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Effects of symmetry breaking in the performance and the design of Quantum Approximate Optimisation Algorithm (QAOA).

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1 Introduction

Quantum mechanics is the theory that best explains the physical phenomena that occur between interacting particles in atomic or subatomic level. In such levels, the theory of classical physics is not accurate. Feynman [1] was the first to propose the creation of a computer that will be based on quantum mechanics as a tool for simulating physics. The goal was to invent a machine that would be better for the specific task than its classical counterpart. Since then, a lot of research regarding the creation and effectiveness of such machines has been executed. Many researchers begun to invent and propose algorithms that can run on quantum machines with the aim to take advantage of their computational power, even before the creation of a quantum computer. The main goal in the early years was to provide quantum algorithms that prove that the quantum advantage exists by trying to find good aPPROximate solutions for problems that are difficult to be solved with classical machines [2]. Today, we can say that the main intention is to find if quantum computers can be useful for solving real-world problems using most of the times NISQ (Noisy intermediate-scale quantum) devices [42].The algorithms that are used in such devices are called Variational Quantum Algorithms. In this work, we want to make a proposal regarding possible improvements that can be implemented in a specific type of Variational Quantum Algorithms. We will mainly focus on the Quantum Approximate Optimisation Algorithm (QAOA).

The rapid evolution of the Quantum Computing field has led to the creation of new methods that are used to tackle many different kinds of problems. Those methods were experimentally tested on near-term quantum machines. A successful class of algorithms that emerged were the Variational Quantum Algorithms (VQAs). Their main characteristic is that they are hybrid quantum-classical. This means that they contain both a quantum and a classical part that are combined. The quantum part uses a quantum processor that produces a quantum state that depends on some parameters β, γ. Then, the classical processor is used to classically optimise the specific parameters. The goal is to find more efficient solutions and extract more information in different types of tasks that are difficult for classical algorithms. Some examples are classical combinatorial optimization [7] [8], quantum chemistry problems [33] [40] or simulation of quantum physics [37] [38]. We also have to mention, that they are one of the tools that may prove that the quantum advantage exists [36].

VQAs use a target Hamiltonian, for which we want to approximate its ground state (the state that has the minimum energy). This corresponds to the cost function of the problem that we want to solve. The cost function can be naturally mapped to a Hamiltonian that corresponds to actual physical interactions. The Hamiltonians that are used, are constructed based on the type and the constraints of the problem. The minimization procedure is achieved by generating a quantum state that depends on some real parameters (β, γ) using a quantum processor. Then the specific state is measured to compute its expectation value in respect with the problem Hamiltonian. Those results are passed to a classical processor and classical

algorithms are utilised to optimize the parameters and feed them back to the quantum processor.

As we mentioned, VQAs depend on the parametrisation of a quantum circuit. However, we cannot be sure about the performance of those algorithms as different aspects may affect their accuracy or their speed. Moreover, when quantum devices are used, the noise extracted from near-term quantum machines is increased and the possible solutions are affected. Although the selection of a good ansatze remains crucial and most of the research is made with symmetry preserving ansatzes [11] [12], as the problems that are addressed contain symmetries which must be used in order to obtain more efficient solutions. This is useful because the space in which the algorithm must search for possible solutions, is reduced. This fact, most of the times leads to getting better solutions in less time.

In this work we want to investigate the use of ansatzes that break the symmetries of the target Hamiltonian inspired by the work of Choquette et al. [6]. Our main intention is to investigate if the use of a symmetry breaking term can lead us to solutions that were not reachable otherwise. In addition, Bravyi et al. [35] proved that the preservation of a symmetry in procedures like QAOA may cause problems in the accuracy of the results. This claim was based on the fact that symmetries make the good variational states very entangled, but low-depth circuits cannot generate highly entangled states. Moreover, we want to check if the performance of the algorithm in terms of time and accuracy can be improved. We mainly focused on quantum target Hamiltonians and simulation of quantum evolution. Another interesting aspect that we intend to investigate is how fast, in terms of the size of the quantum circuit, we can move the search space of the algorithm to a new eigenspace (different than the initial one). This corresponds to the minimum depth needed in order to move from the eigenspace that the initial state lives, to another eigenspace. The fidelity of the states that are produced from the optimisation procedure with each of the eigenspaces of the problem, denotes the eigenspace that each state lives in. If we find which is the maximum amount of fidelity that we can move to a new eigenspace for one layer of the quantum circuit we can determine the minimum number of layers needed in order to generate states that will completely belong to the new eigenspace. This can be crucial in problems where the target ground state lives in an eigenspace different than the one of the initial state. Such problems can highlight possible drawbacks that may arise from using symmetry preserving ansatzes. That is because symmetries are created from some symmetry operators that commute with the Hamiltonian. This naturally creates a set of eigenspaces in the system that must be preserved. As a result, the evolution with a symmetry preserving operator will be limited to the specific eigenspaces. More specifically it will be limited to one of the subspaces that will be created (the one from where the evolution will start).

One of our initial intentions was to create a method that would help us achieve an efficient block diagonalisation of a Hamiltonian using symmetry groups from group theory (cyclic, reflection and dihedral group). This helped us to denote the differences in the block diagonalisation of a Periodic and an Open Boundary Hamiltonian. We also compared our method with the one that Tavakoli et al. [3]. In [3] they use the block diagonalisation to make the computations for the evaluation of semidefinite relaxations for bounding the set of quantum correlations in finite dimensional Hilbert spaces, easier. Their method is interesting because they create block diagonalised matrices without using complicated terms from group theory. The specific method aims to take advantage of the symmetries that are created via abelian groups, with the aim to provide a general method for block diagonalisation. More specifically

they want to achieve a block diagonalisation that will be irreducible. For the implementation of the optimisation procedure, we will utilise a model that is similar to QAOA as we will use a term that slightly breaks the symmetry of the target Hamiltonian, with the intention to approximate its ground state. We must mention that we use a quantum cost function instead of a classical cost function. We mainly focused on exploiting the differences between the evolution with a symmetry breaking and a symmetry preserving term. We also demonstrated possible advantages of using a symmetry breaking ansatze and we tried to find the minimum circuit depth needed to reach a block that will be different than the block of the initial state. We proved analytically that this will be possible using a symmetry breaking term and we also performed some numerical experiments that enhanced this assumption. The way to find the minimum depth needed was to compute the maximum quantity of fidelity that can be moved through blocks in one step of a QAOA procedure. The main research questions that we want to answer in this work are:

1. What are the effects of using a symmetry breaking term for the evolution of an optimisation procedure based on QAOA with a quantum cost function?

2. What are the advantages of using such a term for the evolution in the specific optimisation procedures?

3. Is it possible to move the search space of the optimisation procedure to a new eigenspace and if yes, which is the maximum quantity (in terms of fidelity) that we can move to a new eigenspace for $p = 1$ (p denotes the number of layers of the quantum circuit that is used in the procedure)?

4. Which is the minimum circuit depth required in order to to produce states that will completely belong to a new eigenspace?

This work is organised as follows. Section 2 contains the Preliminaries needed in order develop our model. In Section 3 we discuss our approach for getting the block structure of a Hamiltonian and compare it with other existing approaches. We also make a small introduction to why the breaking of symmetries can be useful for optimization problems. In Section 4 we analyze the implementation of our model and provide the results. In Section 5 we make an analytical explanation on the maximum amount of fidelity that can be moved to a new block starting from a known initial state that lives in a different block. Finally, Section 6 contains the conclusion and some ideas for future work.

2 Preliminaries

As we mentioned in the previous section, this work is based on the effect that Symmetries have on finding optimal solutions for various problems. We want to investigate if the breaking of symmetries in a Hamiltonian may lead to a space where better solutions may exist. In this section we will introduce some basic concepts that will be necessary to prove the validity of our model.

2.1 Hamiltonians and Ground state problem

The specific work is mainly focused and based on the notion of Hamiltonian matrices. The problems that we are investigating are based on finding the ground state of a specific Hamiltonian

matrix. The ground state for each system is the one that produces the lowest possible energy. This is one of the reasons that the specific problem can be mapped to combinatorial optimisation problems. In such problems the goal is to minimise (or maximise) a specific objective function and is similar to approximating the ground state energy of specific Hamiltonian. The ground state is the eigenvector of a Hamiltonian matrix that corresponds to its lowest possible eigenvalue.

2.1.1 Hamiltonian Matrix

In physics and more specifically in quantum mechanics, Hamiltonians are considered operators that give us information about the total energy (e.g. kinetic and potential) of a specific system. As we mentioned, the eigenvalues of the system are equivalent to states with a well defined energy. Hamiltonians are also related to the evolution of the system and the equivalence of the energy and time. This means that they describe the time evolution of a closed quantum system (Schrödinger equation).

In finite dimension, the Hamiltonian matrix is equal to the coefficients H_{ij} [19]. We can compute the elements of this matrix by using the following formula

$$H_{ij} = \langle i|H|j\rangle \tag{1}$$

where H is the Hamiltonian function which is known. The main characteristic that a matrix must have to be considered Hamiltonian is

$$H_{ij}^{\dagger} = H_{ij} \tag{2}$$

which means that Hamiltonians are Hermitian operators (H_{ij} denotes the whole Hamiltonian matrix), thus they have real eigenvalues due to the spectral theorem. This is reasonable as energies must be represented by real numbers The way that the time independent Hamiltonian matrix defines the evolution of a system through time is the following. Let us suppose that we are at a specific state $|\psi(t_0)\rangle$ at time t_0. We want to find the state of the system described by a Hamiltonian matrix H at time t_1. We can compute that by applying a unitary operator to the initial state like

$$|\psi(t_1)\rangle = U(t_1)|\psi(t_0)\rangle \tag{3}$$

but from the Schrödinger equation, we know that

$$U(t_1) = e^{-iH\Delta t} \tag{4}$$

where $\Delta t = t_1 - t_0$ in our case. For $U(t_1)$ we also know that

$$U(t_1)^{\dagger} = U(t_1)^{-1} \tag{5}$$

since it is unitary (the above equation holds for every t).

All the above information and especially how a quantum system evolves through time will be extremely useful for this work. As we mentioned, our work is based on the ground state problem and the evolution of a quantum system, which is a way to compute it, and finally reach the minimum energy of a system that is described by a specific Hamiltonian.

2.1.2 Applications of the Ground state problem

As we mentioned in Section 2.1, a state of a quantum mechanical system is called its ground state when it corresponds to the lowest energy that can be produced from this quantum mechanical system. This means, that it is the state which is related to the lowest eigenvalue of the Hamiltonian. In some of our experiments we investigated systems that contained more than one ground states. In this case the ground state is called degenerate.

The ground state problem is considered one of the most exciting and difficult to tackle problems [21] and many different methods have been developed for solving it. In the specific problem, both classical and quantum Hamiltonians can be used depending on the type of application.

The fields that the ground state problem can be applied are many. One of them is the understanding of physically relevant quantum phenomena through the simulation of quantum physics and quantum circuits [23] [25]. Another really important field that the ground state problem has been applied is quantum chemistry. More specifically, an example of such a problem in quantum chemistry is the calculation of the ground state molecular energy of specific molecules [22]. Another field where we have applications is mathematics and more specifically in factoring [24]. An adiabatic algorithm [20] was proposed for the specific case, but there are also other methods that can map a problem to a ground state preparation instance. We have to mention that the Quantum Approximate Optimisation Algorithm (QAOA) [8] was inspired from the Quantum Adiabatic Algorithm [20]. We will explain their relationship in Section 2.2 Finally, many combinatorial optimisation problems like MAX-CUT or SAT can be solved by creating an efficient mapping to ground state preparation problems [5] [6] [8]. The specific examples use procedures inspired by QAOA which is a Variational Quantum Algorithm, most of the times, implemented in near-term devices.

2.1.3 Implementation on near-term devices

Near term devices are those that can handle computations for small number of qubits or shallow circuit depth. Those devices do not contain efficient error-correction and that is one of the reasons they cannot contain circuits of higher depth and higher number of qubits. They belong to the Noisy Intermediate Scale Quantum (NISQ) era [42]. The main goal is to see if we can achieve something really useful in NISQ era. In general, the ultimate goal would be to reach an era of full-scale or universal quantum computing.

Near-term devices cannot efficiently solve large, real world (quantum) problems [27] [36]. Even perfect quantum computers cannot solve efficiently most real world (quantum) problems (e.g. those that belong to the $QMA - complete$ class). That is the reason why we are searching for heuristic approaches that can produce good approximate solutions that can be better than those produced from classical approaches. In order to achieve this, Variational Quantum Algorithms (VQAs) are used. As we described in previous sections, those methods contain both a quantum and a classical part. More specifically, a set of parameters is inserted in a quantum device which uses a sequence of gate operators in order to produce a quantum state. This state is measured in order to obtain its energy. Then this value is passed on the classical computer which optimises the parameters and then send them back to the quantum computer to calculate the new expected energy. Such approaches can be used to solve both

classical optimisation [8] and quantum problems [37] [40] (in chemistry or in physics). The main advantage of such algorithms is that they can efficiently use near-term devices as the quantum computational power they demand is not high. Moreover the error that is produced is tolerable [36].

Based on the emergence and the rapid development of near-term devices, we decided that we must focus on VQAs and check if we can contribute to the exploration of their abilities. In this work we use a Variational Quantum Algorithm that is based on Quantum Approximate Optimisation Algorithm (QAOA). The target and the evolution Hamiltonian that we are using, are Quantum. Our main goal is to check if the procedure can be improved by using an evolution Hamiltonian that breaks the symmetries of the problem Hamiltonian. In general, we investigate the effects that such a modification may provoke.

2.2 Quantum Approximate Optimization Algorithm (QAOA)

The Variational algorithm we decided to use in this work is the Quantum Approximate Optimization Algorithm (QAOA). In this section we will make a description of how those algorithms work. As we mentioned, the specific algorithm takes advantage of the near-term devices as it contains both a classical and a quantum part. There is also a relation to the adiabatic algorithm [20]. In the adiabatic algorithm we start from the ground state of a Hamiltonian that is easy to produce (H_M) (this is one similarity with QAOA since most of the times the initial state corresponds to the ground state of the Mixing Hamiltonian). The goal is to find or approximate the ground state of another Hamiltonian that its ground state is generated much harder (H_P). In general, the Adiabatic theorem states that when the system is in the ground state of a Hamiltonian, it will stay in a ground state if the time dependent Hamiltonian ($H(t) = (1-t/T)H_M + (t/T)H_P$) is modified slowly. That is why a huge amount of time is required in order to get efficient solutions. The main similarity with QAOA comes from the fact that if we had a huge amount of time (layers) available, then by using Trotterized evolution (alternating unitary operators of H_M, H_P as in QAOA) we can find some parameters (angles) that will lead us to a good approximation of the ground state. However we have to mention that in QAOA when the number of layers is increased, most of the times we get better solutions. This does not necessarily hold for the Quantum Adiabatic Algorithm. Moreover, the number of layers (depth) needed to obtain a good approximation using QAOA is much smaller. The algorithm was first introduced by Fahri et al. [8] and was initially used to solve combinatorial optimisation problems. The main goal is to approximate the ground state of a target Hamiltonian.

2.2.1 Procedure Description

The way that QAOA works is quite simple. It was introduced as a way to solve combinatorial optimisation problems [8]. Combinatorial optimisation problems contain a set of satisfiability clauses that are in one-to-one correspondence with the objective function,

$$C(z) = \sum_{a=1}^{m} C_a(z) \tag{6}$$

with z being a bit string. We know that $C_a(z) = 1$ if z satisfies clause a and 0 in all other cases. This means that if $C_a(z) = 0$ then the bit string z is a solution that cannot be accepted

from the constraints of the problem. We want to create a Hamiltonian which will be diagonal in the computational basis based on the objective function of the problem to be solved. In general the specific Hamiltonian can be written as,

$$H_P = \sum_{z \in \{0,1\}^n} C(z) = |z\rangle\langle z| \tag{7}$$

with z being the states that represent a candidate solution. More specifically, in order to write H_P in terms of Pauli Z operators we can replace every bit of the solution (z_i) to a matrix like $z_i \mapsto 2^{-1}(\mathbb{I} - Z_i)$, with $\mathbb{I}$ representing the identity matrix and Z_i the Pauli Z matrix acting on qubit i. Then we can write the Hamiltonian as the sum of all the local terms of the problem.For instance, for the MAXCUT problem H_P can be written as:

$$H_P = \frac{1}{2} \sum_{j,l \in Edges} \mathbb{I} - Z_j Z_l. \tag{8}$$

The goal in optimisation problems is to minimise or maximise the objective function, depending on the type of the problem. We want to correlate the objective function with an operator which is diagonal in the computational basis. This unitary operator will depend on one parameter γ

$$U(H_P, \gamma) = e^{-i\gamma H_P}. \tag{9}$$

with H_P being the problem Hamiltonian associated with the objective function of the problem to be solved.

We must also define an operator H_M which will be the sum of Pauli X operators,

$$H_M = \sum_{k=1}^{n} \sigma_k^x. \tag{10}$$

We have to create a new unitary operator that will depend on a new parameter β,

$$U(H_M, \beta) = e^{-i\beta H_M}. \tag{11}$$

In order for the algorithm to work we need an accurate initial state. Most of the times we use the superposition over of all basis states,

$$|\psi_0\rangle = (\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle))^{\otimes n}. \tag{12}$$

The state that we want, is prepared by applying the aforementioned unitaries one after the other like,

$$|\psi(\vec{\beta}, \vec{\gamma})\rangle = U(H_M, \beta_p)U(H_P, \gamma_p) \dots U(H_M, \beta_1)U(H_P, \gamma_1)|\psi_0\rangle \tag{13}$$

with p denoting the circuit depth that we will set. When we increase it, we will most likely get a better approximation of the ground state of the problem Hamiltonian but we will need higher computational power. There is a trade-off between accuracy and time.

We now have all the terms we need to approximate the ground state of a Hamiltonian.

We start by applying the initial state that we formed to a quantum computer (quantum circuit) and we prepare a quantum state that depends on the initial parameters $\vec{\beta}, \vec{\gamma}$. We then measure the specific state in the computational basis in order to get the energy that it produces by computing its expectation value by

$$\langle \psi(\vec{\beta}, \vec{\gamma}) | H_P | \psi(\vec{\beta}, \vec{\gamma}) \rangle \tag{14}$$

where H_P is the Hamiltonian that is related to the objective function of the problem, as our goal is to approximate the ground state of the specific Hamiltonian. We then put the state in a classical optimiser. The optimiser produces a new set of parameters $\vec{\beta}', \vec{\gamma}'$. The next step is to put those parameter to the quantum circuit to get a new state. We repeat this procedure until convergence. The goal is to minimise Equation 14 by finding the optimal parameters $\vec{\beta_{opt}}, \vec{\gamma_{opt}}$.

2.2.2 Hamiltonians Used

The Hamiltonians that are used in the QAOA, and more specifically for the creation of the quantum circuit are the problem or target Hamiltonian, and the mixing Hamiltonian. Here we will describe the special characteristics of the Hamiltonians that are required in the procedure. We have to mention that in our implementation we will use an additional Hamiltonian which will be used for the evolution of the system, because we will mainly focus on a quantum cost function instead of a classical one We will describe our implementation in more detail in Section 4.

Problem Hamiltonian: It is the Hamiltonian that is created based on the objective function of the problem that we want to solve (most of the times it is a combinatorial optimisation problem). The specific Hamiltonian will be denoted most of the times by H_P, and its unitary operator will depend on a parameter γ. The ground state that we want to approximate is the ground state of the specific Hamiltonian. In the classical QAOA this Hamiltonian is also used for the evolution of the system which is achieved by Equation 13.

Mixing Hamiltonian: The specific Hamiltonian is usually denoted by H_M and in most cases it is a sum of Pauli X operators as described above (for the cases where the cost function is classical). It is selected by the user depending on the problem Hamiltonian. This is useful in our case as we use quantum cost functions. It is crucial to select a good mixing Hamiltonian as this will make the procedure more accurate. If the mixing Hamiltonian is not selected properly then the algorithm will not manage to produce a good approximation of the ground state of the problem Hamiltonian. One significant condition is that it must not commute with the problem Hamiltonian.

Finally, we also have to mention that a good selection must be made for the initial state. Most of the times it is chosen to be the superposition of all basis states [8]. However, this depends on the two Hamiltonians and the type of the problem. It is crucial to select a good initial state as this will speed up the procedure.

2.2.3 QAOA Circuits

The QAOA needs a quantum circuit in order to produce a state and then measure its expectation values. We must first start from the initial state, which most of the times is equal to the

superposition of all the basis states. We can achieve this superposition by applying a Hadamard gate to each qubit. Then, we must apply the unitary that will be related to the problem Hamiltonian. The structure of this gate will defer, depending on the type of problem that we want to solve. However, we can say that it will be represented by a two-qubit gate. This means, that the gate must be applied to every pair of qubits that our system contains. Moreover, the specific unitary will depend on parameter γ. Finally, we must create the Mixing Hamiltonian. We will suppose that it will be equal to the sum of Pauli X operators. In order to put this in a quantum circuit, we must apply to each qubit a rotation in the X basis that will depend on a parameter β. After the creation of the initial state, the unitaries of the mixing and the problem Hamiltonian will alternate in the circuit depending on the depth (p = number of layers) that we will choose.

2.2.4 Applications

After the publication of the original QAOA procedure by Fahri et al. [8], many variations were created that intended to improve the performance of the method and to test it in different types of problems [5] [6] [7].

In this work we mainly used QAOA as a tool to investigate the effects of using an Open Boundary Hamiltonian in 1 spatial dimension with nearest-neighbors interactions for the evolution of the system. Our main purpose was to investigate whether such a modification may improve the performance of an algorithm like QAOA. We will describe the method that we used for our experiments in Section 4.

2.3 Symmetry groups (Group Theory)

One of the main parts of this work is related to efficient block diagonalisation of Hamiltonians in order to get accurate insights regarding how the breaking of symmetries will affect the evolution in an optimisation procedure using algorithms similar to QAOA. In order to achieve this, we decided that it will be useful to use symmetry groups from group theory. Another interesting aspect is that the symmetry groups are used to create the different eigenspaces that span the whole space of the system. This applies to any operator (Hermitian or Unitary) that acts on the whole space. We use those groups to create a block structure of a Hamiltonian. Each block that is formed corresponds to a different eigenspace. Those eigenspaces contain all the eigenstates of the Hamiltonian including its ground state. This is crucial for our work as our intention is to move around different eigenspaces in order to be able to better approximation of the ground state of the Hamiltonian for the cases that it does not located in the same eigenspace with the initial state of the algorithm.

Groups are sets that can contain an abstract number of elements. However, a set must satisfy some specific axioms in order to be a group. We can consider a set G and an operator $\cdot$ that creates an element of G by using two other elements of G. The first axiom is that the set must contain an identity element. This means that there exists an element $d \in G$, that for every other element $m \in G$, it is true that $m \cdot d = m$ and $d \cdot m = m$. The group can only contain one identity element. The second axiom states that an inverse element must exist in the set. This means that for every element $m \in G$ it also exist an element $n \in G$ for which it is true that $m \cdot n = d$, with d denoting the identity element that was defined above. If

this holds, n is the inverse of m and it can be denoted as m^{-1}. The final axiom is related to associativity. This is related to the order of operations in the set. In order for the set to satisfy the third axiom it must be true that for every $m, n, j \in G$, it holds that $m \cdot (n \cdot j) = (m \cdot n) \cdot j$. Groups are algebraic structures whose characteristics and behaviors are analysed by group theory.

The groups offering the easiest analysis are the cyclic group, the reflection group and the dihedral group. We made experiments with all groups but in the implementation of our model we mainly focused on the cyclic group. This is because it is simpler to use, and it also commutes with the Hamiltonians that we are using. Moreover, it is generated by one element and this allows us to use only the group generator for the block diagonalisation of the Hamiltonians. We will analyze the characteristics of all groups in this section.

2.3.1 Cyclic Group

We will start from the cyclic group [17]. It is an abelian group, which means that all the elements of the group commute with each other and also the group generator commutes with the Hamiltonians that we used in our model. In addition, it has one group generator from which we can find all the other elements of the group. We can achieve this, by applying a multiplication with the group generator depending on how many elements of the group we want. This means, that all the elements can be computed by getting the power of the group generator g^i for $i = 2, 3, \ldots, n$ (with $n =$ number of qubits in our case. We say that the group is of order n and $g^n = e$ (neutral element of the group), where n is the smallest positive integer for which this happens). Another interesting characteristic of all groups is that always one of its elements must correspond to the identity matrix. This means that the groups that we used belong to the finite cyclic groups. We will analyze how the formation of the cyclic group is achieved, in the next section.

2.3.2 Reflection Group

Another group of interest was the reflection group [18]. This group is considered as discrete which means that there exits only one element that can be formed from a specific perturbation, so the group contains only one generator, and is created from a set of reflections that depend on a hyperplane. As we mentioned, the reflection group contains only two elements(one of them is the group generator). The other element is the identity matrix which results from the multiplication of the generator with itself. We must also mention that the generator commutes with the Hamiltonians that we used. We will analyze how the reflection group is formed in the next section.

2.3.3 Dihedral Group

Finally, the other group that we wanted to investigate was the dihedral group. The specific group is formed from a combination of cyclic (rotations) and reflection groups. It is a finite group (similar to cyclic group) and it corresponds to the group of symmetries that leave invariant a regular $n - gon$ in the plane. An important difference of the specific group type is that it is not abelian in general cases. This means that the elements of the group do not commute with each other. This is one of the reasons that the computations, experiments and formation of the specific group type is more difficult and this also enhances our choice of using the cyclic group in our model. Moreover, for the same reason, the way that it is formed is a

little bit different and more complex. We can say that a dihedral group D_n is constructed by a rotation r (that has order n as we denoted in the explanation of the cyclic group) and a reflection s (that has order 2 as we explained above). The formula that specifies the generators of the dihedral group is the following:

$$D_m =< r, \sigma : r^n = 1, s^2, r^{-1} = srs > \tag{15}$$

We will analyze how we used the dihedral group for numerical experiments in the next section.

2.3.4 Motivation of selection

We demonstrated numerical experiments with all three group types. We first created groups of specific order (equal to the number of qubits on which the Hamiltonian acts) in order to get a block diagonalisation of the Hamiltonian. As we mentioned, in the implementation of our model we preferred to use the cyclic group due to its characteristics. The most important fact was that it is an abelian group (all the elements of the group commute with each other and this allows us to use only the group generator in the experiments) and it also commutes with the Hamiltonian we used (since we construct it translationally invariant), which means that they share an eigenbasis. When two operators (M, N) share an eigenbasis we know that there exists an eigenbase $|\psi_j\rangle$ for which the following is true:

$$M|\psi_j\rangle = m|\psi_j\rangle, N|\psi_j\rangle = n|\psi_j\rangle$$

with m, n being the eigenvalues of M, N respectively. This makes the procedure of the change of basis (block diagonalisation) of the Hamiltonian that we want to perform much easier and with less computations. The results and the procedure we followed in our implementation will be explained in Section 3.

2.4 Mean Field Theory

Mean field theory is a way to go from a many-body problem to a one-body problem. It is a rough approximation which is useful in some cases of interest but however does not capture the entanglement structure. This means that we consider the interactions of specific individual components while for the remaining ones we use an average over the existing interactions [16]. More specifically, this means that we are not taking into account the entanglement that exists between the interacting qubits. The main advantage of the specific method, is that it can be used to get an idea of how the system evolves without having to make difficult computations that may be almost impossible to implement in classical machines. Because of this, it can be used to roughly estimate the ground state of a Hamiltonian, even if it is applied to a large number of qubits. As we mentioned, this is crucial as we do not need a quantum machine to approximate the ground state and the ground state energy of a Hamiltonian. In our case, this was useful as we utilised it as a tool to make an approximation of the ground state of a Hamiltonian in order to compare it with the ground state approximation when being at the wrong symmetry sector. We proved in Section 4 that even the mean field solution achieved a much better approximation to the ground state than the case where the algorithm searched in the wrong symmetry sector.

The way to compute the mean field solutions is by splitting the Hamiltonian in local terms. Every qubit can be associated with a state which is denoted as follows.

$$|\psi\rangle = \cos(\theta)|0\rangle + e^{-i\phi}\sin(\theta)|1\rangle \tag{16}$$

The mean field solution is produced from the optimisation of the parameters (angles) θ_i and ϕ_i. Since we want to find the lowest energy of the system (within product states), it will be a minimisation problem.

Each qubit is characterised by two real parameters. So, if we have N qubits then the number of parameters that we will have to optimise will be $2N$. We intend to find the angles for vector ψ that when applied to local Hamiltonian will give us the lowest possible value. It is obvious that the result we will get for the energy of the Hamiltonian with the mean field solution cannot be lower than the lowest eigenvalue of the Hamiltonian. This happens because the lowest eigenvalue of a Hamiltonian is equal to its ground state (lowest) energy. More specifically, with the mean field solution we are trying to find the minimum energy from a subset of valid states of the original Hamiltonian. As a result, when we increase the subsets we can only get decreased values for the energy. The equation that is used for the computation of the energy is:

$$E_i = \langle\psi_i|H|\psi_i\rangle \tag{17}$$

This is the amount that we have to minimise by finding the appropriate parameters (angles) for ψ_i. We computed the mean field solution for a Hamiltonian of the Qauntum Heisenberg model (H). We then computed the ground state energy of H in order to know the difference with the mean field solution. The next step was to extract the blocks of the block diagonalised Hamiltonian (we will describe the procedure in Section 3). We observed that the lowest energy of the blocks that do not contain the ground state of the Hamiltonian is much higher than the mean field solution (results are demonstrated and explained further in Section 4). This implies, that in an optimisation procedure (QAOA) with the goal of approximating the ground state of a Hamiltonian, the results will not be efficient if the evolution is done by a symmetry preserving Hamiltonian when the eigenspace of the initial state is not the same with the one that contains the ground state. This happens because when we use a periodic boundary (symmetry preserving) Hamiltonian for the evolution, we cannot move to another eigenspace during the optimisation procedure. We will explain this in detail in Section 4, where we will analyse the method that we used and the results from the experiments that we performed.

In addition, we made an experiment of finding the mean field solution for a specific system using H and 2 qubits. This means that we had to optimize 4 parameters. The algorithm we used for the optimization was COBYLA.

In order to get better insights from our results we decided to plot the resulting parameters in the bloch sphere. We used two different instances of Hamiltonians of the same type H and for 100 iterations of the optimization procedure. The different colours and shapes in the bloch sphere denote different pairs of parameters (angles) that produced the optimal energy values when applied to the Hamiltonian. We decided to plot the pairs in the bloch sphere because all the states produce the same energy amounts.

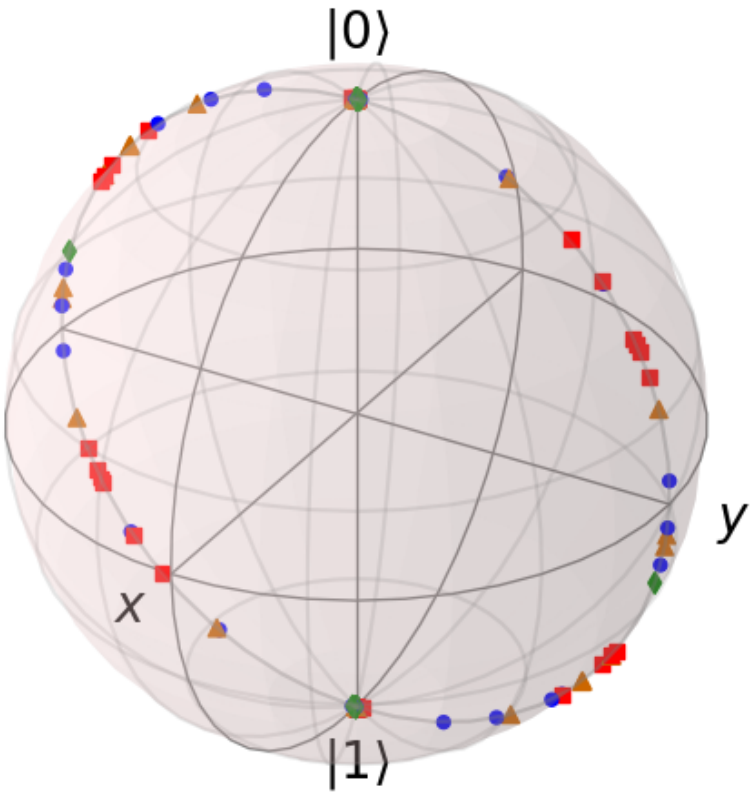


Figure 1: Pairs of optimal parameters for different iterations of the optimization procedure for finding the Mean Field Solution, represented in the Bloch Sphere. The combinations of shapes and colours denotes different optimal pairs from the various iterations.

It can be observed from Figure 1 that all the pairs that were part of the optimal solution are symmetric and can be considered as anti-polar points. By finding the Mean Field Solution we wanted to demonstrate why the symmetry breaking evolution is important. The breaking of symmetries may lead us to better solutions than the preservation of symmetries in the optimisation procedure as it can helps us explore wider areas of the Hilbert space.

2.5 Quantum Heisenberg Model

The Hamiltonians that we used in our experiments were based on the Quantum Heisenberg Model [13]. This can be considered as a statistical mechanical problem, mainly used in the study of magnetic systems. The difference form other similar methods is that the spins of those systems are treated quantum mechanically.

The general form of this Hamiltonian is the following:

$$H = \sum_{j=1}^{N} (J_x \sigma_j^x \sigma_{j+1}^x + J_y \sigma_j^y \sigma_{j+1}^y + J_z \sigma_j^z \sigma_{j+1}^z) \tag{18}$$

where $\sigma^x, \sigma^y, \sigma^z$ represent the Pauli matrices, J_i denotes the coupling constants of the model (related to the strength of the interactions) and N is the number of qubits on which the

Hamiltonian is implemented.

More specifically, the Hamiltonian that we used is identical to ZZX model. The type of the model depends on the values of the coupling constants J_i. For example, if all coupling constants have different values, then we have the Heisenberg XYZ model while if $J_x = J_y = J_z$, the model is called Heisenberg XXX. Our Hamiltonian has the following form:

$$H_{ZZX} = \sum_{j}^{N} (-0.5\sigma_j^x \sigma_{j+1}^x - \sigma_j^y \sigma_{j+1}^y - \sigma_j^z \sigma_{j+1}^z) \tag{19}$$

In the experiments that we performed we used $J_x = -0.5 \neq J_y = J_z = -1$. The signs of the coupling constants are important for the type of the model. If $J_i > 0$ the ground state is ferromagnetic while when $J_i < 0$ the ground state is antiferromagnetic.

The specific Hamiltonian (especially the antiferromagnetic case), can be solved easily and can exploit the properties that the breaking of symmetries has. Moreover, the Quantum Heisenberg Model is quite difficult to be analyzed classically, especially for higher dimensions. By higher dimensions we mean when the Hamiltonian acts on a big number of qubits and as a result the dimensions of the Hilbert space are higher. Another important fact is that the specific model, is widely used to solve classical combinatorial optimisation problems or to check the performance of different types of VQAs [14] [15].

3 Block diagonalization

We mentioned in Section 1 that one of the parts of this work was to find a method to perform en efficient block diagonalisation of Hamiltonian matrices. In order to achieve this we used abelian groups that are described in Section 2.3. We have to state in this section that for simplicity we will use terms from group and representation theory interchangeably.

In this section we will demonstrate how we implemented this procedure, by analyzing the steps that we followed. We will use an example in order to make the explanation simpler. Lets assume we have four qubits. This means that the possible quantum states in the computational basis will have the following form.

$$\begin{gathered}|0000\rangle, |0001\rangle, |0010\rangle, |0011\rangle, \\ |0100\rangle, |0101\rangle, |0110\rangle, |0111\rangle, \\ |1000\rangle, |1001\rangle, |1010\rangle, |1011\rangle, \\ |1100\rangle, |1101\rangle, |1110\rangle, |1111\rangle\end{gathered}$$

Cyclic Group: In general, the permutation for the generator of the cyclic group is implemented in the following way

$$V_c|abcd\rangle \longmapsto |bcda\rangle$$

while for the example that we used for 4 qubits the result will be:

$$
\begin{aligned}
|0000\rangle &\longmapsto |0000\rangle, |0001\rangle \longmapsto |0010\rangle \\
|0010\rangle &\longmapsto |0100\rangle, |0011\rangle \longmapsto |0110\rangle \\
|0100\rangle &\longmapsto |1000\rangle, |0101\rangle \longmapsto |1010\rangle \\
|0110\rangle &\longmapsto |1100\rangle, |0111\rangle \longmapsto |1110\rangle \\
|1000\rangle &\longmapsto |0001\rangle, |1001\rangle \longmapsto |0011\rangle \\
|1010\rangle &\longmapsto |0101\rangle, |1011\rangle \longmapsto |0111\rangle \\
|1100\rangle &\longmapsto |1001\rangle, |1101\rangle \longmapsto |1011\rangle \\
|1110\rangle &\longmapsto |1101\rangle, |1111\rangle \longmapsto |1111\rangle
\end{aligned}
$$

We can see that for some states the permutation leads to the same state. The above states form the generator of the cyclic group for the case of 4 qubits. As we mentioned in Section 2.3 the order of the group (number of elements) is equal to the number qubits. We also mentioned that all the other elements of the group can be computed from the generator of the group as

$$\{V_c, V_c^2, V_c^3, V_c^4\} \tag{20}$$

with V_c being the group generator. It is important to mention that all the group elements commute ($[H, V_c] = 0$) with the Hamiltonians that we used, which means that they share an eigenbasis (for every r). Moreover, it is important to mention that because of the commutation relation, they have common eigenvectors. That is one of the reasons that allows to use only the generator of the group to change the basis of the Hamiltonian.

We must also compute the eigenvalues of the group generator in order to perform the change of basis for the Hamiltonian. We know that all the elements of the group are unitary matrices. As a result, for every $|\lambda_i| = 1$ and $\lambda_i = e^{i\phi}$. From all the above we can derive that:

$$
\begin{aligned}
V_c^4 = 1 \Rightarrow \\
\lambda^4 = 1
\end{aligned}
$$

and we finally have that $\lambda = \pm 1$ or $\lambda = \pm i$. Those different values of λ represent the four eigenspaces (blocks) of the cyclic group that will be used in the change of basis (diagonalisation) of the Hamiltonian.

Moreover, we know that the eigenvalues of the cyclic group generator have a specific multiplicity. This multiplicity is quite important as it is equal to the size of each block. This means that if the eigenvalue $\lambda = 1$ has multiplicity 6, then the size of the eigenspace (block) that corresponds to the specific eigenvalue will be a square matrix of size 6×6.

Reflection Group: A similar procedure must be followed for the reflection group. First, we must explain how the reflection group generator is created, using the states that were mentioned above. The generator of the specific group is created from the following permutation.

$$V_s|abcd\rangle \longmapsto |dcba\rangle$$

The states that we used in our example for 4 qubits will be modified as,

$$|0000\rangle \longmapsto |0000\rangle, |0001\rangle \longmapsto |1000\rangle$$
$$|0010\rangle \longmapsto |0100\rangle, |0011\rangle \longmapsto |1100\rangle$$
$$|0100\rangle \longmapsto |0010\rangle, |0101\rangle \longmapsto |1010\rangle$$
$$|0110\rangle \longmapsto |1001\rangle, |0111\rangle \longmapsto |1110\rangle$$
$$|1000\rangle \longmapsto |0001\rangle, |1001\rangle \longmapsto |0110\rangle$$
$$|1010\rangle \longmapsto |0101\rangle, |1011\rangle \longmapsto |1101\rangle$$
$$|1100\rangle \longmapsto |0011\rangle, |1101\rangle \longmapsto |1011\rangle$$
$$|1110\rangle \longmapsto |0111\rangle, |1111\rangle \longmapsto |1111\rangle$$

while the second element of the group is calculated from the multiplication of the generator with itself (must always be equal to the identity matrix). This means that the group will have the following form

$$\{V_s, \mathbb{I}\}$$

with V_s denoting the generator of the reflection group.

The commutation relation holds for the reflection group as well. This means that the reflection group generator commutes with the Hamiltonian ($[H, V_s] = 0$) and as a result it shares an eigenbasis with it. The difference with this group type is that it contains 2 elements. This implies that we will have

$$V_s^2 = 1 \Rightarrow$$
$$\lambda^2 = 1$$

and $\lambda = \pm 1$. This group type splits the Hilbert space in 2 eigenspaces.

The same things hold for the multiplicity of each eigenvalue. It denotes the size that each eigenspace will have. We will explain in more detail how the block structure diagonalisation is achieved with specific examples in the next section. We will demonstrate the whole procedure that we followed in order to create the blocks for each Hamiltonian.

Dihedral Group: The same procedure becomes much more complex for the case of the dihedral group. The characteristic that makes it more difficult is that the generators of the two groups (cyclic and reflection) do not commute ($[V_c, V_s] \neq 0$). In order to achieve the block diagonalisation, we must use the projector operators of each group. Our goal must be to find an invariant subspace for both cases. As we mentioned, we are allowed to use only the conserved quantity of each group which is the group generator. We know that the sum of Projectors of a matrix is equal to the Identity (span the whole space). This holds for all group generators. As a result, the Projectors for each group generator can represent the Identity.

The generator of the cyclic group can be represented using its orthogonal projectors:

$$V_c = \sum_{i=0}^{n-1} \omega_i \Pi_i \tag{21}$$

We also know that

$$\sum_{i=0}^{n-1} \Pi_i = \mathbb{I} \tag{22}$$

The generator of the reflection group can be represented using its orthogonal projectors with a similar way:

$$V_s = \Pi'_+ - \Pi'_- \tag{23}$$

The two projectors of the reflection group span the whole space and we can say that

$$\Pi'_+ - \Pi'_- = \mathbb{I} \tag{24}$$

We mentioned in Section 2.3, that the elements of the cyclic group are equal to the order of the group. For our case the order is equal to the number of qubits that the Hamiltonian acts on. We denote this number by n. On the other hand, the size of the reflection group is always 2. We know that both group generators (and as a result all the other elements of each group) commute with the Hamiltonians that we use in this work. However, they do not commute with each other.

Our goal is to find the appropriate matrix that will allow us to make the correct change of basis. To achieve this, we must multiply each of the projectors of the group generators together.

$$\Pi_i \times \Pi'_+ = \sum_j \lambda^+_{ij} P^{(j)}_{i\pm} \tag{25}$$

This is the crucial part needed to complete the change of basis of the Hamiltonian. We have to mention that the number of blocks and their size will be different compared to other groups. We will make a detailed description of the next steps in Section 3.1.

3.1 Block formation

The procedure we must follow to get a fine block diagonalisation will be described in detail in this section. The use of symmetry groups is useful as they produce a symmetry-adapted basis, that can block diagonalise operators, forcing them to obey the specific symmetry. This can helps us in several computations by making them simpler. An example of why computations with a block diagonal Hamiltonian are easier is the following

$$e^{iHt} = e^{iU^\dagger HUt} = U^\dagger e^{iH_{BD}t} U,$$

with H_{BD} denoting the block diagonal form of H:

$$H_{BD} = \begin{bmatrix} e^{iB1t} & 0 & 0 & 0 \\ 0 & e^{iB2t} & 0 & 0 \\ 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & e^{iB_kt} \end{bmatrix}$$

The steps that we must follow are identical for the cases of cyclic and reflection group. However, the results that we will get are going to be different due to the different number of projectors that each group generator has.

The first and most crucial part in the procedure of block digonalisation is the creation of the

groups. It is described in detail in the beginning of Section 3. As we explained, it is enough to use only the conserved quantity of the group (because the specific groups can be generated by one element) in order to achieve the appropriate change of basis. The steps that we must implement are:

- We begin by using the group generator in order to change the basis of our initial Hamiltonian (H).
$$H_{gr_i} = V_g^\dagger H V_g \tag{26}$$
with V_g being the group generator either for the cyclic or the reflection group.

- Then we must get the sum, and divide it by the length of the group (2 for the reflection group and n for the cyclic group). The equation for one of the groups will be:
$$H_{gr} = \frac{\sum_{i=0}^{n-1} V_{g_i}^\dagger H V_{g_i}}{n} \tag{27}$$
We must mention that we can understand if the block diagonalisation will be efficient from this matrix already, despite the fact that the block structure is not clear. We will discuss the differences regarding the specific matrix for different cases Section 3.2.

- The next step is to get the eigendecomposition of the group generator. We need this to determine which of the eigenvectors correspond to the same eigenvalues. The matrix of the eigenvectors is important because it is the one we need in order to get a fine block diagonalisation. In order to achieve this, we must change the original order of the specific matrix by putting together the eigenvectors that correspond to the same eigenvalues.

- Finally, we use the ordered matrix that contains the eigenvectors of the group generator in order to perform the block diagonalisation of the Hamiltonian using the matrix that we created in the previous step, with the change of basis using all the group elements. We expect that the resulting matrix will preserve the block structure.
$$H_{sym} = M_{ord}^\dagger H_{gr} M_{ord} \tag{28}$$
with M_{ord} being the ordered matrix of the eigenvectors that we described in the previous step.

We have to mention that the specific procedure holds for every Hamiltonian H. This happens because the block diagonalisation procedure depends only on the group type. As a result, we can derive that the number of blocks and the structure of the resulting matrix (size of blocks) will be the same for every initial Hamiltonian. That is the reason we made some experiments using random Hamiltonians. The results are demonstrated in Section 3.1.1. We also evaluate another method for block diagonalisation that was proposed by Tavakoli et al. [3] in Appendix A.

3.1.1 Experiments on various Hamiltonians using different group types

For the visualisation of the specific experiments we used matrix plots in which the blocks are easily distinguished. It is also an efficient way for the cases where the matrix of the Hamiltonian is large (big number of qubits).

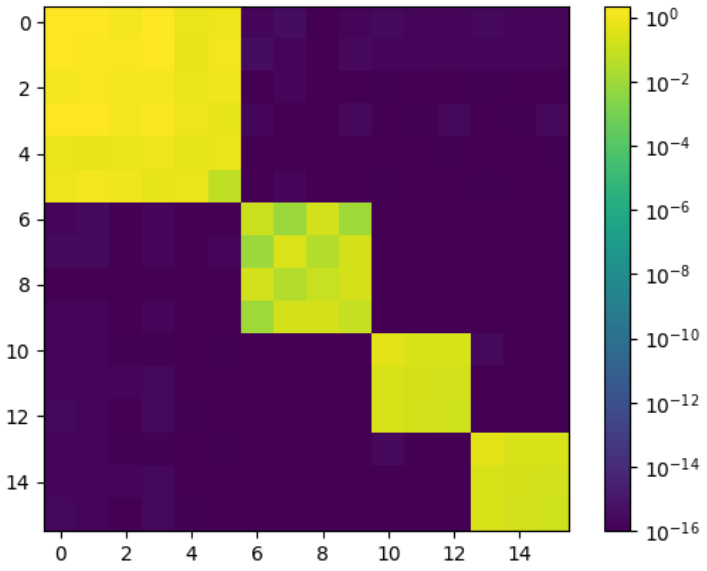


Figure 2: Matrix plot for a diagonalised Hamiltonian (random) that acts on 4 qubits, using cyclic group for the change of basis. The number of blocks that are created, is equal to the number of qubits that the Hamiltonian acts on.

Figure 2 contains the matrix plot for a random Hamiltonian that has been diagonalised in order to get its block structure. The specific Hamiltonian acts on 4 qubits and we used the cyclic group to perform the change of basis. We can see that the blocks can be easily distinguished. In addition, the number of blocks is equal to the number of qubits, when the cyclic group is used for the diagonalisation. This is distinguishable in Figure 2.

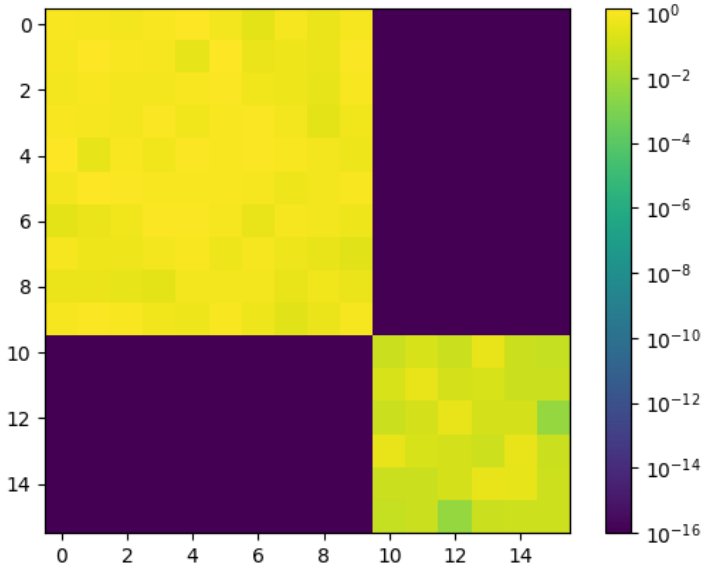


Figure 3: Matrix plot for a diagonalised Hamiltonian (random) that acts on 4 qubits, using reflection group for the change of basis. The number of blocks is two which is what we expected for the specific case.

Figure 3 contains the matrix plot of a random Hamiltonian that has been diagonalised using the reflection group. The Hamiltonian acts on 4 qubits but this time we used the reflection group for the change of basis. The blocks can be seen in the Figure. The difference compared to Figure 2 is the number of blocks and their size. As we mentioned in Section 3, the number of blocks is always 2 when the reflection group is used for the diagonalisation. As we expected, the size of the blocks are larger.

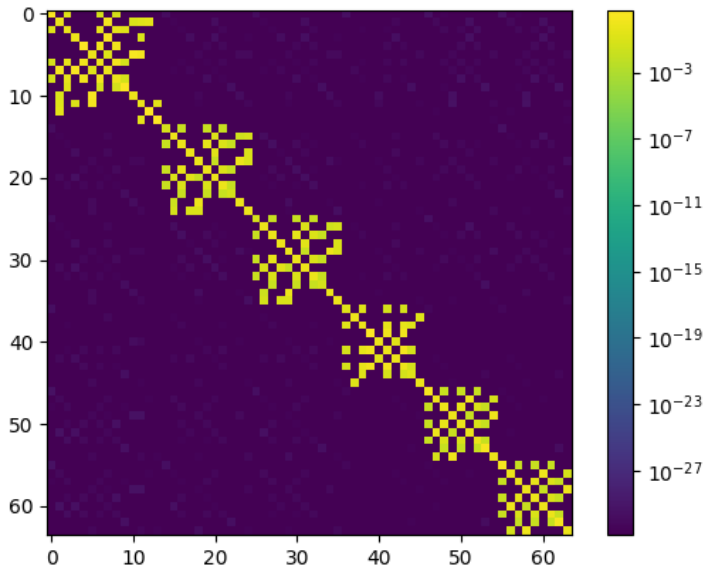


Figure 4: Matrix plot for a diagonalised Hamiltonian based on the Quantum Heisenberg model that acts on 6 qubits, using cyclic group for the change of basis. The number of blocks is equal to the number of qubits that the Hamiltonian acts on. The checkerboard pattern indicates that we can create a better block diagonalisation by separately re-applying the procedure for each block .

Figure 4 contains the matrix plot for a Hamiltonian based on the Quantum Heisenberg model with periodic boundaries after the diagonalisation. The specific Hamiltonian is larger compared to those used in Figures 2, 3 as it acts on 6 qubits. The group type that was used for the change of basis was the cyclic group. In Figure 4, the blocks are clearly distinguishable. It can be observed that the number of blocks is again equal to the number of qubits.

From Figures 4, 5 we can also derive another interesting deduction. The Hamiltonian that was used in Figures 2 was formed randomly while the one used in Figures 4, 5 is the quantum Heisenberg Hamiltonian which we use in most of our experiments. The group type that was used for their change of basis is the cyclic group. We can see that the structure (number of blocks and their size) does not differ. This confirms that creation of the block structure for a Hamiltonian depends only on the group type that will be used in order to achieve it. In Figure 5, the blocks and their size seem different but this is not the case. This happens because the values of the specific Hamiltonian are quite low in specific eigenspaces. That is why for the final two blocks all the values are close to 0. There are ways that keep the characteristics of the Hamiltonian unaffected, and help us in the visualisation of the block structure. However, the actual result of the block diagonalisation is not affected and that is why we preferred to plot it that way. The actual blocks are denoted with the small red squares in Figure 5.

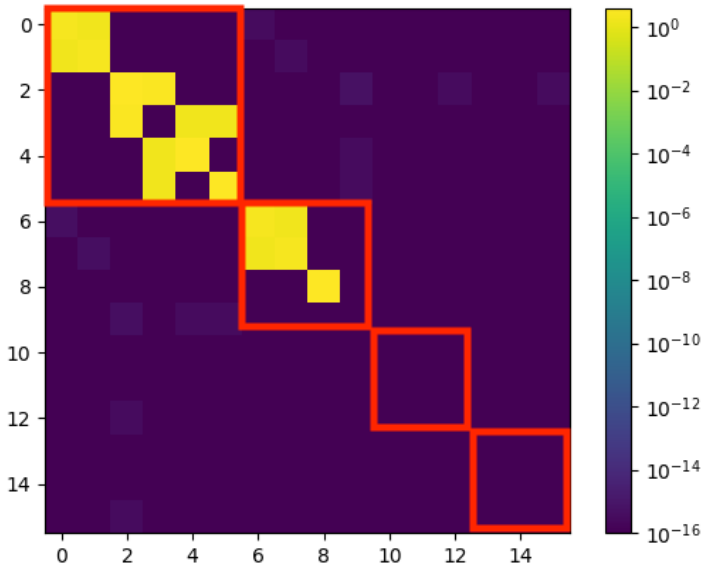


Figure 5: Matrix plot for a diagonalised Hamiltonian based on the Quantum Heisenberg model that acts on 4 qubits, using cyclic group for the change of basis. The last two blocks are not distinguishable in the figure, as the elements in some eigenspaces have values equal to 0.

We also made the same procedure using the reflection group for the change of basis. The results are demonstrated in Figure 6. We can see that for this case (using the reflection group in a Hamiltonian based on the Quantum Heisenberg model) the results are identical to the previous cases (reflection group but with random Hamiltonian). This happens because for the two eigenspaces represented from the specific group (those for eigenvalues 1 and -1) the values are greater than 0 and this is visible in the plot. This plot assures the dependency of the formation of the block structure only from the type of the group that we use.

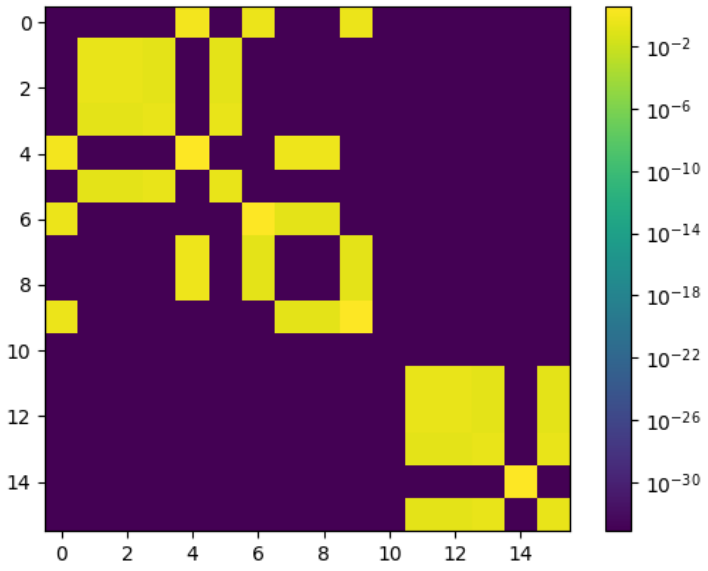


Figure 6: Matrix plot for a diagonalised Hamiltonian based on the Quantum Heisenberg model that acts on 4 qubits, using reflection group for the change of basis. Both groups are distinguishable in this case.

This implies that the use of those group types for the change of basis of the Hamiltonian in order to derive their block structure is universal. It holds for every Hamiltonian that we want to use (there are some exceptions for open boundary Hamiltonians where there are small blocks outside the main diagonal that are not zero, but the general structure remains).

As we mentioned, we used the same procedure to make experiments using the dihedral group. The block diagonalisation for the specific group type is more difficult and complex than for the previous cases. This happens because we need both the cyclic and the reflection group generators. Those generators do not commute, and as a result we must follow a different procedure to achieve the block diagonalisation, as we described in Section 3.1.

The resulting matrix after the change of basis will be different from the previous cases as the number of blocks and their size must be a combination of the two groups. We will have some combinations from the two eigenspaces that are common between the two groups (those that correspond to eigenvalues 1 and -1) and the remaining will be filled by the eigenspaces that exist only in the cyclic group (those that correspond to eigenvalues i and $-i$).

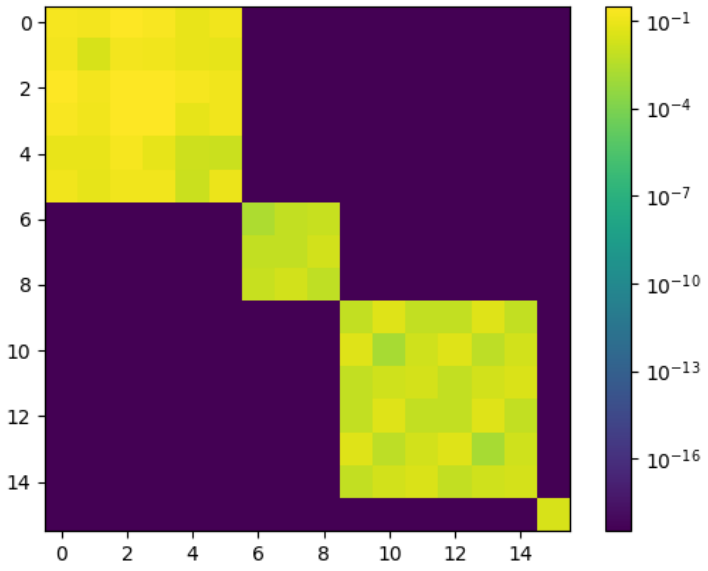


Figure 7: Matrix plot of a diagonalised Hamiltonian (random) that acts on 4 qubits. Dihedral group was used for the change of basis. The number of blocks is equal to the qubits that the Hamiltonian acts on, but the size of each block is different compared to the case of the cyclic group.

Figure 7 contains the matrix plot after the diagonalisation procedure of a random Hamiltonian that acts on 4 qubits.

3.2 Differences between Periodic and Open Boundary Hamiltonians

One of the most important aspects of the block diagonalisation procedure is the effect that it has on different types of Hamiltonians. We mainly focused on two types, regarding their boundaries. They are separated to Periodic and Open Boundary Hamiltonians. More specifically, by Periodic Boundary Hamiltonian we mean that each qubit that the Hamiltonian acts on, is interacting with its neighboring one. It can be written as

$$H_{PBC} = \sum_{i=0}^{N-1} H_{i,i+1} \tag{29}$$

with N denoting the total number of qubits that the Hamiltonian acts on, and including interactions between the last and the first qubit of the system. Those interactions take part in a $1D$ lattice. We chose the $1D$ lattice because with this way the model will become simpler by avoiding more complex interactions. In addition, we did not want to add complexity that would not give us actual insights or improve the quality of our final results and conclusions.

The difference of the Open Boundary Hamiltonian is that it contains a term that slightly breaks the symmetry of the Periodic Boundary Hamiltonian. This means, that in the example that we mentioned above, the interactions between the fourth and the first qubit will not exist. As a result, the interactions that we will have, will be

$$H_{OBC} = H_{PBC} - H_{N-1,0} \tag{30}$$

with $H_{n-1,0}$ being the term that slightly breaks the symmetry of the Periodic Boundary Hamiltonian.

The first thing that we will investigate in this work is the difference of the aforementioned types of Hamiltonians in the block diagonalisation procedure using the groups that were mentioned in Section 2.3. The procedure from which we achieve the change of basis is described in detail in Section 3.1. The main difference between the two Hamiltonians can be derived from the first change of basis where we have

$$H_{gr} = V_c^{\dagger} H V_c \tag{31}$$

with V_c being the cyclic group generator (the same holds for the reflection group generator). The specific matrix (H_{gr}) is different when $H = H_{PBC}$ and $H = H_{OBC}$.

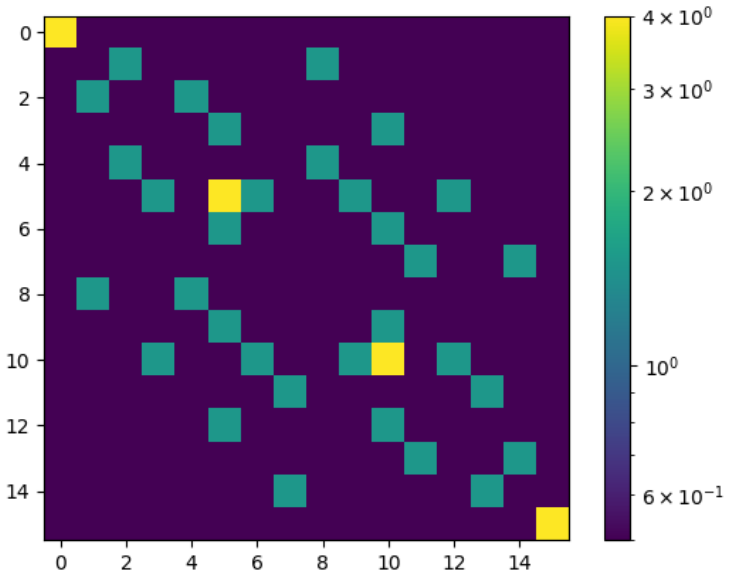


Figure 8: Matrix plot for the change of basis of a Hamiltonian (H_{ZZX}) that acts on 4 qubits with Periodic Bpundary conditions. Cyclic group generator was used for the change of basis. The specific matrix has a structure that will produce perfect blocks in the next change of basis.

Figure 7 contains H_{gr}, in the case where $H = H_{PBC}$. It can be observed from Figure 7, that the specific matrix has a specific structure, as it contains zero and non-zero values in specific positions. From this structure we can derive that when we proceed to the next step in order to complete the block diagonalisation, we will get a fine formation of blocks, without other non-zero entries.

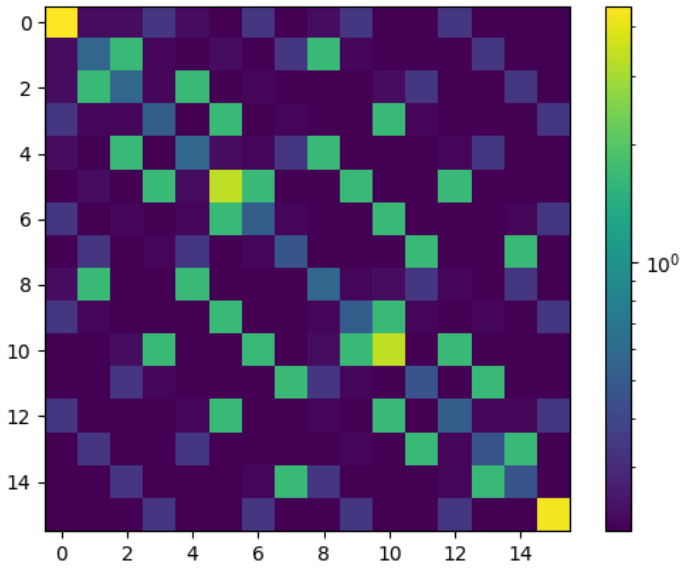


Figure 9: Matrix plot for the change of basis of a Hamiltonian (H_{ZZX}) that acts on 4 qubits and has Open Boundaries. Cyclic group generator was used for the change of basis. We have more non-zero elements and the structure of Figure 8 is not preserved. As a result, non-zero elements will exist in the block diagonalised Hamiltonian, outside the main blocks.

Figure 9 contains the same matrix but this time $H = H_{OBC}$. As you can see, the two matrix plots do not have exactly the same structure. In Figure 9, the structure is not preserved. There are elements that are close to zero, and are spread in different positions. This implies that the symmetry of the Hamiltonian we used, was slightly broken (the values are really close to zero, which is a small difference compared to Figure 8). From this plot we can understand that the matrix we will get after the next step of the Block diagonalisation procedure, will not be a perfectly diagonalised matrix. This will happen because there are going to be small blocks outside the main diagonal which will have low value, but non-zero elements. The same will hold for every symmetry group.

3.2.1 Breaking of Symmetries

The main goal of this work is to use a Hamiltonian that will not exactly preserve a symmetry to approximate the ground state of the corresponding symmetry preserving Hamiltonian using a quantum cost function. We implemented this in a QAOA procedure which we will analyse in detail in Section 4.

As we discussed in this Section, the Open Boundary Hamiltonians (do not preserve a symmetry) have a different diagonalised form than the Periodic Boundary Hamiltonians. More specifically, Open Boundary Hamiltonians, do not have a strict block structure. This means that there are elements outside the block diagonal which are not zero. Small blocks are created with low values that slightly break the symmetry. This characteristic is the one that enables us to search in new symmetry sectors when using the Open Boundary Hamiltonian for the evolution in an optimisation procedure like QAOA.

4 Experiments and Results

The main goal of this work is the implementation of an optimisation procedure that will use a Hamiltonian that will not preserve a symmetry (only up to some extent) for the approximation of the ground state of a symmetry preserving Hamiltonian. Our procedure is based on the Quantum Approximate Optimisation Algorithm which is described in Section 2.2. It is not a classical QAOA procedure as we made some modifications that we will explain in Section 4.1.

From this experiments, we intended to extract evidence that will prove the advantages of using an open boundary Hamiltonian to approximate the ground state of the problem Hamiltonian with a quantum cost function. One of the main expected advantages is that it will be possible to find better approximations for Hamiltonians where the symmetry preserving method fails. An example is Hamiltonians for which their ground state lies in a different eigenspace than the eigenspace of the initial state. Moreover, we also wanted to check whether it is possible with the specific method to reach states that do not completely live in the initial eigenspace.

4.1 Procedure description

The procedure that we followed is based on the Quantum Approximate Optimisation Algorithm (QAOA). The QAOA procedure is explained in detail in Section 2.2. Our method begins by an educated guess of the initial state, as it is important for the result of the optimisation procedure. It is crucial to choose an initial state that will be easy to prepare. The initial state depends on the mixing Hamiltonian that is used. In our experiments, we mainly used the $|11\ldots1\rangle$ state (ground state of the mixing Hamiltonian). The Hamiltonians that we need in our method are three. We need one mixing Hamiltonian which we must select properly and depends on the type of the target Hamiltonian. Moreover, we have to set a target Hamiltonian and a Hamiltonian for the evolution of the system. The objective function in our experiments is quantum and that is the reason why we must properly select the mixing Hamiltonian (it must not commute with the problem Hamiltonian).

Although we have to mention that our implementation has some differences and some necessary modifications compared to the original QAOA procedure. The specific algorithm was introduced as a way to solve combinatorial optimisation problems [8], thus the cost function was classical. As we mentioned, we want to use an open boundary Hamiltonian to approximate the ground state of a periodic boundary Hamiltonian. We need one Mixing Hamiltonian and one target Hamiltonian like in the original QAOA procedure. However, we also need a Hamiltonian for the evolution of the system which will be the open boundary version of the target Hamiltonian. This happens because the cost function that we have is quantum. We can observe that when the problem and the evolution Hamiltonians are quantum, there is not a periodic behavior for the values of the parameters $\vec{\beta}, \vec{\gamma}$ that we want to optimise. Another difference is that we did not use a quantum circuit to produce the quantum state. We used a simulation using matrix exponentials that can be utilised as an alternative to the quantum circuit creation. The procedure can be considered a trotterized evolution. In order to have more accurate results we should have included Trotter error but we decided that it would be better to ignore it in our experiments. Moreover, another modification is that we use a classical optimiser to find the best initial parameters before the calculation of the quantum state. The goal is to begin with a good approximation from the first layer of the quantum circuit. Another difference is related to

the selection of the initial state. The proposed initial state according to the authors that first proposed QAOA [8], is the $|+++++\ldots\rangle$. However, we have to mention that the objective function in [8] is classical. In the experiments that we performed, we used the ground state of the mixing Hamiltonian. We had to use a different mixing Hamiltonian than the one that is proposed in [8] as it commuted with the problem Hamiltonian.

In order to improve the performance of the optimisation algorithm that we propose, we found the local-optimum parameters for $p = 1$ where p denotes the depth of the quantum circuit. More specifically, we used our simulation of the quantum circuit only with $p = 1$, in order to get a quantum state, then measure it, and finally use the classical optimiser (COBYLA) to optimise the parameters. We run this procedure 20 times, to gain an efficient local optimum. We used the parameters that produced the optimal energy as the initial parameters of our optimisation method. The initial parameters that we used for the specific procedure were chosen randomly.

Now we have all that we need in order to implement our method. As initial parameters we use the local-optimum parameters which were calculated with the method described above. Using those parameters we executed our simulation of the quantum circuit using exponential matrices in order to obtain the quantum state and measure it. The next step is to use the classical optimiser (COBYLA [46]) to optimise the real parameters $(\vec{\beta}, \vec{\gamma})$ and choose those that minimise the expectation value of the quantum state. We picked the specific classical optimiser because it is deterministic (the output depends only on the inputs as there is no randomness) and it is a consistent method that is easy to be applied and has satisfying results in similar problems [6]. This is achieved by calculating the expectation value of the produced state. The optimal parameters that are produced from one layer, are used as the initial parameters in the next one. With this way we ensure that we will start the optimisation procedure for the next layer with parameters that generate a good solution. In the next iteration, the number of layers p of the quantum circuit is increased, most of the times, by 1. The increase in the number of layers of the quantum circuit usually increases the accuracy in the result but more computational power and time is needed for the computation. The maximum number of layers that we used was 11. Moreover, we used an observation of Zhou et al. [7] according to which, when the number of layers is high we can increase the number by more than 1 as the improvement that we expect when we increase it by 1 is not crucial. This is useful as we can save computational resources and computational time.

The goal was to check the performance of the QAOA algorithm using an open boundary Hamiltonian for the evolution. In order to evaluate the quality of solutions we used both the expected energy and the fidelity of the generated state with the ground state of the Hamiltonian. The fidelity is calculated via the following equation:

$$F = |\langle\psi(\vec{\beta}, \vec{\gamma})|GS\rangle|^2 \tag{32}$$

with GS representing the ground state of the problem Hamiltonian. We also wanted to check how the produced states get modified when the open boundary Hamiltonian is used for the evolution. That is why we computed the fidelity of the produced quantum state with each of the eigenspaces that are produced using the cyclic group. The specific fidelity values were calculated by the following equation:

$$\langle Pr_i\rangle = \langle\psi(\vec{\beta}, \vec{\gamma})|Pr_i|\psi(\vec{\beta}, \vec{\gamma})\rangle \tag{33}$$

with Pr_i denoting the orthogonal projector that corresponds to the eigenvalue i of the cyclic group and represents a specific eigenspace. By calculating those fidelities, we were able to verify that when the open boundary Hamiltonian is used for the evolution of the system, the quantum states that are generated do not lie in only one eigenspace. That allowed us to make comparisons with the case where the periodic boundary Hamiltonian is used for the evolution.

4.2 Hamiltonians used

As we mentioned, we need three Hamiltonians for the implementation of the optimisation procedure. We need one problem (target) and one mixing Hamiltonian which are the Hamiltonians that a typical QAOA procedure needs. In addition, we need a different Hamiltonian for the evolution of the system. The characteristic of this Hamiltonian is that it is not symmetry preserving and it is used for the approximation of the ground state of the target Hamiltonian.

4.2.1 Problem (Target) Hamiltonian

The problem Hamiltonian we used in our experiments is based on the Quantum Heisenberg model and is explained in detail in Section 2.5. It has the following form and it is called ZZX Hamiltonian:

$$H_{ZZX} = \sum_{j}^{n} (J_x \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \sigma_j^z \sigma_{j+1}^z) \tag{34}$$

where n is the number of qubits where the Hamiltonian acts on and J_x is the coupling constant of the model.

We chose the specific Hamiltonian as it can be solved easily and can help us explore the advantages that our method has. The Quantum Heisenberg Model is difficult to be solved classically. Moreover, it is widely used to solve classical combinatorial optimisation problems and it is also utilised to check the performance of many variational quantum algorithms.

4.2.2 Mixing Hamiltonian

The mixing Hamiltonian must be chosen wisely in order to obtain better performance of the algorithm. The mixing Hamiltonian that we used in our experiments was the sum of local Pauli Z gates and has the following form:

$$H_M = \sum_{j=1}^{n} Z_j \tag{35}$$

where n is the number of qubits where the Hamiltonian acts on.

We chose the specific mixing Hamiltonian as it must not commute with the target Hamiltonian and this holds in the specific case. We observed that when the coupling constant J_x is higher, the ground state energy of the problem Hamiltonian is lower and the two matrices (mixing and problem Hamiltonian) commute more. The specific observation holds for negative coupling constants. From this we can imply that when the two matrices commute more, the approximation of the ground state becomes more difficult. The initial state that we chose was the ground state of the mixing Hamiltonian ($|11\ldots1\rangle$).

4.2.3 Evolution Hamiltonian

The Evolution Hamiltonian is related to the target Hamiltonian as it must be its open boundary version. More specifically, we must add to the periodic boundary Hamiltonian a term that will slightly break its symmetry. If the target Hamiltonian has the following form,

$$H_P = \sum_{j=0}^{n} H_{j,j+1} \tag{36}$$

then the evolution Hamiltonian will be,

$$H_E = H_P - H_{n-1,0} \tag{37}$$

with n being the number of qubits that the Hamiltonian acts on. We know that the norm of the symmetry breaking term ($H_{n-1,0}$) will be smaller than the norm of H_P. This means that the norm of the blocks of diagonal elements will be larger than the norm of the off diagonal elements. More specifically it will be approximately n times larger. This will also have an effect on the minimum number of layers that the quantum circuit must have in order to move the search space to a new eigenspace, as we will see in Section 5. This breaking of symmetries is the one that allows us to move in different eigenspaces during the optimisation procedure.

4.3 Characteristics of the experiments

To summarise, the main parts of the algorithm that we use are the following:

- Initial state:
$$|\psi_0\rangle = |1\rangle^{\otimes n}. \tag{38}$$
It corresponds to the ground state of mixing Hamiltonian (H_M) and n denotes the number of qubits that the Hamiltonians act on.

- Evolution:
$$|\psi_p(\vec{\gamma},\vec{\beta})\rangle = e^{-i\beta_p H_M} e^{-i\gamma_p H_E} \dots e^{-i\beta_1 H_M} e^{-i\gamma_1 H_E} |\psi_0\rangle \tag{39}$$
with H_E denoting the evolution Hamiltonian and H_M the mixing Hamiltonian.

- Objective function:
$$E_p(\vec{\gamma},\vec{\beta}) = \langle\psi_p(\vec{\gamma},\vec{\beta})|H_P|\psi_p(\vec{\gamma},\vec{\beta})\rangle \tag{40}$$
with H_P denoting the problem Hamiltonian. We also evaluated the results in terms of fidelity using Equation 32.

- Initial parameters: Generated by finding the local optimum parameters by running the algorithm for $p = 1$, with p denoting the number of layers.

We must also mention that we use the cyclic group to create the eigenspaces that divide the Hilbert space in different blocks by changing the basis of the problem Hamiltonian. The eigenspaces that are created correspond to the eigenvalues of the cyclic group generator.

In this section, we are going to describe the experiments that we performed and modifications we made in order to evaluate different characteristics of the algorithm. We tested the performance of the algorithm with different number of qubits. More specifically we have

executed experiments using from 3 to 8 qubits.

Moreover, we tested the performance with different initial parameters. We tried with random initial parameters (in the region $(-\pi, \pi)$), with all of them being 0, and with the local optimum parameters which we calculated with the procedure described above. The last technique provided better results and because of that, in the experiments that we demonstrate in this work, we use it for the generation of the initial parameters.

Another interesting modification which we made was related to the parameters that we must use when the number of layers of the quantum circuit is increased. We used the optimal parameters that were produced from the previous layer as the initial for the next layer. However, when the number of layers (p) increases, two additional parameters must be added. We made two tests for generating the additional parameters. We tried putting them as 0s and we also generated them randomly. When those parameters are 0s we ensure that the optimal solution for the additional layer will be at least equal to the optimal solution that produced for the previous layer. Most of the times we used the 0s choice, we were trapped in local minimums and the results were not satisfying. This is reasonable as with this strategy we reduce the search space for the next layer as we search for solutions only near to the optimal solution produced from the previous step. This happens because if we set the additional parameters to 0 the corresponding unitaries will be the identity matrix. The random choice produced better results.

In order to verify our claims regarding the differences of using an open boundary Hamiltonian for the evolution of this optimisation procedure we had to compare it with an evolution with a periodic boundary Hamiltonian. Because of that, we will demonstrate the produced results for both cases and we will compare their differences.

4.3.1 Eigenspace of Initial state

It is important to find the eigenspace of the initial state. This corresponds to the eigenspace that the ground state of the mixing Hamiltonian lies. For our case, the ground state of the mixing Hamiltonian lives in the eigenspace that corresponds to eigenvalue 1. Those eigenspaces are formed using the cyclic group.

For our work, this is of high importance, as our experiments are based on it. We implemented two different experiments related to the eigenspace of the ground state of the target Hamiltonian and the eigenspace of the initial state that we used. The first, was with the ground state of the target Hamiltonian being in the same eigenspace with the initial state and the other with the two states being in different eigenspaces. Especially for the second type, the advantages of using an open boundary Hamiltonian for the evolution are clear as the evolution using periodic boundary conditions cannot reach an efficient approximation of the ground state. This happens because without the symmetry breaking factor, we cannot change the eigenspace where the algorithm searches for possible solutions. As a result, all the produced states will completely lie in the eigenspace from which we started which is equivalent to the eigenspace of the ground state of the mixing Hamiltonian. We expect this to change when we use the open boundary Hamiltonian for the evolution. With the symmetry breaking term, we can search in other eigenspaces for possible states. The goal will be to reach the eigenspace where the ground state of the target Hamiltonian lies or to check if we can increase its fidelity with the

specific eigenspace. Taking this into account, we expect that the use of a symmetry breaking Hamiltonian will improve the results of the algorithm both in terms of fidelity and in terms of the lowest energy produced.

4.4 Implementation and Results

In this section, we will describe the experiments that we implemented and we will demonstrate the results and the plots that we produced. We executed many experiments by alternating the values of the different variables that define the implementation and the method used.

In most of the experiments we used negative coupling constants in the Hamiltonians. This means that we have an anti-ferromagnetic model. We made some experiments with positive coupling constants but the results were worse than expected. There are indications that it is more difficult to compute the ground state energy in a ferromagnetic model (positive coupling constants), because the states that represent it are anti-parallel and this leads to a ground state that will be a superposition of those anti-parallel states [41]. We only demonstrate the results using positive coupling constants for low number of qubits (3), because for that case the ground state was not in the same eigenspace with the ground state of the mixing Hamiltonian. For low number of qubits the ferromagnetic model does not causes us problems in the approximation of the ground state.

In addition, we implemented experiments using different number of qubits. The number of qubits we utilised was 3-6 (we also made experiments with 8 qubits but the results did not provide new findings). It is useful to see how the behavior of the model changes when the number of qubits is increased.

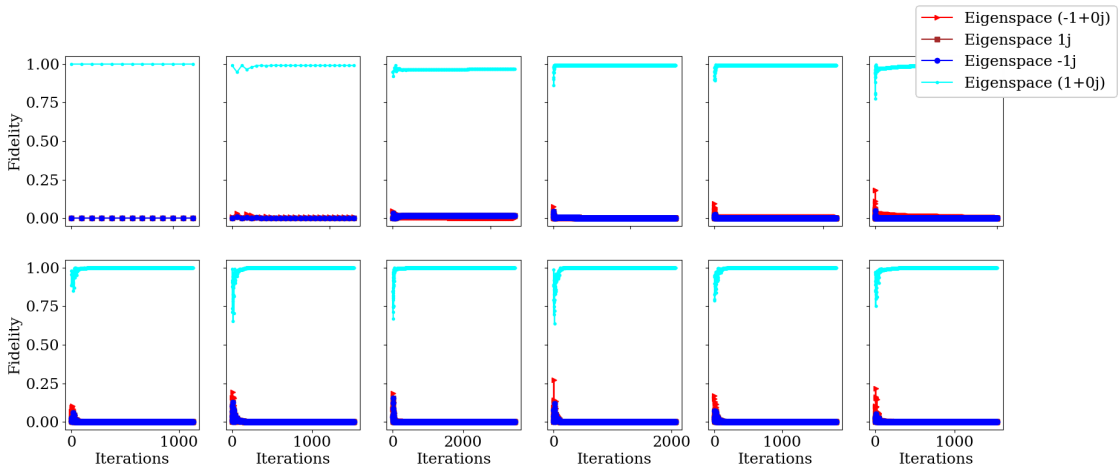
Moreover, we made some experiments using a target Hamiltonian that contains a ground state that lives in a different eigenspace than the initial state. The improvements for this case were clearer. However, for this case, the Hamiltonian used had a degenerate ground state. We had to make some modifications in order to create a Hamiltonian without a degenerate ground state.

We have to mention that for all the experiments that we performed, we made comparisons by alternating between open and periodic boundary Hamiltonians for the evolution of the system. By this comparison, we can highlight the advantages from the use of an open boundary Hamiltonian. The experiments and the results are demonstrated in detail in the following subsections.

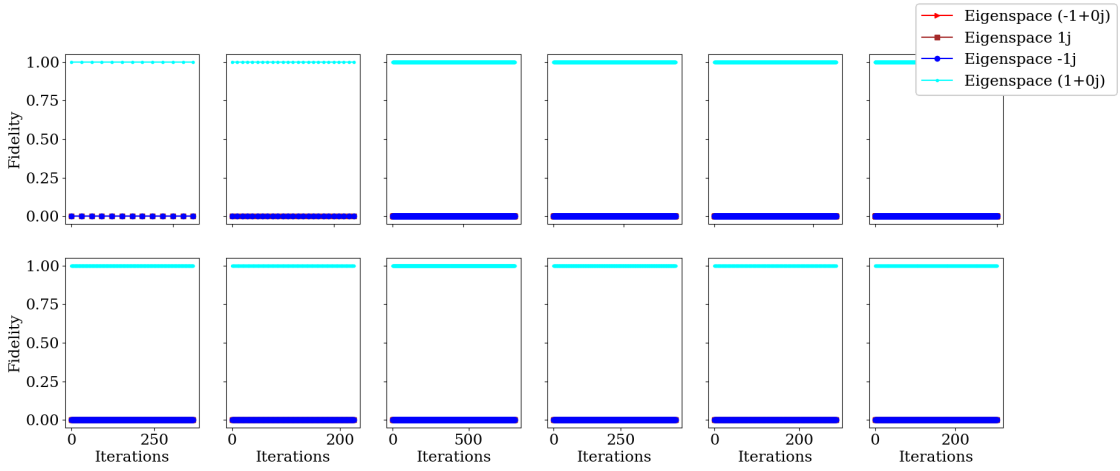
4.4.1 Results for even number of qubits

In this section we demonstrate the results from the experiments with even number of qubits. The variables that were used (initial parameters, initial parameters when the number of layers is increased, total number of layers, Hamiltonians used) for the experiments and their selection, were described in previous sections.

The first experiments that we made were with Hamiltonians that act on 4 qubits. For the specific case, the results were efficient when using the open boundary Hamiltonian for the evolution. The same holds when the periodic boundary Hamiltonian is used.



(a)



(b)

Figure 10: (a) Each subplot of the Figure corresponds to the values of the fidelity of the produced state with every eigenspace, at each iteration of the model, for every layer, using the Open Boundary Hamiltonian for the evolution. The eigenspace of the initial state is the one corresponding to eigenvalue 1 of the cyclic group. The ground state of the Hamiltonian is also in the same eigenspace. However, we can see that all eigenspaces are explored as their fidelities with the produced states are ≥ 0 through all iterations. We can also denote that as the amount of energy of the produced states decreases, the fidelity of the eigenspace that contains the ground state increases. Moreover, we can see that for small number of layers, the fidelity of the produced state with the eigenspaces that do not contain the ground state, is higher than for more layers. This is reasonable, as the quality of solutions is worse for small number of layers. The number of qubits that the Hamiltonians act on is 4. The first subplot is for $p = 0$ (number of layers) and then p is increased by 1. The final plot corresponds to $p = 11$.
(b) Each subplot of the Figure corresponds to the values of the fidelity of the produced states with every eigenspace, for each iteration of the model, for every layer, using the Periodic Boundary Hamiltonian for the evolution. We can see that only one eigenspace is explored in this case. The subplot for $p = 0$ is the same with the rest of the subplots for larger p. This indicates that all the states that are produced in all iterations for every layer completely belong to the same eigenspace. This is a crucial difference compared to the previous case where the Open Boundary Hamiltonian was used for the evolution. The number of qubits that the Hamiltonians act on is 4. The first plot is for $p = 0$ (number of layers) and then p is increased by 1. The final plot corresponds to $p = 11$.

Figure 10 (a) contains the results for open boundary evolution and Figure 10 (b) for the periodic boundary evolution. Both plots contain the evolution of the fidelity of the produced states with every eigenspace, after each iteration of the classical optimisation procedure, for every layer of the quantum simulation. We decided to plot the fidelity of the produced quantum states with each of the eigenspaces that were formed from the cyclic group. This is useful as it helps us understand if the algorithm searches for possible solutions in more eigenspaces than the eigenspace of the initial state. The specific plots are for Hamiltonians that act on 4 qubits.

The differences between the two subplots are clear. In Figure 10 (a), where the symmetry breaking Hamiltonian is used for the evolution, we can see that the algorithm generates states that do not belong only in the eigenspace of the ground state of the mixing Hamiltonian. All the eigenspaces were explored with this method. In addition, we can denote that the minimum energy that is produced approaches the ground state energy of the system. This is a huge difference in the case of the evolution with the periodic boundary Hamiltonian. We can see that the only eigenspace that is explored, is the one that contains the ground state of the mixing Hamiltonian (initial state). The results were satisfying, but this was only because the ground state of the target Hamiltonian was in the same eigenspace with the eigenspace of the ground state of the mixing Hamiltonian. Moreover, for the specific model, the preservation of symmetries seems to have positive effects.

Another interesting thing we can derive, is the fact that when more eigenspaces were explored the produced energy was higher, which means that the quality of the solution is worse. This is reasonable for the case where the ground state is in the same eigenspace with the ground state of the mixing Hamiltonian. Another interesting observation from Figure 10, is that the number of iterations needed for the Periodic Boundary evolution to produce the optimal state at each layer are less compared to the Open Boundary evolution. This can be explained because with an Open Boundary Hamiltonian, the algorithm searches in a bigger space. We will not include the plots for the Periodic Boundary evolution, as in Figure 10 (b), in the following Figures because the results are exactly the same and there are no new findings.

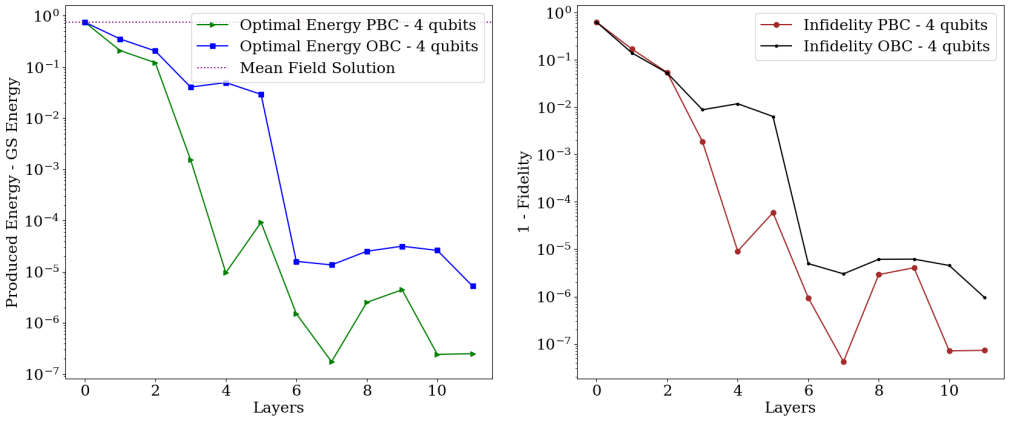


Figure 11: The Hamiltonians used act on 4 qubits and the eigenspace of the ground state is the same with the eigenspace of the initial state. The left subplot contains the difference between the ground state energy of the problem Hamiltonian and the optimal energy produced for each layer of the optimisation procedure when using the periodic and the open boundary boundary evolution. The mean field solution is also plotted. Both methods provided good solutions that clearly outperformed the mean field solution. However, with the periodic boundary evolution the results were slightly better as the produced energy was lower and the model converged to a satisfying solution in less layers.
The right subplot contains the infidelity of the generated optimal states with the ground state of the problem Hamiltonian at each layer for both the periodic and the open boundary evolution. The observed fidelities are satisfying for both models as they are really close to 1. The performance of the periodic boundary evolution is slightly better.

The results were as expected. The main advantage of the evolution with the symmetry breaking Hamiltonian is that we can explore more eigenspaces and the optimisation procedure can be driven to paths that contain better solutions when the preservation of symmetry limits us from generating good solutions in more complex models. However, we have to mention that for the specific experiment, the performance of the symmetry preserving evolution, in terms of iterations of the classical optimisation procedure and the layers needed to reach a good approximation, is better. This is reasonable as with the specific procedure the search space is reduced, compared to the case of the symmetry breaking evolution. This can be clearly seen in Figure 11. The differences between the two approaches are small. It can be observed that when the open boundary Hamiltonian is used, the model converges after 6 layers, while for the case of the symmetry preserving evolution it converges between 4 and 5 layers.

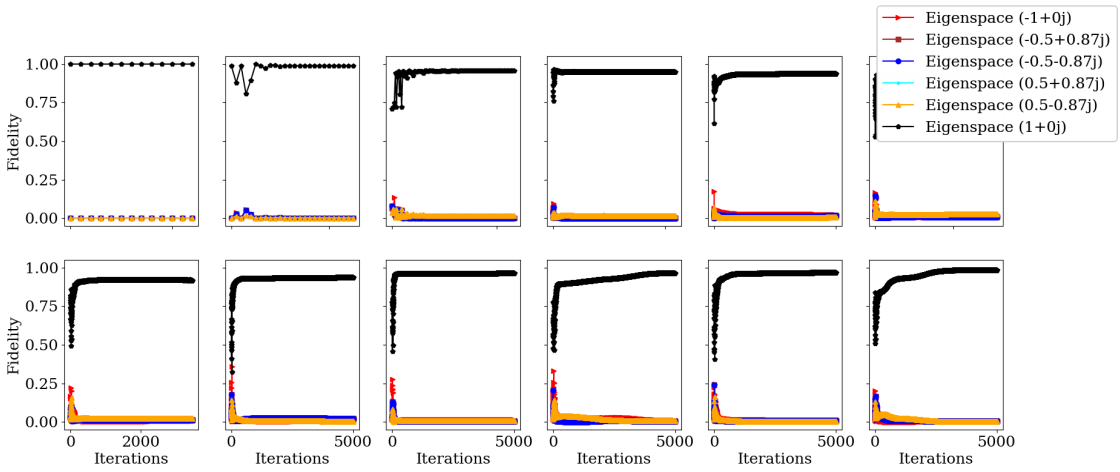


Figure 12: Each subplot of the Figure corresponds to the values of the fidelity of the produced state with every eigenspace, at each iteration of the model, for every layer, using the Open Boundary Hamiltonian for the evolution. The eigenspace of the initial state is the one corresponding to eigenvalue 1 of the cyclic group. The ground state of the Hamiltonian is also in the same eigenspace. The number of qubits that the Hamiltonians act on is 6. The findings are similar to those presented in Figure 10 for 4 qubits. The first subplot is for $p = 0$ (number of layers) and then p is increased by 1. The final plot corresponds to $p = 11$. For 6 qubits, the eigenspaces that do not contain the ground state of the Hamiltonian, are explored more. It is interesting to observe that the fidelity of the produced states with the eigenspace that contains the ground state is always close to 1. It is also clearer that when the produced energy is higher (worse), the fidelity of the equivalent state with the eigenspace that contains the ground state, becomes lower.

Figure 12 contains the same plots but this time for Hamiltonians that act on 6 qubits. The results are identical with the case of 4 qubits. We can see that now more eigenspaces exist. The number of eigenspaces that are created using the cyclic group, depends on the number of qubits that our system acts on. An interesting thing that we can derive from the specific plots is that the states that are produced have higher fidelity with the eigenspaces that do not contain the ground state. Especially for specific layers (e.g. $p = 7$), the produced states, for the first iterations of the classical algorithm, have fidelity close to 0.5 with the eigenspace that contains the ground state. From this we can derive that when the number of qubits is increased, the fidelity of the produced states with the eigenspace of the ground state can be reduced more.

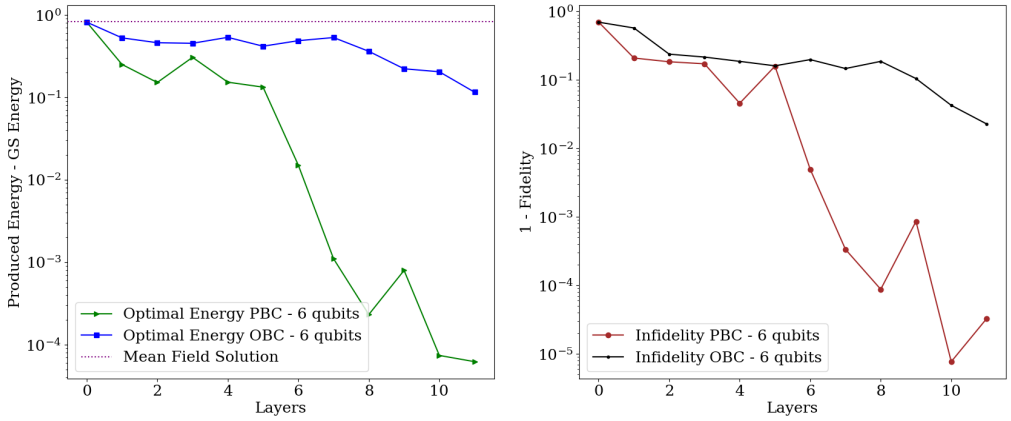


Figure 13: The Hamiltonians used act on 6 qubits and the eigenspace of the ground state is the same with the eigenspace of the initial state. The left subplot contains the difference between the ground state energy of the problem Hamiltonian and the optimal energy produced for each layer of the optimisation procedure when using the periodic and the open boundary boundary evolution. The mean field solution is also plotted. The proposed solutions are worse than those for 4 qubits as we expected. We can notice that the optimal energy produced from the open boundary evolution is clearly better than the mean field solution but it is not as good as the one for 4 qubits. Moreover the difference with the optimal energy of the periodic boundary evolution is higher.
The right subplot contains the infidelity of the generated optimal states with the ground state of the problem Hamiltonian at each layer for both the periodic and the open boundary evolution. The fidelity of the optimal state produced from the open boundary evolution is close to 1 but clearly the same amount for the periodic boundary evolution is better.

Figure 13 is identical to Figure 11 but this time for 6 qubits. We can see that the quality of solutions is worse than the solutions for 4 qubits, as we expected. Moreover, the difference in the convergence to a good solution between the two approaches is increased compared to Hamiltonians that act on 4 qubits. In this case, we can clearly denote that the performance of the periodic boundary evolution is better than the one of the open boundary evolution, both in terms of optimal energy produced and in terms of fidelity. However, the optimal energy produced with the open boundary evolution is close to the ground state and it is much better than the mean field solution.

4.4.2 Results for odd number of qubits

The performance of our approach was worse when the Hamiltonian had a degenerate ground space. This happens when the Hamiltonian acts on odd number of qubits. For those cases we had to make some modifications in order to compute the actual fidelity of the approximated ground state with the degenerate one. More specifically, we summed the fidelity of the generated states with each of the ground states.

Figures 14, 15 contain the results from the experiments that we made with Hamiltonians that act on 5 qubits. The plots are identical to those presented in the previous section.

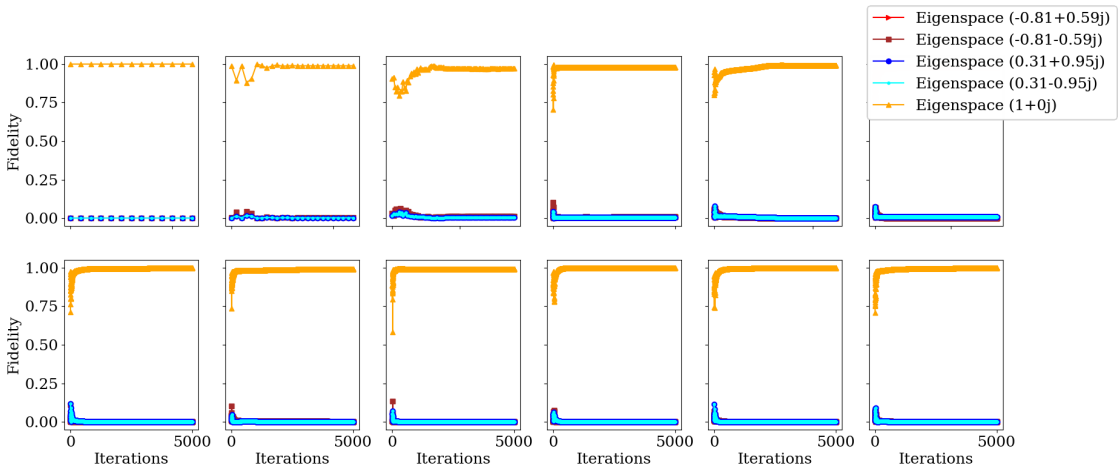


Figure 14: Each subplot of the Figure corresponds to the values of the fidelity of the produced state with every eigenspace, at each iteration of the model, for every layer, using the Open Boundary Hamiltonian for the evolution. This time the Hamiltonian acts on 5 qubits and its ground state is degenerate. The eigenspace of the initial state is the one corresponding to eigenvalue 1 of the cyclic group. The ground state of the Hamiltonian is also in the same eigenspace. We had to make some modifications to produce more accurate results for the fidelity of the generated states with the multiple ground states. The results are identical with those for 4 and 6 qubits. The first plot is for $p = 0$ (number of layers) and then p is increased by 1. The final plot corresponds to $p = 11$. We decided not to include the same plots for the case of Periodic Boundary Hamiltonian as there are no new findings that we can derive from this case, compared to those of 4 and 6 qubits.

We can claim that there is no big difference in the results compared to the Figures for 4 and 6 qubits without a degenerate ground state.

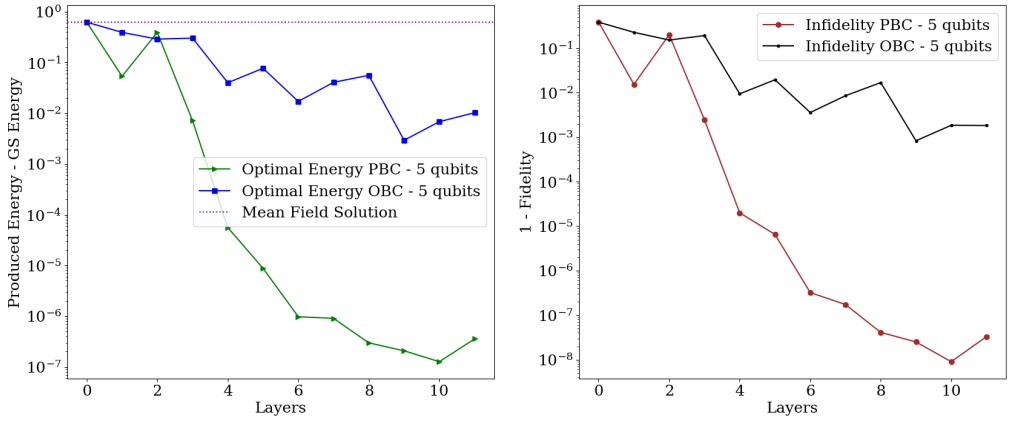


Figure 15: The Hamiltonians used act on 5 qubits and the eigenspace of the ground state is the same with the eigenspace of the initial state. The specific Hamiltonian contained a degenerate ground state and we had to make some modifications to efficiently compute the fidelities. The left subplot contains the difference between the ground state energy of the problem Hamiltonian and the optimal energy produced, for each layer of the optimisation procedure, when using the periodic and the open boundary boundary evolution. The mean field solution is also plotted. The periodic boundary evolution produced an impressively good approximation to the ground state energy of the Hamiltonian, which was better than the same approximation for 4 qubits. The open boundary evolution also produced a good approximation that was much better than the mean field solution but worse than the one produced from the periodic boundary evolution.
The right subplot contains the infidelity of the generated optimal states with the ground state of the problem Hamiltonian, at each layer, for both the periodic and the open boundary evolution. The results are extremely good for the periodic boundary evolution. The fidelity of the optimal state produced from the open boundary evolution is close to 1 but the difference with the optimal state of the periodic boundary evolution is high.

Figure 15 contains the optimal energy that was found at each layer minus with the ground state energy of the target Hamiltonian for evolution both with periodic and with open boundaries. On the right subplot, the infidelities of the produced states with the ground state of the problem Hamiltonian are plotted. The main fact that can be derived from the specific plots is that when the Periodic Boundary Hamiltonian is used for the evolution, the model converges faster and it produces better results. This is identical to the non degenerate cases. The difference in the performance between the two approaches depends on the number of qubits (for smaller number, smaller differences).

Eigenspace of the initial state different than the eigenspace of the ground state.
For all the previous cases, the ground state of the target Hamiltonian was in the same eigenspace with the ground state of the mixing Hamiltonian (initial state). It is interesting to see the results for a case where the ground state of the target Hamiltonian lies on a different symmetry sector compared to the initial state. This happens for the H_{ZZX} Hamiltonian with positive coupling constants that acts on 3 qubits. The ground state of the specific Hamiltonian was degenerate with multiplicity 4. This had a negative impact in the accuracy of the results, as the ground states belonged to more than one eigenspaces. In order to improve the results, we had to break the degeneracy. We achieved this by adding to our Hamiltonian some terms. A

sum of local Pauli Xs to all qubits and a XYZ term

$$H_D = H_{ZZX} + \sum_{j=0}^{2} \sigma_j^x \sigma_{j+1}^x + \sigma_0^x \sigma_1^y \sigma_2^z + \sigma_0^z \sigma_1^x \sigma_2^y + \sigma_0^y \sigma_1^z \sigma_2^x \tag{41}$$

We have to mention that for the specific case, we executed experiments with multiple initial states ($|++\rangle$, $|111\rangle$). We decided to demonstrate the results that were produced using as an initial state the $|111\rangle$. Starting from the specific state enhances the advantages of using a symmetry breaking Hamiltonian for the evolution of the optimisation procedure.

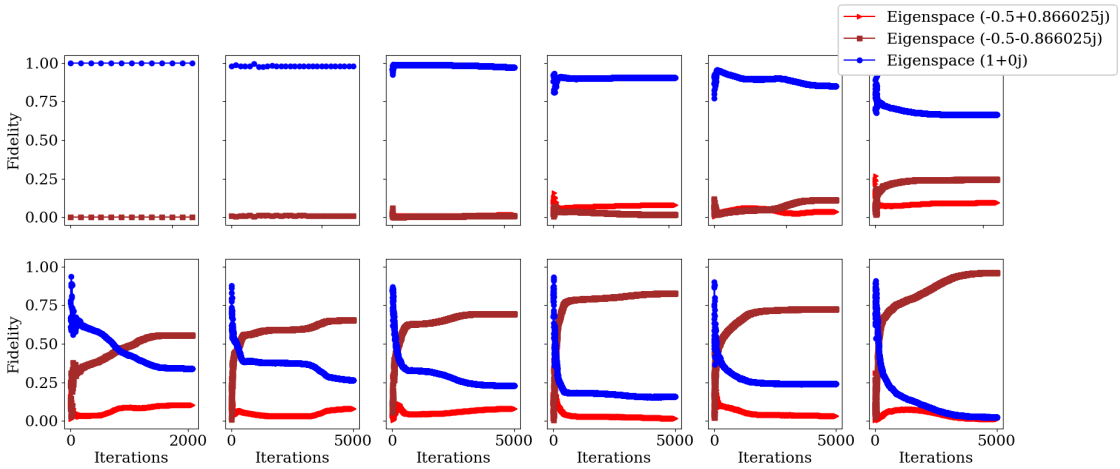


Figure 16: Each subplot of the Figure corresponds to the values of the fidelity of the produced state with every eigenspace, at each iteration of the model for every layer, using the Open Boundary Hamiltonian for the evolution. The number of qubits that the Hamiltonian acts on is 3 and it has positive coupling constants. For the specific case, the eigenspace of the ground state is different than the eigenspace of the initial state. More specifically, the initial state is in the eigenspace that corresponds to eigenvalue 1 while the ground state lies in the eigenspace that corresponds to eigenvalue $0.5 - 0.866i$ It is clear that all eigenspaces are explored. The eigenspace from which we start (eigenspace of the initial state) is different than the eigenspace of the optimal state. We can observe the evolution of the model and how the fidelities change. For less layers, where the quality of solutions is worse, the fidelities of the produced states with the eigenspace that contains the ground state are lower and then as p increases the specific fidelity almost reaches 1. Until $p = 6$ the initial eigenspace has the higher fidelity with the produced states. The first plot is for $p = 0$ (number of layers) and then p is increased by 1. The final plot corresponds to $p = 11$.

Figure 16 represents the evolution of the fidelity of the produced states with all eigenspaces, at each layer of the simulation of the quantum circuit, using the open boundary Hamiltonian for the evolution. It is clear that all the eigenspaces are explored. Because of this, it is possible to get a good approximation of the ground state. Without an evolution with an open boundary Hamiltonian, it would not be possible to get a good approximation. We start from a state that completely belongs to one eigenspace as it can be observed in Figure 16, in the first subplot. As the optimisation procedure evolves, the states that are produced, have higher fidelity with the eigenspace that contains the ground state, while the fidelity with the eigenspace of the initial state is reduced and approaches 0. As we expected, the energy of the generated states improves (decreases), when the fidelity of the produced states with the eigenspace of the ground state,

approaches 1. We can derive that the model begins to produce states that mostly belong to the eigenspace of the ground state for $p \geq 6$, with p denoting the number of layers of the quantum circuit. The left subplot of Figure 17 (a) contains the difference between the optimal energy that was produced after each layer, with the ground state energy, using both the periodic and the open boundary evolution. On the right subplot we have the infidelity of the produced states with the ground state of the problem Hamiltonian for both the periodic and the open boundary evolution. The differences in the results are clear. We can see that the approximation of the ground state when the open boundary Hamiltonian is used, is much better. In addition, the optimal energy produced with the symmetry preserving Hamiltonian is much worse than the mean field solution, which means that the results are bad. Moreover the fidelity of the generated states using the periodic boundary evolution are almost 0 for all layers. On the other hand, it can be observed that the performance of the open boundary evolution clearly improves when the number of layers is increased. This means that if we use more layers in our models we will most probably generate even better solutions. Figure 17 (b) contains the infidelities of the optimal states with the ground state of the Hamiltonian and with all eigenpsaces. From this plot we can notice that the the fidelity of the generated states with the ground state, and with the eigenspace that contains it, are almost identical. Moreover, the model needed 11 layers in order to produce a state with fidelity close to 1 with the eigenspace that contains the ground state.

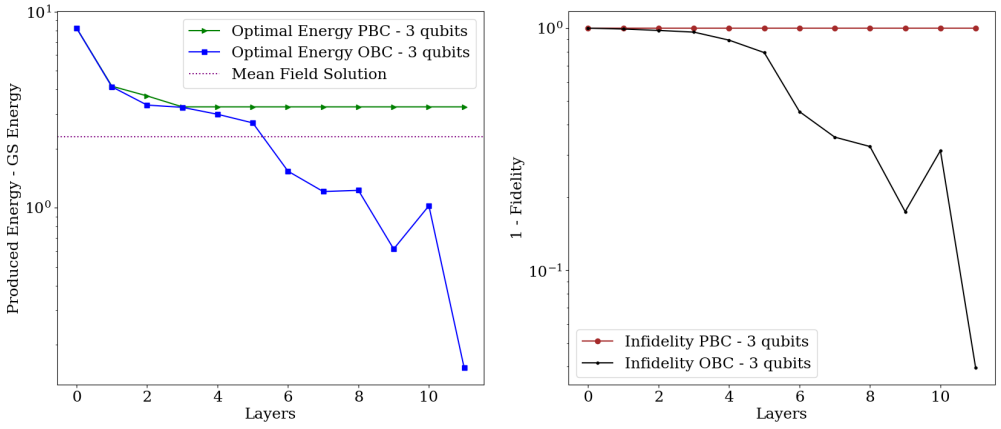
The specific case proves the main advantage of the evolution with an open boundary Hamiltonian. We can get good approximations even when the ground state of the target Hamiltonian is in different eigenspace than the one of the mixing Hamiltonian. It was proven that this was not possible for the periodic boundary Hamiltonian.

4.4.3 Evaluation of Results

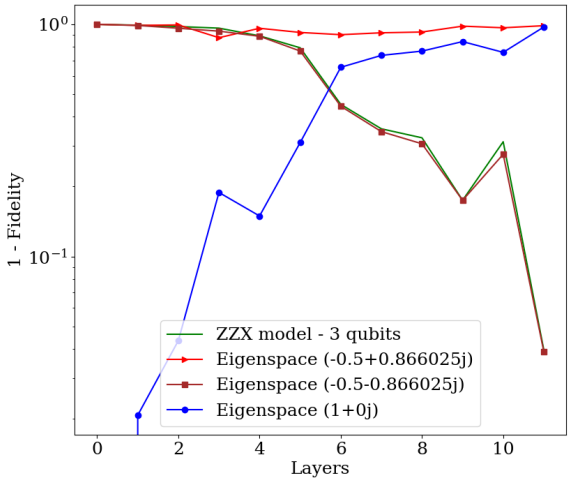
In Section 4.4 we showcased experiments that provided useful findings. Our goal was to answer the objectives that we declared in Section 1. More specifically, the experiments in this section gave us answers for Questions 1 and 2. For all the experiments we followed the same procedure and used the same parameters in order to be as consistent as possible. In all the experiments we used specific values for the coupling constants of the H_{ZZX} Hamiltonian ($j_x = -0.5$, $j_y = -1$, $j_z = -1$) and used the same procedure to generate the initial parameters. Moreover, we made experiments with more qubits, with different methods for initialising the initial parameters, with higher number of layers (p) for the simulation of the quantum circuit, and with modifications in the form of the target Hamiltonian. We decided that it is better not to demonstrate all of them, as the insights they provided were not crucial, and were similar to the cases that we analysed.

The results for most of the experiments that we implemented were satisfying. Most of our initial claims regarding the performance of the symmetry breaking evolution were verified from the results of the experiments. There were experiments whose results were difficult to explain but most of them were not related to the evolution of the system and the Hamiltonian that was used for it (e.g. the bad performance of both models for the ferromagnetic Hamiltonians for more than 4 qubits).

We think that the results we provided are useful in the evaluation of an optimisation procedure using an open boundary Hamiltonian, with the goal to approximate the ground state of a



(a)



(b)

Figure 17: (a) The Hamiltonians used act on 5 qubits and the eigenspace of the ground state is in a different eigenspace than the one of the initial state. The ground state of the Hamiltonian was degenerate and we made some modification to break this degeneracy. The left subplot contains the difference between the ground state energy of the problem Hamiltonian and the optimal energy produced, for each layer of the optimisation procedure, when using the periodic and the open boundary boundary evolution. The mean field solution is also plotted. The open boundary evolution clearly outperforms the periodic boundary evolution in terms of the optimal energy produced. The optimal energy of the periodic boundary evolution was much worse than the mean field solution which means its performance was bad. The optimal energy produced from the open boundary evolution was satisfying. The right subplot contains the infidelity of the generated optimal states with the ground state of the problem Hamiltonian, at each layer, for both the periodic and the open boundary evolution. The fidelity of the optimal state generated from the periodic boundary evolution is always close to 0. The performance of the open boundary evolution is promising.
(b) This plot contains the infidelities of the optimal states produced at each layer with the ground state of the Hamiltonian and with all eigenpsaces. The eigenspace that contains the ground state is the one that corresponds to eigenvalue $-0.5 - 0.866i$ of the cyclic group generator. The eignespace of the initial state is the one that corresponds to eigenvalue 1. It can be observed, that the fidelity of the generated states with the ground state and with the eigenspace that contains it, are almost identical. Moreover, the fidelity with the eigenspace of the initial state is reduced when the quality of solutions improves.

symmetry preserving Hamiltonian. From the experiments we enhanced our hypothesis that we can explore more solutions and avoid local optima where it is necessary and useful. It was clear that when we used the symmetry breaking Hamiltonian for the evolution of the system, we searched in an enlarged space as more eigenspaces were explored. This can be useful in many problems especially in cases where the preservation of symmetries leads us to local minima. In addition, we saw that when a periodic boundary Hamiltonian is used for the evolution, it is not possible to move to a different eigenspace. We can derive that the use of a symmetry preserving evolution is not efficient, as many times it is possible to get stuck in local minima. However, there is a difference in the layers and the time that the system needs to converge to an efficient approximation. The approach where a periodic boundary Hamiltonian is used, converges faster and most of the times gives us more accurate solutions especially for larger number of qubits. Despite this fact, we have to mention, that the margins are low. Moreover, there are many different techniques that can improve the symmetry breaking procedure and make it more efficient. In general, we can say that the advantages of the specific approach are clear. It can be useful in a wider area of problems than the original approach with a symmetry preserving evolution. Finally, due to the fact that the symmetry breaking evolution allows us to search for possible solutions in more eigenspaces, it may improve the performance of the algorithm even when the target ground state is in the same symmetry sector with the initial state, in more complicated models. This was proved in the work of Choquette et al. [6].

5 Minimum number of layers to produce states that will belong to a new eigenspace

In the optimisation procedure with an open boundary evolution, the states that are produced belong to one or more eigenspaces. In order to find the eigenspace that each produced state belongs, we must compute its fidelity with each of the projectors that represent the different eigenspaces. One of the main goals of the experiment was to determine the maximum amount of fidelity that can be moved to a new block (eigenspace), for one step of the optimisation procedure, using a Hamiltonian that does not preserve a symmetry. This will help us determine the minimum depth of the quantum circuit that will be necessary in order to completely move (change our search space) to a new eigenspace or at least produce states that will not only belong to the initial eigenspace. This amount is really useful, as it can help us in an optimisation procedure where the change of the eigenspace is necessary. Moreover, we have to mention, that this is not possible when we are using a symmetry preserving Hamiltonian for the evolution.

5.1 Evolution using Open Boundary Hamiltonian

In this section our goal is to answer Questions 3 and 4 that were stated in Section 1. As we mentioned, when the periodic boundary Hamiltonian is used in the optimisation procedure, the search space that the algorithm scans for possible solutions is reduced to a specific eigenspace. As a result, solutions that do not completely belong to the specific eigenspace are not explored. This may have a negative effect in the quality of the solutions that are produced, as it is possible to be limited from local optima.

We begin by defining the Hamiltonians that we want to examine. We have one Hamiltonian that has periodic boundaries and one with open boundaries. The general form of the

periodic boundary Hamiltonian is,

$$H_{PBC} = \sum_i H_{i,i+1}$$

while for the Open Boundary Hamiltonian we have,

$$H_{OBC} = H_{PBC} - H_{n-1,0}$$

with $H_{n-1,0}$ denoting the term that breaks the symmetry. We also know that when a group is used in order to create the block structure of the Hamiltonian for H_{PBC}, perfect blocks will be created. This does not hold for H_{OBC} as there will be parts outside the main blocks, that will have non-zero entries.

Our intention is to use H_{OBC} in order to be able to produce solutions that will not lie only in the eigenspace of the initial state. We know that this is not possible using H_{PBC} for the evolution. We assume that we start from a state

$$|\psi_0\rangle = \sum_{k=0}^{k-1} a_k |\psi^{(k)}\rangle$$

where k denotes the size of a specific block that the specific state lives in and $|\psi^{(k)}\rangle$ the eigenstates of block k. We also know that $\|\overrightarrow{\mathrm{a}}\|^2 = 1$. If we choose to start the evolution using H_{PBC} we will have:

$$e^{iH_{PBC}t}|\psi_0\rangle = \sum_{k=0}^{k-1} a'_k |\psi^{(k)}\rangle$$

But this, will leave us in the same eigenspace, as we know that $\|\overrightarrow{\mathrm{a}}'\|^2 = 1$ and also the inner product of the two is equal to 1 ($\langle\overrightarrow{\mathrm{a}}, \overrightarrow{\mathrm{a}}'\rangle = 1$). This means, that the two vectors are parallel since their norms are equal to 1. We also now that H_{PBC} commutes with the generator of the cyclic group (as a result they share an eigenbasis). This does not hold for H_{OBC} and the group generator.

What we want to investigate is what happens when we use H_{OBC} for the evolution. In this case we have:

$$e^{iH_{OBC}t}|\psi_0\rangle = \sum_{k} a''_k |\psi^{(k)}\rangle$$

This time we are not sure regarding the result of the inner product of the vectors $\overrightarrow{\mathrm{a}}, \overrightarrow{\mathrm{a}}''$. We can assume that there will be a lower bound like:

$$\|\langle\overrightarrow{\mathrm{a}}, \overrightarrow{\mathrm{a}}''\rangle\| \geq f(N)$$

The main objective that we wanted to test in the specific work is the effects of using an Open Boundary Hamiltonian for the evolution of the system, in a variational algorithm. The problem can be explained more formally like:

Consider a symmetry group G and a Hamiltonian H that commutes with a representation of G (G-invariant), an operator (mixing Hamiltonian) H_m that commutes with a representation of G (G-invariant) and a Hamiltonian h which does not commute with a representation of G (not

G-invariant) with $H_{OBC} = H - h$. Let us assume that $|h| = O(1)$. We want to approximate a state $|\psi_{final}\rangle$ starting from a state $|\psi_{init}\rangle$ that is in a different symmetry sector. Our ultimate goal will be to determine an upper bound for the quantity of fidelity of the produced state with a new eigenspace for a quantum circuit with 1 layer. This may allow us to make an assumption regarding the minimum number of layers needed for the quantum circuit in order for the produced quantum state to completely belong to a new block.

The quantity that we want to compute, mainly depends on the number of qubits that the Hamiltonian acts on, the initial state that we will choose, and the projectors of the symmetry sectors that are related to the symmetry group that we will use. As we mentioned in Section 3, we know the different structure of Hamiltonians after the block diagonalisation procedure. More specifically, H will only contain the blocks, h will not have a block structure and as a result, H_{OBC} will preserve the block structure but it will also have small blocks outside the main diagonal, with non-zero elements. We also know that the norm of the main blocks will be much larger than the norm of the secondary blocks.

The evolution of such a system can be achieved by using the following equation,

$$|\psi\rangle = e^{-iH_{OBC}t}|\psi_0\rangle. \tag{42}$$

We will mainly focus on the term $e^{-iH_{OBC}t}$. This term can be written as

$$e^{-iH_{OBC}t} = e^{-iH_{PBC}t}e^{iH_{n-1,0}t}e^{-i[H_{PBC},H_{n-1,0}]\frac{t^2}{2}}\dots \tag{43}$$

since H_{PBC} does not commute with $H_{n-1,0}$. This equation is a result of the Baker-Hausdorff formula [30]. We can derive that the amount of fidelity that can be moved to a new block in the evolution procedure only depends on the term $e^{iH_{n-1,0}t}$. This is because we already know that the term $e^{-iH_{PBC}t}$ cannot be used for the change of eigenspace as we observed in the previous section. We also know from Euler's formula, Taylor expansion and Maclaurin series [31] that the following holds

$$e^{-iht} = \cos(t)\mathbb{I} - i\sin(t)h \tag{44}$$

for any t and when $h^2 = 1$. For our matrices this does not hold, but we can get an insight regarding the maximum amount of fidelity that we will be able to move to a new block, for a single layer of the quantum circuit. The computation of an exponential is in general a difficult task. To make the computations easier, we can find the coefficients of the specific exponential matrix by using the polynomial of the exponential and the characteristic polynomial. We can use the Cayley-Hamilton Theorem [29] in order to find them. In our case, the exponential will be of the form

$$e^{iht} = A\mathbb{I} + Bh + Ch^2 + Dh^3 \cdots + Kh^{k-1} \tag{45}$$

and our goal will be to find the corresponding values for A, B, C, D, $\dots$, K, with K denoting the size of matrix h. We will explain in detail how we can compute those quantities for our Hamiltonians in the next section.

5.1.1 Cayley-Hamilton Theorem

In order to compute the coefficients that we described above, we can use the Cayley-Hamilton Theorem [29]. The specific theorem states that every matrix can be expressed as the polynomial

produced from the characteristic polynomial of the matrix with degree $n-1$ (for matrices with size $n \times n$). The characteristic polynomial of a matrix h with size $n \times n$ is the function

$$f(\lambda) = \det(h - \lambda \mathbb{I}_n) \tag{46}$$

with λ_0 being an eigenvalue of h if and only if $f(\lambda_0) = 0$. Moreover, we know that $f(\lambda)$ is a polynomial with degree n (equal to the size of h) and has the form

$$f(\lambda) = (-1)^n \lambda^n + (-1)^{n-1} \mathrm{Tr}(h) \lambda^{k-1} + \cdots + \det(h) \tag{47}$$

with $\det(h)$ being the constant term because of the following relation

$$f(0) = \det(h - 0\mathbb{I}_n) = \det h.$$

It is also useful to define the matrix polynomial. We know that for a matrix h with size $n \times n$ we have:

$$P(h) = \sum_{i=0}^{n} a_i h^i = a_0 \mathbb{I} + a_1 h^1 \dots a_n h^n \tag{48}$$

with the eigenvalues of h being the roots of $P(h) = 0$.

More specifically, Cayley-Hamilton theorem states that a square matrix will satisfy its own characteristic polynomial equation. This means that it is possible to replace the eigenvalues (λ_i) of the matrix, with the matrix itself, and this will be equal to 0 as well.

$$P(h) = h^n + a_{n-1} h^{n-1} + \cdots + a_1 h + a_0 \mathbb{I} \tag{49}$$

The main consequence of the Cayley-Hamilton theorem is that any analytic function of a matrix h with size $n \times n$ can be rewritten as a polynomial with degree at most $n-1$ like,

$$P(h) = a_{n-1} h^{n-1} + \cdots + a_1 h + a_0 \mathbb{I} \tag{50}$$

with the constant term being $a_0 = \det(h)$ and $a_{n-1} = Tr(h)$.

Given all the above, we know that we can write the exponential matrix of a matrix h with size $n \times n$ like,

$$e^{iht} = a_0 \mathbb{I} + a_1 hi + \cdots + a_{n-1} h^{n-1} i^{n-1} \tag{51}$$

with the eigenvalues of h ($\lambda_1, \dots \lambda_n$) known.

This means that the coefficients ($a_0, \dots a_{n-1}$) can be determined from the following equations:

$$\begin{gathered} e^{i\lambda_1 t} = a_0 + a_1 \lambda_1 i + \cdots + a_{n-1} (\lambda_1 i)^{n-1} \\ \vdots \\ e^{i\lambda_n t} = a_0 + a_1 \lambda_n i + \cdots + a_{n-1} (\lambda_n i)^{n-1} \end{gathered}$$

From Euler's Formula we know that: $e^{ix} = \cos x + i \sin x$. We can write:

$$\begin{gathered} e^{i\lambda_1 t} = \cos(\lambda_1 t) + i \sin(\lambda_1 t) \\ \Rightarrow \cos(\lambda_1 t) + i \sin(\lambda_1 t) = a_0 + a_1 \lambda_1 i + \cdots + a_{n-1} (\lambda_1 i)^{n-1} \\ \vdots \\ e^{i\lambda_k t} = \cos(\lambda_n t) + i \sin(\lambda_n t) \\ \Rightarrow \cos(\lambda_n t) + i \sin(\lambda_n t) = a_0 + a_1 \lambda_n i + \cdots + a_{n-1} (\lambda_n i)^{n-1} \end{gathered}$$

From the above equations we can determine the values of all the coefficients. We can derive that they will be related to $\cos(\lambda_j t)$ and $\sin(\lambda_j t)$ so they will have a periodic behavior.

5.1.2 Vandermonde Matrix

Another way to compute the coefficients $(a_0, \ldots, a_{n-1})$ mentioned in the previous section, is to use the Vandermonde Matrix [28]. The specific matrix is used for polynomial interpolation at a set of points and is denoted as follows:

$$V = \begin{bmatrix} 1 & x_1 & x_1^2 & \ldots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \ldots & x_2^{n-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n-1} & x_{n-1}^2 & \ldots & x_{n-1}^{n-1} \end{bmatrix}$$

The specific matrices have a determinant that can be easily computed:

$$\det(V) = \prod_{1 \le i < j \le n} (x_j - x_i).$$

In order to find the coefficients of a Polynomial using the Vandermonde Matrix, we have to use a specific set of points (inputs and outputs). In general, the coefficients can be found from the following equation:

$$[a_0, a_1, \ldots, a_n]^T = V^{-1}[y_1, y_2, \ldots y_n]^T$$

In our case we have:

$$e^{iht} = a_0 I + a_1 hi + a_2 h^2 i^2 + \cdots + a_{n-1} h^{n-1} i^{n-1}$$

$$\begin{bmatrix} 1 & h_1 i & h_1^2 i^2 & \ldots & h_1^{n-1} i^{n-1} \\ 1 & h_2 i & h_2^2 i^2 & \ldots & h_2^{n-1} i^{n-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & h_n i & h_n^2 i^2 & \ldots & h_n^{n-1} i^{n-1} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

More specifically we can write the above as:

$$\begin{bmatrix} 1 & \lambda_1 i & \lambda_1^2 i^2 & \ldots & \lambda_1^{n-1} i^{n-1} \\ 1 & \lambda_2 i & \lambda_2^2 i^2 & \ldots & \lambda_2^{n-1} i^{n-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & \lambda_n i & \lambda_n^2 i^2 & \ldots & \lambda_n^{n-1} i^{n-1} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{bmatrix} = \begin{bmatrix} e^{i\lambda_1 t} \\ e^{i\lambda_2 t} \\ \vdots \\ e^{i\lambda_n t} \end{bmatrix}$$

With this equation, we can find the appropriate values for the coefficients $a_0, \ldots, a_{n-1}$.

Taking those into account, we can derive that it is important to compute the inverse of the Vandermonde Matrix. As we know, the inverse of a matrix is related to its determinant. The Vandermonde Matrix has a specific form for its determinant which is much more simple for squared Vandermonde Matrices which is identical to our case. We can derive, that the Vandermonde determinant is non-zero, if and only if all x_i are distinct. This is important because if the determinant is zero then we cannot invert the matrix.

5.1.3 Coefficients of the Polynomial for Exponential Matrix

In the previous sections we described the methods we can use in order to calculate the values of the coefficients for the polynomial form of the exponential matrix. As we mentioned, it is really useful to find those coefficients as we are interested in computing the value of the exponential $e^{iH_{n-1,0}t}$. We intend to use this exponential to calculate the resulting state from the evolution of the system, using the term that breaks the symmetry of the Periodic Boundary Hamiltonian. By this, we will be able to determine the maximum amount of fidelity that can be moved to a new eigenspace using one layer of the quantum circuit in a QAOA procedure.

We know that we can write $e^{iH_{n-1,0}t}$ as a polynomial like

$$e^{iH_{n-1,0}t} = a_0 I + a_1 H_{n-1,0} i + \cdots + a_{n-1} H_{n-1,0}^{n-1} i^{n-1} \tag{52}$$

with n representing the number of qubits that the Hamiltonian acts on. For simplicity, we can assume that $n = 4$ in our experiments. Using one of the methods described above we can efficiently calculate all the coefficients $a_0, \dots a_3$ of the polynomial. From the analytical explanation, and by using the Cayley-Hamilton theorem, we saw that the values of the coefficients depend on some cosines and sines. More specifically those cosines and sines depend on the eigenvalues of the Hamiltonian that we are using, which are constant, and on t which can take multiple values. Due to the fact that the values depend on cosines and sines we know they will have a periodic behavior. As a result, it is not necessary to make experiments using infinite values for t. When those coefficients change, the exponential matrix $e^{-iH_{n-1,0}t}$ is going to change, and this will have an effect of the resulting state, as it is computed from the following equation:

$$|\psi'\rangle = e^{-iH_{3,0}t}|\psi_0\rangle \tag{53}$$

for $n = 4$. The next step is to compute the fidelity of the resulting state $|\psi'\rangle$ with the projectors that are formed from a representation of a symmetry group G. In our experiments we prefer to form the eigenspaces using the cyclic group. The fidelity values will determine which is the maximum amount that can be moved to a new block (different than the one that the initial state belongs).

5.2 Moving in new blocks

We made an actual experiment in order to determine which is the maximum amount of fidelity that can be moved to a new eigenspace (different than the eigenspace of the initial state). We utilised the breaking symmetry term $H_{n-1,0}$ of the periodic boundary Hamiltonian that we used in our previous experiments. The periodic boundary Hamiltonian is the ZZX Hamiltonian of the Quantum Heisenberg Model,

$$H_{ZZX} = \sum_{j}^{n} (J_x \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \sigma_j^z \sigma_{j+1}^z) \tag{54}$$

with $n = 4$. The breaking symmetry term of the above Hamiltonian contains only the connections of the last qubit (3) with the first (0). It has the following form

$$H_{3,0} = J_x \sigma_3^x \sigma_0^x + \sigma_3^y \sigma_0^y + \sigma_3^z \sigma_0^z \tag{55}$$

with $J_x = -0.5$, $J_y = -1$ and $J_z = -1$. For the implementation of the experiment we also need an initial state. We chose to use the ground state of the sum of Pauli Z matrices for 4 qubits which is equal to $|1111\rangle$ because it is easy to compute and find the eigenspace that it belongs. Another advantage is that the specific state is the one that we used as an initial state in most of the experiments.

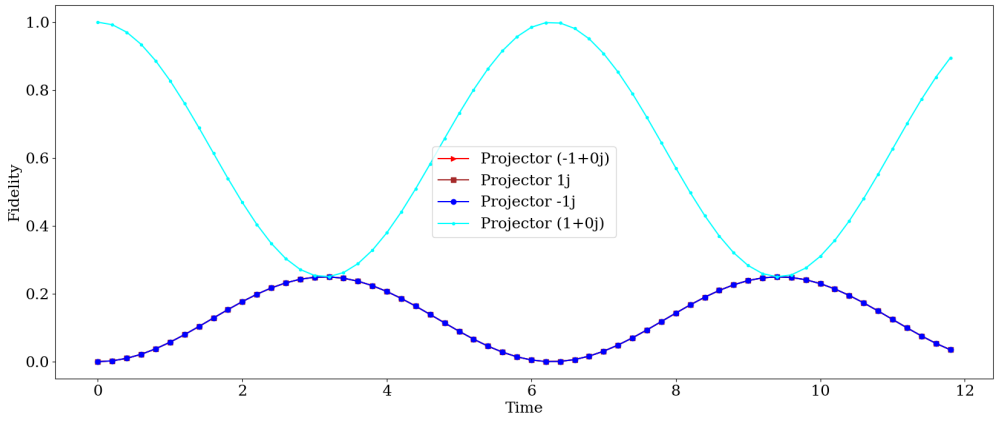
5.2.1 Maximum amount of fidelity that can be moved to new block

In the previous section we described all the necessary steps that are necessary to implement the experiment. We used the following equation

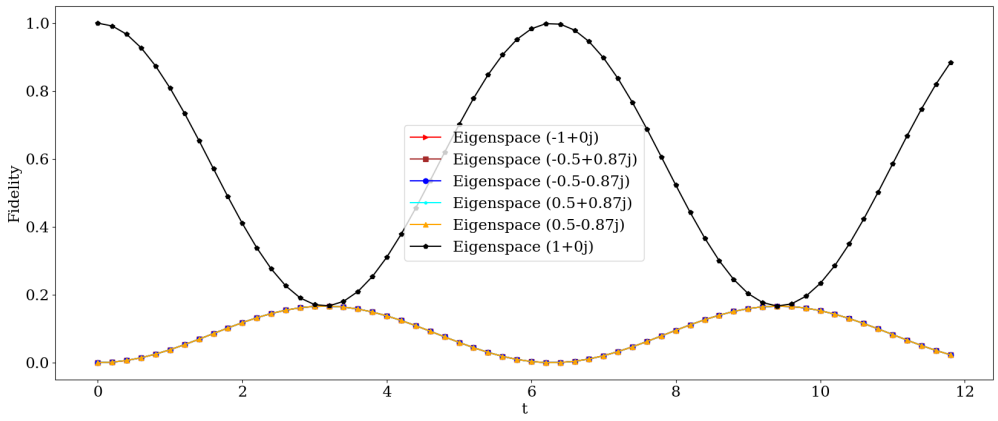
$$|\psi'\rangle = e^{-iH_{3,0}t}|\psi_{init}\rangle \tag{56}$$

to compute a new state $|\psi'\rangle$, that was produced from the evolution with a symmetry breaking term. We used different values for t at each iteration. The next step was to compute the fidelities of all the resulting states with the projectors of eigenspaces. We know that the initial state we used, belongs to the eigenspace that corresponds to eigenvalue 1 of the cyclic group generator. This means that we want to check the fidelity of the resulting states with the other three projectors. This quantity will correspond to the maximum amount of fidelity that can be moved to a new eigenspace in an optimisation procedure (e.g. QAOA).

Figure 18 contains the results from the experiments that we implemented using the method that we described above. There are two plots that correspond to different number of qubits. In Figure 18 (a) we used a Hamiltonian that acts on 4 qubits, while in Figure 18 (b) we used a Hamiltonian that acts on 6 qubits.



(a)



(b)

Figure 18: (a) Results that represent the fidelity of the resulting states that are produced for different values of t with the projectors that are formed from the cyclic group generator (the fidelities of the resulting states with the new eigenspaces are all equal, and that is why only one line is visible). The Hamiltonian that was used for the evolution acts on 4 qubits. The maximum amount of fidelity that can be moved to a new eigenspace is almost 0.25. The periodic behavior is also clear.
(b) Results that represent the fidelity of the resulting states that are produced from different values of t with the projectors that are formed from the cyclic group generator (the fidelities of the resulting states with the new eigenspaces are all equal, and that is why only one line is visible). The Hamiltonian that was used for the evolution acts on 6 qubits. The maximum amount of fidelity that can be moved to a new eigenspace is almost 0.17 and the periodic behavior is again clear.

We can clearly see that the values of the fidelities are periodic as expected. We can also observe that the maximum amount of fidelity that can be moved to a new eigenspace is not the same for different number of qubits. When the number of qubits increases, the maximum amount of fidelity that can be moved is reduced. We can notice that the maximum amount of fidelity that is moved to a new block for 4 qubits it is close to 0.25 while for 6 qubits is almost 0.17. Those quantities are equal to $\frac{1}{4}$ and $\frac{1}{6}$ respectively. As a result, we can denote that the maximum amount of fidelity that can be moved to a new eigenspace is close or almost equal to $\frac{1}{n}$, with

n being the number of qubits that the Hamiltonian acts on. However, this is not proven yet as it holds only for a quantum circuit with 1 layer.

Through the experiments that we performed, we were able to determine the maximum amount of fidelity that can be moved to a new eigenspace (different than the one of the initial state) for a quantum circuit with depth (number of layers) 1. This amount is almost equal to $\frac{1}{n}$ with n being the number of qubits that the Hamiltonian acts on. This quantity is useful, as it may help us determine the minimum number of layers that the quantum circuit must have, in order to produce states that will completely belong to a new eigenspace. This can be a crucial observation as it can be utilised to save computational resources and time, by using exactly the necessary layers.

Based on the results from the numeric experiments that we made, we can make an assumption that if we increase the number of layers, the quantity that will be moved to a new block will be proportional to the maximum quantity that was moved with 1 layer. If this holds, we will be able to get states that will completely belong to a new eigenspace using at least n layers, with n denoting the number of qubits that the Hamiltonian acts on. However, this assumption is not valid and we cannot prove that this will hold as we are not sure about what happens when the number of layers increases. That is why we must make more experiments using deeper circuits.

6 Conclusion and Future Work

To conclude, we investigated the performance and the results from the implementation of an optimisation procedure, based on Quantum Approximate Optimisation Algorithm on a minimisation problem of approximating the ground state of a quantum Hamiltonian. The objective function that we used was quantum. The interesting aspect of the specific method, is that it uses an open boundary Hamiltonian (Hamiltonian that does not preserve a symmetry) for the evolution of the system. The main advantage that erupts from such a method is that we are able to search for possible solutions in different eigenspaces than the one of the initial state of the problem. As a result, we are able to avoid getting stuck in local minimums. With the experiments that we performed, we proved that using an open boundary Hamiltonian for the evolution of the procedure, it is possible to change the eigenspace and thus get much better solutions in problems where the ground state is in a different eigenspace than the eigenspace of the initial state. Using a periodic boundary Hamiltonian (preserves a symmetry) for the evolution in the same problem, the result was quite bad, as we stacked in a local minimum after few iterations. We also performed experiments using both methods in problems where the ground state of the Hamiltonian was in the same eigenspace with the one of the initial state. We noticed that despite the fact that the ground and the initial state were in the same eigenspace, when we used the open boundary Hamiltonian for the evolution, the algorithm produced states that did not completely belong to this eigenspace. This means, that it searched for solutions in different eigenspaces as well, while the periodic boundary evolution only produced solutions that completely belonged to the target eigenspace. The results produced with the open boundary evolution were satisfying. Although we have to mention that in terms of performance (time and iterations needed), in the specific experiments, the periodic boundary evolution was more efficient. This is reasonable as the space where it searches for solutions was much smaller compared to the one of the open boundary evolution. However, if

the same method was applied to a more complex model, like the one utilised in [6], maybe the symmetry breaking evolution would have better results. Another important aspect of the specific work, was to determine the maximum quantity (in terms of fidelity) that we can move to a new eigenspace (different than the one of the initial state) for 1 layer of the quantum circuit. This quantity corresponds to the fidelity of the produced state with the projectors of the different eigenspaces that are created from a symmetry group G. It is important, because it can helps us determine the minimum depth (number of layers) of the quantum circuit required, to produce states that will completely belong to a new eigenspace. We managed to find analytically the values that the specific quantity depends on, and to compute them for specific examples. In the experiments that we performed, we saw that the fidelity of the produced states follow a periodic behavior and the values depend on $cosine$ and $sine$ of the eigenvalues of the Hamiltonian and time t. Another interesting observation, was that it is related to the number of qubits that the Hamiltonian acts on, as for the experiments that we run, the value was almost equal to $\frac{1}{n}$ with n being the number of qubits for 1 layer of the quantum circuit.

Despite the fact that we managed to produce some useful results with the experiments that we implemented, there are many suggestions for future work. First, more experiments can be performed using more qubits and bigger depth (number of layers) for the quantum circuit. Another improvement that can be implemented is the use of the original QAOA procedure by constructing an actual quantum circuit instead of using exponentials. This may help us implement a similar procedure in an actual near-term device. It will be useful to test the specific method for the approximation of the ground state in more complicated models than the Quantum Heisenberg Model, in order to test its performance and evaluate the effects of symmetry breaking evolution. We can also use different terms for breaking the symmetry of the problem Hamiltonian and test if this will have an effect in the quality of the produced results. In addition, it is really important to perform more experiments for the maximum amount of fidelity that can be moved to another block with a quantum circuit that will have more layers. This can help us check if our claim regarding the minimum depth required to completely move to a new eigenspace, is valid. On top of that, by running such experiments with a deeper quantum circuit, we will be able to derive more insights regarding the performance and the efficiency of the method for moving around blocks. We also expect that the specific, or a similar method, can be implemented to real-world problems that could not be solved efficiently with the existing methods. We proved in Section 4.4.2, that it helps us avoid local minimums, and explore larger spaces. There is also the work of Bravyi et al [35] that highlights some drawbacks from the preservation of symmetries. This can be enhanced by the fact that algorithms used in near-term quantum devices are improving, and their accuracy becomes even better. Thus we expect that more problems will be solved using quantum algorithms. An example is the work made by Huggins et al. [33], where they used Variational Quantum Algorithms in near term devices for computations in quantum chemistry, which were infeasible a few years before. Moreover, new techniques of error suppression [34], [39] in such devices are explored. As a result, we expect that techniques such the one that is proposed in this work, will be useful and implemented on actual problems.

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A Evaluation of method in [3]

Tavakoli et al. in [3], propose a different way to achieve a block formation for a Hamiltonian. It is an interesting method as they try to perform a block diagonalisation of Hamiltonians without using complicated group theory that may prove difficult to understand. This makes their method simpler. Their goal is to propose an algorithm that will perform an irreducible representation of for each of the blocks that the matrix will have. This means that they first use an initial change of basis to achieve a partial block diagonalisation. This will create some isotypic components that will divide the vector space in different eigenspaces. Then, they intend to use another change of basis in order to make each isotypic components irreducible (create smaller blocks that cannot be reduced). They state that with two random Hamiltonians and an abelian group we can perform a block diagonalisation. They only use the abelian group for the initial change of basis of the Hamiltonians (in order to create the partial isotypic components). The different isotypic components that the matrix contains are handled individually. As we will explain in our implementation of their method, they use one Hamiltonian to change the basis of the other.

$$\begin{pmatrix} L_{11}(Y_1^T Y_1) & L_{12}(Y_1^T Y_2) & \dots & L_{1m}(Y_1^T Y_m) \\ L_{21}(Y_2^T Y_1) & L_{22}(Y_2^T Y_2) & \dots & L_{2m}(Y_2^T Y_m) \\ \vdots & \vdots & & \vdots \\ L_{m1}(Y_m^T Y_1) & L_{m2}(Y_m^T Y_2) & \dots & L_{mm}(Y_m^T Y_m) \end{pmatrix}$$

This is the most important matrix that the authors use to change the basis of the Hamiltonian. According to their intuition, this matrix always have a specific structure, thus it can be used to change the basis of the corresponding isotypic of the Hamiltonian. In order to achieve the irreducible representation this matrix must only contain small identity-like matrices. The authors of [3] chose to focus on the change of basis of the first isotypic component for simplicity.

We will make a description of how their method work and we also want to check if it holds for every Hamiltonian. Hence, the exposition until the end of section will be taken from [3]. For simplicity, we can suppose that we have a matrix Λ that is constructed by using the elements that the first block (isotypic component) L^1 contains like:

$$\Lambda = L_1 \otimes \mathbb{I} = \begin{pmatrix} L^1_{11} \otimes \mathbb{I} & L^1_{12} \otimes \mathbb{I} & \dots & L^1_{1m} \otimes \mathbb{I} \\ \vdots & & & \vdots \\ L^1_{m1} \otimes \mathbb{I} & L^1_{m2} \otimes \mathbb{I} & \dots & L^1_{mm} \otimes \mathbb{I} \end{pmatrix}, L \in \mathbb{R}^{m \times m}$$

and in order to find the new change of basis for the irreducible representation we can begin by finding the spectral decomposition of the specific matrix. From this we can get a diagonal matrix that will contain the eigenvalues of L^1 that are independent from the change of basis,

$$D \otimes \mathbb{I} = \begin{pmatrix} \lambda_1 \otimes \mathbb{I} & 0 & 0 & 0 \\ 0 & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \lambda_m \otimes \mathbb{I} \end{pmatrix}$$

where λ_1, λ_m are the eigenvalues of L^1.

The main intention is to find the matrix which will manage to perform a change of basis to D, but by keeping it diagonal. It is not possible to find a non-trivial unitary change of

basis for this task, because if the change of basis is diagonal, the eigenvalues will change. We must try to create a matrix that will have a form like

$$Y = \mathbb{I} \otimes U = \begin{pmatrix} U & 0 & 0 & 0 \\ 0 & U & 0 & 0 \\ 0 & 0 & U & 0 \\ 0 & 0 & 0 & U \end{pmatrix}.$$

This means, that if we make an attempt to change the basis of D using Y, we will get a new matrix which will be:

$$Y^\dagger D Y = \begin{pmatrix} U^\dagger \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_1 \end{pmatrix} U & 0 \\ 0 & U^\dagger \begin{pmatrix} \lambda_m & 0 \\ 0 & \lambda_m \end{pmatrix} U \end{pmatrix}$$

The small matrices that are formed in $Y^\dagger D Y$ can be simplified as they are proportional to identity like

$$U^\dagger \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_1 \end{pmatrix} U = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_1 \end{pmatrix}$$

and this will hold for every U. The main question is if this change of basis will hold for more general Y, that will leave it invariant.

If all of the things that we described above hold for a more general matrix Y, then the following must be correct.

$$(Y_1^T Y_m)(Y_2^T Y_m)^T = Y_1^T Y_2$$

We performed an experiment using the specific procedure with a random Hamiltonian that acts on 4 qubits. The result that we expected and that would prove that the specific procedure holds for general cases, was identical to the initial matrix L.

The procedure that we followed to check if their claims are accurate for more general cases started by creating two random Hamiltonians that contain 4 qubits. We also made them Hermitian. Then, we used one of the abelian groups (cyclic) in order to perform the first change of basis for our Hamiltonians. The next step was to compute the eigenvectors of one of the two Hamiltonians (after the change of basis with the cyclic group), which is utilised to change the basis of the other. We are going to focus on one of the blocks, as we mentioned. We choose the group which has a diagonal that is proportional to identity. For our Hamiltonian, it had the following form,

$$\begin{pmatrix} 0.07 & 0 & 0.08 & 0.15 & -0.26 & 0.02 \\ 0 & 0.07 & 0.15 & -0.08 & 0.02 & 0.26 \\ 0.08 & 0.15 & 0.23 & 0 & -0.2 & 0.01 \\ 0.15 & -0.08 & 0 & 0.23 & -0.01 & -0.2 \\ -0.26 & 0.02 & -0.2 & -0.01 & -0.3 & 0 \\ 0.02 & 0.26 & 0.01 & -0.2 & 0 & -0.3 \end{pmatrix}$$

From this, we can create the matrix that can change the basis of this block. The goal is to find the appropriate change of basis for the irreducible representation by using the elements of the corresponding isotypic component. They achieve this by putting its first rows in a new matrix in a diagonal form like

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.08 & 0.15 & 0 & 0 \\ 0 & 0 & 0.15 & -0.08 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.26 & 0.02 \\ 0 & 0 & 0 & 0 & 0.02 & 0.26 \end{pmatrix}$$

This corresponds to the matrix Y, from the description of the method in [3] which contains the elements of U in a diagonal form. We use this matrix in order to change the basis of the block (isotypic component). We expect that the result will be similar to the matrix L of [3] which contains parts that are proportional to identity. The results were

$$\begin{pmatrix} 0.068 & 0 & 0.029 & 0 & 0.068 & 0 \\ 0 & 0.068 & 0 & 0.029 & 0 & 0.068 \\ 0.029 & 0 & 0.007 & 0 & 0.004 & -0.008 \\ 0 & 0.029 & 0 & 0.007 & 0.008 & 0.004 \\ 0.068 & 0 & 0.004 & 0.008 & -0.02 & 0 \\ 0 & 0.068 & -0.008 & 0.004 & 0 & -0.02 \end{pmatrix}$$

As it can be observed, it contains parts that are not proportional to identity. This means that the proposed method does not hold for a random Hamiltonian that acts on 4 qubits. Another way to understand this, is by checking if the following equation holds

$$(Y_1^T Y_m)(Y_2^T Y_m)^T = Y_1^T Y_2.$$

In our case, we have to check this by using Y_1, Y_2, Y_3 and more specifically, according to [3] we know that

$$Y_1^T Y_2 = \begin{pmatrix} 0.08 & 0.15 \\ 0.15 & -0.08 \end{pmatrix}$$
$$Y_1^T Y_3 = \begin{pmatrix} -0.26 & 0.02 \\ 0.02 & 0.26 \end{pmatrix}$$
$$Y_2^T Y_3 = \begin{pmatrix} -0.2 & 0.01 \\ -0.01 & -0.2 \end{pmatrix}$$

We then have to normalise those matrices and check if the following equality holds

$$Y_3^T Y_2 = (Y_1^T Y_3)^T (Y_1^T Y_2).$$

If the above equation is correct, then the multiplication between $Y_3^T Y_2$ and $Y_2^T Y_3$ must return the identity matrix which is not the case as the result we got was

$$(Y_3^T Y_2)(Y_2^T Y_3) = \begin{pmatrix} 0.45 & 0.89 \\ -0.89 & 0.45 \end{pmatrix}$$

The above results prove, that the specific method does not hold for the case of two random Hamiltonians that act on 4 qubits. This means it is not a general method that can be used for the irreducible block diagonalisation of an arbitrary Hamiltonian. That is why we decided to use another method for the change of basis procedure in our experiments that was described in Section 3.