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Searching for quantum circuits preparing maximally multipartite entangled states

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Streszczenie In this work genetic programming is applied to the problem of generating maximum entanglement in multi-qubit systems of different structures. We provide quantum circuits that prepares multipartite entangled states in systems consisting of up to 8 qubits. We present results pertaining to the minimum size of a quantum circuit preparing a maximally entangled multi-qubit state in cases of reduced sets of quantum gates that correspond to spin chain quantum systems.

Keywords: quantum systems, multi-qubit systems.

1. Introduction

There is a significant difference between the classical and quantum information theory. Theory of quantum information provides a number of unique concepts which have no classical analogue. These concepts make quantum information theory a more complex field of research and enable to develop techniques that cannot be formed within limits of the classical theory.

One of the key resources in the quantum information theory is entanglement [1, 2]. Most generally the nature of entanglement is that two particles can be connected and can influence each other instantly regardless of the distance separating them. In particular that means that a change of state of one of the particles, such as its measurement, can cause changes to the state of the other particle. Such connection cannot be explained in terms of the classical theory.

In mathematical terms, state $|\psi\rangle$ is separable if it can be represented as a tensor product of two states:

$$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle. \tag{1}$$





If a state cannot be written as in Eq. 1 it is called an entangled state. In the case of a system consisting of more than two subsystems, one can introduce a definition of an m-separable state.

Definition 1 State $|\psi\rangle \in \mathbb{C}^{2^n}$ is m-separable if it can be represented as a tensor product of m states and cannot be represented as a tensor product of m + 1 states

$$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \otimes |\psi_3\rangle \otimes \ldots \otimes |\psi_m\rangle, \tag{2}$$

where $|\psi_i\rangle \in \mathbb{C}^{2^{n_i}}$, $i = 1, \dots, m$ and $\sum_{i=0}^m n_i = n$.

Even though the definition of the basic criteria determining whether a state of a complex system is entangled or not is not difficult [3, 4] a systematic way of determining a quantitative measure of entanglement is not provided. Since there is no clear definition of quantitative value of entanglement for multipartite entanglement, there exists a number of non-equivalent entanglement measures. Moreover, it is not easy to distinguish bipartite entanglement between the subsystems from truly multipartite entanglement.

In bipartite systems we can introduce a number of entanglement measures such as entropy of the Schmidt numbers and teleport capacity from distillation. In a 2-qubits system states which maximize all that features are $|\psi^{\pm}\rangle = (|00\rangle \pm |11\rangle)/\sqrt{2}, |\phi^{\pm}\rangle = (|01\rangle \pm |10\rangle)/\sqrt{2}$ called Bell basis states. Such determinism in selecting the maximally entangled states is possible only in the case of bipartite states. In the case of systems consisting of many particles divided into two subsystems the maximally entangled states are the ones with maximally mixed reduced states.

Definition 2 State $\rho \in D(\mathcal{X} \otimes \mathcal{Y})$, dim $(\mathcal{X}) \ge \dim(\mathcal{Y}) = n$ is maximally entangled if and only if the reduced state is maximally mixed: $\operatorname{Tr}_{\mathcal{X}}(\rho) = 1/n$ i.e. $S(\operatorname{Tr}_{\mathcal{X}}(\rho)) = n$.

Any generalization of Bell states such as $|\psi\rangle = |00...00\rangle + |11...11\rangle$ in more than tree-partite systems leads to states that are proven not to be maximally entangled in the sense of multipartite entanglement [5, 6, 7]. Lack of any scalable structure of maximally entangled states makes it hard to find any representatives for complex systems. Multipartite states has been characterized [8] and known results in this field are obtained using numerical optimization methods [9, 10]. The optimization problem was rigorously characterized using a statistical mechanics framework with analysis of the entanglement frustration problem and the process of entanglement generation by Facchi et al. [11, 12, 13, 14]. In this paper we use genetic programming(GP) for this purpose [15, 16, 17].

The key matter in this paper is to look for maximally entangled states. In such a case it is vital to distinguish maximally entangled states from other states. We use the notion of maximum multipartite entanglement introduced by Facchi et al. [7].

Definition 3 State $|\psi\rangle \in \mathbb{C}^{2^n}$ is called maximally multipartite entangled state if it is maximally entangled according to every bipartition.

What is important in the context of our work is that we do not necessarily need a perfect entanglement measure to perform a successful numerical optimization. Numerical search is based on a fitness function which gives some kind of estimation of multipartite entanglement and reaches its maximum only for maximally entangled states. We only need a function with some basic properties essential for finding maximally entangled states.

The most useful measure of entanglement for such a purpose is the one with possibly small equivalence class for the maximum value of entanglement. Considering computational complexity and equivalence classes of a number of entanglement measures we decided to use algebraic sum of von Neumann Entropy measure over all possible bipartitions of a system.

Definition 4 We call the generalized von Neumann entropy of a state $|\psi\rangle \in \mathbb{C}^{2^n}$ an algebraic sum of von Neumann entropy over all possible bipartitions:

$$E_{VN}^{(n)}(|\psi\rangle\langle\psi|) = \sum_{(\mathcal{X},\mathcal{Y})} E_{VN}(tr_{\mathcal{X}}(|\psi\rangle\langle\psi|)), \qquad (3)$$

where $(\mathcal{X}, \mathcal{Y})$ is a bipartition of a system, and $\dim(\mathcal{X}) \ge \dim(\mathcal{Y})$.

Using algebraic sum is known as an estimation of multipartite entanglement and was considered in the work of Facchi et al. [7] for introduction the notion of maximally multipartite entangled states. This measure reaches its maximum only for maximally entangled states. Thus such a measure is sufficient in the discussed application.

Every class of maximally entangled states consists of many states. In this paper we try to find states with the possibly simplest algebraic representation i.e. pure states with a small number of non-zero coefficients in their vector representations. We assume that states generated by a simple quantum circuit have a simple structure. This assumption makes it reasonable to search for possibly simple quantum circuits which generate maximally entangled states instead of searching in the space of all states. Such an approach enables us to research the minimum size of a quantum circuit which generates maximum entanglement. Considering the ability of a circuit to generate maximum entanglement, it is vital to take the structure of a system into consideration. Related work focuses only on states [9, 10, 18] or considers a systems where every pair of qubits can interact[19]. Physical implementation of such systems is definitely not the easiest to control. In this paper we, additionally, consider spin chain systems.

This paper is organized as follows. In section 2. we describe the basic measures of entanglement considered suitable for GP. In section 3. we explain the mechanism of a selected optimization method. All the obtained results are gathered in section 4.. In section 5. we provide conclusions.

2. Measures of entanglement

Quantum entanglement is a highly non-intuitive feature of the physical world and there is no systematic way of measuring it. One of the necessary conditions for an entanglement measure is LOCC monotonicity [20]. It is based on physical criteria determining which state is more entangled. Roughly speaking if state $|\psi\rangle$ can be transformed into state $|\psi'\rangle$ under LOCC, then state $|\psi'\rangle$ cannot be more entangled. The states which can be obtained by an invertible LOCC operation are considered equally entangled and form LOCC-orbits. However, this criterion is not strict and allows to define a number of non-equivalent measures.

2.1. Entanglement measures of bipartite systems

One can use various measures of entanglement to quantitatively determine entanglement. In the context of this paper the most interesting ones are computable measures of entanglement. The most basic measures of entanglement are designed for bipartite cases. Most of such measures are based on separability criteria. In this paper we recall two of them, considered the most suitable for the discussed problem. One of such measures is Negativity, defined as

$$E_{Neg}(\rho) = \sum_{\lambda < 0} |\lambda|, \qquad (4)$$

where λ are the eigenvalues of the partial transpose of the density operator ρ . In the case of a quantum system consisting of 2 qubits a state is separable if and only if the partial transpose of the density matrix does not contain negative eigenvalues in its spectrum. Thus, every eigenvalue can be considered as an entanglement witness. Moreover, it is proven that the sum of all the negative eigenvalues is monotonic under LOCC.

Another measure of entanglement - von Neumann entropy of Schmidt numbers - is based on a different criterion. One of the fundamental measures of



entanglement is distillable entanglement (E_d) that for pure states is equal to von Neumann entropy of the reduced state of either subsystem. For pure states it holds that $\text{Tr}_Y(|\psi\rangle\langle\psi|) = AA^{\dagger}$, where A is the coefficients matrix of state $|\psi\rangle$ (i.e. $|\psi\rangle = \text{vec}(A)$) Thus we have:

$$E_{VN}(|\psi\rangle\langle\psi|) = E_d(|\psi\rangle\langle\psi|) = S(\operatorname{Tr}_Y(|\psi\rangle\langle\psi|)) = S(AA^{\dagger}) = -\sum \lambda_i \log_2 \lambda_i, \quad (5)$$

where S is the von Neumann entropy. In other words, the matrix of coefficients of every separable state has only one singular value. When a state becomes entangled, the number of Schmidt numbers increases and thus increases its entropy which is proven to be LOCC monotonic.

It is worth noting that in this paper we use entanglement measures to evaluate entanglement of pure states. In this case every function proven to be LOCC monotonic for pure states is sufficient.

2.2. Entanglement measures of multipartite systems

In the case of a quantum system consisting of more than two subsystems, computing the measure of entanglement is more complex. In systems with more than two subsystems state tensors have the order grater that 2. In such a case there is no unambiguous way to compute eigenvalues or singular values.

To establish a multipartite measure of entanglement, one can use generalizations of Schmidt decomposition. Other family of measures is the generalization of determinants called hyperdeterminants. Also, one can build a measure by investigating entanglement of reduced states. By applying the partial trace any multipartite system can be reduced to a bipartite systems and estimated using a bipartite entanglement measure.

Another approach is to create a measure of entanglement of a complex system with the use of a known measure for simpler systems. Using a bipartite entanglement measure, one can obtain the value of entanglement between two subsystems. By summation over all the possible decompositions into two subsystems one can obtain a value which provides information on multipartite entanglement.

$$E_{\gamma}(\rho) = \sum_{\gamma = \lambda \cup \sigma} E_2(\rho_{\lambda,\sigma}), \tag{6}$$

where γ is a set representation of subsystems. The key advantage of this method is using measures that are already developed. However, using tools created this way, it is not easy to distinguish between bipartite entanglement and truly multipartite entanglement.

It is not obvious how to characterize multipartite entanglement. LOCCmonotonicity does not provide total order in space of states and when two different LOCC-orbits are not related there is no way to determine which one of them



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is more entangled. As a result, different measures may create opposite relations between such orbits. Some examples of maximally entangled states that may be characterized differently are the GHZ state $|\psi_{GHZ}\rangle = |000\rangle + |111\rangle$ and the W state $|\psi_W\rangle = |001\rangle + |010\rangle + |100\rangle$. In going from GHZ to W states the geometric measure, the relative entropy of entanglement, and the bipartite entanglement all increase monotonically, whereas the three-tangle and bi-partition negativity both decrease monotonically. Details can be found in [21]. Since there are many non-equivalent measures of entanglement and all of them are designed in order to provide as much information about states as possible, measures that distinguish more orbits preserving LOCC-monotonicity are more useful.

The key matter in this paper is to look for maximally entangled states. This means that we need to use the measure of entanglement with possibly the smallest equivalence class with the maximum entanglement measure value. Moreover, different approaches to computing multipartite entanglement may determine different kinds of entanglement. There is no characterization for systems containing more than 4 qubits and we can only rely on our intuition in order to decide which approach is the most useful to describe the distribution of multipartite entanglement. Measures used in this work are based on bipartite entanglement mainly because of its computational complexity and scalable properties. On comparing all the discussed measures, we decided that the von Neumann entropy of Schmidt numbers will best serve this purpose.

3. Genetic programming

Considering the known entanglement measures, obtaining the quantitative value of entanglement is computationally complex. This makes searching for the global maximum of an entanglement measure rather improbable to succeed in analytical terms. During the maximization of any measure one can face a number of problems, mainly large search space of possible circuits and non-linear form of the fitness functions. This makes numerical methods, especially those which are based on the Monte Carlo method, very suitable for this problem. One can choose from a number of methods from this family. There is no comparison of such methods but the nature of genetic programming suggests that it is adequate to this problem.

Genetic programming belongs to the family of search heuristics inspired by the mechanism of natural evolution. In genetic algorithms each element of a search space being candidate for a solution is encoded as a representative of a population. Every member of a population has its unique genetic code, this code is its representation in optimization algorithm. Searching for the optimal solution is done by modification of genetic code due to rules of the evolution such as mutations,

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selections, crossovers and inheritance. Mutators are functions that change single elements of genetic code of a population member randomly. Cross-overs implement mechanism of inheritance. This function divides parental genetic codes and create a new genetic code. In every iteration of the algorithm all members of the population are evaluated using fitness function. Then using the selector function the set of the best members is obtained and used to create a new generation of a population using mutation and cross-over functions. This makes genetic programming especially usable when parts of genetic code represents features of elements of search space and can be interchanged between elements independently. In such case GA is expected to find features that occur in well fitted representatives and mix them in order to find the best possible combination.

In order to apply the Genetic Algorithm it is necessary to define a population, fitness function, methods of crossing-over, mutation and selection. In the case of optimization of quantum circuits generating entanglement the population consists of quantum circuits. The most convenient way to represent computation in a quantum circuit is a sequence of quantum gates. Every quantum gate can be approximated using the gates from a set of universal quantum gates. In this work we use a set containing the Hadamard gate H, the $R(\pi/4)$ (called $\pi/8$ gate) gate and the controlled-NOT gate CNOT (Eq. 7) [22]. However, initial experiments suggest that the $R(\pi/4)$ gate is not necessary for generating maximally entangled states. Thus, in order to simplify the resultant state, we consider a set containing only H and CNOT gates when the obtained entanglement is maximal.

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1\\ 1 & -1 \end{pmatrix}, CNOT = \begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0 \end{pmatrix}, R(\pi/4) = \begin{pmatrix} 1 & 0\\ 0 & e^{i\pi/4} \end{pmatrix}$$
(7)

As our goal is to find a circuit which prepares as much entangled state as possible, our fitness function is the entanglement measure of the prepared state. In this case computing fitness of a quantum circuit requires obtaining the output state and then computing its value of a chosen measure of entanglement.

While customization of population representation and fitness function unavoidably relies on the optimization problem, other parameters of genetic programming such as crossover and mutation methods are universal. When treating quantum circuits as strings of integers representing quantum gates one can use various, already developed methods.

Having that every quantum circuit is represented as a sequence of quantum gates as its genetic code, all evolution mechanisms acts on this sequence. Methods

of crossing-over join parts of parental circuits with high value of multipartite entanglement of resulting state. Mutators change single gate in well-fitted circuits.

Entanglement of a state in a quantum circuit evolves during applying gates successively. One can suspect that this evolution in optimal circuits progresses monotonically [19] and entanglement is increasing in particular segments of the circuit independently. This makes genetic programming with methods enabling to exchange parts of the circuit between different circuits generating high entanglement by the use evolution mechanisms a good candidate for the optimization method.

Using genetic algorithms for constructing quantum algorithms is known [23]. Our problem is very similar, although we do not have any fixed prospective result of the algorithm. We demand a circuit which prepares maximally entangled states with respect to a selected measure.

4. Results

In this work we investigate systems consisting of up to 8 qubits. In each case we analyze the possibility of connecting qubits in two different ways. Firstly we define a completely connected system as a system in which we are able to act on every pair of qubits. It means that the set of all available CNOT gates is equal to $\{CNOT(i; j) : i \neq j\}$, where CNOT(i, j) is a controlled NOT gate acting on *i*-th and *j*-th qubit. Possibility of applying the Hadamard gates and the phase gates are independent of changes of possible qubit connections while H gate acts on one qubit only. By a spin chain system we mean a system where we are able to act on pairs of nearest neighbors in a chain. In such a case the set of available CNOTS gates is $\{CNOT(i; j) : |i - j| = 1\}$.

4.1. Analysis of the 3-qubits case

The structure of 3 qubit entanglement is well known. By the analysis of prior results [21] one can expect the algorithm to generate the GHZ state $|\psi_{\text{GHZ}}\rangle = |000\rangle + |111\rangle$. This state is maximally entangled in respect to the von Neumann entropy of Schmidt numbers measure. The GA engine returns a number of circuits preparing it. The minimal obtained circuit contains 3 gates. Such a circuit can be created regardless of available connections.

4.2. Analysis of the 4-qubits case

In the case of a system containing 4 qubits the classification of entanglement is developed and it is known that pure states can be entangled in nine different





Rysunek 1: A quantum circuit preparing a maximally entangled state in the 3qubits case.

ways[24]. Higuchi and Sudbery [25] have proved that there is no 4-qubits pure state with all its marginal density matrices completely mixed, which means that the hypothetical maximum of von Neumann entropy measure is unreachable. However they found a highly entangled state $|HS4\rangle = \frac{1}{\sqrt{6}}(|100\rangle + |0011\rangle + \omega(|1001\rangle + |0110\rangle) + \omega^2(|1010\rangle + |0101\rangle))$, where $\omega = 1/2 + i\sqrt{3}/2$ is the third root of unity. This state is known to be a local maximum [26] and is also conjectured to be a global maximum [25] according to the von Neumann entropy measure. As pointed out in [19] it is not possible to prepare the HS4 state using CNOT and H gates.

By applying the GA it is possible to get a circuit preparing state $|\psi_4\rangle = \frac{1}{2}(|0000\rangle + |0110\rangle + |1011\rangle + |1101\rangle)$ with a high value of entanglement measure equaling $E_{VN} = 9$.



Rysunek 2: A quantum circuit preparing a highly entangled state $|\psi_4\rangle$ in the 4-qubits case.

The state obtained that way is not as much entangled as HS4, but it has a much simpler form and physical implementation of a circuit preparing such a state is much more likely. Thus, such a state could be useful in quantum algorithms that require highly entangled 4-qubits states.



4.3. Analysis of the 5-qubits case

Classification of entanglement in case of 5-qubits systems is a subject of ongoing research. However some maximally entangled states, such as the BSSB5 state $|\psi_{BSSB5}\rangle = \frac{1}{2}(|001\rangle|\phi^{-}\rangle + |010\rangle|\psi^{-}\rangle + |100\rangle|\phi^{+}\rangle + |111\rangle|\psi^{+}\rangle)$ have been studied. This state was researched by Muralidharan and Panigrahi, however no simple quantum circuit for preparing this state was introduced. Similar states with corresponding circuits were introduced in [19]. The minimal circuit in a system with complete connections obtained by the application of the GA is of length 8 and has the form presented in the Figure 3.



Rysunek 3: Quantum circuits preparing maximally entangled states in the 5qubits case.

All resulting circuits of this length contain at least one gate acting on nonneighbor qubits i.e. the connection graph of every circuit has at least one vertex of degree 3 which is not possible in a spin chain system. Thus, when using the spin chain system, the number of gates must be greater than 8. In order to find a spin chain system circuit generating a maximally entangled state we reduce the set of available CNOT gates to the ones acting on neighbor qubits and we apply the GA. The best solution includes 10 gates.

4.4. Analysis of the 6-qubits case

When we consider a completely connected system in the 6-qubits case the number of gates necessary to generate the maximally entangled state is 12 (best known result is 13 [19]). Reduction of the number of quantum gates in the circuit caused a reduction of the number of non-zero coefficients in the resulting state from 32 to 16. In the spin chain case the best found solution consists of 17 quantum gates.



Rysunek 4: Quantum circuits preparing maximally entangled states in the 6qubits case

4.5. Analysis of the 7-qubits case

In the 7-qubits case the possibility of preparing a maximally entangled pure state is an open problem. The best known result is presented in work [27], where the authors tried to minimize the purity of a state. In this work we introduce states with equal value of purity and greater value of von Neumann entropy and the circuits preparing them. In the systems containing up to 6 qubits the set of available gates contained the H and CNOT gates. In the case of 7 qubits introducing the phase gates allowed us to generate states with higher value of entanglement measure. In order to achieve a wide range of states we use two phase gates: $R(\pi/3)$ and $R(\pi/4)$. In the 7-qubits case the hypothetical value of the entanglement measure for a maximally entangled state is $E_{VN} = 154$. Circuits without the phase gates produce an entangled state with the value of von



Neumann entropy equal to $E_{VN} = 151$, whereas circuits containing the phase gate produce a state with the value of von Neumann entropy equal to $E_{VN} = 151.65$. This result has been obtained both in the case of the complete connection system and in the spin chain system. Numerical results suggest that Borras conjecture, that there is no pure maximally entangled 7-qubit state, is correct.



Rysunek 5: Quantum circuits preparing a highly entangled state in the 7-qubits case.

4.6. Analysis of the 8-qubits case

It is known that for systems containing more than 7 qubits there is no pure maximally entangled state [27]. The value of entanglement measure E_{VN} for hypothetical a maximally entangled state is 372, which in this case is the upper bound for von Neumann entropy. The best solution found within circuits without the phase gates is 362. In this paper we introduce a quantum circuit generating a highly entangled state with entanglement measure $E_{VN} = 363.13$. The minimum size of circuits generating such states is 30 and 40 quantum gates for both the complete and spin chain systems respectively.

4.7. More complex systems

Analysing systems that contain more than 8 qubits is very time-consuming. Our analysis suggests that in the most basic case, when a circuit contains only the H and CNOT gates the best achievable value of the von Neumann entropy measure is 821 and 1866 for 9 and 10 qubit systems respectively. Because of computation complexity, the optimal size of quantum circuits obtained during this work are not reliable.

5. Concluding remarks

In this paper we have presented the results obtained by using the genetic algorithm to generate quantum circuits preparing maximally entangled states. In our work we presented a new approach to discussed problem. This approach allows us to find both maximally entangled states and quantum circuits generating them. In this way gives us new possibilities of analysing the process of generating multipartite maximum entanglement.

The main feature of a quantum circuit that gives us some information about generated state is its size. In our work put the main interest in the minimal number of quantum gates needed to obtain a circuit which manages to generate a maximally entangled state. The number of basic gates needed to generate maximum entanglement provide insight into the difficulty of this process. The computation performed by us shows that the size of the circuit grows exponentially with the size of a system. If we treat the gates used in our work as the elementary operations, we find out that the complexity of all quantum algorithms using generation of multipartite entanglement is exponential. It means that all hypothetical quantum algorithms which are supposed to bring essential computational speed-up, which use multipartite entanglement may be practically inefficient.

The size of a circuit is interesting both in the context of minimal complexity of a circuit generating the maximum entanglement and in the obtaining of maximal-





Rysunek 6: A quantum circuit preparing a highly entangled state in the 8-qubits case.

ly entangled states itself, because the complexity of the algebraic representation of a resulting state increases with the number of gates in a circuit.

Additionally considering both complete systems and spin chains independently gives us an opportunity to compare this structures. Obtained results show that the simulation of dynamics of a complete system using spin chain system brings exponential growth of the number of quantum gates needed. We do not



provide any proof of the general rule, although shown example suggests that this problem should occur for every algorithm that utilise multipartite entanglement. This means that quantum systems of informatics based on spin chains may be exponentially less efficient than systems where interaction between all pairs of qubits are possible.

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Szukanie układów kwantowych generujących maksymalnie wielocząstkowo splątane stany

Streszczenie

Praca skupia się na możliwości generowania stanów wielocząstkowo maksymalnie splątanych w układach kwantowych. Przedstawione zostały wyniki zastosowania algorytmów genetycznych do szukania układów kwantowych generujących takie stany. Praca zawiera dyskusję dotyczącą metod tworzenia funkcji przybliżających miarę splątania wielocząstkowego, w szczególności sposobów opartych na miarach dla systemów dwudzielnych. Przyjmujemy, że stan jest maksymalnie wielocząstkowo splątany jeśli jest maksymalnie splątany względem każdego możliwego podziału systemu. Poza problematyką doboru odpowiedniej miary splątania zostały poruszone zagadnienia związane z zastosowaniem algorytmów genetycznych do optymalizacji układów kwantowych. Rezultaty, które zostały zaprezentowane, dotyczą dwóch rodzajów systemów. Oprócz systemów pozwalajacych na oddziaływanie pomiędzy dowolnymi cząsteczkami dodatkowo rozpatrywany jest przypadek łańcucha spinowego, w którym oddziałują jedynie sąsiednie cząsteczki. Zamieszczone w pracy układy kwantowe przedstawiają przykładowe obwody dla systemów składających się z maksymalnie 8 qubitów.