Variational Quantum Eigensolvers (VQE)

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Introduction

What is VQE?

The Variational Quantum Eigensolver (VQE) is a quantum/classical hybrid algorithm:

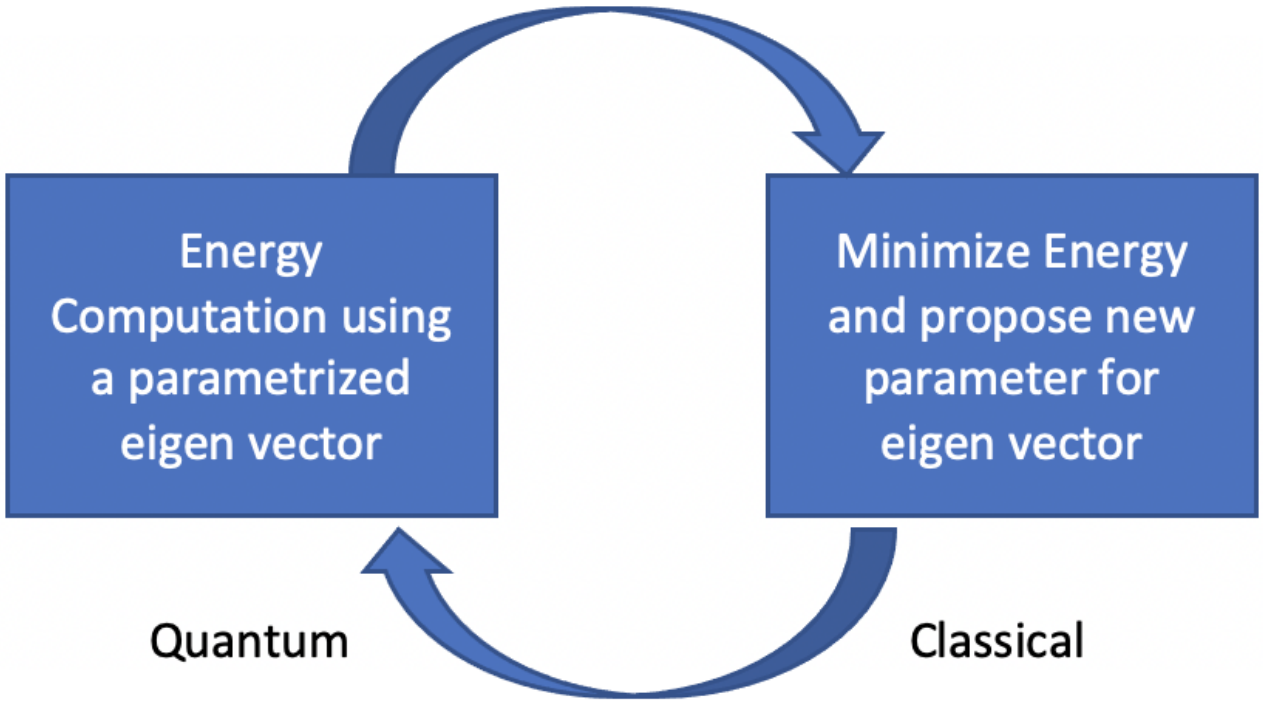
(a) that can be used to find eigenvalues of a (often large) matrix H.

(b) H is typically the Hamiltonian of some system.

(c) a quantum subroutine is run inside of a classical optimization loop.

Introduction

VQE is a hybrid quantum/classical algorithm because it works by variationally determine the ground state energy of the Hamiltonian of the system by employing a classical as well as a quantum computer.



Hamiltonian

The **Hamiltonian** of a system is an operator corresponding to the total energy of the system. For the purposes of this presentation we assume that we are able to get the Hamiltonian from a domain expert. It has the following characteristics:

(a) H is Hermitian

(b) H can be uniquely decomposed into a linear combination of pauli matrices such that the coefficients are all real.

Example: Hubbard model Hamiltonian

$$H = -t \sum_{<i,j>} \sum_{\sigma} t_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} c^{\dagger}_{i,\uparrow} c_{i,\uparrow} c^{\dagger}_{i,\downarrow} c_{i,\downarrow}$$

Recap of Pauli Matrices

The **Pauli Matrices** form a basis for the real vector space of 2×2 Hermitian matrices.

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The **Hamiltonian** can be decomposed into the linear combination of Pauli matrices using the Jordan-Wigner scheme or the Bravi-Kitaev scheme.

Solution plan

The algorithm proceeds in the following stages:

(a) Express the Hamiltonian in computational basis i.e. in terms of a linear combination of Pauli matrices.

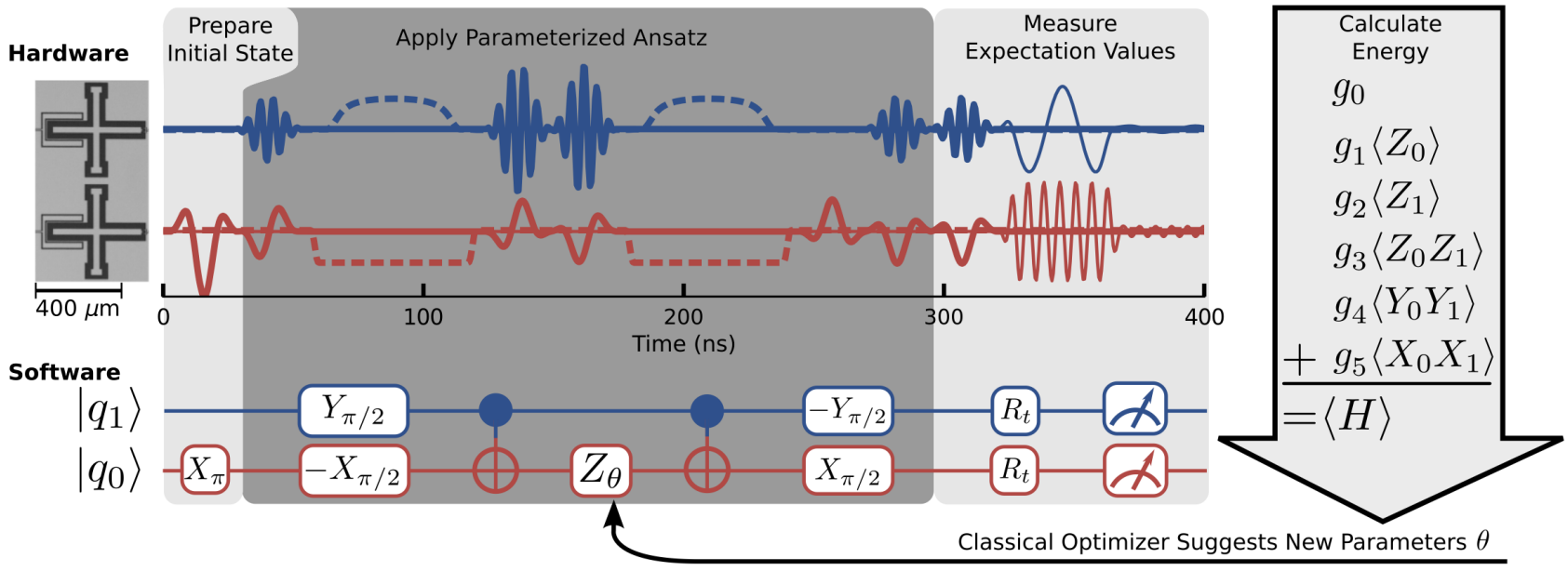
(b) Create a trial wave function(**ansatz**) of the form $\left|\psi(\vec{\theta})\right\rangle$, where $\vec{\theta}$ is a parameter. Initialize $\vec{\theta} = \vec{0}$, randomly, or on the basis of classical precomputation.

(c) Represent ansatz as a quantum circuit.

(d) Using current parameters (in ansatz), $\vec{\theta}$, repeatedly execute the circuit, each time performing an individual measurement of one of the pauli operators in H. After a sufficient number of circuit executions (shots), the averages of the resulting data converges to the expectation values of the operators.

(e) Check convergence. If the average energy has decreased by a small enough value determined to be converged, exit.

Quantum Circuit



Note: Here the R_t gates are rotation operations.

Calculating expectation value

When using a statevector simulator, $\langle\Psi|H|\Psi\rangle$ can be calculated by performing the matrix multiplication.
On a quantum computer we must do the following:

(a) Get quantum register into the state you want to compute the observable of (Pauli string)

(b) Transform the current basis such that the computational basis is rotated onto the measurement basis

(c) Measure quantum register in the computational basis

(d) Compute probabilities for each eigenvector from the counts

$$\langle\Psi|H|\Psi\rangle = \sum_i \lambda_i \mathbb{P}_i$$

The ansatz

In the VQE algorithm, a state $\left|\psi(\vec{\theta})\right\rangle$ is parametrized by action of a quantum circuit $U(\vec{\theta})$ on an initial state $|\phi\rangle$. i.e.

$$\left|\psi(\vec{\theta})\right\rangle = U(\vec{\theta})\,|\phi\rangle$$

The interesting thing about this expression is that even if $|\phi\rangle$ is a simple product state and $U(\vec{\theta})$ is a shallow quantum circuit, $\left|\psi(\vec{\theta})\right\rangle$ can contain complex many-body interactions.

We can represent $U(\vec{\theta})$ as a concatenation of parametrized quantum gates in the form:

$$U(\vec{\theta}) = U_1(\vec{\theta})U_2(\vec{\theta})....U_n(\vec{\theta})$$

The Ansatz

In fact, forming the ideal ansatz is the most critical aspect of the VQE algorithm. We will be discussing some standard proposals for setting up the ansatz later, but formulating the ansatz correctly and reducing the search space of the parameters is an area of active research.

The Variational Principle

Theorem

Given ψ, the expectation value of the Hamiltonian represents an upper bound to the exact ground state energy,i.e.

$$\langle\psi| H |\psi\rangle \geq E_0$$

Proof:

Let $|\psi\rangle = \sum_\alpha C_\alpha |\psi_\alpha\rangle$. Therefore,

$$\langle\psi|\psi\rangle = \left\langle \sum_\beta C_\beta \psi_\beta \middle| \sum_\alpha C_\alpha \psi_\alpha \right\rangle = \sum_{\alpha,\beta} C_\beta^* C_\alpha \underbrace{\langle\psi_\beta|\psi_\alpha\rangle}_{\delta_{\alpha\beta}} = \sum_\alpha |C_\alpha|^2 = 1$$

The Variational Principle - Proof Contd.

Using the Schrodinger's equation $H\psi = E\psi$,

$$\langle\psi|\, H\, |\psi\rangle = \sum_{\alpha,\beta} C_\beta^* C_\alpha E_\alpha \left\langle \psi_\beta \middle| \psi_\alpha \right\rangle = \sum_\alpha E_\alpha |C_\alpha|^2$$

But $E_\alpha \geq E_0$,

$$\implies \langle\psi|\, H\, |\psi\rangle \geq \sum_\alpha E_0 |C_\alpha|^2 = E_0 \geq \sum_\alpha |C_\alpha|^2 = E_0$$

Note: ψ is normalized $\implies \langle\psi|\psi\rangle = 1$

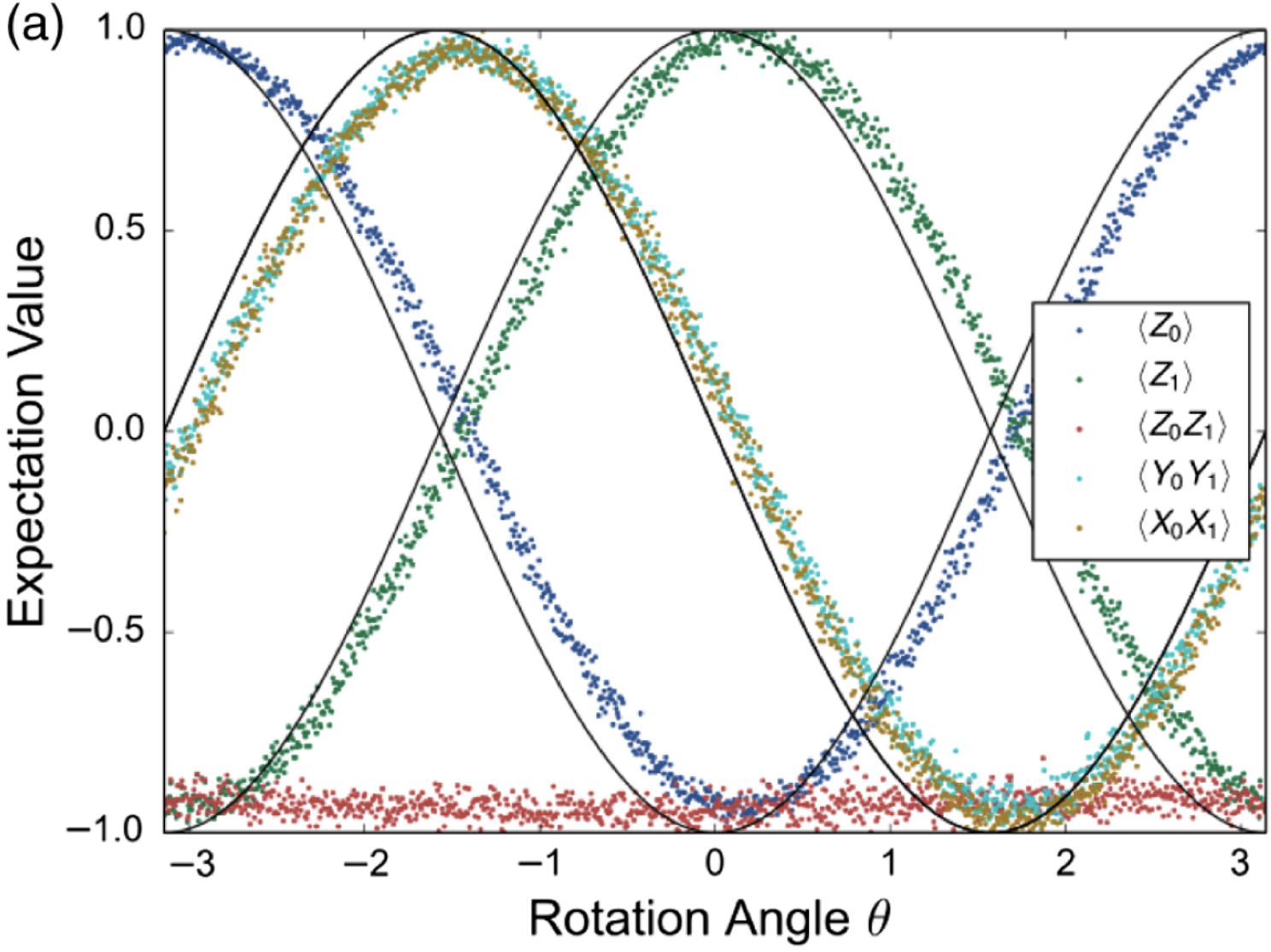
Expectation of Hamiltonian (Energy) calculation

In fact, forming the ideal ansatz is the most critical aspect of the VQE algorithm. We will be discussing some standard proposals for setting up the ansatz later, but formulating the ansatz correctly and reducing the search space of the parameters is an area of active research. Given an ansatz, the expectation of Hamiltonian (Energy) is given by:

$$E(\vec{\theta_0}) = \left\langle \psi(\vec{\theta_0}) \right| H \left| \psi(\vec{\theta_0}) \right\rangle \geq E_0$$

Note: In the beginning, θ_0 is initialized to a certain value and an ansatz is created. After the first round of energy calculation, subsequent $\theta_k, k \geq 1$ are proposed by the classical optimizer.

Expectation of terms in Hamiltonian by $\vec{\theta}$



Choice of $\vec{\theta}$

(a) $\text{len}(\vec{\theta}) \leq \mathcal{O}(poly(N))$ i.e. the number of parameters stays small as the system grows.

(b) $U(\vec{\theta})$ needs a decomposition into at most a number of quantum operations that is polynomial in N.

Note: Here $N \times N$ is the size of the Hamiltonian.

Choice of Ansatz

(a) UCC

(b) Hamiltonian variational

(c) ADAPT-VQE

UCC

Inspired by quantum chemistry, the variational state is prepared using a unitary evolution under a sum of fermionic terms.

$$|\Psi_T\rangle = e^T |\Psi_I\rangle$$

where

$$T = \sum_{p<q} (T_{pq} c_p^\dagger c_q - H.c.) + \sum_{p<q,r<s} (T_{pqrs} c^\dagger c_q^\dagger c_r c_s - H.c.)$$

Often, e^T is implemented using a Trotter-Suzuki method for a small number of Trotter steps.

$$e^{(A+B)} = lim_{n\to\infty} \left(e^{\frac{A}{n}} e^{\frac{B}{n}} \right)^n$$

Hamiltonian variational

The Hamiltonian variational ansatz sets out to resolve the issues of UCC. Building the variational state using rotations by terms in the Hamiltonian reduces ansatz circuit depth.

$$|\Psi_T\rangle = \prod_{b=1}^{S} \left[U_u\left(\frac{\Theta_U^b}{2}\right) U_h(\Theta_h^b) U_v(\Theta_v^b) U_u\left(\frac{\Theta_U^b}{2}\right) \right] |\Psi_I\rangle$$

Where $U_X(\Theta)$ approximates $e^{i\Theta h_x}$ for $X \in \{U, h, v\}$ in the Hamiltonian. We again use Trotterization, but only for U_h. The choice of Ψ_I is also important and is often a Slater determinant or the Hartree Fock state.

ADAPT-VQE

The key idea is to systematically grow the ansatz by adding fermionic operators one-at-a-time, such that the maximal amount of correlation energy is recovered at each step.

$$|\Psi^{ADAPT(\epsilon)}\rangle = (e^{\hat{\tau}_N})(e^{\hat{\tau}_{N-1}})...(e^{\hat{\tau}_2})(e^{\hat{\tau}_1})|\Psi_{HF}\rangle$$

where $\hat{\tau}_i$ comes from a pool of one and two (and possibly three and four) body operators.
Selecting which operator goes in the ansatz is done by computing the gradient for each operator in the pool and taking the largest.

$$\frac{\partial E^{(n)}}{\partial \Theta_N} = \langle \Psi^{(n)} | [\hat{H}\hat{A}_N] | \Psi^{(n)} \rangle$$

Notes on Optimization

Quoting the authors from the original VQE paper: *"For the classical optimization step of our integrated processor we implemented the Nelder–Mead (NM) algorithm, Although in general NM can fail because of the deterioration of the simplex geometry or lack of sufficient decrease, the convergence of this method can be greatly improved by adopting a restarting strategy. Although other DS methods, such as the gradient descent, can perform better for smooth functions, these are not robust to the noise, which makes the objective function non-smooth under experimental conditions. NM has the ability to explore neighbouring valleys with better local optima, and likewise this exploring feature usually allows NM to overcome non-smoothnesses. We verified that the gradient descent minimization algorithm is not able to converge to the ground state of our Hamiltonian under the experimental conditions, mainly due to the Poissonian noise associated with our photon source and the accidental counts of the detection system, while NM converged to the global minimum in most optimization runs."*

Nelder-Mead Optimizer

(a) Initialize with a random start point.

(b) Construct a set of vertex points, evaluate the function value at each of these points and finally rank them from best (lowest function value) to worst.

(c) Find the centroid of all points leaving aside the worst.

(d) Use the centroid to calculate a new reflection point.

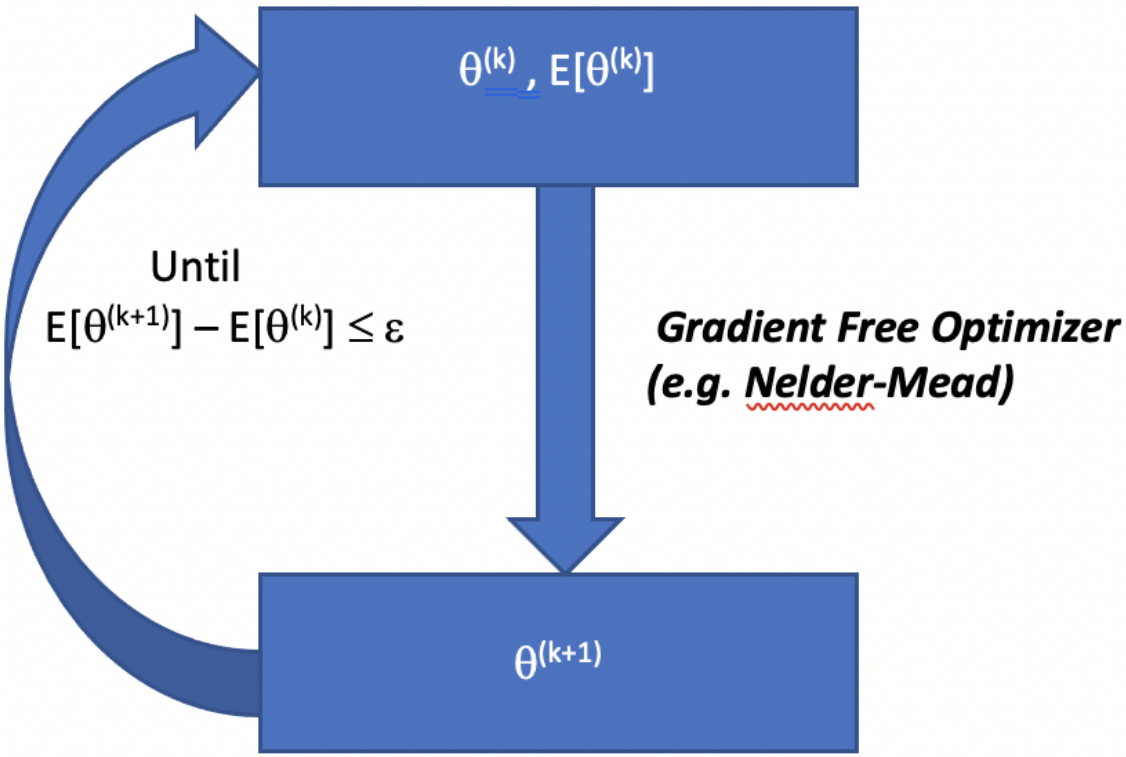
(e) Depending on new value of the function at this point, we either perform an expansion or contraction operation to move towards the minima.

Nelder-Mead Optimizer

Click for Demo of Nelder Mead

The closed loop optimization process

The following diagramatic representation outlines the closed loop process that runs between the optimizer and the quantum computer.



Advantages of VQE

(a) VQE seeks to find optimal parameters in a fashion that is blind to control errors (some hardware stuff).

(b) VQE is robust due to adaptive nature of the algorithm.

(c) Compared to PEA, VQE achieves better Chemical Accuracy at low cost.