Quantum Chemistry using Quantum Computers

\[ \begin{align*}
\sigma_{g \uparrow} &: |1\rangle - R_z(\frac{\pi}{2}) - R_z(-\frac{\pi}{2}) \\
\sigma_{g \downarrow} &: |1\rangle - H - H \\
\sigma_{u \uparrow} &: |0\rangle - H - R_z(\theta) - H \\
\sigma_{u \downarrow} &: |0\rangle - H - H
\end{align*} \]
From the Molecular Hamiltonian to Qubits Hamiltonians

- Molecular Hamiltonian with $M$ nuclei, $N$ electrons

\[ H_e = -\sum_i \frac{\nabla_i^2}{2} - \sum_{i,J} \frac{Z_I}{\|\mathbf{r}_i - \mathbf{R}_J\|} + \frac{1}{2} \sum_{i \neq j} \frac{1}{\|\mathbf{r}_i - \mathbf{r}_j\|} \]

$r_i$: coordinate nuclei

- Hamiltonian in second quantization form

\[ H_e = \sum_{p,q} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s \]

\[ h_{pq} = \int dx \phi_p^*(x) \left( -\frac{\nabla^2}{2} - \sum_I \frac{Z_I}{\|r - \mathbf{R}_I\|} \right) \phi_q(x) \]

\[ h_{pqrs} = \int dx_1 dx_2 \frac{\phi_p^*(x_1) \phi_q^*(x_2) \phi_s(x_1) \phi_r(x_2)}{\|x_1 - x_2\|} \]

- Mapping the Fermion Fock space into qubits bosons by (for instance) store the occupation number of an orbital in the $|0\rangle$ or $|1\rangle$ state of a qubit:

\[ |f_{M-1}, \ldots, f_0\rangle \rightarrow |q_{M-1}, \ldots, q_0\rangle \quad \text{Linear combination of Slater Det. becomes superposition of qubit states} \]

- Hamiltonian in the qubit space as sum of Pauli matrices

\[ H = c_1 I I I I + c_2 Z Z I I + c_3 X Z X Z + \ldots \]
Variational Quantum Eigensolver

• Ansatz

\[ |\psi(\vec{\theta})\rangle \]

Quantum Chemistry
Real Hardware

• Variational principle

\[ \langle \psi(\vec{\theta}) | H | \psi(\vec{\theta}) \rangle \geq E_0 \]

where \( E_0 \) is the lowest energy eigenvalue of the Hamiltonian \( H \), and \( \vec{\theta} \) is a vector of parameters used to construct the qubit state.

• Uses a classical computer to optimize the parameters \( \vec{\theta} \) and a quantum computer to measure the expectation value
Wave Function Ansatz inspired by Quantum Chemistry

UCCSD operator for H2 in the STO-3G basis

$U(\vec{\theta}) = e^{T - T^\dagger}$

$T = \sum_i T_i$

😌 Accurate
رمزیت Bad scaling for the number of gates
Wave Function Ansatz from heuristic approach

- The heuristic ansatz wavefunction is:

\[ |\psi(\theta)\rangle = R_y(\theta_D) U_{ent} \cdots R_y(\theta_1) U_{ent} R_y(\theta_0) |00\ldots0\rangle \]

where \( R_y(\theta_i) \) is a rotation around axis \( y \) (generated by the Pauli matrix \( Y \)) on all qubits, and \( U_{ent} \) is an entangling block (CNOTs between neighbors).

Very compact ☺️

Lost of the chemical meaning 😞
Variational Quantum Eigensolver

Fermionic problem

\[
H_q = \sum_\alpha h_\alpha P_\alpha = \sum_\alpha h_\alpha \bigotimes_{j=1}^{N} \sigma_j^{\alpha_j}
\]

Classical cost function

Mapping

Mapping

qubit Hamiltonian

\[
calculate \text{ energy } \quad E = \sum_\alpha h_\alpha \langle \Psi(\vec{\theta}) | P_\alpha | \Psi(\vec{\theta}) \rangle \geq E_{\text{exact}} \\
\text{ adjust parameters } \quad \vec{\theta}
\]

classical computer

\[
\text{prepare trial state (choosing ansatz)} \quad |\Psi(\vec{\theta})\rangle \\
\text{measure expectation values} \quad \left\langle \Psi(\vec{\theta}) \bigotimes_{j=1}^{N} \sigma_j^{\alpha_j} | \Psi(\vec{\theta}) \right\rangle
\]

\[
\text{optimize} \quad \vec{\theta}^* \\
\text{solution} \quad \vec{\theta}^*
\]

quantum computer
The Variational Quantum Eigensolver
The Variational Quantum Eigensolver

- The Hamiltonian is a sum of Pauli strings, each with its coefficient:

\[ H = c_1 IIII + c_2 ZZII + c_3 XZXZ + \ldots \]

- Pick one Pauli string to measure it:

\[ H = c_1 IIII + c_2 ZZII + c_3 XZXZ + \ldots \]
The Hamiltonian is a sum of Pauli strings, each with its coefficient:

\[ H = c_1 I I I I + c_2 Z Z I I + c_3 X Z X Z + \ldots \]

- Measure the Pauli string

\[ \langle \Psi | X Z X Z | \Psi \rangle \]
Non-unitary ansatz for VQE

\[ |\Psi^J(\vec{\theta})\rangle = J |\Psi(\vec{\theta})\rangle \]

- We can study non-unitary operators if we divide the expectation value of the Hamiltonian by the normalization of the state. The estimated energy on the state is now

\[ E = \frac{\langle \Psi^J(\vec{\theta}) | H | \Psi^J(\vec{\theta}) \rangle}{\langle \Psi^J(\vec{\theta}) | \Psi^J(\vec{\theta}) \rangle} = \frac{\langle \Psi(\vec{\theta}) | J^\dagger H J | \Psi(\vec{\theta}) \rangle}{\langle \Psi(\vec{\theta}) | J^\dagger J | \Psi(\vec{\theta}) \rangle} \]

- We use a Quantum Monte-Carlo inspired operator to introduce some qubit correlation outside of the quantum computer; this acts as a ‘projector’ reducing the contribution of unphysical states
Jastrow operator

- The operator is inspired by the one-body and two-body Jastrow factors

\[
J = J_1 + J_2
\]

\[
J_1 = \exp \left[ - \sum_{i=1}^{N} \alpha_i Z_i \right]
\]

\[
J_2 = \exp \left[ - \sum_{i<j=1}^{N} \lambda_{ij} Z_i Z_j \right]
\]

- This would add an exponentially growing number of measurements! So instead we use the linearization

\[
J(\vec{\alpha}, \vec{\lambda}) = 1 - \sum_{i=1}^{N} \alpha_i Z_i - \sum_{i<j=1}^{N} \lambda_{ij} Z_i Z_j
\]

- This only adds a polynomial number of parameters (and additional measurements)

Mazzola et al. PRL 123, 130501 (2019).
Procedure

• Choose a hardware efficient ansatz (rotations on each qubit, blocks of entangling CNOTs)

• Given a set of parameters (rotation angles), initialize the wavefunction on the quantum computer

• Measure the Pauli strings composing \( J^\dagger H J \) and \( J^\dagger J \)

• Calculate the expectation value

\[
E = \frac{\langle \Psi(\vec{\theta}) | J^\dagger H J | \Psi(\vec{\theta}) \rangle}{\langle \Psi(\vec{\theta}) | J^\dagger J | \Psi(\vec{\theta}) \rangle}
\]

• Optimize all the parameters together (the rotation angles and the coefficients in the Jastrow operator) like in the normal VQE
Dissociation curve for $H_2$
Dissociation curve for $H_2$
The improvement grows with the number of entangling blocks!
The number of total parameters grows as
\[ \alpha \left( N_{\text{qubits}} + N_{\text{qubits}}^2 \right) + \beta N_{\text{blocks}} \]
The method works with all qubit mappings
Conclusions

\[ |\Psi^J(\vec{\theta})\rangle = J |\Psi(\vec{\theta})\rangle \]

- Effective procedure to introduce non-unitary wavefunctions in VQE
- The advantage increases with the number of blocks of the wave function
- Results are robusts with respect to chemistry \(\rightarrow\) qubits mapping
Many Thanks to the Group of 
Ivano Tavernelli 
IBM-Research 
Zurich
Spin-Qubit promise good miniaturization and scale up.
Quantum Computing: present and future applications
Quantum Algorithm Providing Exponential Speed Increase for Finding Eigenvalues and Eigenvectors

Daniel S. Abrams*
Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California 91109-8099

Seth Lloyd†
d’Arbeloff Laboratory for Information Sciences and Technology, Department of Mechanical Engineering, MIT 3-160, Cambridge, Massachusetts 02139
(Received 27 July 1998)

We describe a new polynomial time quantum algorithm that uses the quantum fast Fourier transform to find eigenvalues and eigenvectors of a local Hamiltonian, and that can be applied in cases (commonly found in ab initio physics and chemistry problems) for which all known classical algorithms require exponential time. Applications of the algorithm to specific problems are considered, and we find that classically intractable and interesting problems from atomic physics may be solved with between 50 and 100 quantum bits.
Quantum speedup in solving the maximal-clique problem

Weng-Long Chang,1,* Qi Yu,2 Zhaokai Li,2,3 Jiahui Chen,2,4 Xinhua Peng,2,3,5,† and Mang Feng5,6,7,‡

1Department of Computer Science, National Kaohsiung University of Applied Sciences, Kaohsiung City 80778, Taiwan, China
2CAS Key Laboratory of Microscale Magnetic Resonance and Department of Modern Physics, University of Science and Technology of China, Hefei 230026, China
3Synergetic Innovation Center of Quantum Information and Quantum Physics, University of Science and Technology of China, Hefei 230026, China
4Institute for Quantum Computing and Department of Physics and Astronomy, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1
5Synergetic Innovation Center for Quantum Effects and Applications, Hunan Normal University, Changsha 410081, China
6State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, China
7Department of Physics, Zhejiang Normal University, Jinhua 321004, China

(Received 16 October 2017; published 29 March 2018)

The maximal-clique problem, to find the maximally sized clique in a given graph, is classically an NP-complete computational problem, which has potential applications ranging from electrical engineering, computational chemistry, and bioinformatics to social networks. Here we develop a quantum algorithm to solve the maximal-clique problem for any graph $G$ with $n$ vertices with quadratic speedup over its classical counterparts, where the time and spatial complexities are reduced to, respectively, $O(\sqrt{2^n})$ and $O(n^2)$. With respect to oracle-related quantum algorithms for the NP-complete problems, we identify our algorithm as optimal. To justify the feasibility of the proposed quantum algorithm, we successfully solve a typical clique problem for a graph $G$ with two vertices and one edge by carrying out a nuclear magnetic resonance experiment involving four qubits.
EU Quantum Technology Flagship 1.3 billions euros up to 2028

**2016**
- **PREPARATORY STEPS**
  - 04/2016: Announcement in EU Cloud Initiative
  - 09/2016: Set-up of the QT Flagship High Level Steering Committee
  - Intermediate report (02/2017)
  - Final report (09/2017)

**2018**
- **RAMP UP PHASE**
  - Flagship Coordination & Support Actions: 0.5 m€ (2017) + 2 m€ (2018)
  - Flagship Research & Innovation Actions: 130 m€ (2018)

**2019**
- **QUANT-ERA**
  - QuantERA (01/2018): 26 countries, 36 m€ (1/3 EU)
  - QuantERA II (2020 - tbc): FET call: 10 m€

**2020**
- **FULL IMPLEMENTATION**
  - Series of QT calls
  - EU Quantum Key Distribution Network

*pending adoption under the next multi-annual framework programme

- **CYBERSECURITY**
  - H2020 LEIT ICT QKD Testbed call (2019): 15 m€
Representative list of players. A very active ecosystem!