Quantum Chemistry on Quantum Annealers

March 2019
What We Do
Materials Discovery

Developing advanced materials to solve large scale industrial problems for displays + lighting
Organic Light Emitting Diode (OLED)

Light from organic pigments sandwiched between electrodes
Closed Loop Development with Customer Feedback

In-house end-to-end testing from materials discovery up to production testing

Materials Discovery
- Quantum Simulations
- Production Testing
- Synthesis
- Validation

Detailed Specifications
MP Ready Materials
- Tool Builders
- Panel Makers
- OEMs
Our Materials Discovery Platform
Advanced computation + simulation + ML/AI

Properties
- Vapor pressure
- Optical constants
- Electronic structure
- Film forming
- Crystallinity
- Etc.

Structure

Computational Design
Quantum Simulations
Machine Learning

CPU
GPU
QPU (Quantum Processing Unit)
Example: Aerelight for Print™
Flexible OLED module for print + packaging
Example: ConducTorr™ for Transparent Display
Automotive Demonstration
Quantum Chemistry
Why do we care?

Understanding and prediction of the Structure -> Property relationship
Overview of Quantum Chemistry on a Quantum Computer

\[ H = \sum_{ij} C_i^j a_j^\dagger a_i + \sum_{ijkl} C_{ij}^{kl} a_k^\dagger a_l^\dagger a_j a_i \]

Generate a fermionic Hamiltonian

\[ H = \sum \hat{P}_i \]

Transform into spin basis (function of Pauli Operators)

\[ |\psi(\theta)\rangle = \exp(\hat{T} - \hat{T}^\dagger) |\psi_0\rangle \]

Construct Ansatz (UCC)

\[ \hat{T} = \hat{T}_1 + \hat{T}_2 + \cdots \]

\[ \hat{T}_1 = \sum_{ij} C_i^j a_j^\dagger a_i \quad \hat{T}_2 = \sum_{ijkl} C_{ij}^{kl} a_k^\dagger a_l^\dagger a_j a_i \]
Variational Quantum Eigensolver

\[ \hat{H} = \sum \hat{P}_i \quad \text{Where } \hat{P}_i = \prod \sigma_j^n, \ n = \{x,y,z\} \ & j = \text{qubit index} \]

\[ E_0 \leq \sum \langle \Psi_i | \hat{P}_i | \Psi_i \rangle \quad \text{Where } \Psi \text{ is wavefunction of the ith Pauli word} \]

With serial processing, time scales linearly with number of Pauli words

BK transformation generates \( O(N^4) \) Pauli words

Hidden Consequences

Is this “kink” a hardware problem or theory problem?

Kandala et al. (2017) Nature 549, 242-246
Broken symmetry GHF between 1.5 Å – 1.6 Å, as it transitions from singlet to triplet.
Quantum computers cannot directly encode

$$U = \exp(T_1 + T_2 + \cdots)$$

Trotterized

$$U \approx \left(\exp\left(\frac{T_1}{M}\right)\exp\left(\frac{T_2}{M}\right)\cdots\right)^M \quad M \geq 1$$

Even simplest fermionic operators are lengthy combination of Pauli terms

$$\begin{align*}
a_5^+a_4^+a_3a_2 - a_2^+a_3^+a_4a_5 \\
i \frac{1}{8} (x_2y_4 + z_1x_2z_3y_4 - y_2x_4 - z_1y_2z_3x_4 - y_2x_4z_5 - z_1y_2z_3x_4z_5 + x_2y_4z_5 + z_1x_2z_3y_4z_5)
\end{align*}$$

Lengthy combinations of Pauli terms increases quantum circuit depth

Qubit Coupled Cluster Method

\[ \Psi(\tau, \omega) = \hat{U}(\tau) |\omega\rangle \]

General form of qubit methods

\[ \hat{U}(\tau) = \prod_k^N \exp \left( \frac{i \tau_k \hat{P}_k}{2} \right) \]

\( \hat{P} \) is Pauli word entanglers

\[ E(\tau, \omega) \leq \langle \omega | U(\tau)^\dagger \hat{H} U(\tau) |\omega\rangle \]

Variational search for ground state

https://pubs.acs.org/doi/abs/10.1021/acs.jctc.8b00932
PES Curve for LiH & H₂O
Quantum Chemistry on Quantum Annealers

We have developed a quantum solver for quantum chemistry on a quantum annealer.

**Universal Gate**
- IBM Q (20 qubits)

**Quantum Annealer**
- D-Wave 2000Q (2048 qubits)

Annealer is suitable for solving binary optimization problems (not applicable for quantum chemistry)
Qubit Transformation and Domain Folding

\[ \theta \in [0, \frac{\pi}{2}) \]

\[ \varphi \in [0, \pi) \text{ or } [0, \frac{\pi}{2}) \]

\[ \tau \in [0, \pi) \text{ or } [0, \frac{\pi}{2}) \]

\[ z_i \rightarrow \cos \theta_i \]
\[ x_i \rightarrow \cos \varphi_i \sin \theta_i \]
\[ y_i \rightarrow \sin \varphi_i \sin \theta_i \]
Solution on Quantum Annealer

1. Transform Pauli words to Ising model
2. Generate J and H Couplings
3. Anneal Solution
4. Classically Optimize
PES Curves Solved on Quantum Annealer

\[ E, E_h \]

\[ \text{H}_2\text{O}/6-31G \]

\[ \text{RHF} \]

\[ \text{Exact} \]

\[ R(\text{O-H}), \text{Å} \]

\[ -76 \]

\[ -75.9 \]

\[ -75.8 \]

\[ -75.7 \]

\[ -75.6 \]

\[ -75.5 \]

\[ -228 \]

\[ -228.5 \]

\[ -229 \]

\[ -229.5 \]

\[ -230 \]

\[ \text{C}_6\text{H}_6/STO-6G \]

\[ \text{RHF} \]

\[ R(\text{C-C}), \text{Å} \]

\[ 0.8 \]

\[ 1 \]

\[ 1.2 \]

\[ 1.4 \]

\[ 1.6 \]

\[ 1.8 \]

\[ 2 \]
Benefit of the use of the annealer

**Ideal Ising machine**

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<th>Success rate, %</th>
<th>No folding</th>
<th>(1,0)</th>
<th>(3,0)</th>
<th>(1,1)</th>
<th>(1,2)</th>
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<td>2.05 Å</td>
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**D-Wave 2000Q**

<table>
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<th>Success rate, %</th>
<th>No folding</th>
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Where Are We Today
Started to test industrial problems

We are here!

We have demonstrated industrial relevant size simulations on quantum hardware