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Abstract

In this work, we read the quantum adiabatic approach of change of Hamiltonian which is known as Adiabatic quantum computing(AQC) alongwith Variational quantum eigen solver(VQE) to study "Adiabatically Assisted Variational Quantum Eigensolver" (AAVQE) algorithm which is an hybrid classical-quantum algorithm to solve optimization problems in current quantum computers. We also read some examples of implementation of AQC and VQE.

1 Introduction

Quantum algorithms were first designed to model quantum circuits for particular problems which were often related to classical computation. Two of the most relevant instances of this original approach are the algorithms given by Grover [1] and Shor[2] . Both of them exploited the advantage of quantum superposition and parallel processing using quantum circuits. Furthermore, the quantum circuit must be designed in such a way that it transforms an initial quantum state into a final state which encodes the solution to the problem.

The above circuit approach can be categorized as the "digital" or "gate" model to quantum Computing. In parallel to the gate model, there is a separate class of quantum computing models that are relevant for chemistry applications. This separate class of approach is sometimes termed as an "analog" approach to quantum computing. Adiabatic quantum computation (AQC) is a good example of it. These analog models consists of quantum algorithms that are used to find solution for eigen value and optimisation problems. Since the initial proposal by Richard Feynman [3], a number of advancements have been made in desiging quantum circuit models and developing quantum algorithms to solve these problems. Here, we will focus on this adiabatic approach of computation and connect it with other proposed algorithms later .

2 Quantum Computation by Adiabatic Evolution

This idea of quantum computation using adiabatic approach was first proposed back in 2000 by Frahi, gutmann and Sipser [4]. They presented a quantum algorithm based on adiabatic evolution of Hamiltonian for solving instances of the satisfiability problem(SAT). This approach is also termed as Adiabatic quantum computing(AQC). In this methodology, the evolution of the quantum state is governed by a time-dependent Hamiltonian which is changed from an initial Hamiltonian (of which ground state is easy to construct) to the final Hamiltonian(of which ground state is the solution of a computationally interesting problem). To ensure that the system evolves into the desired final ground state, the evolution must be done slowly enough. Moreover, the required evolution time also depends on the minimum energy difference between the two lowest states of the interpolating Hamiltonian and we will discuss this soon. The adiabatic quantum computing(AQC) is based on the principle of quantum adiabatic theorem.

So, lets begin with the adiabatic theorm and the formulation of adiabatic evolution.

2.1 Adiabatic Therom

A quantum system evolves according to the Schrödinger equation

$$i\frac{d}{dt}|\psi(t)>= H(t)|\psi(t)\rangle$$

and the adiabatic theorem tells us how to follow this evolution if H(t) is slowly varying. We define a paramter s = t/T as the rate of change of evolution where T being the total evolution time which controls the rate at which H(t) varies and $0 \leq s \leq 1$. Consider a smooth one-parameter family of Hamiltonians H'(s)

$$H(t) = H'(t/T) = H'(s)$$

Define the instantaneous eigenstates and eigenvalues by:

$$H(s)|l;s\rangle = E_l(s)|l;s\rangle$$

and $|\psi(0)\rangle$ is ground state of H'(0), that is

$$|\psi(0)\rangle = \left|\langle l=0; s=0|\psi(T)\rangle\right|$$

According to the adiabatic theorem, if the gap between the two lowest levels, $E_1(s) - E_0(s)$, is strictly greater than zero for all $0 \leq s \leq 1$, then

$$\lim_{T\to\infty} \left|\langle l=0; s=1|\psi(T)\rangle\right| = 1$$

This implies that if T is big enough, the existence of a nonzero gap guarantees that $|\psi(t)\rangle$ obeying the Schrodinger Equation remains very close to the instantaneous ground state of H(t) for all t from 0 to T .
A closer look at Adiabatic theorem tells us, if we take Total time large enough as below

$$T >> \frac{max_s \left|\langle\psi_1|\frac{dH(s)}{ds}|\psi_0\rangle\right|}{g_{min}^2}$$

,we can write

$$\left|\langle l=0; s=1|\psi(T)\rangle\right| \approx 1$$

The numerator in formulation of T corresponds to the transition amplitude between the ground state and the first excited state, and the denominator is the minimum gap of the system

$$g_{min} = min_s(E_1(s) - E_0(s))$$

2.1.1 Adiabatic Evolution

Consider an system which follows adiabatic evolution linearly:

$$H(t) = (1 - t/T)H_B + (t/T)H_P$$

or

$$H'(s) = (1 - s)H_B + sH_P$$

where s = t/T and $0 \leq s \leq 1$
H(t) is defined for t between 0 and T is slowly varying.
H_B is the starting Hamiltonian of which ground state is easy to construct
H_P is the given problem Hamiltonian whose ground state encodes the problem solution.

Given the total evolution time T condition in section 2.1, the adiabatic theorem states that the initial ground state of H_B will evolve to the ground state of H_P i.e. the desired solution of the problem. The theorem indicates that the source of error is related to the possibility of jumping from the ground state to the first excited state, which is can occur either because the amplitude for such a process is large or due to a very small gap. In this language, hard problems are associated to adiabatic evolution where the gap becomes exponentially small.

3 Variational Quantum eigensolver(VQE) Algorithm

Despite developments in quantum algorithms and optimization of resource requirements, many of the algorithms have hardware requirements which are far beyond the capability of near-term quantum computers. As with the increase of size of physical system, dimension of the problem increases exponentially. So determining efficient solution of large eigenvalue problem is must. The known pre-existing algorithm Quantum phase estimation(QPE) offers exponentially speedup but requires $O(p^{-1})$ operations to obtain an estimate with precision p. In addition, to maintain the time coherency of quantum computer (which is determined by the necessity of $O(p^{-1})$ successive application of e^{-iHt}), the QPE algorithm can require millions or billions of quantum gates for practical application [5][6].

In 2014, Peruzzo and Mc- Clean et al. put forward a hybrid quantum-classical algorithm under the name Variational quantum eigensolver(VQE)[7] designed to find variational solutions to eigenvalue and optimization problems while utilizing both quantum and classical resources. These type of algorithm which utilises both classical and quantum computers are called Hybrid Quantum classical algorithm(HQC). VQE is the first proposed example of HQC. Furthermore, VQE has notable property that it can run on any quantum device, making it a candidate for exploring the performance of early quantum computers. Moreover, VQE has a modular design which gives scope of enhancement in individual component and thus overall performance gain. VQE is major algorithm of interest in recent past year.

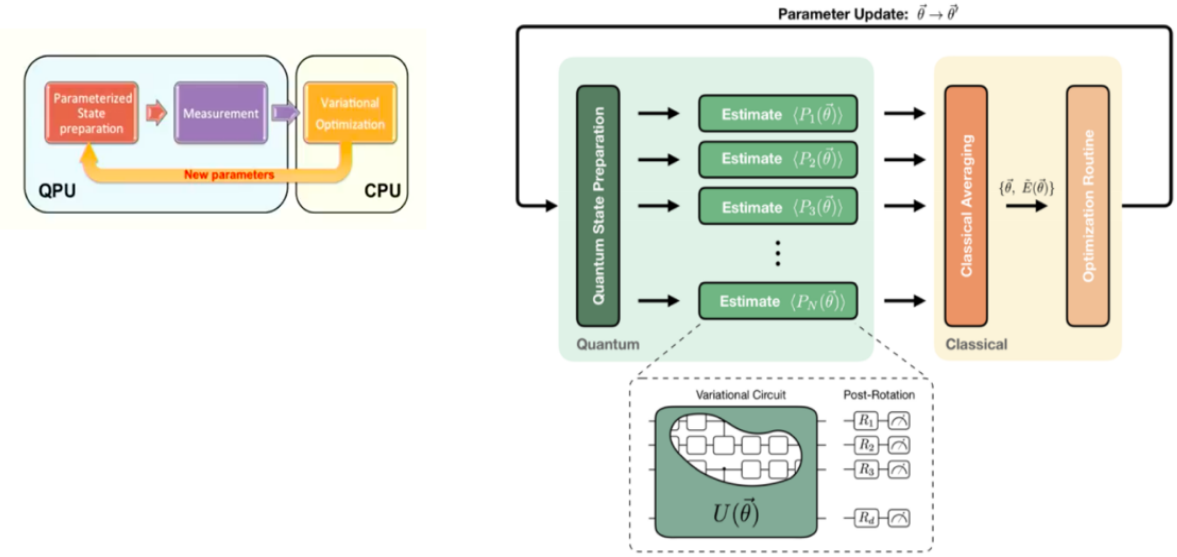

Figure 3.1: Illustration of VQE algorithm [8]

Figure 3.1 shows the quantum computer is used to prepare a set of parameterized quantum states followed by applications of rotations depending on the Pauli term of the Hamiltonian to be measured. The classical computer then takes the individual estimates of the Pauli term expectation values $\langle P_i(\theta) \rangle$ and averages them to compute a single value $E(\theta)$. This cost function value is fed into an optimization routine, which produces an updated set of parameters θ input for the quantum circuit in the next optimization loop. This procedure is repeated until the energy converges.

The Algorithm can be divided into following steps:

1. Parameterised State preparation: Take an easy to prepare initial state $|\psi_0\rangle$ and prepare a param-

eterised quantum state $\psi(\vec{\theta})$ as an output of wisely parameterised quantum circuit where $\vec{\theta}$ can be any adjustable experimental $\langle H(\vec{\theta}\rangle$ or gate parameter.

2. Energy Estimation: The expectation value of the energy $\langle H\rangle(\vec{\theta})$ is estimated using a Hamiltonian averaging procedure.

3. Variational Optimisation: The parameter $\vec{\theta}$ of the quantum state are updated using a classical non-linear optimisation scheme.

4. Iterate this procedure until convergence in the value of the energy. The parameters $\vec{\theta}$ at convergence define the desired state.

A brief sketch of different approaches used in individual steps is shown as in figure 3.2

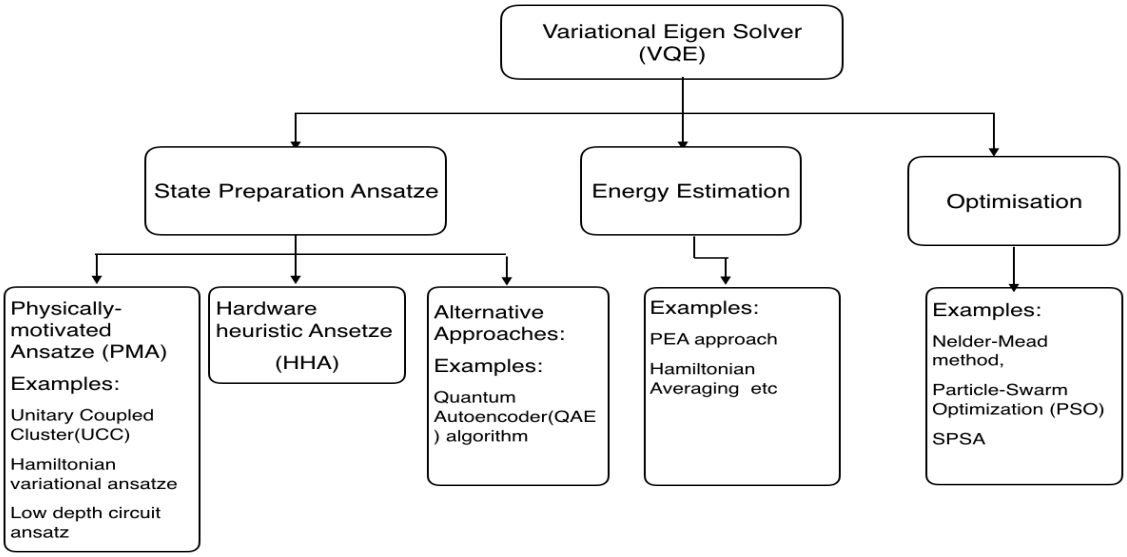

Figure 3.2: Various Approaches used in VQE

The main feature of VQE is that it gives flexibility to choose parametrised trial state to approximate eigenstates of target Hamiltonian. So the ansatz for state preparation is one of common ground of interest. Among the state ansatz listed in figure , UCC and Hamiltonian variational ansatz is most used in recent past. Besides state ansatz, the efficiency and accuracy of VQE can be enhanced by optimisation step of algorithm. Along with usage of different optimization methods, variations of the optimisation step have also been put forward since VQE was first introduced.

In the section 4 , we will read Adiabatically Assisted Variational Quantum Eigensolver (AAVQE) method which breaks the optimization into easier, smaller parts and shows promising results .

3.1 Implementation of VQE in recent works

Below are some works in recent past years which used VQE as computational quantum algorithm

1. Ground state molecular energy for He–H^+ [7]: Alberto Peruzzo et al. proposed and implemented VQE algorithm by combining a small-scale photonic quantum processor with a conventional computer. They experimentally demonstrated the feasibility of this approach with an example from quantum chemistry calculating the ground state molecular energy for He–H^+ within chemical accuracy.

2. Quantum Implementation of Unitary Coupled Cluster for simulating the electronic structure of He–H+ [9]: Yangchao Shen et al. provided the first experimental implementation of the unitary version of the coupled cluster ansatz (UCC) on trapped ion quantum system. They performed a simulation on the electronic structure of a molecular ion ($He–H^+$), where the ground-state energy surface curve was probed. The paper shows the agreement of experimental data with the energy calculated by the exact diagonalization of the full matrix of Hamiltonian within the accuracy limit.

3. Energy spectrum of the H_2 molecule:[10] J. I. Colless, et al. demonstrated a complete implementation of the Variational Quantum Eigensolver (VQE) augmented with a novel Quantum Subspace Expansion(QSE) algorithm, to calculate the complete energy spectrum of the H_2 molecule with near chemical accuracy. In this paper, they also showed QSE mitigate the effects of incoherent errors, potentially enabling larger-scale quantum simulations without the need for complex error-correction techniques.

4. Energy surface of molecular hydrogen: [11]P. J. J. O'Malley et al. used a programmable array of superconducting qubits to compute the energy surface of molecular hydrogen using two distinct quantum algorithms. They experimentally executed the unitary coupled cluster(UCC) ansatz using the variational quantum eigen- solver. The implementation predicted the correct dissociation energy to within chemical accuracy of the numerically exact result. In Addition they compare experimentally the results with canonical quantum algorithm which consists of Trotterization[12] and quantum phase estimation[29] . They showed VQE method is more robust to certain errors in comparison to Canonical quantum algorithm and is promising for preparing molecular ground-states for quantum simulation.

5. Potential Energy surface of small molecules H_2, LiH and BEH_2:[14] Abhinav Kandala et al. implemented VQE approach combined with a compact encoding of fermionic Hamiltonians[28] and a robust stochastic optimization routine[16] to determine the ground state energy for molecules of increasing size up to BEH_2. They showed that results for H_2, LiH and BEH_2 and find the method has more deviation with increasing size of molecule.

7. Quantum simulation of the deuteron binding energy [17] Dumitrescu et al. performed quantum simulation of the deuteron binding energy on quantum processors accessed via cloud servers. They used a Hamiltonian from pionless effective field theory at leading order and designed a low-depth version of the unitary coupled-cluster ansatz. They used variational quantum eigensolver algorithm and compute the binding energy to within a few percent. It is first step towards scalable nuclear structure computations on a quantum processor via the cloud.

8. Addressing hard classical problems with Adiabatically Assisted Variational Quantum Eigensolvers [19]: Garcia-Saez et al presented a hybrid classical-quantum algorithm which is an enhancement of VQE to solve optimization problems in current quantum computers. They combine the basic idea of this variational quantum eigensolvers (VQE) with adiabatic change of the Hamiltonian. They used this approach to solve both quantum Hamiltonians and hard classical problems .

In the next section, we will read the implementation and results of Adiabatically Assisted Variational Quantum Eigensolvers (AAVQE) in more detail.

4 Adiabatically Assisted Variational Quantum Eigensolver (AAVQE)

4.1 Introduction

Since when Variational Quantum eigensolver (VQE), the first clasical Quantum Algorithm, has been introduced, a lot of work on this algorithm has been done by different researchers . They have not only come up with results in different scenarios but its variations also. The main reason of its popularity is due to modular design of algorithm which give flexibility and scope of continuous improvement. With same ideology, A.Garcia-Saez and J. I. Latorre came up with an extension of VQE algorithm based on adiabatic approach discussed in section 1 for solving optimization problems in current quantum computers. The motive of this new algorithm is to circumvent the problem of facing very small gradients in the classical optimization step of a VQE, while being able to run in current hardware efficient devices. They benchmarked this Adiabatically assisted variational quantum eigensolver (AAVQE) algorithm[19] on quantum Hamiltonians and hard classical problems.

4.2 THE AAVQE ALGORITHM

We can define quantum algorithm as a collection of steps from a state which is easy to prepare to another state which encodes the solution to a problem. But finding a reasonable path to connect both states, given the exponential size of the Hilbert space, is a daunting task. It is possible that, given the exponential size of the Hilbert space, VQE may get lost in parameter space in search of minimum as quantum circuit need to deal with tiny gradients. On the other hand, adiabatic quantum evolution always find its way to solution and can be optimised to pick an efficient path. So it can be combined with VQE to have better solution.

The method breaks the optimisation step of VQE algorithm into several timesteps of adiabatic evolution and employs a parameterised Hamiltonian of the form as below(see section 2.1.1)

$$H(s) = (1-s)H_0 + sH_P$$

where H_0 is initial Hamiltonian for which ground state is easy to prepare and H_P encodes the solution of the problem. s is interpolation parameter and takes values between 0 and 1 .

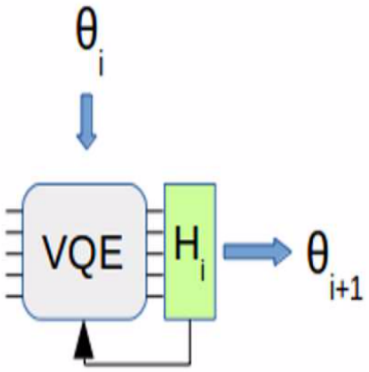

Figure 4.1: Scheme of AAVQE algorithm

Lets define some terminology for the illustration of scheme of algorithm as shown in figure 5.1.

As at each step s_i , quantum circuit of VQE needs to be initialized with a classical set of parameters . Let $\theta_{s_i}^{(0)}$ and $\theta_{s_i}^{(f)}$ are the initial and final parameter set of ith step respectively.

We can define the scheme as below:

1. Initialise the parameter set $\theta_{s0}^{(0)}$ for the quantum circuit of VQE and prepare the parameter set for ground state of simple Hamiltonian as $\theta_{s0}^{(f)}$. The set $\theta_{s0}^{(0)}$ can be chosen randomly.

2. At every step s_i , VQE needs the quantum circuit to be initialized with a classical set of parameters $\theta_{si}^{(0)}$. At each step it minimises the intermediate Hamiltonian H_i .

3. After minimization is complete the quantum circuit is defined by the trained final set of parameters $\theta_{si}^{(f)}$

4. The final parameters that deliver the optimal minimum for the Hamiltonian at any step s_i are passed as initial parameters for the next one, that is $\theta_{si}^{(f)} = \theta_{si+1}^{(0)}$

5. And we iterate this up to desired evolution time steps.

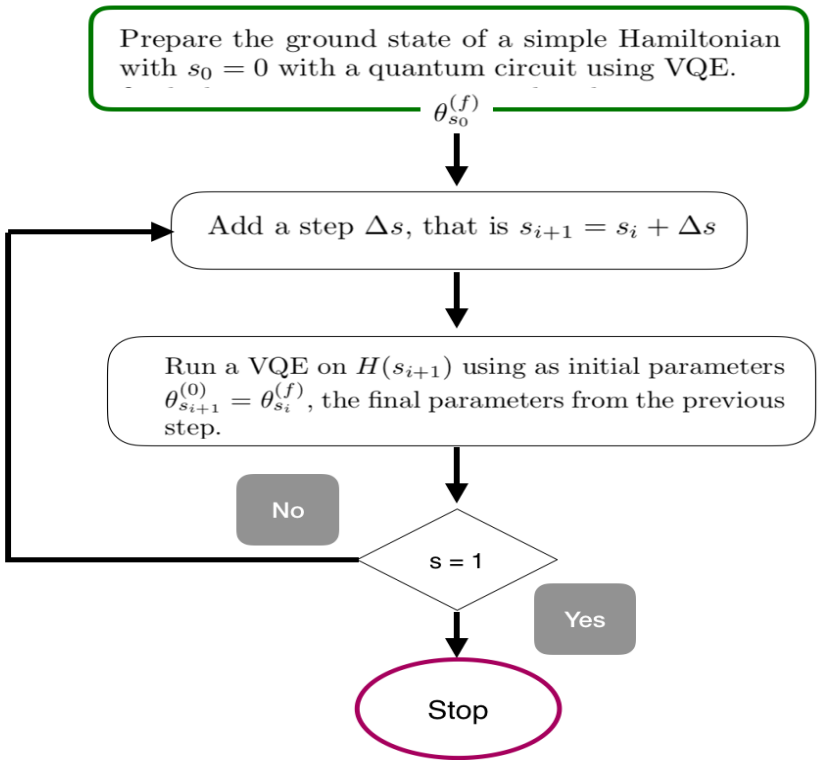

Figure 4.2: Flow diagram of AAVQE algorithm

Lets note that we don't do any real time dynamic adiabatic evolution , but we use the concept of adiabatic evolution in which interpolation parameter is used to adjust the Hamiltonian from one VQE run to the next. Moreover, as long as the gap of H(s) does not become too small (see Section 2.1),the ground state of H(s) will lie close to the ground state of the Hamiltonian H(s+Δs) in the subsequent step .

In the next subsection, we will see advantages of AAVQE algorithm.

4.3 Advantages of AAVQE

The below are few major benefits of AAVQE:

1. As AAVQE can use any type of Hamiltonian evolution(non-linear also) and has no relation with problem Hamiltonian, it can be used with any kind of problem. This broadens the scope of AAVQE to both classical and Quantum problems.

2. AAVQE also provides the scope of performance enhancement by giving two tunable options as below:
(*i*) The number of discretization steps of the adiabatic evolution of H(s) is a matter of choice.
(*ii*) Second, the classical optimization method used to find the gradient towards the ground state is also a choice in the hands of the programmer.

3. It is also possible to apply non-linear adiabatic evolution, but linear evolutions is mostly used because it restricts the scaling factor of used number of gates as linear.

4. It is also arguable that with larger system size, the problem of finding a good path to the final solution gets exponentially worse and AAVQE may have an advantage over VQE as the system size gets larger. In that case, an adiabatic strategy may be mandatory.

4.4 Results

The paper[19] includes the implementation of AAVQE to both quantum(ground state of XX spin chain) and classical NP-complete problem(Exact Cover) and compares the results with standard VQE implementation. In both of problems, exactly same quantum circuit and parameter set has been used. It shows the flexibility of AAVQE for solving optimization problems.

4.4.1 Optimisation of quantum problem

The paper shows total evolution of XX spin chain with N =4, $\Delta = 0.05$ and simultaneous perturbation stochastic approximation(SPSA) for optimisation.

The implementaion gives following results:

1. VQE takes less number of iterations and performs well. While AAVQE outputs similar results, but takes more iteration steps.

2. AAVQE may not converge in some instances in last stages and get stuck in local minima. But it is less probable with respect to VQE.

To solve the convergence problem, the Adiabatic evolution gives the option to store each previous parameter set because of discretisation of time T. One may restart the optimisation at best solution of near problem H(s_i). Moreover, one may stop the optimisation upon convergence, reducing the numerical effort for each value of s_i.

4.4.2 Optimisation of classical problem

The AAVQE method is used to obtain solutions of hard instances of EXACT COVER problem(an NP-complete problem).

The following results are found from calculations:

1. With N =4 and N =8, the final state encodes the correct solution, however the intermediate states may have large deviation from ground state of H(s).

2. They compute the adiabatic evolution of 200 hard instances with N = 16. and plotted the histogram of finding solution with respect to the value of s. They used 100 iterations of the VQE for each values of s (with Δ s = 0.05) and almost all instances are solved in less than 100 VQE iteration.

3. They found the same results with N=20

4. According to paper, for the same instances, they were unable to find a valid set of parameters of the VQE to solve or even approximate these problems.

5 Examples of implementation of Adiabatic Quantum computing

AQC has been applied to classical optimization problems that lie in the complexity class NP. For example, studies have been performed on satisfiability[4], Exact Cover[20], 3-regular 3-XORSAT and 3-regular Max-Cut[21], random instances of classical Ising spin glasses[22], protein folding[23][24] and machine learning [25] [26]. AQC has also been applied to structured and unstructured search, search engine ranking and artificial intelligence problems arising in space exploration. In this section,we will read some of proposed methodologies and works in detail..

5.1 Adiabatic Quantum Simulation of Quantum Chemistry[27] :

Ryan Babbush, Peter J. Love and Aspuru-Guzik designed a scalable method for quantum computation of molecular properties using quantum adiabatic algorithm. They described how to map electronic structure Hamiltonians to 2-body qubit Hamiltonians with a small set of physically realizable couplings. They divided the method into three sections:

(a) Second Quantisation; The procedure begins with second quantized formulation of the molecular electronic structure in which Hamiltonian is represented with fermionic creation and annihilation operators.

(b) Qubit Representation: Second, give mapping by converting the fermionic Hamiltonian to a qubit Hamiltonian using the Bravyi-Kitaev transformation.[28][29] The Bravyi-Kitaev transformation offers a middle ground in which both parity and occupancy information are stored non-locally, so neither can be determined by measurement of a single qubit. Both parity and occupancy information can be accessed by acting on a number of qubits that scales as the logarithm of the number of qubits. This logarithmic scaling makes the proposed mapping of electronic structure to a 2-local qubit Hamiltonian efficient.

(c) Hamiltonian Gadgets: At last step, use gadgets for locality reduction. Hamiltonian gadgets provide a method for embedding the eigen- spectra (and sometimes eigenvectors) of an n-qubit "target" Hamiltonian.

They showed the implementation of this method with an example of Hydrogen molecule.

5.2 Adiabatically parameterised states preparation ansatz for VQE[30]:

The main idea behind this parametric state anstaz is combination of Adiabatic theorem and Variational theorem. The most common considered form of adiabatic evolution can be defined in below format :

$$H_s = A(s)H_i + B(s)H_P$$

where B(s) = (1 -A(s)) and A(0)= B(1) = 0 and A(1) = B(0) =0 and t $\in$ [0,T]

Here, we consider all paths f $\in$ F(T) for values of A(s) and B(s) from 0 to 1 and we take that optimal path in F(T) that minimises the expectation value of final state. The expectation value of final state can be written as functional of the path $\langle H \rangle[f]$

$$\langle H_P \rangle[f] = \langle \psi[f]|H_p|\psi[f]\rangle$$

This functional minimization may be changed into a standard minimization by parameterizing the path f by a set of parameters θ, and performing an optimization on the parameters θ that determine the path.

The main reason behind using variational approach is that in realistic situation, its hard to get a good estimate of minimum gap and the system may have de-coherence. It is known that for systems experiencing de-coherence or de-phasing on the timescale of evolution, slowest possible evolution is not optimal in preparing the ground state of final problem Hamiltonian[31][32][33]. Thus variational principles helps to get optimised parameters without taking care of above mentioned problems.

Moreover, this ansatz is capable of preparing states which can not be efficiently prepared or sampled from classically using only a small number with the currently available methods [34]

5.3 Equivalence of Adiabatic Quantum Computation to Standard Quantum Computaion [35]:

Dorit Aharonov,Seth Lloyd et al. showed that standard quantum computation can be efficiently simulated by adiabatic computation and thus model of adiabatic computation is polynomially equivalent to the standard model of quantum computation.

6 Conclusion

In this work, we studied the Quantum adiabatic approach along with Variational quantum eigensolver. We also studied one recently introduced method AAVQE which splits the optimistaion step of VQE with help of adiabatic evolution. The adiabatic approach has pitfalls of slow time evolution and of not leading to optimal solution if the system experiencing de-coherence but on the other hand it gives us an assurance of always finding a path to the problem hamiltonian if total evolution time is large enough. In general, we dont expect that quantum computing, including AQC, can provide efficient solutions to NP-Complete problems in the worst case [36]. However, there may exist sets of instances of some NP-Complete problems for which AQC can find the ground state efficiently, but which defy efficient classical solution by any means. If this is the case then AQC is certainly of considerable scientific interest, and likely of great industrial importance.

7 Acknowledgement

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