Scaling of the energy and entropy errors in quantum circuits

Author: Josep Lumbreras Zarapico
*Facultat de Física, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain.**

Advisor: José Ignacio Latorre

Abstract: Quantum algorithms based on simulating states of a quantum system cannot simulate these states without an error. This work studies the relations between the error of an approximated quantum circuit that simulates the ground state of a Hamiltonian and the error of the energy and Von Neumann entropy of this state. In addition, we relate the errors with the gate cost of the approximated quantum circuit using the Solovay-Kitaev theorem.

I. INTRODUCTION

Over the past few years, quantum computing has become more plausible due to the great advances in technology. In particular, quantum computers will have a huge impact in simulations of large quantum systems, since the data stored on them scale logarithmically with the dimension of the Hilbert space. In order to simulate the dynamics of a quantum system it is necessary to prepare certain states of a many-body Hamiltonian in a quantum circuit. However, in the gate model of quantum computing, one of the main issues is that the set of quantum gates is limited and most of the algorithms will carry an error with respect to ideal ones. Specifically, quantum algorithms for ground state preparation are able to approximate the ground state of the system with a certain non zero error.

In this paper we study the relations between the error of an approximated quantum circuit and the errors of the energy and Von Neumann entropy of the approximated states. In the first part of the paper we present the Solovay-Kitaev theorem and give an expression for two close unitary operators. Then, we present the relations between the errors of a quantum circuit and the energy and entropy of the simulated states. Finally we check the relations using a classical simulation.

II. APPROXIMATE UNITARY OPERATORS

Let $\mathcal{H}$ be a complex Hilbert space, and $X : \mathcal{H} \to \mathcal{H}$ be a bounded linear operator. Its *operator norm* is defined as

$$\|X\| = \sup_{||\psi\rangle|=1} |X\,|\psi\rangle\,|, \tag{1}$$

where $|\cdot|$ denotes the standard vector norm. The operator norm induces a distance in the group of unitary operations $U(n)$. Thus, a unitary operator $\tilde{U}$ approximates the unitary operator U with precision ϵ if

$$\|\tilde{U} - U\| = \mathcal{O}(\epsilon). \tag{2}$$

Also, $\tilde{U}$ is called an ϵ-approximation for U.

Since $U^\dagger U = I$, if $\tilde{U}$ is a "good" approximation for U it follows that

$$\tilde{U}U^\dagger = I + \epsilon B \tag{3}$$

for some sufficiently small $\epsilon > 0$ and matrix B with norm $\|B\| \leq 1$. Note that this expression is an ϵ - approximation for the identity, $\|\tilde{U}U^\dagger - I\| = \mathcal{O}(\epsilon)$.

Since $\tilde{U}$ and U are unitary, Eq. (3) should also be unitary. Imposing that condition to the terms of order ϵ, implies that $B^\dagger + B = 0$. So, it is useful to define $A = iB$ and the condition will be $-A^\dagger + A = 0$, which means that A is hermitian. Thus, Eq. (3) can be expressed as

$$\tilde{U}U^\dagger = I - i\epsilon A. \tag{4}$$

The term $i\epsilon A$ gives a small change to a vector, so, since I is unitary, the operator of Eq. (4) is almost a unitary operator. In order to achieve a unitary operator we would need to develop terms of higher order in ϵ. The resulting operator is the exponential function of a matrix, i.e.

$$\tilde{U}U^\dagger = e^{-i\epsilon A}. \tag{5}$$

Equivalently, $\tilde{U}$ can be expressed in terms of U as $\tilde{U} = e^{-i\epsilon A}U$ for some hermitian matrix A. Calculating the operator norm of $\|e^{-i\epsilon A}U - U\|$, we find that $\tilde{U}$ is a ϵ-approximation for U.

III. SOLOVAY-KITAEV THEOREM

In classical computing a universal set of logic gates is a set that can implement any Boolean function. In quantum computation the notion of universal set is quite different since the operations are elements of the unitary group $U(n)$. Given a finite set of quantum gates it is not possible to achieve an arbitrary unitary operation because the group $U(n)$ is uncountable and a finite sequence of gates is countable. Instead, a set of quantum

*Electronic address: joseplumbreraszarapico@gmail.com

gates will be universal if it can implement any unitary operation with a given error. More precisely, a *universal set of quantum gates* is a set $\mathcal{G}$ of unitary operators such that for any unitary operator U and error $\epsilon > 0$, there exists an ϵ-approximation for U, $g_1 \cdots g_n$, with $g_i \in \mathcal{G}$ and $n < \infty$.

Apart from the finite set of gates, near term quantum computers will be restricted by the numbers of operations. Moreover, these operations must be done in a fault-tolerant way, and fault-tolerant constructions are typically available only for a limited number of gates (e.g., the Clifford group gates and $\pi/8$ gate [1]). For those reasons, it is important to find efficient ways of implementing quantum algorithms with a limited set of quantum gates.

The Solovay-Kitaev theorem states that any universal set of quantum gates can approximate any unitary operation quickly and with a good precision. In the simplest form, the theorem states:

Theorem 1 (Solovay-Kitaev)**.** *Let $\mathcal{G}$ be a universal set of quantum gates in* SU(2) *closed under inversion. Then for any error $\epsilon > 0$ and $U \in$ SU(2), there is a sequence of elements $g_1, ..., g_l \in \mathcal{G}$ such that $\|U - g_l \cdots g_1\| \leq \epsilon$ with $l = \mathcal{O}(\log^c(1/\epsilon))$ and $c \approx 4$.*

The proof of the theorem does not give us any practical construction of the approximated unitary, but it tells us that it is possible to achieve efficient constructions of the desired unitary with a given set of gates. For example, quantum algorithms like Shor's can be broken into a sequence of m quantum gates $U_1, \cdots U_m$. A reasonable assumption is that each quantum gate can be approximated with an accuracy of $\epsilon > 0$ using $\mathcal{O}(1/\epsilon)$ quantum gates from the given set [2]. Then, if we want to approximate the entire sequence to an accuracy of $\epsilon > 0$, each gate should be approximated to an accuracy of $\mathcal{O}(\epsilon/m)$, and the total length of the approximation would be $\mathcal{O}(m^2/\epsilon)$, a quadratic increase in the original size of the circuit. The Solovay-Kitaev theorem provides that each quantum gate can be approximated with $\mathcal{O}(\log^c(m/\epsilon))$ quantum gates, and the total length of the circuit would be $\mathcal{O}(m \log^c(m/\epsilon))$. Thus the theorem reduces the total length from a quadratic to a polylogarithmic increase over the original size.

Solovay announced the theorem in 1995 for the case SU(2) but he did not publish it. In 1997, Kitaev proved the theorem independently for the general case $SU(d)$ in a review paper [3]. Later Kitaev, Shen and Vylaly showed an alternative proof where the constant c was reduced to 3 [4]. In particular, the best value for the constant c that we can achieve is 1 [5], and it was proved that for a particular choice of the set of gates the optimal value for c can be achieved [6].

IV. ENERGY ERROR

Throughout this paper, let H be a $d \times d$ Hermitian matrix that represents some quantum Hamiltonian, and let E_0 be the ground energy of this Hamiltonian with $|\psi_0\rangle$ its eigenstate.

Since the choice of the set of gates is limited, the implementation of most quantum algorithms for ground state preparation of a Hamiltonian will carry an error. Hence, the ground energy of the simulated state will not be exactly the ground energy of the system. The number of gates that are required for the quantum circuit is related to the error with respect to the ideal one, so these three quantities can be related: number of gates, error of the circuit and error of the energy.

The Solovay-Kitaev theorem states that is possible to find the approximated circuit, so our work will be to relate the error of the approximated circuit with the error of the approximated eigenvalue of the target state. Using the results of the previous sections, we prove the following result:

Theorem 2. *Given a universal set of quantum gates $\mathcal{G}$ closed under inversion, a Hamiltonian H, and error $\epsilon > 0$ it is possible to find a quantum circuit $\tilde{U}$ such that it can simulate an approximation for the ground state $|\tilde{\psi_0}\rangle$, with an error of the energy of $\mathcal{O}(\epsilon^2)$ in a gate complexity of*

$$\mathcal{O}(\log^c(1/\epsilon)) \tag{6}$$

for some constant c, $c \leq 4$.

Proof. To prove this result we will need to use the Solovay Kitaev theorem and standard perturbation theory. Suppose that exists a quantum circuit U such that

$$U |0\rangle^{\otimes d} = |\psi_0\rangle . \tag{7}$$

Then using the Solovay-Kitaev theorem we have that is it possible to find an ϵ-approximation $\tilde{U}$ for U in the sense of Eq. (2) using $\mathcal{O}(log^c(1/\epsilon))$ gates from our set $\mathcal{G}$.
Using the calculations of the previous section, the approximated $\tilde{U}$ can be expressed as $\tilde{U} = e^{-i\epsilon A}U$ for some bounded Hermitian matrix A, ($\|A\| < 1$). Expanding $\tilde{U}$ with the usual definition of the matrix exponential to the first order on ϵ, we can calculate the approximated state $|\tilde{\psi_0}\rangle$ of the exact ground state

$$|\tilde{\psi_0}\rangle = \tilde{U} |0\rangle^{\otimes d} = |\psi_0\rangle - i\epsilon A |\psi_0\rangle + \mathcal{O}(\epsilon^2). \tag{8}$$

Recall that since A is bounded, this $|\tilde{\psi_0}\rangle$ is a ϵ-state close to $|\psi_0\rangle$. Finally, it suffices to compute the energy of the state $|\tilde{\psi_0}\rangle$ as $\tilde{E_0} = \langle\tilde{\psi_0}| H |\tilde{\psi_0}\rangle$. Using that $E_0 = \langle\psi_0| H |\psi_0\rangle$,

$$\tilde{E_0} = E_0 + \epsilon^2 \langle\psi_0| AHA |\psi_0\rangle . \tag{9}$$

The terms of order ϵ have cancelled thanks to the hermicity of A and the change of sign produced by the conjugation of the factor i. Thus, the result $|\tilde{E_0} - E_0| = \mathcal{O}(\epsilon^2)$ follows.

□

The Solovay-Kitaev theorem does not give us the construction of the approximated circuit, but if the quantum circuit has a certain error with respect to the ideal one, this result still guarantees the quadratic improvement in the error of the energy compared to the error of the circuit. Moreover, fixing the number of gates of the set, this result tells us the order of the error of the energy that we can achieve with an approximated quantum circuit.

V. ENTROPY ERROR

Let $\mathcal{H}$ be a bipartite Hilbert space for two subsystems A and B i.e $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. The entanglement between the systems A and B of a quantum state can be measured using the Vonn Neumann entropy. Since $|\tilde{\psi_0}\rangle$ is an approximate state for $|\psi\rangle$, the entropy of $|\tilde{\psi_0}\rangle$ will carry an error respect to $|\psi\rangle$. Let ρ_0^A be the corresponding density matrix of the state $|\psi_0\rangle$ for the subsystem A, i.e,

$$\rho_0^A = \mathrm{Tr}_B \, |\psi_0\rangle \langle\psi_0| \, . \tag{10}$$

The Vonn Neumann entropy for the state $|\psi_o\rangle$ can be computed as

$$S_0 = -\operatorname{Tr} \rho_0^A \log_2 \rho_0^A = -\sum_i \lambda_i \log_2 \lambda_i, \tag{11}$$

where λ_i are the eigenvalues of ρ_0^A. In fact, it is possible to choose the logarithm in another base because all logarithms are related up to a constant factor.

In order to relate the Von Neumann entropy $\tilde{S_0}$ of the state $|\tilde{\psi_0}\rangle$ with S_0 and the number of gates of the approximated circuit $\tilde{U}$, we prove the following result:

Theorem 3. *Given a universal set of quantum gates $\mathcal{G}$ closed under inversion, a Hamiltonian H, and error $\epsilon > 0$ it is possible to find a quantum circuit $\tilde{U}$ such that it can simulate an approximation for the ground state $|\tilde{\psi_0}\rangle$, with an error of the Von Neumann entropy of $\mathcal{O}(\epsilon)$ in a gate complexity of*

$$\mathcal{O}(\log^c(1/\epsilon)) \tag{12}$$

for some constant c, $c \leq 4$.

Proof. Using the same construction as in Th. 2, we can find an ϵ -approximation $\tilde{U}$ of the ideal circuit, that produces an approximated state $|\tilde{\psi_0}\rangle$. In order to compute $\tilde{S_0}$ it is useful to compute the density matrix of $|\tilde{\psi_0}\rangle$,

$$\tilde{\rho_0^A} = \rho_0^A + i\epsilon \operatorname{Tr}_B(-A\,|\psi_0\rangle\langle\psi_0| + |\psi_0\rangle\langle\psi_0|\,A) + \mathcal{O}(\epsilon^2). \tag{13}$$

Note that the terms of order ϵ does not cancel, thus $\|\tilde{\rho_0^A} - \rho_0^A\| = \mathcal{O}(\epsilon)$. Let $\lambda_0, ..., \lambda_m$ and $\tilde{\lambda_0}, ..., \tilde{\lambda_m}$ be the eigenvalues of ρ_0^A and $\tilde{\rho_0^A}$ respectively. Then the eigenvalues can be related:

$$\tilde{\lambda_i} = \lambda_i + \epsilon c_i + \mathcal{O}(\epsilon^2) \tag{14}$$

where c_i is some constant such that $|\tilde{\lambda_i} - \lambda_i| = \mathcal{O}(\epsilon)$, and the terms of higher order on ϵ are ignored. Finally, it suffices to compute the terms $\lambda_i \log_2 \lambda_i$. Expressing $\log_2 \tilde{\lambda_i} = \log_2(\lambda_i(1 + \epsilon c_i/\lambda_i))$ and using the Taylor expansion for the logarithm we find that:

$$\tilde{\lambda_i} \log_2 \tilde{\lambda_i} = \lambda_i \log_2 \lambda_i + c_i \epsilon \log_2 \lambda_i + c_i \epsilon + \mathcal{O}(\epsilon^2) \tag{15}$$

Then summing over all the terms $\tilde{\lambda_i} \log_2 \tilde{\lambda_i}$ the result $|\tilde{S_0} - S_0| = \mathcal{O}(\epsilon)$ follows. □

The results of Th. 2 and Th. 3 are given for the ground state as the target state to simulate but they can be generalized to other quantum states. Preparing excited states of a Hamiltonian seems to be more difficult and most of the existing quantum algorithms are focused on ground state preparation.

VI. SIMULATIONS FOR THE ENERGY AND ENTROPY

In this section we are going to check Th. 2 and Th. 3 with a numerical simulation for a particular Hamiltonian. To carry out the simulation it is important to choose a Hamiltonian such that we can calculate the exact ground energy and the exact Von Neumann entropy. For the simulations we have chosen the Heisenberg Hamiltonian without a transversal field and constant equal weights,

$$H = \sum_i \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z. \tag{16}$$

Note that the approximated circuit $\tilde{U}$ produces a state $|\tilde{\psi_0}\rangle$ ϵ-close to the ground state, so, instead of finding the approximate circuit, it suffices to implement the state $|\psi_0\rangle$ and calculate $\tilde{E_0}$ and $\tilde{S_0}$. With this Hamiltonian we have calculated the ground state $|\psi_0\rangle$ for the specific cases of 4,6 and 8 qubits using standard programming techniques. With the ground state calculated, the state $|\tilde{\psi_0}\rangle$ is generated with the following expression

$$|\tilde{\psi_0}\rangle = \frac{|\psi_0\rangle + \epsilon\,|\phi\rangle}{|\,|\psi_0\rangle + \epsilon\,|\phi\rangle\,|} \tag{17}$$

where $|\phi\rangle$ is a random state equivalent to the $A\,|\psi_0\rangle$ term of Eq. (8).

In order to find how the error of E_0 and S_0 scale, we will suppose that they scale as $O(\epsilon^k)$ for some exponent k. Then, calculating E_0 and S_0 with different values of ϵ, the exponent k can be computed using the following linear regressions

$$\log|\tilde{E_0} - E_0| = k_E \cdot \log(\epsilon) + c_E, \tag{18}$$

	k_E	k_S
4 qubits	1.9986	0.9975
6 qubits	1.9988	1.0123
8 qubits	1.9988	1.0851

TABLE I: *Values for the coefficients k_E and k_S of the linear regressions of Eqs. (18-19) using the results from Fig. 1 and Fig. 2.*

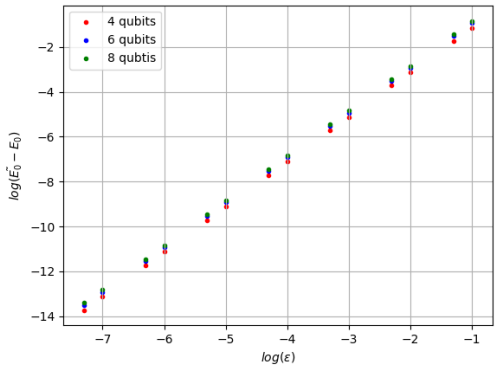

FIG. 1: *Ground energy errors for the Hesienberg Hamiltonian for 4,6 and 8 qubits. The error ϵ and energy error $|\tilde{E}_0 - E_0|$ are shown in a logarithmic scale. The energy error scales like $\mathcal{O}(\epsilon^2)$ for all cases.*

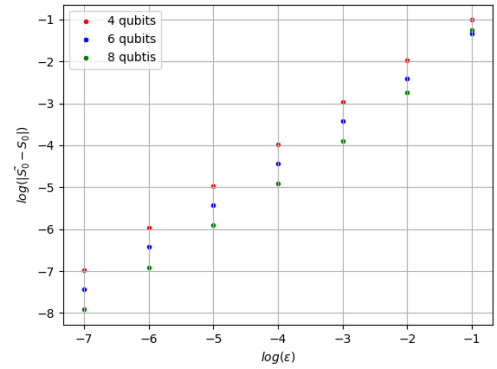

FIG. 2: *Ground entropy errors for the Heisenberg Hamiltonian for 4,6 and 8 qubits. The error ϵ and entropy error $|\tilde{S}_0 - S_0|$ are shown in a logarithmic scale. The entropy error scales like $\mathcal{O}(\epsilon)$ for all cases.*

$$\log|\tilde{S}_0 - S_0| = k_S \cdot \log(\epsilon) + c_S, \tag{19}$$

where c_S and c_E are some constants. The values of k_E and k_S are the exponent of $\mathcal{O}(\epsilon)$. These values are shown in Table I. The simulations plotted in Fig. 1 and Fig. 2 have been averaged over 100 times.

From the values of k_E, we see in a clear way that the error of the ground energy scales like $\mathcal{O}(\epsilon^2)$. For the error of the Von Neumann entropy, the values of k_S show that the entropy error scales like $O(\epsilon)$. Moreover, Fig. 1 and Fig. 2 show that there is no dependence on the number of qubits. These results prove the dependencies of the errors established in Th. 2 and Th. 3.

VII. GATE COMPLEXITY

In order to check the gate complexity of Th. 2 and Th. 3 we will use the Variational Quantum Eigensolver (VQE) algorithm [7] for the case of the Heisenberg Hamiltonian of Eq. (16) with 4 qubits. The VQE algorithm consists on:

1. Prepare a quantum circuit $U(\vec{\theta})$ depending on k parameters, $\vec{\theta} = (\theta_1, \cdots, \theta_k)$. Pick an initial state $|0\rangle^{\otimes n}$, a set of initial parameters for $\vec{\theta}$, and compute the state $|\tilde{\psi}\rangle = U(\vec{\theta})\,|0\rangle^{\otimes n}$.
2. Measure the expectation value $\tilde{E}_0(\vec{\theta}) = \langle\tilde{\psi}|\,H\,|\tilde{\psi}\rangle$.
3. Use a classical minimization algorithm to minimize the value of $\tilde{E}_0(\vec{\theta})$.
4. Repeat the steps until convergence.

According to the variational theorem of quantum mechanics we will get always $\tilde{E}_0 \geq E_0$. Increasing the gate complexity of the trial circuit $U(\vec{\theta})$, we will check the value of the constant c of Eq. (6) measuring the energy error $|\tilde{E}_0(\vec{\theta}) - E_0|$.

The choice of the quantum circuit $U(\vec{\theta})$ is arbitrary, but not all circuits can produce the desired state. Our choice of the circuit is based on the universal set of quantum gates $\mathcal{G} = \{H, T, CNOT\}$ [5], where H denotes the Hadamard gate, T the $\pi/8$ gate and $CNOT$ the controlled-NOT gate. The H and T gates can produce the following rotations over the Bloch sphere:

$$R_{\hat{n}}(\alpha) = THTH \text{ and } R_{\hat{m}}(\alpha) = HTHT, \tag{20}$$

where $\hat{n}$ and $\hat{m}$ are the normalized axis $\vec{n} = (\cos\frac{\pi}{8}, \sin\frac{\pi}{8}, \cos\frac{\pi}{8})$ and $\vec{m} = (\cos\frac{\pi}{8}, -\sin\frac{\pi}{8}, \cos\frac{\pi}{8})$ respectively. The angle α is defined by $\cos(\alpha/2) = \cos^2\pi/8$, and it is an irrational multiple of 2π [8], thus successive iterations of these rotations can fill up the interval $[0, 2\pi)$ along their respectively axis. The main idea of the implementation is that any quantum gate acting on a single qubit $U \in \mathrm{U}(2)$ can be decomposed as

$$U = e^{i\alpha} R_{\hat{r}}(\beta) R_{\hat{s}}(\gamma) R_{\hat{r}}(\delta), \tag{21}$$

for any non-parallel real unit vectors $\hat{r}$, $\hat{s}$ and an appropriate choice of $\alpha, \beta, \gamma, \delta \in \mathbb{R}$. So, using the rotations $R_{\hat{n}}$ and $R_{\hat{m}}$ it is possible to achieve any quantum gate $U \in \mathrm{U}(2)$.

The scheme of Fig. 4 shows the basic building block of our quantum circuit. In order to study the error of the circuit with the number of gates, we have implemented the VQE algorithm as shown in Fig. 3 with the classical optimizer Nelder-Mead method from the standard Python library SciPy. The depth of the circuit denoted d, is the number of times that is repeated the circuit of Fig. 4 in the VQE implementation of Fig. 3. In order to estimate the value of the constant c we have implemented the

VQE algorithm for $d = 1, \cdots, 7$ and computed the energy error for each case. The results obtained are shown in Fig. 5. The results for $d = 1, 2$ are not shown because there was not convergence in the energy error. Note that each d increases the number of gates by 20, so, the total gate complexity of Fig. 3 is given by $l = 8 + 20d$.

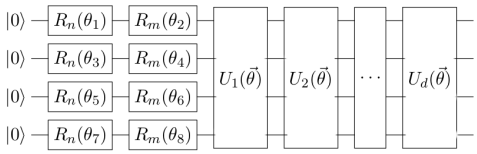

FIG. 3: *Implementation of the quantum circuit for the VQE algorithm. The general gates U_i corresponds to the circuit of Fig. 4.*

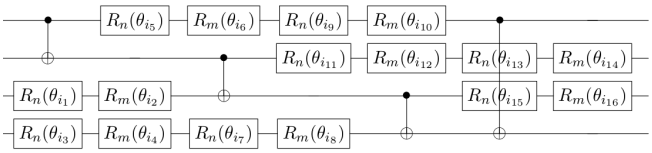

FIG. 4: *Circuit for the implementation of the VQE algorithm of Fig. 3. This circuit has 16 free parameters corresponding to the R_n and R_m rotations.*

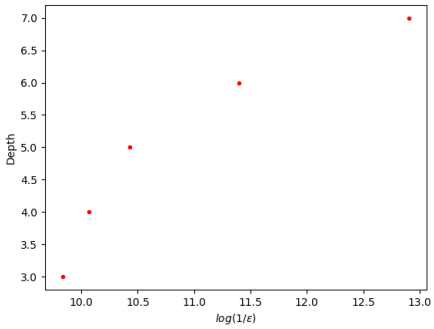

FIG. 5: *Depth of the circuit of Fig. 3 as a function of* $\log(1/\epsilon)$ *with ϵ the energy error. The behaviour of the curve shows that* $\log^c(1/\epsilon)$ *scales with $c \leq 1$.*

The results show that the value of c scales like $c \leq 1$, according to Th. 2 and Th. 3. Recall that the best value that the Solovay-Kitaev theorem can achieve is $c = 1$, however for particular cases we can achieve a better result (e.g the trivial case of approximating an operation that is in the given set).

VIII. CONCLUSIONS

Simulating a quantum state of a Hamiltonian with an ϵ-approximated quantum circuit will produce a state with a quadratic improvement $\mathcal{O}(\epsilon^2)$ in the error of the energy. The error of the Von Neumann entropy will scale with the same order of $\mathcal{O}(\epsilon)$. Moreover, the dependencies of the errors does not depend on the number of qubits, they depend only on the ϵ-approximated quantum circuit.

Given a universal set of quantum gates, the Solovay-Kitaev theorem relates the number of gates that would cost achieving an approximation for a unitary operator with the error of the approximation. Using this relation in Th. 2 and Th. 3 we related the errors of the energy, entropy and circuit with the number of gates that would cost the implementation of the circuit. Implementing the VQE algorithm for the Heisenberg Hamiltonian with 4 qubits we have found the desired scaling stated in Th. 2 and Th. 3 with a value of $c \leq 1$.

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