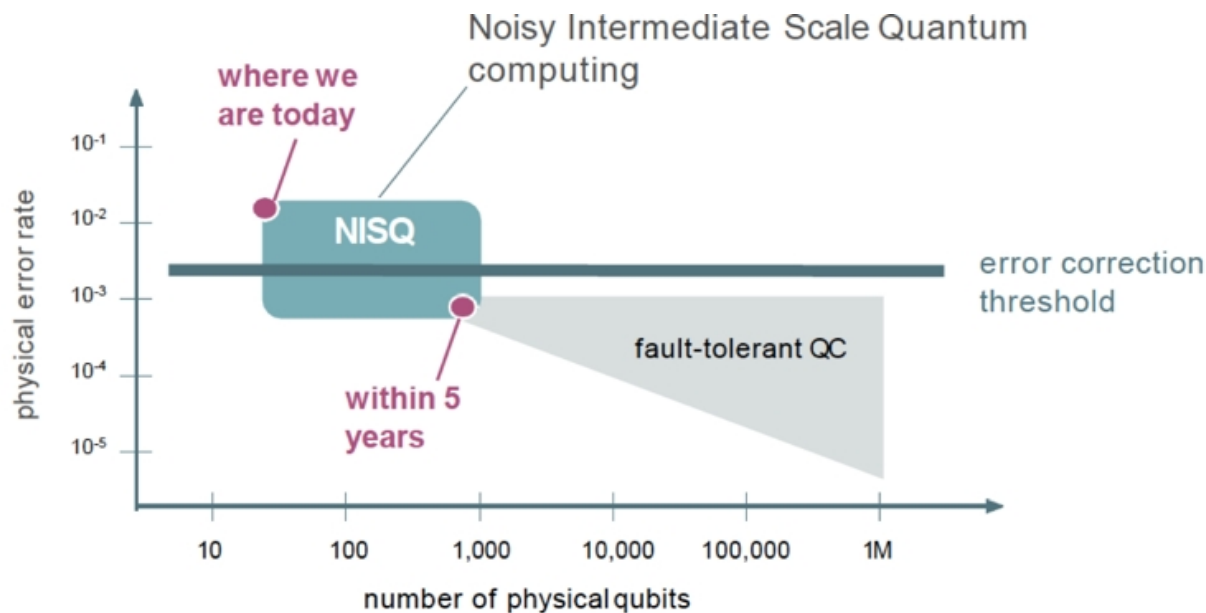# Ch7: The Variational Quantum Eigensolver
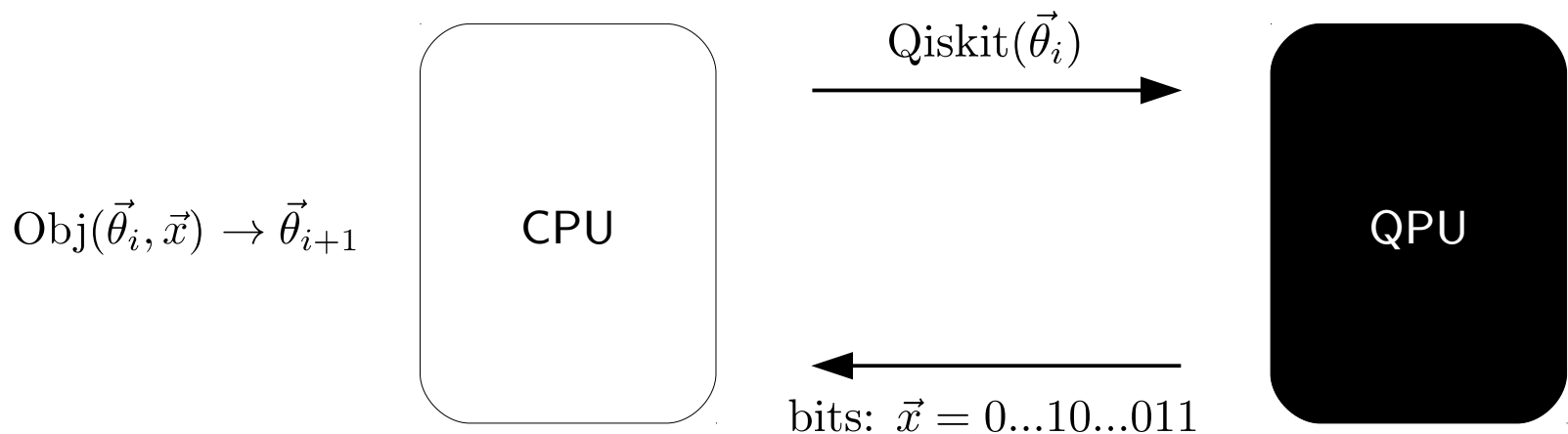
The NISQ era

In the last few lectures we have shown that noise is a critical part of today's quantum programming. It will remain critical for many years even as hardware continues to improve. This means there is a need for programming models that can be robust to QPU errors.

"Quantum computing in the NISQ era and beyond" Preskill, 2018 https://arxiv.org/abs/1801.00862

Variational optimization

The variational quantum eigensolver (VQE) is a key example of the so-called hybrid quantum/classical or variational quantum algorithms. In the variational paradigm, the parameters of a quantum program are learned with the following feedback loop:

$$\text{Obj}(\vec{\theta}_i, \vec{x}) \rightarrow \vec{\theta}_{i+1}$$

CPU

$$\text{Qiskit}(\vec{\theta}_i)$$

QPU

$$\text{bits: } \vec{x} = 0...10...011$$

where we used an objective function to update parameters used to generate a Qiskit programme.

Variational optimization

Note that this is a non-trivial optimization for several reasons:

- We have "sampling errors" where we may not have run enough trials
- We are optimizing over a noisy landscape due to quantum noise

Thus variational optimization for quantum programming is an optimization of a parametrized distribution over a noisy landscape.

NISQ application areas

As we will see throughout the class, this method can be used to make noise robust quantum algorithms for applications in:
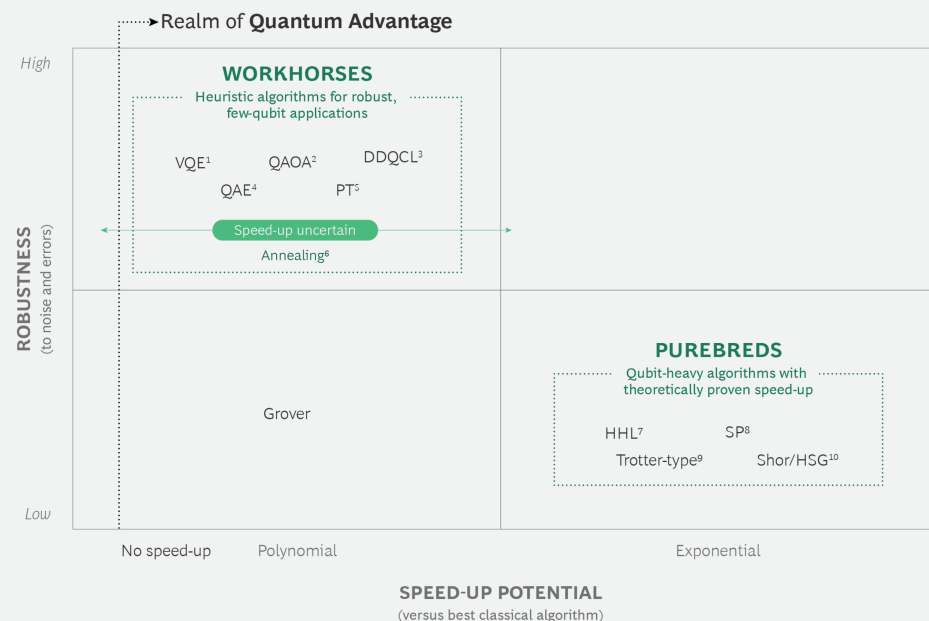
- Quantum chemistry (e.g. VQE)
- Machine learning (e.g. QNN)
- Optimization (e.g. QAOA)
- ...

No free lunch

While variational algorithms are more noise robust it is often an open research question as to how robust they are and/or what speedup they may give.

EXHIBIT 8 | Workhorse Algorithms Will Dominate During the NISQ Era

Sources: BCG analysis; expert interviews.
[1]Variational quantum eigensolver.
[2]Quantum approximate optimization algorithm.
[3]Data-driven quantum circuit learning for generative modeling in machine learning tasks.
[4]Quantum auto encoder, a compression algorithm for quantum data.
[5]Population transfer between computational states with similar energies for search and reverse annealing optimization.
[6]Optimization by quantum annealing as an alternative to circuit-based algorithms.
[7]Linear-system-solving algorithm devised by Harrow, Hassidim, and Lloyd.
[8]Semidefinite programming.
[9]Trotter-based algorithms for molecular simulation and adiabatic state preparation.
[10]Algorithms exploiting hidden-subgroup symmetries such as Shor's algorithm.

The variational quantum eigensolver

The VQE algorithm shows how we can use variational quantum programming to find the smallest eigenvalues and eigenvectors of large matrices, in fact some can be exponentially large !
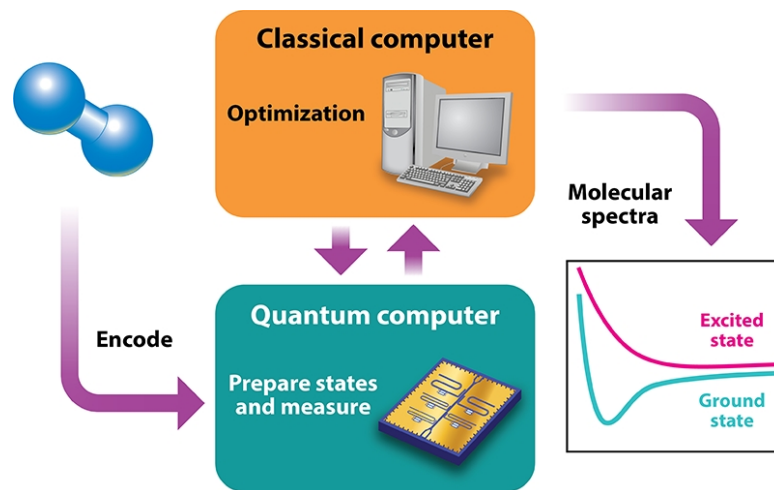
For example, in chemistry, the minimum eigenvalue of a Hermitian matrix characterizing the molecule is the ground state energy of that system.

Eigen problem

An eigen problem is given a representation of a matrix A find λ_0 and $\vec{x}_0$ the smallest eigenvalue and corresponding eigenvector of A.

The variational principle

Let H be a $2^n \times 2^n$ hermitian complex matrix with eigenvalues $\{\lambda_i\}$ (ordered by size from smallest to largest) and eigenvectors $\{\vec{x}_i\}$. Then for any vector $|y\rangle$ (complex and size 2^n):

$$\frac{\langle y|H|y \rangle}{\langle y|y \rangle} \geq \lambda_0$$

Equality of the above holds only when $|y\rangle = |\vec{x}_0\rangle$.

Proof of variational principle

As H is hermitian its eigenvectors are orthogonal and so we can expand $|y\rangle$ in the eigenstates of H:

$$|y\rangle = \sum_i c_i |\vec{x}_i\rangle$$

where the sum coefficients are complex numbers. Thus:

$$\langle y|y\rangle = \sum_{i,j} c_i^* c_j \langle \vec{x}_i | \vec{x}_j \rangle = \sum_i |c_i|^2$$

due to the orthogonality of the eigenvectors, and:

$$\langle y|H|y\rangle = \sum_{i,j} c_i^* c_j \langle \vec{x}_i |H| \vec{x}_j \rangle = \sum_{i,j} c_i^* c_j \lambda_j \langle \vec{x}_i | \vec{x}_j \rangle = \sum_i \lambda_i |c_i|^2$$

Proof of variational principle

We then have:

$$\frac{\langle y|H|y\rangle}{\langle y|y\rangle} = \frac{\sum_i \lambda_i |c_i|^2}{\sum_i |c_i|^2} \geq \frac{\lambda_0 \sum_i |c_i|^2}{\sum_i |c_i|^2} = \lambda_0$$

This gives us a method for VQE.

Algorithm

1 – Let $\mathrm{Qiskit}(\vec{\theta_i})$ be a quantum program that produces some state $|y(\vec{\theta_i})\rangle \equiv U(\vec{\theta_i})|y\rangle$ from an input state $|y\rangle$.

2 – Run the program and measure the expectation value $\langle y(\vec{\theta_i})|H|y(\vec{\theta_i})\rangle$.

3 – As $|y(\vec{\theta_i})\rangle$ is a normalized vector, we know the expectation value is $\geq \lambda_0$. Thus use a classical non-linear optimizer to update $\vec{\theta_i} \to \vec{\theta_{i+1}}$ in order to minimize $\langle y(\vec{\theta_i})|H|y(\vec{\theta_i})\rangle$.

4 – Repeat previous steps until convergence, this will then approach λ_0 from above.

VQE for non-hermitian matrix

Q1: Doesn't this only work for hermitian matrices ?

A1: It is easy to generalise as for any square matrix A:

$$C = \begin{pmatrix} 0 & A \\ A^\dagger & 0 \end{pmatrix}$$

is hermitian.

Expectation values

Q2: How to calculate $\langle y(\vec{\theta_i})|H|y(\vec{\theta_i})\rangle$? (When working with Qiskit we can only measure the Z observable ?)

A2: We need a decomposition of H in terms of Pauli operators X, Y, Z.

<u>Example</u>: Let: $H = Z_0 + X_1 Z_0$

$\rightarrow$ First run and measure statistics on qubit-0:
```
qc.measure(0,0)
```
$\rightarrow$ Then run and append:

```
qc.h(1)  # Convert Z measurement to X measurement
qc.measure(1,1)
qc.measure(0,0)
```

$$\langle y(\vec{\theta_i})|H|y(\vec{\theta_i})\rangle = \langle y(\vec{\theta_i})|Z_0|y(\vec{\theta_i})\rangle + \langle y(\vec{\theta_i})|X_1 Z_0|y(\vec{\theta_i})\rangle$$

The electronic structure problem

VQE was introduced in the context of a quantum chemistry simulation known as the electronic structure problem.

In this problem one is given a description of a molecule – represented by its Hamiltonian, and then we are asked to find the molecule's ground state and ground state energy.

State evolution

A molecule is a quantum system with state $|\psi\rangle$. The time evolution is given by a unitary evolution operator as well – assuming there are no time-dependant interactions:

$$U(t) = e^{-iHt/\hbar}$$

H is the Hamiltonian of the system and it describes the dynamics of the molecule.

H is a fixed hermitian operator whose details are given by the dynamics of the physical system.

In general: $H = T + V$, where T and V represent respectively the kinetic and the potential energy of the system.

Energy eigenstates and eigenvalues

Because H is hermitian we can decompose H into a basis formed by its eigenvalues and eigenvectors:

$$H = \sum_E E |E\rangle\langle E|$$

These are referred to as the energy eigenstates and energies of the system. The smallest energy is called the ground state energy and is associated with the ground state eigenvector.

The ground state tells us the most stable structure of the molecule which is useful for determining chemical properties like reaction rates.

Energy eigenstates and eigenvalues

Evolution in quantum mechanics is described by the Schrödinger equation:

$$i\hbar \frac{d|\psi\rangle}{dt} = H|\psi\rangle$$

Thus for any energy eigenstate:

$$\frac{d|E\rangle}{dt} = \frac{-iH}{\hbar}|E\rangle = \frac{-iE}{\hbar}|E\rangle \qquad \Rightarrow \qquad |E\rangle \rightarrow e^{-iEt/\hbar}|E\rangle$$

Evolution is just multiplication by some overall phase factor. In fact general evolution for a time independent Hamiltonian is given by:

$$|\psi\rangle \rightarrow e^{-iHt/\hbar}|\psi\rangle$$

Hamiltonian of a molecule

Given a set of nuclear charge N_i and a number of electrons the Hamiltonian describing their interactions is — in atomic units:

$$H = -\sum_i \frac{\nabla_{R_i}^2}{2M_i} - \sum_i \frac{\nabla_{r_i}^2}{2} - \sum_{i,j} \frac{N_i}{|R_i - r_j|} + \sum_{i,j>i} \frac{N_i N_j}{|R_i - R_j|} + \sum_{i,j>i} \frac{1}{|r_i - r_j|}$$

$$\underbrace{\phantom{-\sum_i \frac{\nabla_{R_i}^2}{2M_i}}}_{\substack{\text{Nuclear} \\ \text{kinetic}}} \underbrace{\phantom{\sum_i \frac{\nabla_{r_i}^2}{2}}}_{\substack{\text{Electronic} \\ \text{kinetic}}} \underbrace{\phantom{\sum_{i,j} \frac{N_i}{|R_i - r_j|}}}_{\substack{\text{Attraction} \\ \text{to nucleus}}} \underbrace{\phantom{\sum_{i,j>i} \frac{N_i N_j}{|R_i - R_j|}}}_{\substack{\text{Nuclear} \\ \text{repulsion}}} \underbrace{\phantom{\sum_{i,j>i} \frac{1}{|r_i - r_j|}}}_{\substack{\text{Electronic} \\ \text{repulsion}}}$$

R_i : nuclear position r_i : electronic position M_i : nuclear masses

This is called the first quantization form. Typically chemists then make the Born-Oppenheimer approximation by assuming nuclei are classical point charges with fixed positions R_i.

Mapping into Pauli representation

In second quantization form we project the electronic Hamiltonian into a spin-orbital basis. Thus instead of talking about real space positions we talk about occupations of discrete orbitals:

$$H = \sum_{p,q} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

Where:

- $a_i^\dagger$ is the creation operator
- a_i is the annihilation operator

This means roughly that $h_{pq} a_p^\dagger a_q$ is the transition probability for a single electron to go from orbital *q* to orbital *p*, and $h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$ is the transition probability for a pair of electrons to go together from orbitals *r* and *s* to orbital *p* and *q*.

Mapping into Pauli representation

This is sufficient as all operations in this system are pairwise – Coulomb – interactions. There are no natively n-body interactions for $n > 2$.

Electrons are fermions and so their $a_i^\dagger$ and a_i form a fermionic algebra with the following commutations rules:

$$\left\{a_p^\dagger, a_r\right\} = a_p^\dagger a_r + a_r a_p^\dagger = \delta_{p,r} \rightarrow aa^\dagger = 1 - a^\dagger a$$

$$\left\{a_p^\dagger, a_r^\dagger\right\} = \left\{a_p, a_r\right\} = 0 \rightarrow aa = a^\dagger a^\dagger = 0$$

Mapping to qubit representation

Ideally we would hope to use our qubits to represent the occupations of the molecular orbitals.

The Pauli exclusion principle states that each orbital can have at most two electrons.

This would require $2N_e$ qubits for N_e electrons:

2 electrons
in 1$^{\text{st}}$ orbital

$$|\psi\rangle = |01\overbrace{10}...\rangle$$

1 electron in
0$^{\text{th}}$ orbital

Mapping to qubit representation

We can then represent the creation and annihilation operators as:

$$Q^- |0\rangle = 0 \qquad\qquad Q^+ |0\rangle = |1\rangle$$
$$Q^- |1\rangle = |0\rangle \qquad\qquad Q^+ |1\rangle = 0$$

Where we have a Pauli operator representation:

$$Q^- = |0\rangle\langle 1| = \frac{1}{2}(X + iY)$$

$$Q^+ = |1\rangle\langle 0| = \frac{1}{2}(X - iY)$$

However these don't immediately obey the fermionic anti-commutation relations.
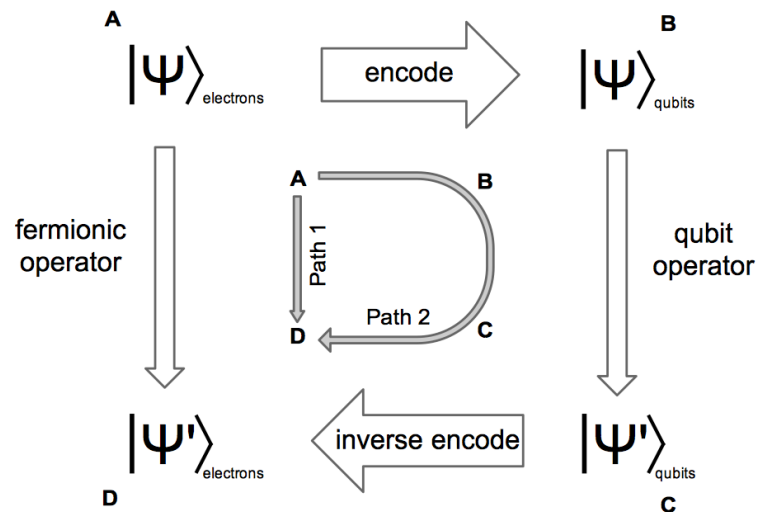
Mapping to qubit representation

What's going on here is that fermions have properties that qubits don't. Namely that if you swap two fermions then you are suppose supposed to acquire a phase – this is called the symmetrization postulate.

To capture this we can define the Jordan-Wigner transform:

$$a_p^\dagger = \left(\prod_{n<p} Z_n \right) Q_p^+ \qquad a_p = \left(\prod_{n<p} Z_n \right) Q_p^-$$

- Jordan-Wigner transform $\rightarrow$ O(n) Pauli operators per fermonic operator
- Bravyi-Kitaev transform $\rightarrow$ O(log n) Pauli operators per fermonic operator

Choosing an ansatz

Once we have a Pauli operator representation we must choose an ansatz.

Example: Variationally prepared state

Let $|\psi(\vec{\theta})\rangle = e^{-iV(\vec{\theta})}|0\rangle$ where $V(\vec{\theta})$ is an adiabatic evolution into H e.g. :

$$V(\vec{\theta}) = A(\vec{\theta})H_0 + B(\vec{\theta})H$$

with H_0 an initial simple Hamiltonian like: $H_0 = \sum_i X_i$,

H our target Hamiltonian with Pauli decomposition, and $\theta \in [0,1]$ a function of t with $A(0) = B(1) = 1$.

Adiabatic theorem says that if we do it slowly enough we will stay near the ground state. So we let VQE pick our annealing schedule mapping $e^{-iV(\vec{\theta})}$ into our parametrized gate set.

Summary

The Variational Quantum Eigensolver

Used for the electronic structure problem in quantum chemistry

1. MOLECULAR DESCRIPTION

e.g. Electronic Structure Hamiltonian

$$H = \sum_{i,j<i}^{N_n} \frac{Z_i Z_j}{|R_i - R_j|} + \sum_{i=1}^{N_e} \frac{-\nabla_{r_i}^2}{2} - \sum_{ij}^{N_n, N_e} \frac{Z_i}{|R_i - r_j|} + \sum_{i,j<i}^{N_e} \frac{1}{|r_i - r_j|}.$$

2. MAP TO QUBIT REPRESENTATION

e.g. Bravyi-Kitaev or Jordan-Wigner Transform

e.g. DI-HYDROGEN

$$\begin{aligned}
H = {}& f_0 \mathbb{1} + f_1 Z_0 + f_2 Z_1 + f_3 Z_2 + f_1 Z_0 Z_1 \\
& + f_4 Z_0 Z_2 + f_5 Z_1 Z_3 + f_6 X_0 Z_1 X_2 + f_6 Y_0 Z_1 Y_2 \\
& + f_7 Z_0 Z_1 Z_2 + f_4 Z_0 Z_2 Z_3 + f_3 Z_1 Z_2 Z_3 \\
& + f_6 X_0 Z_1 X_2 Z_3 + f_6 Y_0 Z_1 Y_2 Z_3 + f_7 Z_0 Z_1 Z_2 Z_3
\end{aligned}$$

3. PARAMETERIZED ANSATZ

e.g. Unitary Coupled Cluster Variational Adiabatic Ansatz

$$\frac{\langle \varphi(\vec{\theta})| H |\varphi(\vec{\theta})\rangle}{\langle \varphi(\vec{\theta})|\varphi(\vec{\theta})\rangle} \geq E_0$$

4. RUN Q.V.E. QUANTUM-CLASSICAL HYBRID ALGORITHM

QUANTUM PROCESSOR

PREPARE QUANTUM STATE (θ)

MEASURE TERM 1 → $\langle H_1 \rangle$

MEASURE TERM 2 → $\langle H_2 \rangle$

MEASURE TERM N → $\langle H_N \rangle$

CLASSICAL PROCESSOR

SUM TERMS → $\sum_i \langle H_i \rangle$

CLASSICAL OPTIMIZATION OF ANSATZ PARAMETER: θ

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Wecker, D., et al. (2015). Progress towards practical quantum variational algorithms. *Physical Review A*, 92(4), 042303.
McClean, J. R. et al. (2015). The theory of variational hybrid quantum-classical algorithms. *arXiv:1509.04279*.
Peruzzo, A., et al. (2014). A variational eigenvalue solver on a photonic quantum processor. *Nature communications*, 5.