Variational Quantum Eigensolver

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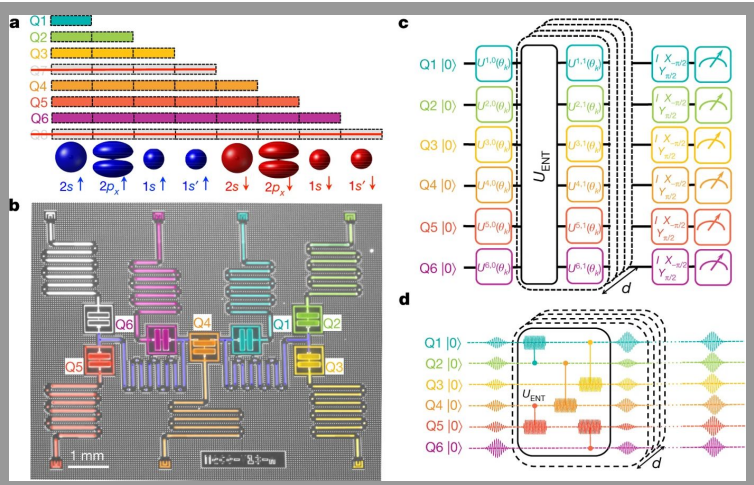
Introduction



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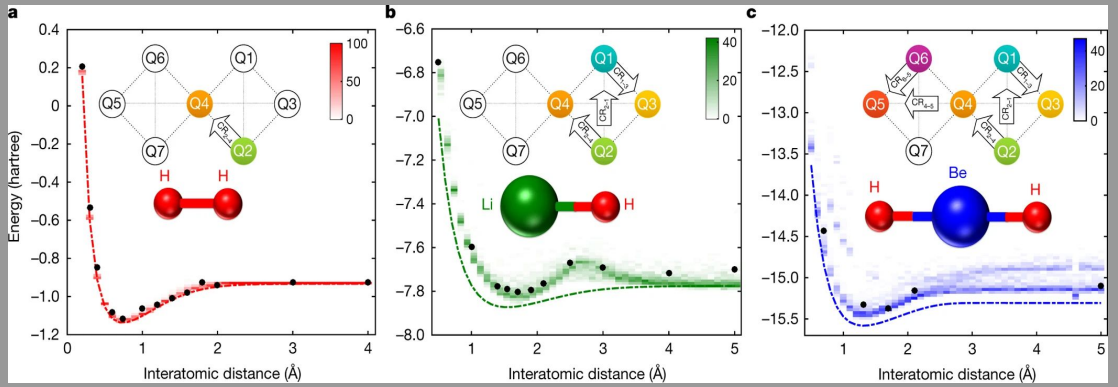

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Introduction: Stating the problem

We want to solve the following problem:

Given an Hamiltonian H we want to approximate the ground state energy by solving the following optimization problem:

$$\min_\theta \langle \psi(\theta) | \mathcal{H} | \psi(\theta) \rangle$$

Using the variational principle, we have that:

$$\lambda_\theta = \langle \psi(\theta) | \mathcal{H} | \psi(\theta) \rangle \geq \lambda_{\min} = E_{gs}$$

So by minimizing this value we get an approximation of the minimum eigenvalue of the Hamiltonian.

Introduction: Variational Method

Consider the eigenvector $|\psi_i\rangle$ of a matrix $\mathcal{H}$ which is invariant under the transformation $\mathcal{H}$ up to a constant (the eigenvalue of $|\psi_i\rangle$). Therefore:

$$\mathcal{H}|\psi_i\rangle = \lambda_i|\psi_i\rangle$$

Considering that the matrix $\mathcal{H}$ is Hermitian, we have that all eigenvalues are real, thus: $H = \sum_{i=1}^{N} \lambda_i |\psi_i\rangle\langle\psi_i|$ the expectation value of $\mathcal{H}$ given an arbitrary state is:

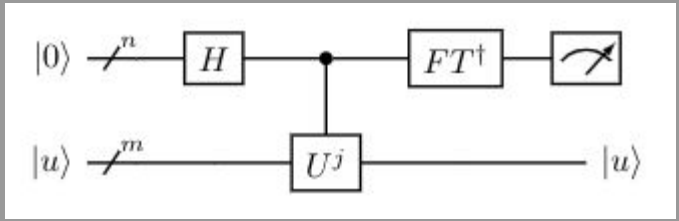
$$\langle H\rangle_\psi = \langle\psi|\mathcal{H}|\psi\rangle = \langle\psi|\sum_{i=1}^{N}\lambda_i|\psi_i\rangle\langle\psi_i||\psi\rangle \quad = \sum_{i=1}^{N}\lambda_i\langle\psi|\psi_i\rangle\langle\psi_i|\psi\rangle = \sum_{i=1}^{N}\lambda_i|\langle\psi_i|\psi\rangle|^2$$

$$\lambda_{\min} \leq \langle H\rangle_\psi = \langle\psi|\mathcal{H}|\psi\rangle = \sum_{i=1}^{N}\lambda_i|\langle\psi|\psi_i\rangle|^2$$

Thus the expectation value of any wave function will always be at least the minimum eigenvalue associated with $\mathcal{H}$. This method thus is usually used to estimate the ground state of an Hamiltonian.

Introduction: Quantum Phase Estimation (QPE)

We know that using QPE, we can solve the previous problem, but this would need a high-depth circuit and low-noise Quantum Computers. In order to obtain the eigenvalue with accuracy of **n** bits with probability of success at least 1 - ε, we choose:



$$p = \log\left(2 + \frac{1}{2\epsilon}\right)$$

$$t = n + \log\left(2 + \frac{1}{2\epsilon}\right)$$

Thus we need to find alternatives that can be implemented on near-term devices.

Variational Quantum Eigensolver

VQE: Algorithm

1) Create an ansatz $|\psi(\theta)\rangle$

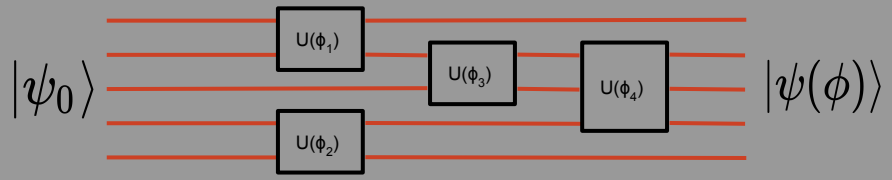
2) Decompose the Hamiltonian into Pauli Strings of polynomial size $\mathcal{H} = \sum_\alpha h_\alpha P_\alpha \qquad P_\alpha = \sigma^{\alpha_1} \otimes \ldots \sigma^{\alpha_N}$

3) Evaluate the Hamiltonian using the chosen ansatz $\langle \mathcal{H} \rangle (\theta) = \langle \psi(\theta) | \mathcal{H} | \psi(\theta) \rangle \quad = \sum_\alpha h_\alpha \langle \psi(\theta) | P_\alpha | \psi(\theta) \rangle$

4) Using the value of the first step, minimize the expectation value with respect to the parameter θ using a classical optimizer.

VQE: Variational Forms (Ansatz)

It is needed to construct a quantum circuit for the ansatz, for this we will use parametrized quantum circuits with a fixed form which will help us to explore a part of the Hilbert space that (hopefully) is useful for our problem. Thus we have two conflicting goals:



$$U(\phi)|\psi\rangle = |\psi(\phi)\rangle$$

- We want to generate any state $|\psi\rangle \in \mathbb{C}^{2^n}$
- We want to use as few parameters as possible and of polynomial size.

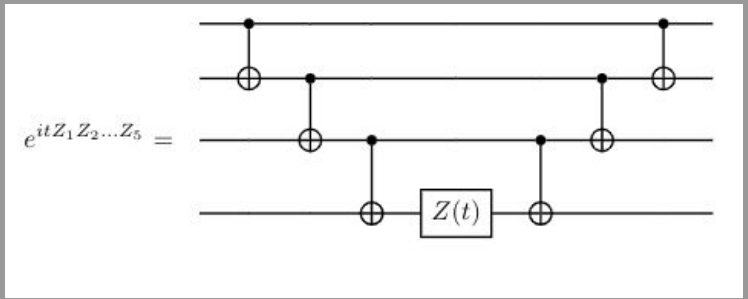
VQE: Domain Specific Ansatz

Suppose we want to calculate the ground state of a molecule, then we know a priori how many particles are on the circuit. Thus we limit the variational for that only produces particle preserving transformations reducing the number of parameters needed.

$$|\psi(\theta)\rangle = U(\theta)|\phi\rangle = e^{T(\theta)-T^\dagger(\theta)}|\phi\rangle$$

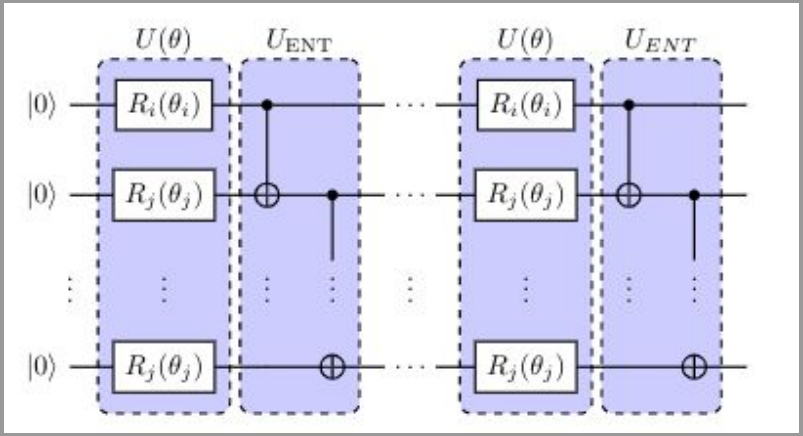
$$T_1(\theta) = \sum_{i\in\text{occ},\, j\in\text{unocc}} \theta^{(j)}_{(i)} a_j^\dagger a_i$$

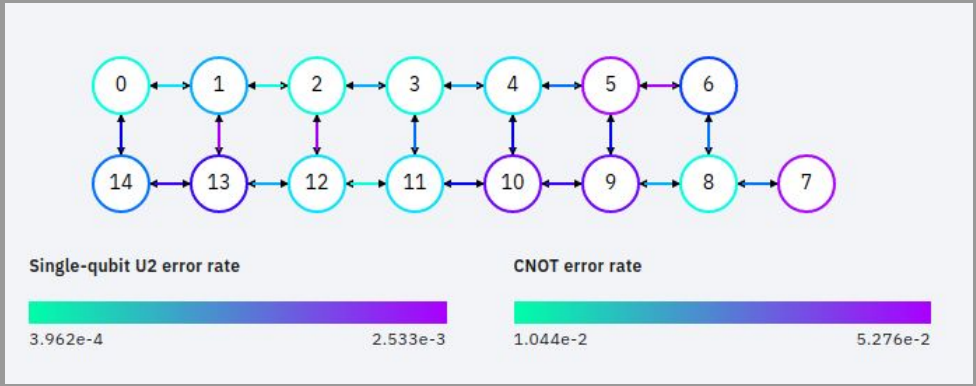
$$T_2(\theta) = \sum_{i,j\in\text{occ}\,,\, k,l\in\text{unocc}} \theta^{(k,l)}_{(i,j)} a_k^\dagger a_l^\dagger a_i a_j$$



VQE: Hardware Efficient Ansatz

For this kind of ansatze we choose gates and coupling strategies that are efficient for the device that we are working on, this fixes the depth problem from the domain specific ansatze, making us control the depth that we are working on. Two common ones are R_Y R_Z or R_Y followed by an entangling block that is commonly used by CNOT gates.





IBMQ Melbourne

VQE Demo

Applying to Chemistry

Chemistry with Qubits

We want to find the lowest energy of the following Hamiltonian (after the Bohr-Oppenheimer Approximation):

$$\mathcal{H} = \overbrace{\sum_{i=1}^{K} -\frac{1}{2}\nabla_i^2 + V(r_i)}^{\mathcal{H}_1} + \overbrace{\sum_{1\leq i\leq j\leq K} \frac{1}{|r_i - r_j|}}^{\mathcal{H}_2}$$

$$\Psi(x_1, \dots x_K) \propto \det \begin{pmatrix} \psi_1(x_1) & \psi_1(x_2) & \dots & \psi_1(x_k) \\ \vdots & \vdots & \vdots & \vdots \\ \psi_K(x_1) & \psi_K(x_2) & \dots & \psi_K(x_k) \end{pmatrix}$$

$$t_{pq} = \langle p | \Big(-\frac{\nabla^2}{2} + V \Big) | q \rangle$$

$$u_{pqrs} = \langle p, q | \Big(\frac{1}{|r_i - r_j|} \Big) | r, s \rangle$$

$$\mathcal{H} = \sum_{i=1}^{K} \sum_{p,q=1}^{N} t_{pq} |p\rangle\langle q|_i$$

$$+ \sum_{1\leq i\neq j\leq K} \sum_{p,q,r,s=1}^{N} u_{pqrs} |p\rangle\langle r|_i \otimes |q\rangle\langle s|_j$$

Chemistry with Qubits: Second Quantization

The second-quantization approach often results in a simpler simulation Hamiltonian and require fewer qubits. Given a set of N orbitals ψ_1 , ... , ψ_N , the second quantized Hamiltonian is:

$$\mathcal{H} = \sum_{p,q=1}^{N} t_{pq} c_p^\dagger c_q + \sum_{p,q,r,s=1}^{N} u_{pqrs} c_p^\dagger c_q^\dagger c_r c_s$$

$$\mathcal{F} = \bigoplus_{k=0}^{N} \mathcal{H}_{k,N}$$

$$c_i^\dagger \left| \ldots n_i \ \ldots \right\rangle = (1 - n_i) \, (-1)^{\sum_{j<i} n_j} \left| \ \ldots \ n_i + 1 \ \ldots \right\rangle$$

$$c_i \left| \ldots n_i \ \ldots \right\rangle = n_i \, (-1)^{\sum_{j<i} n_j} \left| \ \ldots \ n_i - 1 \ \ldots \right\rangle$$

$$\{c_i^\dagger, c_j\} = \delta_{ij} \ , \ [c_i, c_j] = [c_i^\dagger, c_j^\dagger] = 0$$

The second quantization can be written in terms of qubits using one of the Fermion-to-qubit mappings.

Fermion-to-qubit mapping

Since we are working with qubits and not fermions, we should have a 1-on-1 mapping between fermions and qubits. Let's begin with the case for only one fermion:

$$c^\dagger |0\rangle = |1\rangle \qquad c^\dagger |1\rangle = 0$$

$$c |0\rangle = 0 \qquad c |1\rangle = |0\rangle$$

$$c^\dagger \to \sigma^+$$

$$c \to \sigma^-$$

$$c_i^\dagger | \ \ldots n_i \ \ldots \ \rangle = (1 - n_i) (-1)^{\sum_{j<i} n_j} | \ \ldots \ n_i + 1 \ \ldots \ \rangle$$

$$\sigma^Z |n_i\rangle = (-1)^{n_i} |n_i\rangle$$

$$c_i^\dagger \to \prod_{j<i} \sigma_j^Z \sigma_i^+$$

$$c_i \to \prod_{j<i} \sigma_j^Z \sigma_i^-$$

Fermion-to-qubit mapping: Jordan-Wigner Mapping

From the example, we find the following mapping:

$$c_i^\dagger \rightarrow \prod_{j<i} \sigma_j^Z \sigma_i^+ \qquad\qquad c_i \rightarrow \prod_{j<i} \sigma_j^Z \sigma_i^-$$

This is called Jordan-Wigner Mapping and was discovered in the 20s, and it recovers fermionic algebra. There's a inherent problem that for increasing i, this operator becomes increasingly non-local with O(N)-local interactions, this leads to larger circuits and more measurements.

Fermion-to-qubit mapping: Parity mapping

Another mapping is the parity mapping, which is still O(N)-local but simplify the number of qubits needed, let's see an example:

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} a+b+c+d \\ b+c+d \\ c+d \\ d \end{pmatrix}$$

Fermion-to-qubit mapping: Bravyi-Kitaev

Another one is the Bravyi-Kitaev map which is O(log N)-local and uses a binary tree rule to encode fermionic modes:

$$\beta_{2^{x+1}} = \left(\begin{array}{c|ccc} & 1 & 1 & \dots \\ \beta_{2^x} & 0 & 0 & \dots \\ & 0 & 0 & \dots \\ \hline 0 & \multicolumn{3}{c}{\beta_{2^x}} \end{array}\right)$$

1 qubit

$$(1)$$

2 qubits

$$\left(\begin{array}{c|c} 1 & 1 \\ \hline 0 & 1 \end{array}\right)$$

4 qubits

$$\left(\begin{array}{cc|cc} 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{array}\right)$$

$$c_j^\dagger \equiv X_{U(j)} \otimes \Pi_j^+ \otimes Z_{P(j)} = \frac{1}{2}\left(X_{U(j)} \otimes X_j \otimes Z_{P(j)} - iX_{U(j)} \otimes Y_j \otimes Z_{P(j)}\right)$$

$$c_j \equiv X_{U(j)} \otimes \Pi_j^- \otimes Z_{P(j)} = \frac{1}{2}\left(X_{U(j)} \otimes X_j \otimes Z_{P(j)} + iX_{U(j)} \otimes Y_j \otimes Z_{P(j)}\right)$$

Qubit Tapering

Another way to reduce the number of qubits is to taper symmetries. Consider the following Hamiltonian:

$$H = h_1\, IXIY \;+\; h_2\, XZZX \;+\; h_3 XZYZ$$

And an operator that is a symmetry of the Hamiltonian:

$$P_0 = XIII \qquad [H, P_0] = 0$$

We know the eigenvalues of P_0, thus we can remove the first qubit:

$$H = h_1\, XIY \;\pm\; h_2\, ZZX \;\pm\; h_3 ZYZ$$

LiH Demo

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