Quantum Computing Algorithms in Sustainable Energy Production

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Quantum computing has several promising prospects. With its dependency on quantum computing large, previously unsolvable, problems could be solved. In this research, semi-systematic literature analysis was used to discover popular quantum algorithms with a possible application in sustainable energy production. The algorithms are categorised into two different groups, the quantum chemical simulations algorithms and the quantum optimisation algorithms. The quantum chemical simulations can be used for simulating molecules, allowing better materials and technologies to be discovered for sustainable energy production. The optimization algorithms have a focus on optimising efficiency in energy production by regulating the energy flow of a grid or smart storage of energy. One major theme that haunts all algorithms is current hardware limitations, with all algorithms requiring more processing power than currently available. In addition, most algorithms require careful consideration of initial parameters, meaning that real-world situations need to be represented in the algorithms properly. If these challenges are overcome, quantum computing could enhance sustainable energy production significantly.

Additional Key Words and Phrases: quantum computing, algorithms, quantum circuits, qubits, sustainable energy production

1 INTRODUCTION

1.1 Background of quantum computing

Quantum computing provides high computational power, less energy consumption, and exponential speed over classical computers [1]. These statements have been made multiple times in the past, however, it is still ambiguous to many people how quantum computing can benefit modern technologies. A good understanding of quantum computing and classical computing is needed to shed light on this subject.

Paul E. Ceruzzi [2003] describes classical computing as the following: “It is a system: an arrangement of hardware and software in hierarchical layers.” [2]. Software in this case refers to a description of methods or handling that the computer needs to take, while the hardware is the one performing the method.

The first computers of the 20th century could not even complete calculations on their own. They needed a lot of theoretical knowledge to be used correctly, while nowadays, computers can solve anything almost instantly. Alan Turning was the first to create a computer with software, allowing the general public to use computers themselves. Allowing users without extensive knowledge of computers and operations to use a computer [1]. Over time, the hardware and software components improved to allow even more complicated calculations, eventually resulting in the computers we have today.

As opposed to classical computing, quantum computing, as described before, can have large advantages, severely speeding up calculations. Quantum computers operate on a recent, popular field of physics called: quantum physics. During the development of circuits, a natural route was to decrease the size of certain components. However, during this process, certain circuit elements stopped working as intended. Classical physics had no explanation for these phenomena, resulting in the need for quantum physics and, subsequently, quantum computing [1].

Quantum computing provides large advantages in certain problems due to their use of something called ’quantum bits’. Quantum bits use the same logic as bits used by classical computing, however, these quantum bits are made up of small particles like atoms, electrons, photons, and ions. These particles can also be stacked, allowing for parallel computations, resulting in smaller circuits with larger computational power [1].

Quantum computers make use of quantum algorithms. These algorithms are essentially instructions to follow for each calculation. This definition also applies to classical algorithms, however, quantum algorithms are specifically created for quantum computers. As mentioned before, quantum computers use quantum physics, resulting in the need for new algorithms specifically created for quantum computers. Quantum algorithms can be visualised using quantum circuits, these circuits will show a general path that the computer will take during the calculation.

1.2 Background of sustainable energy production

Sustainable energy in its most commonly used definition was first introduced in 1987. With risks regarding fossil fuels and other forms of unsustainable energy getting more apparent each day, large efforts were put into ensuring a better distribution of clean and other forms of energy [15]. These efforts have only increased over the decades since its first official definition, with the European Union having set the binding renewable energy target to 42.5% for all its members [16].

Sustainable energy production allows for a reduction in greenhouse gasses, resulting in a decrease in global climate change and a decreased risk of rising sea levels [17]. These factors show the importance of sustainable energy production and how it could hope to preserve our current way of living. Referring to the large risks related to non-sustainable energy sources.

1.3 Application of quantum computing algorithms in sustainable energy production

With quantum computers requiring a very large amount of energy, considerations about their cost-effectiveness need to be made. Especially with recent regulations trying to limit energy usage [16]. This is why, conversely, this technology could help to resolve its issue, increasing sustainable energy production beyond its current limits. In order to analyse the application of quantum computing algorithms in sustainable energy sources the following steps will be taken. First, a problem statement will be produced along with main research questions this paper will answer. In section 3, the

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methodology used to approach the research is discussed, followed by the results from this research in section 4 to 7. Lastly, a summary containing all relevant points in the paper and conclusion regarding future uses, research and key points is included. As mentioned, the problem statement will be discussed next.

2 PROBLEM STATEMENT

Quantum computing is still a foreign concept to a lot of people. This paper will strive to elucidate the practical uses of quantum computing in a very relevant topic today: sustainable energy. There is a severe lack of research regarding the use of quantum computing for this specific purpose, which is why this paper will analyse three to five quantum algorithms, clarify how these algorithms work, and use this knowledge to discover how they can be useful towards sustainable energy production. By knowing how the algorithms work, more in-depth knowledge regarding their uses and limitations can be given. Using this information, research questions regarding the problem can be produced.

2.1 RESEARCH QUESTION

The problem statement above can be contrived into the following research questions:

(1) Which algorithms could prove to be useful for solving problems related to sustainable energy production?
(2) What advantages and disadvantages does the functionality of the selected algorithms cause when applied in sustainable energy production?
(3) What applications do the selected quantum algorithms have in sustainable energy production?

Each research question will be handled separately, however, the results of each research question will be necessary to answer the next question. In this way, a clear path towards the final and most important research question can be reached. Which is the actual implementation of current quantum computing algorithms in sustainable energy production.

2.2 Goals

The ultimate goal of this paper is to elucidate the uses of quantum computing algorithms in sustainable energy production. This will allow for more focus to be put on using quantum computing for other relevant problems encountered in society and providing a theoretical implementation of current algorithms.

3 METHODOLOGY

To answer the research question a semi-systematic literary review will be necessary. Although systematic literature reviews are often the most accurate, it is not feasible to include all articles related to this topic in the literature review. Due to this reason, a semi-systematic review was chosen, since the topic is relatively broad. Based on other literature reviews which are 8 pages long, 7-12 articles will be used and assessed for this review. In addition, due to the fast development of quantum technology, the papers will be limited to the last 10 years to preserve relevancy, foundational papers and highly relevant papers providing important insights will be excluded from this rule. Below, a step-by-step plan is shown for answering the different research questions.

First, several articles about the different uses of quantum algorithms will be gathered. These algorithms will then be filtered upon their uses and placed into several categories. These categories will represent their field of use and possible applications. Based on these findings useful algorithms will be selected which provide meaningful contributions to sustainable energy production, leading to an answer to research question 1.

Next, the selected quantum algorithms will be thoroughly analysed. The quantum circuit principles behind each algorithm will be explained, allowing for a better understanding of their advantages and disadvantages.

Using the findings of research questions 1 and 2, a clear answer to applying quantum algorithms in sustainable energy production can be given. The answer will be categorised based on the findings of question 1, and theoretical uses of the algorithms will be provided based on the answers to question 2, allowing for both the advantages and disadvantages of each algorithm to be discussed.

Lastly, the key findings of each research question will be discussed, along with the common themes, trends, and gaps identified in the literature. Following this, the implications of this research and future trends/research will be discussed.

4 QUANTUM COMPUTING ALGORITHMS FOR SUSTAINABLE ENERGY PRODUCTION

To answer the question *"Which algorithms could prove to be useful for sustainable energy production?"*, a literary analysis was done. This literary analysis was done by selecting multiple papers within the last 5 years. These papers were selected using terms such as quantum computing algorithm, sustainable energy production, or a mixture of these terms. These search specifications lead to 20 papers within this field. After reading these papers, a selection was made based on their relation and relevance to the current topic. Review papers were a main priority in this selection. The papers were selected to include most methods of sustainable energy production. Since most papers did not include certain types of sustainable energy production, like fusion energy [4]. In addition, processes related to sustainable energy production an sustainable energy handling were also included to form a complete picture of all its potential uses [8, 10]. Perhaps most importantly, research about the functionality of the algorithm is very important, papers which include this will naturally be more relevant for answering the questions. All steps criteria mentioned above resulted in 8 distinct papers. These 8 papers will be the basis for the findings in this research and refer to reference [3-10].

In Figure 1 an overview of the mentions for each type of algorithm can be seen. The four algorithms seen below were mentioned in most papers, with the QAOA and the VQE algorithms being mentioned more often. Since the difference in mentions is not significant, it will not be assumed that these algorithms are more useful.

Consequently, according to the papers chosen in this literary research (summarised in Figure 1), the best quantum computing algorithms for application in sustainable energy production are the Variational Quantum Eigensolver (VQE), Quantum Phase Estimation

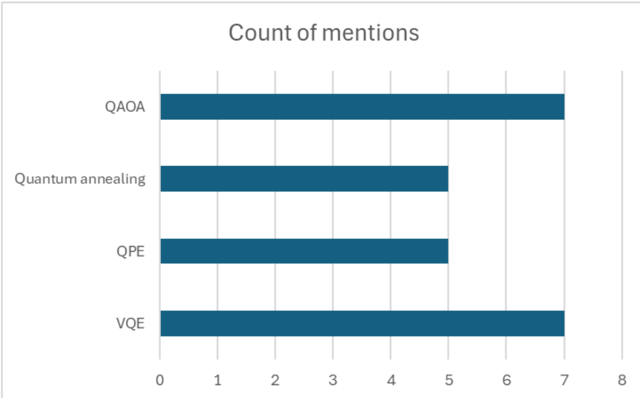

Fig. 1. Mention count

(QPE), Quantum Annealing, and the Quantum Approximate Optimisation Algorithm (QAOA). All quantum computing algorithms will henceforth be referred to by their abbreviated form where applicable.

To clarify the aforementioned algorithms, a classification will be applied. The algorithms can be categorised into two distinct classifications: quantum chemical simulation algorithms and quantum optimisation algorithms. Both the VQE and the QPE algorithms are chemical simulation algorithms, while quantum annealing and the QAOA are quantum optimisation algorithms.

As the name suggests, quantum chemical simulation algorithms can be used to simulate chemical processes. Unlike ordinary computing algorithms, quantum algorithms have the ability to simulate quantum chemistry [5]. Quantum chemistry is a branch of theoretical chemistry that deals with the application of quantum mechanics for predictions of molecular structures and chemical reactivity of chemical systems [11]. Applications of quantum chemistry in sustainable energy production are related to general advances in the used materials, for example for more efficient solar panels due to improved thermodynamic properties [3, 5].

Quantum optimisation algorithms, on the other hand, are better suited towards optimising current technologies [8]. A useful application of these technologies is, for example, in energy grid optimisation. Allowing these algorithms to calculate the placement of renewable energy sources and energy grid planning, energy will be transported and stored optimally, allowing for a minimum amount of energy leakage [7].

The four selected algorithms will now be assessed carefully. This assessment consists of analysing the quantum circuits and operations corresponding to the four algorithms. This will allow for a general consensus to be reached towards its uses based on the functionality of the algorithms.

5 FUNCTIONALITY OF QUANTUM CHEMICAL SIMULATION ALGORITHMS

Quantum chemical simulation algorithms allow for the discovery and improvement of materials used in sustainable energy production. However, to find the limit of this technology, more details about its functionality are needed, allowing for a more complete answer to the question, "*What advantages and disadvantages does the functionality of the selected algorithms cause when applied in sustainable energy production?*".

This will be done by going through the steps taken by the algorithm. This information will be used to analyse its potential applications and limitations. Some initial findings are already listed, which are then expanded upon in section 7.

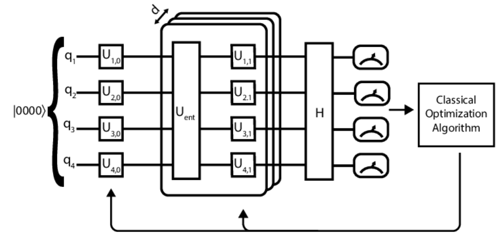

Fig. 2. VQE quantum circuit [20]

5.1 Variational Quantum Eigensolver

The Variational Quantum Eigensolver is a hybrid algorithm consisting of both quantum and classical computing components. It attempts to find the ground state energy of a molecule, which is essential towards creating chemical simulations [3].

Figure 2 by Robert de Keijzer et al. [2021] represents an example of a quantum circuit for the VQE algorithm. This quantum circuit contains all operations mentioned below. This quantum circuit can be used to better understand the operations performed by the algorithm. Note that H followed by the scale symbol represents a measurement and the squares refer to operations undertaken by the algorithm.

The functionality of this algorithm can be described in several steps. First, the molecular system is described. This system consists of the energies and interactions of electrons in the molecule.

Next, a parameterised quantum state is prepared. This state represents the problem scope and tries to make an initial guess of the ground state of a molecule. This initial state can be selected by trial and error, or by using quantum circuits. In addition, This initial guess is modifiable, allowing for changes to be made throughout the calculation process. Following this, an estimate of the previously mentioned ground state can be found by performing measurements over repeatedly run quantum circuits [3]. This can be seen in Figure 2, represented by the 4 different lines, each representing one qubit.

Afterwards, a classical computer uses the acquired ground state to update the initial guess, modifying the value to something that is closer to the actual ground state. The quantum computer then repeats the previously mentioned steps until the ground state energy is produced. This ground state energy can then be used to create precise chemical simulations [12].

This combination of quantum computing and classical computing limits the need for excessive hardware requirements. In fact, some problems regarding small molecules have already been solved using the VQE algorithm. This characteristic also allows the VQE algorithm to be used on NISQ, which are quantum computers with a small amount of qubits. These quantum computers are still influenced by noise, meaning they are not fault-tolerant [13]. However, the hardware still needs to be improved to provide useful applications for larger problems [12].

One large limitation of the VQE algorithm is the choice of the initial parameterized quantum state [3, 12]. This choice can limit the performance of the algorithms significantly, suggesting that more research needs to be done to find a good initial parameterized quantum state. More limitations and advantages of this algorithm will be discussed in section 7.

5.2 Quantum Phase Estimation

The QPE algorithm shares some properties with the VQE algorithm due to several overlapping operations. However, unlike the VQE algorithm, which is a hybrid quantum algorithm consisting of both quantum and classical computing, the QPE algorithm is an approach relying completely on quantum computing. In quantum chemistry, the result from the algorithm can be used to determine molecular energies [3].

Figure 3 by Stephen Diadamo et al. [2021] shows all operations of the QPE algorithm in a quantum circuit. Note that U^{2^0} until $U^{2^{n-1}}$ refer to the controlled unitary operations on the initial guess. And QFT_n^{-1} refers to the inverse Quantum Fourier Transform, which allows the algorithm to find the correct result. These steps will be explained below.

First, an initial quantum state is defined. This quantum state represents an initial guess of the expected result. Next, other qubits are put into superposition. Following this, controlled unitary operations will be applied to the qubits that were used to define the initial quantum state. Lastly, an inverse Quantum Fourier Transform (QFT) is performed on the qubits that have their states in superposition [3]. This last step allows the

The qubits will then be observed and measured, allowing for the result to be found. The result represents the energy level of the molecule. By using the knowledge gained in this calculation, further calculations can be made by the algorithm to find the ground state and even the excited states of molecules, the advantages of this will be described in section 7.

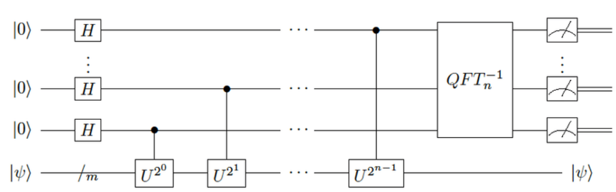

Fig. 3. QPE quantum circuit [21]

Another advantage of this algorithm is that it allows for very accurate calculations of the eigenvalue, assuming that the quantum computer is fault-tolerant. However, unlike the VQE algorithm which also uses classical computing, the sole reliance on quantum computers limits this method for the foreseeable future. A large amount of qubits is needed to arrive at satisfactory results due to the superpositioning of qubits and eigenstate initiation. In addition, current quantum computers are not close to being fault-tolerant, creating a large problem for future applications.

6 FUNCTIONALITY OF QUANTUM OPTIMISATION ALGORITHMS

6.1 Quantum Annealing

Quantum annealing is most useful for solving combinatorial optimisation problems. These optimisation problems require the minimisation of a cost function [5]. This algorithm achieves its purpose through the usage of quantum mechanics.

The previously mentioned optimisation problem is also known as a Quadratic Unconstrained Binary Optimisation (QUBO) problem or Ising problem. To solve the problem, the ground state needs to be found, since the ground state will give the lowest solution to the cost function. In order to find the target ground state, an initial ground state first needs to be set. This assumes that there is a similar problem in which the ground state is known [5].

Next, adiabatic quantum optimisation (AQO) is performed. This entails that the initial ground state is used to approach the target ground state. This step allows for the target ground state to be found using the ground state of an already known system. Next quantum tunneling properties are used to allow the system to discover the global minimum, referring to target ground state. Quantum tunnelling refers to the ability of particles to travel through normal potential energy barriers, allowing it to perform operations which it would need more energy for in classical computing. This concept allows the algorithm to provide more accurate data than classical computing methods.

Both adiabatic quantum optimisation and quantum tunnelling are visualised using Figure 4 by Quantum World Association [2021]. This figure gives a more intuitive overview of how both processes work together to achieve its desired effect.

Lastly, the system is measured to find the final state. This final state should, in an ideal situation, refer to the target ground state. This should be the optimal solution to the originally proposed cost function.

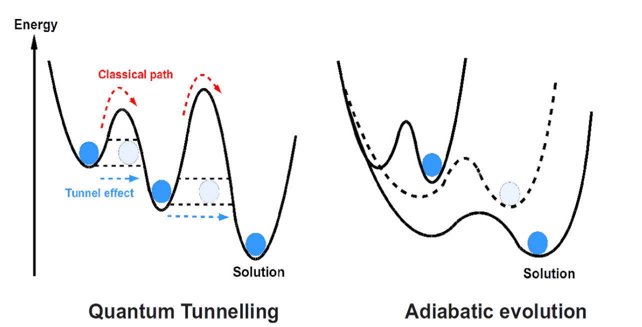

Fig. 4. Quantum annealing visualized [22]

Using this algorithm allows for solutions to very large cost optimisation problems. these problems could only be solved by quantum computing algorithms due to the large hardware requirements in the case of classical computing. However, just like other algorithms, it is limited by current quantum computing hardware, there are some specialised quantum computers which can run these algorithms, however, major progress still needs to be made [9].

6.2 Quantum Approximation Optimisation Algorithm

Just like the VQE algorithm, the QAOA is a hybrid quantum computing algorithm, meaning that operations are performed using both classical and quantum computing. As seen before, this combination diminishes the need for strong processing power of quantum computers. The QAOA also fits into the category of quantum optimisation algorithms since it is also designed to solve combinatorial optimisation problems.

Figure 5 by Ritajit Majumdar et al. [2021] provides an overview of all the steps taken by the algorithm in terms of a quantum circuit. This figure represents a better overview for human understanding.

As is standard with these problems, the combinatorial optimisation problem is encoded as a cost function that needs to be minimised. The minimum of the cost function results in the optimum solution for the optimisation problem, this cost function will be referred to in Hamiltonian form H_C [14].

Next, the quantum state is initialised by putting the relevant qubits into superposition, as seen by the H in Figure 5. Unitary operations will then be applied to all initialised qubits, these operations will use different parameters depending on the problem, resulting in an estimation of the cost function. This estimation is then measured and an optimisation of the used parameters in the unitary operation can be done. After the optimisation, the steps repeat themselves until an optimum solution is found. The optimum solution has been deemed to be found when no significant change in value is discovered or the amount of iterations has reached a predetermined limit [14].

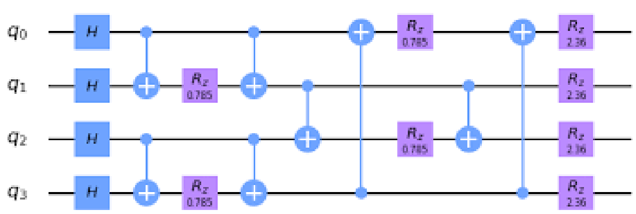

Fig. 5. QAOA quantum circuit [23]

7 APPLICATIONS AND LIMITATIONS OF QUANTUM COMPUTING ALGORITHMS IN SUSTAINABLE ENERGY PRODUCTION

Following the findings of the previous sections an analysis into the uses of these algorithms in sustainable energy production can be made, as well as the advantages and disadvantages of each algorithm. This will be done by focusing on the two categories of algorithms separately. First, quantum chemical simulation algorithms will be discussed, followed by optimisation algorithms.

7.1 Quantum chemical simulation algorithms

As mentioned in research question 1, quantum chemical simulation can help in understanding the properties of current materials and will allow for better simulations of new materials and how they will operate in sustainable energy production [3]. The two algorithms provide a different approach to the problems accompanied by chemical simulations, ultimately leading to varying advantages and disadvantages.

By analysing the selected papers carefully, several key uses of quantum chemical simulation algorithms in sustainable energy production can be found. The first application of this technology in sustainable energy production is its ability to design new materials for fusion reactors [4]. These new materials would provide stronger walls or better conductivity of heat and electricity, providing increased energy production. In the same way, new materials could be created for dams and turbines to provide more efficient energy production.

Another use of the algorithms is for the design of photovoltaic materials and electrocatalysts in energy storage devices [18]. the improvement of photovoltaic materials will help make solar panels more efficient, due to an increase in efficiency when transforming light into energy. Better electrocatalysts would result in an improvement of chemical reactions in the energy storage device. This improvement could result in an increase of lifespan, storage capacity, efficiency, and safety.

One other practical use is the application of quantum chemical simulation algorithms in the creation of catalysts in sustainable energy production [19]. This could help towards converting biomass into biofuel more efficiently, which can be used to create clean energy.

All practical applications above can be achieved by modeling the current materials, this will allow material scientists to discover flaws or useful characteristics of the material. A key issue to this practical application is that it needs a lot of information before the models can be created, meaning that each simulation will cost a lot of time to create. Although a lot of information will be obtained, it will be hard to find useful data in a short amount of time. The information needed refers to the initial guess which was mentioned in research question 2.

Using the information from research question 2, The difference between both algorithms can be carefully considered. Weighing the advantages and disadvantages of its use in sustainable energy.

The main goal of the two algorithms is to find the ground state energy of the studied molecule. This allows chemical simulations to simulate chemical properties, like the thermodynamics or bonds between atoms. Although both algorithms take a different path, the answers provided should deliver the same result.

However, the QPE algorithm has one advantage, it has the ability to calculate the excited state energy of molecules. This excited state energy of a molecule allows chemical simulations to provide abundant information regarding photochemical reactions. Photochemical reactions are central in photovoltaic cells, used in solar panels. Having more knowledge regarding these reactions could improve the performance of photovoltaic cells significantly. Other uses include Electronic Spectroscopy, allowing for more in-depth knowledge regarding the molecular interactions with light, or Reaction Dynamics, which could provide useful information regarding electronic transitions. Leading to a decrease in energy loss and a potential increase in production.

The VQE algorithm approaches the problem by iterating over the problem repeatedly. This is done by selecting an initial state. The performance of the VQE algorithm will be heavily dependant on how close this initial state is to the ground state of the problem. A guess which is far away will result in a slow convergence of the algorithm and an unsatisfactory result [12]. This could be a cause to divert attention away from this algorithm and focus more on an algorithm like the QPE algorithm which does not share this limitation.

Another limitation of the VQE algorithm is the potential bottleneck caused by the classical computing component. This component of the hybrid algorithm allows the algorithm to be performed on small quantum devices called NISQ [13]. This is a large advantage since it can allow results to be gathered even today. However, this classical component could also lead to potential bottlenecks. When quantum computers improve and problem cases continue to expand the classical component will start to lack behind in terms of processing power. When problems reach a certain scale, the VQE algorithm might not be useful anymore. The QPE algorithm, on the other hand, does not have this problem, since it is fully reliant on quantum computing, an assumption can be made that this will allow the QPE algorithm to be more relevant for continued operation, while the VQE algorithm is useful to solve problems today or in the near future which classical computers cannot handle.

The QPE algorithm provides results which are more accurate due to its quantum approach discussed in research question 2. However, this is assuming the quantum computers are fault tolerant. Current quantum computers are not close to being fault tolerant [1], which means that this system can not be used yet. In addition, the amount of resources needed to perform this algorithm is several times higher than the VQE algorithm, meaning large-scale quantum computers are necessary to perform this algorithm.

7.2 quantum optimisation algorithms

As mentioned in research question 1, quantum optimisation algorithms can be used to solve complex problems concerning grid management. The algorithm which is best suited for this task is the QAOA. QAOA will run calculations based on the cost functions of the current grid, and an optimum flow and distribution of energy can be discovered [7]. This optimum solution will result in a grid with minimum energy loss, allowing sustainable energy production sources to transfer their power with the least resistance possible.

The application of this technology should be relatively easy due to the large amount of data currently gathered. With computers containing all the necessary information, this application should not be difficult to implement.

In addition to grid management, another important application of this algorithm is its ability to manage renewable energy sources. This would include finding optimal placement for wind turbines, solar panels and other sources, while also thinking about energy storage and energy transition. QAOA will be able to balance the supply and demand of energy optimally, allowing renewable energy to be used efficiently [7]. When solved correctly using the QAOA, these balance problems should be handled in such a way that almost no excess energy is wasted. In turn resulting in a reduced need for other non-sustainable energy sources.

On the other hand, quantum annealing focuses more on tasks related to the management of resources. Quantum annealing will be able to decide on an optimum mix of renewable and conventional power plant usage to use across a power grid. Quantum annealing could also be useful for scheduling energy usage, allowing energy providers to deal with peak energy demand more efficiently while also integrating renewable energy sources in their planning [8].

The intrinsic difference between the usage of both algorithms comes from their functionality which was further expanded upon in research question 2. Due to the hybrid nature of QAOA, it is more suitable for NISQ devices, allowing for this algorithm to be useful in standard applications today. In addition, QAOA is more flexible in design due to the ease of adjusting the cost Hamiltonian established before starting the algorithm (see research question 2). By adjusting this cost Hamiltonian, changes can be made easily, which is not possible when using quantum annealing.

Just like the VQE algorithm, the performance of the QAOA algorithm is heavily dependent on the initial parameters. This results in a situation in which wrong initial parameters will result in answers which are not correct. In addition, these parameters are very complex and hard to construct, suggesting that faults could happen often [7].

Unlike the QAOA, Quantum annealing is not a hybrid algorithm, relying fully on quantum properties. To use the algorithm, special types of quantum computers need to be used [3], these quantum computers are currently readily available, meaning that they can be used at this moment. However, just like all other algorithms mentioned, it is still limited by current hardware, since more processing power is always needed to solve more complex problems. In addition, quantum annealing is more suitable for wider applications. Quantum Annealing is limited in its approach and can only solve more specific problems. On the other hand, QAOA does not encounter this issue, and, due to its fully quantum nature, is able to solve a wide variety of problems.

8 SUMMARY

In short, the current quantum algorithms have one common factor, the limitation of current technologies. Using currently available resources, the application of the quantum algorithms would not result in satisfying results. Especially with the continuously growing problem scope in energy grid planning and sustainable energy production. For quantum algorithms to provide meaningful and lasting results, severe improvements in hardware and fault tolerance need to be made. Fault tolerance will allow the QPE algorithm to gather more information than the VQE algorithm, allowing for faster development of materials needed in sustainable energy production.

On the other hand, algorithms such as the VQE and the QAOA use hybrid algorithms, consisting of both classical and quantum computing components. This allows the algorithms to be used with NISQ devices, which are devices with smaller amounts of processing power and qubits. This ability allows current quantum computers to use these algorithms to provide meaningful data. However, these hybrid algorithms could prove to be limited in their uses due to possible bottlenecks encountered by using classical computing.

The initial guess is an important factor in all algorithms. This step can influence the result to varying degrees, with algorithms like the Variational Quantum Eigensolver algorithm being affected by it heavily. This area still needs additional research for the algorithm to be used intensively. All points mentioned above summarize the answer to research question 2.

The quantum chemical simulation algorithms can simulate materials to a point which is not possible using conventional computing. This allows for the technology to provide useful help in the production of renewable energy sources. Applications of this algorithm could improve photovoltaic materials, sustainable energy catalysts and more efficient fusion reactors. The quantum optimisation algorithms will be used for efficiently dealing with the produced energy. This can be done by optimising power grid placement, allowing for a more efficient way to transport electricity. This optimization refers to both the placement of the sustainable energy sources and its power lines. Other practical uses are related to balancing the rate of storage and transmission of sustainable energy. If done perfectly, minimal energy is lost in the process, allowing for a better production rate of sustainable energy. This summarizes the answer to research question 3, while the algorithms belonging to both categories are the answer to research question 1.

Quantum computing algorithms prove to have very significant effects in the future, however, due to current limitations, this will not be able to affect current technologies much.

9 FUTURE TRENDS AND CONCLUSION

With the current state of quantum computing, significant results can not be achieved regarding the evolution of sustainable energy production. Severe hardware limitations concerning qubit count and fault tolerance still plague current systems. By improving on these two factors, significant uses for quantum computing in sustainable energy production can be found. Especially when considering the fact that only 4 different quantum algorithms have been analysed. With these 4 algorithms already proving to provide significant progress, other algorithms, which could still be developed or currently exist, should be able to prove even more valuable to sustainable energy production as a whole. With this, The goal of this paper, which is to prove that quantum computing algorithms can be used to improve sustainable energy production, has been reached successfully.

This goal hopefully achieves to satisfy curiosity regarding the uses of quantum computing, allowing for current problems to be analysed using the methods required by quantum computing and testing its effects using current technologies like hybrid algorithms.

An important field for further research is regarding the creation of good initial quantum states of molecular structures. Both the VQE and QPE algorithm rely heavily on this initial quantum state representing the molecule. If a better or easier method of representing a molecule is found, performance of the algorithms will also improve drastically. Resulting in better chemical simulations, in turn providing more information to researchers for better materials.

Another field of further research is regarding the cost of quantum computers. At the moment, quantum computers need a lot of energy and correction. Research needs to be done to find out when quantum computers can actually provide information which is worth the amount of energy and resources spent on the system. By finding a balance in the amount of money spent and saved by some simple quantum computing solutions, further conclusions can be gathered about the possibility of the costs being worth the result.

My recommendation for a continued area of research goes to furthering the understanding of initial parameterized quantum states of molecular structures, allowing for the ability to denote real-world problems in an intuitive way for quantum computing algorithms to solve, improving the performance of future quantum computing algorithms.

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A APPENDIX A

During the preparation of this work the author used Grammarly in order to fix grammatical errors related to spelling and differentiating between American English and British English. After using this tool, the author reviewed and edited the content as needed and takes full responsibility for the content of the work.