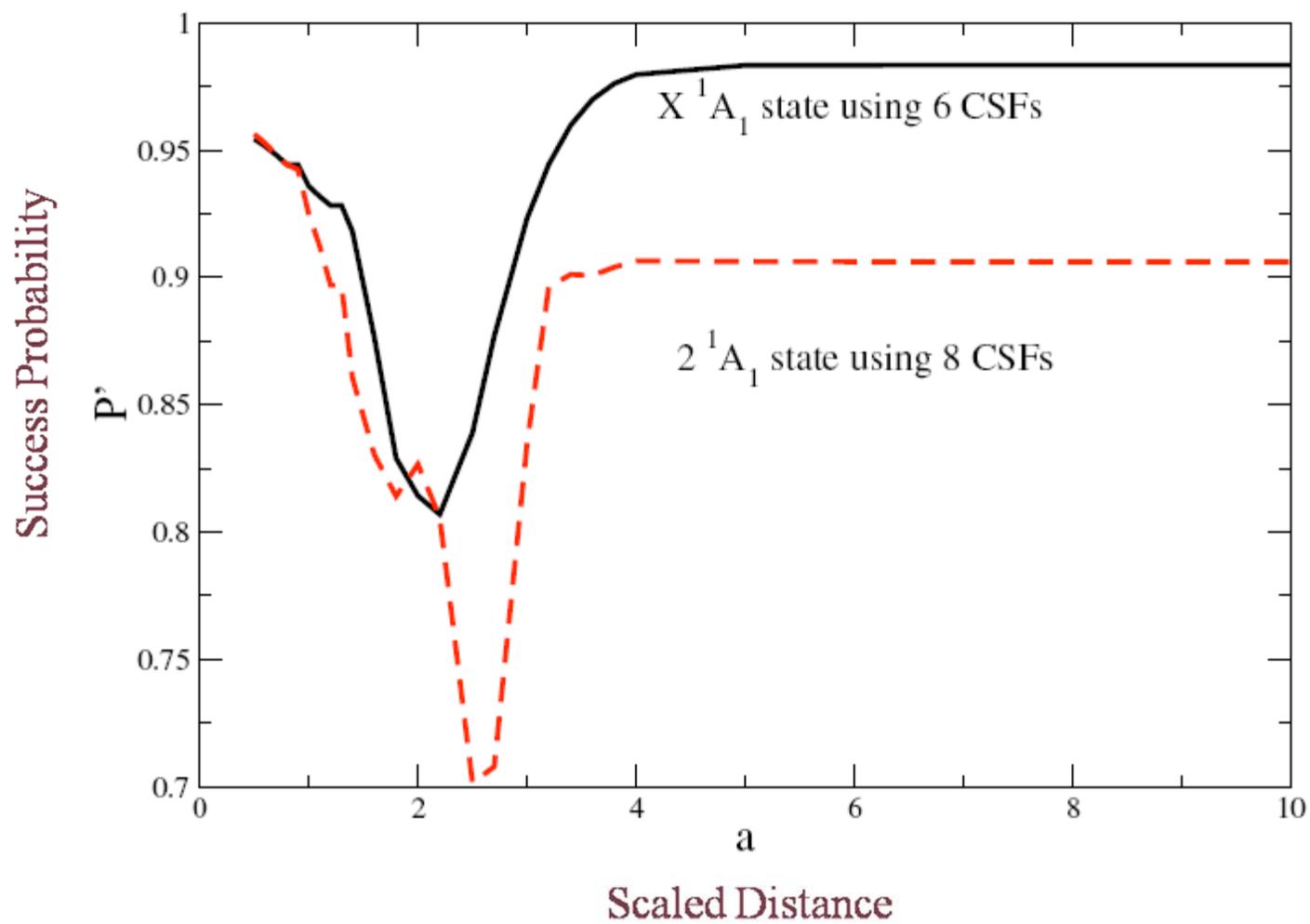
# Continue



$$R_0 = 1.8435 a_0, \ \angle HOH = 110.57 \qquad R = a R_0, a = 0.5 - 10$$

# Continue

# Summary

❑ Using the MCSCF wave function as the initial guess can improve the success probability dramatically, even just a few CSFs.

❑ The method can be generalized to general MRCI scheme and the entire potential energy surface can be explored for ground state and excited states.

❑ Instead of starting from a single element as in the HF wave function, MCSCF method starts from a small matrix. This makes the evolution safer and faster.

❑ The idea can be generalized to Finite element method and any numerical method.