Variational Quantum Circuits for ground state properties of the XXZ model.

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The quantum Heisenberg XXZ model, inspired by Werner Heisenberg's work, is a statistical mechanical model used to study critical points and phase transitions in magnetic systems, where the spins are treated quantum mechanically. Due to the exponential scaling of the Hilbert space dimension with the number of spins, exact diagonalization becomes computationally infeasible for large systems. In this paper, we discuss alternative approaches to obtaining solutions for the ground state of this problem while avoiding exact diagonalization, and we evaluate their validity from an academic perspective. Specifically, we apply the Variational Quantum Eigensolver (VQE) to find solutions for the hamiltonian and we check the validity of the proposed solutions against the exact diagonalization results and against the evolution of a known initial state. The VQE is implemented [1] in Python using PyTorch, leveraging backward automatic differentiation and the Adam optimization algorithm and we check that with a complex enough ansatz, the ground state is found with good accuracy, but with a high number of simulations of the quantum circuit.

I. INTRODUCTION.

The Variational Quantum Eigensolver (VQE) was first developed by [6] and has since garnered significant attention from the research community [8]. This algorithm leverages the variational principle to compute the ground state energy of a hamiltonian, a problem of central importance in quantum chemistry and condensed matter physics. Unlike exact diagonalization, whose computational complexity scales exponentially with the number of particles, the VQE can solve this problem in polynomial time, making it particularly advantageous for large systems.

The VQE process involves defining hamiltonians and parameterized ansatz wavefunctions on a quantum computer to iteratively approximate the ground state energy and the corresponding state. This iterative process combines quantum measurements with classical optimization techniques, earning the VQE its classification as a hybrid quantum-classical algorithm. Notably, the efficiency of this algorithm heavily depends on modern differentiation techniques, which are currently an active area of research. For instance, [5] highlights how proper differentiation techniques can lead to significant computational savings.

Despite its promise, several challenges remain open for investigation. These include quantum error mitigation, the parallelization of quantum hardware, the mitigation of vanishing gradients in differentiation techniques, and understanding how the number of iterations required for a valid approximation scales with the system size. Addressing these challenges is crucial for advancing the practical applicability of the VQE in real-world problems [8]. These lines of research need to be conducted by studying well-known systems whose exact solutions have been previously obtained, like the XXZ model.

The one-dimensional Heisenberg XXZ model for spin-1/2 particles is a cornerstone in the study of quantum magnetism and strongly correlated systems. This model describes a chain of interacting spins where each spin-1/2 particle interacts with its nearest neighbours through anisotropic exchange interactions. Its simplicity and exact solvability make it an ideal testbed for developing and benchmarking new theoretical methods, including tensor networks and quantum algorithms such as the Variational Quantum Eigensolver.

II. COMPUTATIONAL CHALLENGES OF THE XXZ MODEL. EXPONENTIAL GROWTH IN COST.

The hamiltonian of the XXZ model for spin-1/2 particles in 1D is given by:

$$H = -\sum_{i=1}^{L} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z\right) \quad (1)$$

where Δ is the anisotropy parameter and S_i^x, S_i^y, S_i^z are the spin-1/2 operators at site i. Note that we consider periodic conditions, such that $S_{L+1}^x = S_0^x$. The parameter Δ controls the nature of the spin interactions: for $\Delta = 1$, the model reduces to the isotropic Heisenberg antiferromagnet; for $\Delta = 0$, it describes the XX model; and for $\Delta \gg 1$, it approaches the Ising limit [3].

In the XXZ model, when a new particle is added to the system, the Hilbert space dimension is duplicated. Then, since the computational cost of the exact diagonalization grows polynomially with the number of rows [7], it grows as a polynomial of 2^L, where L is the number of fermions in the chain, i.e., exponentially.

As it has been mentioned, the VQE eigensolver is shown to reduce the computational cost to obtain the

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ground state of a complex hamiltonian like the XXZ model. To carry out this algorithm, we need to propose an ansatz circuit with a set of optimization parameters that is expected to be run on quantum hardware. The process consists in running the quantum circuit on a quantum device that reproduces both the ansatz and the hamiltonian, object of study, and performing quantum measurements of the energy and the obtained state. After each measurement, a classical optimization algorithm will update the parameters so that we can figure out the minimum energy and its associate wave function in an iterative way, with a pre-defined convergence criterium. The whole procedure is based in the following statement about the ground state energy E_0:

$$E_0 \leq \langle \Psi(\theta)|E|\Psi(\theta)\rangle \tag{2}$$

where θ is the set of optimization parameters and $\Psi(\theta)$ is any ansatz wave function [6]. The expression on the RHS of the Eq. (2) is the result of the quantum measurement before optimizing the parameters.

Thus, the objetive of this paper is to find the ground state of the L-length spin-1/2 chains with the VQE in order to find the same results that can be obtained through exact diagonalization -or through the Bethe Ansatz [3], such as the bipartite entanglement entropy, the magnetization of the chain in the x, y and z axes and its variance. The obtained results need to explain the different phases that can be analyzed theoretically and that depend on the anisotropy Δ parameter, being this proved for this model in references such as [3].

III. VQE METHODOLOGY AND BENCHMARKING.

Since we don't have available quantum devices to run our ansatzes, we have carried out the whole algorithm in Python code. This implies defining the ansatzes and obtaining their expected values for the energy with matrix operations, for which we have used the `Pytorch` library. We have found this library particularly useful because it includes the optimizer that we use in this paper. On the other hand, to generate de Hilbert spaces for different number of particles and to define the total spin matrices, we have used the library `netket`.

In order to avoid the problem of vanishing gradients [8] and to reach the global minima of our optimization problems, we apply the Adam optimizer [4]. This optimizer will be employed to find the ground state energy for different values of the anisotropy $\Delta \in [-2, 2]$. After a number of iterations, we establish convergence when the difference between two consecutive energy estimates is less than $1e^{-3}$ J and we find the ground state energy and the wave function. The parameters to which the algorithm has converged will be taken as the first approximation of the ansatz in the next step of Δ, that evolves within a set of 21 equally spaced values. In each iteration, we will obtain the entropy of the state and its expected values for the total spin operators S_x, S_y, S_z, that define the magnetization of the system.

If the results are valid, we should be able to explain the main features of the XXZ model, as predicted theoretically in the reference [3]. Therefore, we will obtain the exact wave functions through diagonalization and compare their expected values with those obtained via VQE. Since we are more familiar with *numpy* for diagonalization tasks, we will use this library, which is also useful for computing entropy through trace evaluations. The wave functions obtained with VQE will be compared to the exact wave functions for all Δ using the fidelity measure. Specifically, we will evaluate the expression

$$F = |\langle \Psi_{\mathrm{ED}}|\Psi_{\mathrm{VQE}}\rangle|^2, \tag{3}$$

which should ideally be 1 in the perfect scenario. This will help validate the quality of our ansatzes.

Additionally, we will assess whether our ansatzes are sufficiently complex to follow the time evolution of a given initial state. To do this, we will evolve a fixed initial state with the evolution operator and define a new optimization problem in which the ansatz is tasked with maximizing its fidelity with the exact evolved state. In this case, the optimization parameters will be initialized in two possible ways: randomly or with the values of the previous time step. On the other hand, the initial state will be $|+\rangle^{\otimes L}$ with $L = 5$ and, since the hamiltonian is time independent, its evolution will be defined as follows:

$$|\Psi(t)\rangle = \exp\left(-itH\right)|+\rangle^L \tag{4}$$

IV. VQE IMPLEMENTATION AND RESULTS.

The start point of the VQE is the definition of the ansatz circuit. We have proposed three differente ansatzes with different number of parameters. The first one, consists in the following circuit:

$$|\Psi(\theta)\rangle = \Pi_{i=1}^{L}\left(CNOT^{i,i+1}R_z^i(\theta_i)R_y^i(\theta_i)\right)|1\rangle. \tag{5}$$

This circuit represents the entanglement of the particles with the $CNOT$ gates at nearest neighbours. This is the most efficient in terms of quantum hardware and in terms of the number of optimization parameters, as it has L parameters and only $2L$ rotation matrices R_x, R_y. Notice that the ket $|1\rangle$ represents the state with all the spins up.

The second ansatz introduces the entanglement through the gates $R_{zz}^{i,j}, R_{xx}^{i,j}$ at nearest neighbours [2]:

$$\begin{aligned}|\Psi(\theta)\rangle = \Pi_{i=1}^{L}R_x^i(\theta_{i+3L+1})R_z^i(\theta_{i+2L+1}) \\ R_{xx}^{i,i+1}(\theta_{i+L-1})R_{zz}^{i,i+1}(\theta_i)|1\rangle.\end{aligned} \tag{6}$$

This one needs $4L + 1$ parameters and each execution is proved to need more computational resources. However,

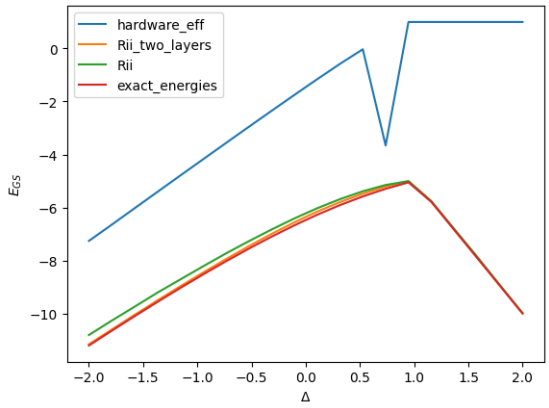

FIG. 1. Energies of the three ansatzes and the exact energy for the ground state against the anisotropy parameter Δ. `hardware_eff` refers to the first ansatz, `Rii` to the second one and `R_ii_two_layers` to the last one.

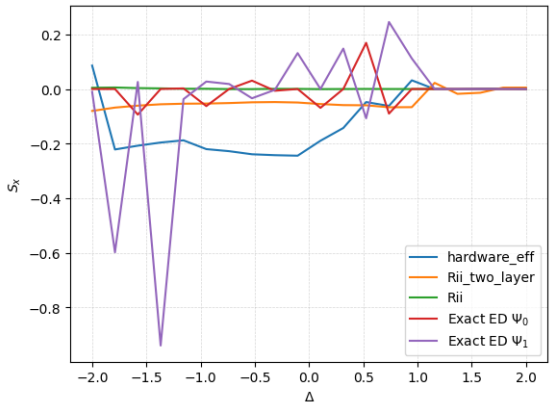

FIG. 2. Total spin S_x expectation value of the three ansatzes and the exact expectation value for the two ground states against the anisotropy parameter Δ. `hardware_eff` refers to the first ansatz, `Rii` to the second one and `R_ii_two_layers` to the last one.

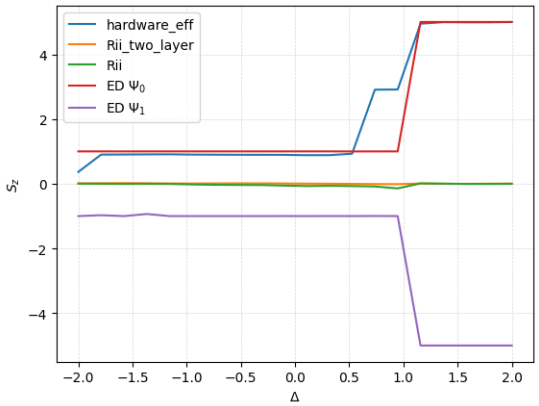

FIG. 3. Total spin S_z expectation value of the three ansatzes and the exact expectation value for the two ground states against the anisotropy parameter Δ. `hardware_eff` refers to the first ansatz, `Rii` to the second one and `R_ii_two_layers` to the last one.

we propose another ansatz, more complex, that applies the same operator twice, but with different parameters. This gives us $8L + 2$ parameters.

If we run the VQE algorithm with the three ansatzes for a chain of $L = 5$ spins, we obtain the results shown in Fig. 1. There, we observe that both the second and third ansatzes yield energies very close to the true ground state energy. The best fit is achieved with the two-layer ansatz. This demonstrates that a circuit with sufficient parameters and a good representation in terms of the interaction range can provide highly accurate approximations to the energy. However, we have shown that with very simple approaches it is difficult to obtain good approximations to the energy, as is the case with the first ansatz.

It´s expected from a valid solution to have fluctuations in the components of the total spin orthogonal to the S_z component, as they don't commute with the hamiltonian, and that´s what we observe in the Fig. 2. Notice that in the exact diagonalization we obtain two ground states. On the other hand, if we plot the expectation value of the magnetization in the z axis for the three ansatzes, we obtain the data from the Fig. 3, where we observe again that the first ansatz doesn't capture well the behaviour of the ground state. Besides that, the fact that both the second and third ansatzes have $S_z = 0$ suggests that they're a uniform superposition of the two ground states of the chain. We validate this intuition plotting the fidelities of the ansatzes in Fig. 4 , where we observe that the sum over the fidelities with the two ground states is very close to 1 for the third ansatz and it shows a worse result for the second ansatz. Nevertheless, in $\Delta = 1$ there is a particular loss of accuracy. This can be explained if we consider that, in this case, the degeneracy for the ground state is $g = 5$ and our ansatzes have components on the ground states that aren't considered in the fidelity. This is the only possible explanation, since in the Fig. 1 the energy eigenvalue is very close to that obtained through exact diagonalization.

Regarding the entropy, we observe in the Fig. 5 that both our ansatzes converge to 1 for $\Delta > 1$, whereas the exact ground states converge to 0. The ground states have null bipartite entropy because they have all the spins aligned. Thus, as the second and third ansatzes are a uniform superposition of both ground states, their entropy needs to be 1, just as it is the bipartite entropy of the following Bell state:

$$|\Psi\rangle \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle). \tag{7}$$

Finally, having checked that the third ansatz is the best approach to the problem, we will evaluate if it's good

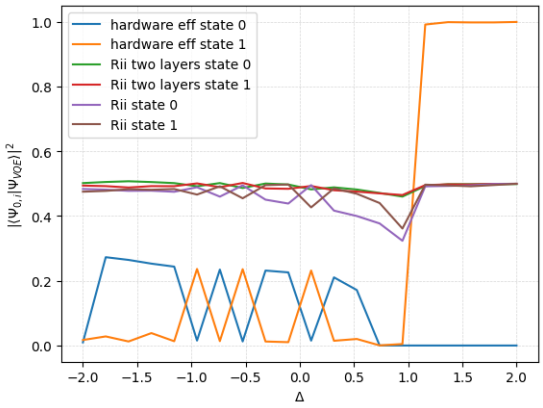

FIG. 4. Fidelity of the three ansatzes with the two ground states against the anisotropy parameter Δ. `hardware_eff` refers to the first ansatz, `Rii` to the second one and `R_ii_two_layers` to the last one.

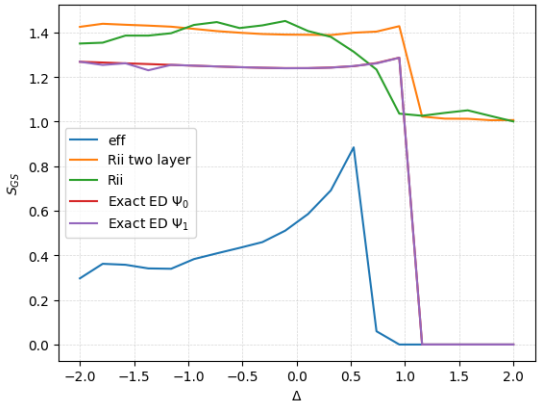

FIG. 5. Entropy of the three ansatzes and the exact entropy for the two ground states against the anisotropy parameter Δ. `hardware_eff` refers to the first ansatz, `Rii` to the second one and `R_ii_two_layers` to the last one.

enough to follow the time evolution described by the Eq. 4. Our optimization algorithm will now minimize the loss function below:

$$Loss = 1 - ||\langle\Psi(\theta)|\Psi(\theta)\rangle||^2. \tag{8}$$

For this, we use again the Adam optimizer and initialize randomly the parameters in $t = 0$. After that, the parameters in each step will be initialized as the parameters obtained in the previous time step, just as we have explained in previous sections. With this, we obtain the data of the Fig. 6 for the fidelity of the time dependent wave function. As it may be noticed, the ansatz with two layers is good enough to follow the time evolution of our state $|+\rangle^{\otimes L}$. However, the number of iterations that the optimizer takes to converge to the state we are looking for has been high during all the simulations.
On the other hand, if we execute the same algorithm but with random initialization for the parameters, the throughput decreases over a 10%. Here we notice the importance of the initialization of our optimization pa-

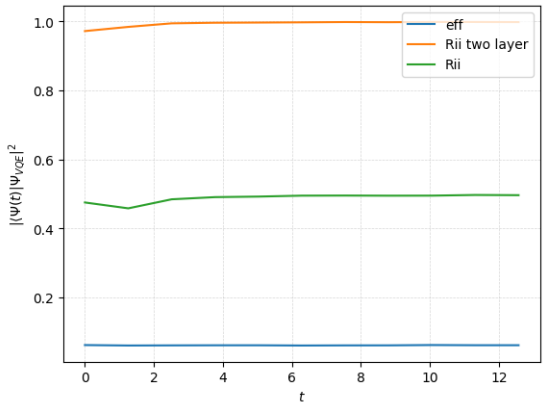

FIG. 6. Fidelity of the time evolved wave function against t. The parameters are initialized with their values at the previous time step.`hardware_eff` refers to the first ansatz, `Rii` to the second one and `R_ii_two_layers` to the last one.

rameters. It is reasonable to expect that if we evolve the wave function only by a small time step, the optimal parameters will remain close to those of the previous step. During this work, we have understood the importance of the complexity of the ansatz in the VQE. If we adapt the complexity of our ansatz to the problem, we will obtain very accurate approximations, as those that are shown in the Fig. 1, where the energy of the third ansatz appears to be an accurate approximation to the ground state energy, that can be almost perfect if we choose a more precise convergence criterion for the optimization. The solution offered by this ansatz gives good insights about the behaviour of the $L = 5$ spin-1/2 chain regarding the bipartite entanglement entropies, the magnetization and the energies. However, the number of iterations required for the optimization algorithm to converge to a precise solution is very high. We find that, to obtain an accuracy of 98.38% for $\Delta = -1.5$ with the third ansatz, 39 iterations are required.

V. OUTLOOK.

Considering these results, and having tried with different initial learning rates for the Adam optimizer with no remarkable results, we find interesting to try different optimization algorithms that may need less iterations to find accurate solutions. Since we don't know the time it takes to perform a big number of quantum simulations and quantum measurements on quantum devices, it would be interesting to do research about it. Besides that, as our simulations have been classical, in that case, we would need to consider the effect of quantum errors, that may increase the number of iterations. This number must be always small enough to make the VQE better than exact diagonalization.

On the other hand, we consider primordial to

know a method to define ansatzes adapted to each problem without needing to compare with exact diagonalization results, as the objective of the VQE is to solve problems that cannot be solved in a finite time with exact diagonalization.

[1] Daniel Del Canto de Guzmán. Code for vqe simulation in google colab. `https://colab.research.google.com/drive/1X7eKgl8vI55HYTAOU8UJkW2DVmwQuk4J`, 2025. Accessed: 2025-02-18.

[2] Trong Duong, Sang T. Truong, Minh Tam, Bao Bach, Ju-Young Ryu, and June-Koo Kevin Rhee. Quantum neural architecture search with quantum circuits metric and bayesian optimization, 2022.

[3] Fabio Franchini. *An Introduction to Integrable Techniques for One-Dimensional Quantum Systems*. Springer International Publishing, 2017.

[4] Diederik P. Kingma and Jimmy Ba. Adam: A method for stochastic optimization, 2017.

[5] Jarrod R McClean, Jonathan Romero, Ryan Babbush, and Alán Aspuru-Guzik. The theory of variational hybrid quantum-classical algorithms. *New Journal of Physics*, 18(2):023023, feb 2016.

[6] Alberto Peruzzo, Jarrod McClean, Peter Shadbolt, Man-Hong Yung, Xiao-Qi Zhou, Peter J. Love, Alán Aspuru-Guzik, and Jeremy L. O'Brien. A variational eigenvalue solver on a photonic quantum processor. *Nature Communications*, 5:4213, 2014.

[7] Phil Romero, Manish Bhattarai, Christian F. A. Negre, Anders M. N. Niklasson, and Adetokunbo Adedoyin. Matrix diagonalization as a board game: Teaching an eigensolver the fastest path to solution, 2023.

[8] Jules Tilly, Hongxiang Chen, Shuxiang Cao, Dario Picozzi, Kanav Setia, Ying Li, Edward Grant, Leonard Wossnig, Ivan Rungger, George H. Booth, and Jonathan Tennyson. The variational quantum eigensolver: A review of methods and best practices. *Physics Reports*, 986:1–128, November 2022.