ICFO Challenge
Team Orange Juice

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1 Spins in the ground state - the Heisenberg XXZ model

1.1 Ground state energy of the XXZ model

For $\Delta > 1$ the system is in the ferromagnetic phase, meaning that all spins face in the same direction. Consequently, the ground states can be simply described as $|0\rangle^{\otimes N}$ or $|1\rangle^{\otimes N}$. The second state can be simply prepared by applying an X-gate to each qubit. By using the HeisenbergModel from qiskit_nature and the estimator primitive, we find perfect agreement for the ground state energy between our simulations and the exact solution $\epsilon_{gs} = -N\Delta/4$ for $\Delta = 4$.

Next, we consider the case with $\Delta = -2$, which belongs to the anti-ferromagnetic phase. We use the NumPyMinimumEigensolver to compute the exact ground state energy at $\epsilon_{gs} \approx -7.46$. To reproduce this result with a VQE, we choose a TwoLocal ansatz with Y-rotations as single-qubit gates and CZ-operations as entangling gates. We further specify the entanglement to be circular. Using the SPSA optimizer with a maximum of 500 iterations, we achieve a ground state energy of around $\epsilon_{gs} \approx -7$, in good agreement with the ideal solution. The optimization process is depicted in Fig. 1.

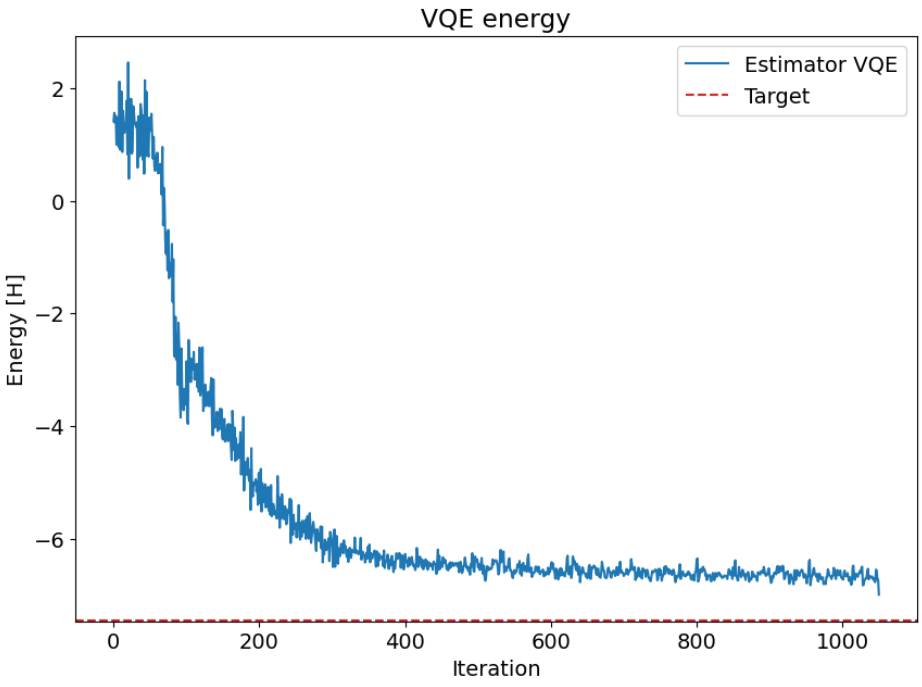

Figure 1: Ground state energy as a function of VQE iterations.

1.2 Ansatz expressibility

Here, we once again use the TwoLocal ansatz, with sca- and full entanglement. Also, we make use of the SPSA, COBYLA and SLSQP optimizers. We select the initial parameters from a uniform distribution for all combinations of ansätze and optimizers. The results for all six different

combinations are shown in Fig. 2. We find that the sca entanglement together with the COBYLA optimizer give by far the best results with the fastest convergence. Also, we noticed that sca entanglement leads to quicker convergence than the regular circular entanglement.

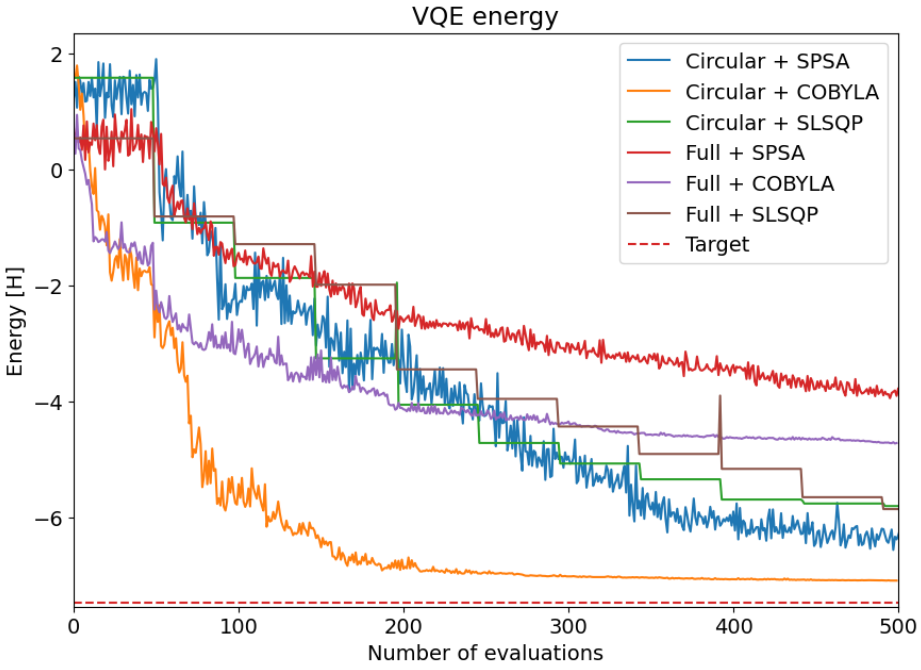

Figure 2: Ground state energy as a function of the number of evaluations during the different optimizations. (Circular refers to the sca entanglement here)

1.3 Phase diagram

To compute the phase diagram, we use the sca + COBYLA VQE to determine the ground state for each value of Δ. Before diving into the magnetic properties, we simply compare the VQE ground state energies to the exact solution. In Fig. 3, we can see that the ideal ground states are only achieved in the ferromagnetic phase.

Next, we use the optimal circuit parameters from the ground state energy calculations to build our state preparation circuits. Instead of naively applying the Estimator to all the observables from the magnetization, staggered-magnetization and nearest-neighbor correlations, we make use of the Sampler. All observables are of the type Z or ZZ and can therefore be reconstructed from the same probability distribution. This way, we only have to use the Sampler once. The results are shown in Fig. 4. We observe the two phase transitions at the critical points $\Delta = -1$ and $\Delta = 1$.

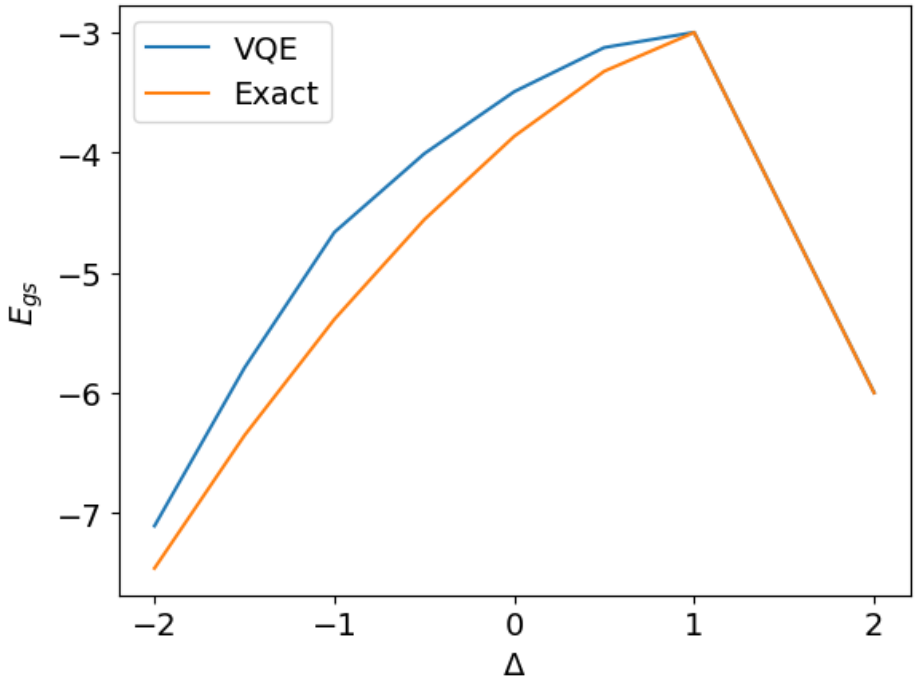

Figure 3: Ground state energie as a function of Δ.

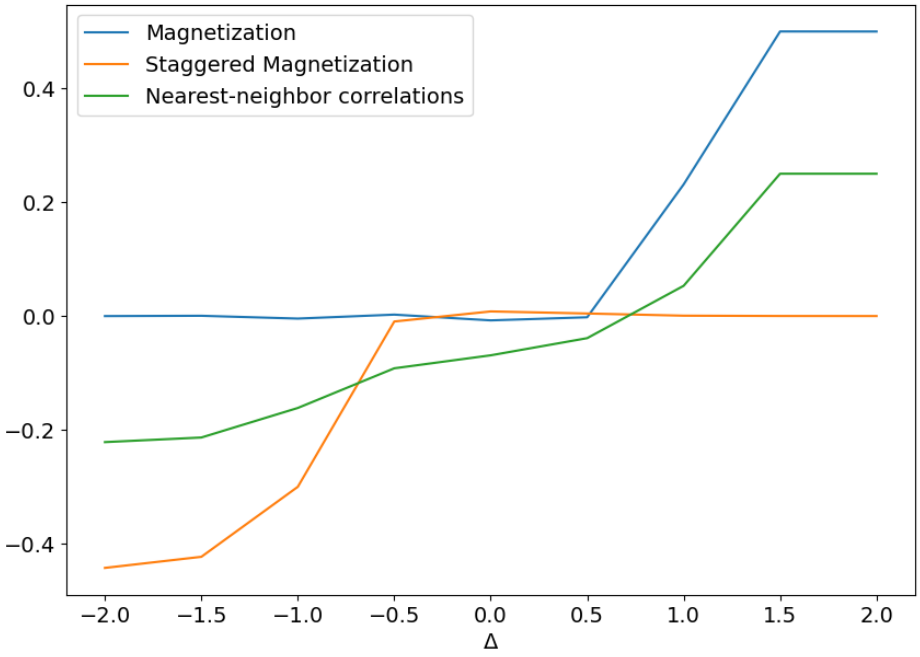

Figure 4: Magnetization, staggered magnetization and nearest-neighbor correlations as a function of Δ.

2 Fermions in excited states - the lithium hydride molecule

2.1 Molecular spectra

To obtain the molecular Hamiltonian, we make use of the PySCF library. We describe the Hamiltonian in the STO-3G basis set according to the task. By using the PySCFDriver, we obtain the Hamiltonian in second quantization. We map this Hamiltonian to a qubit Hamiltonian with the ParityMapping. The obtained Hamiltonian then consists of PauliSumOperators which contain a weighted sum of Pauli strings. From this Hamiltonian, a simulation using the VQE can be performed. However, the Hamiltonian consists of a large amount of Pauli strings (> 600), which is computationally demanding. To reduce the runtime and qubit cost, we utilize the FreezeCoreTransformer, which is used to freeze the inner orbitals. While this approach significantly increases the runtime and storage cost, freezing the wrong orbitals may result in an unphysical model. Further, symmetry transformations in the mapping process can be used reduce the qubit count. By applying these techniques, the original 12-qubit hamiltonian is reduced to an 8-qubit system with < 300 strings.

Due to technical issues, we were not able to make use the UCCSD ansatz with a Hartree-Fock initial state, which would be well-suited for these kinds of problems. Instead, we once again refer to the TwoLocal ansatz (which may violate the conserved quantities).

Before tackling the excited states, we perform ground state calculations using exact diagonalization and VQE like in the first task. Since the VQE generally does not inhibit the nuclear repulsion, we have to manually add the repulsion energy. We observed the best results using the COBYLA optimizer. The exact ground state energies as well as the VQE approximations are depicted in Fig. 5. We find decent agreement for most interatomic distances. Decrepancies might be due to the lack of iterations (long runtime), an unsuited ansatz (as it breaks the particle number conservation). Also, other optimizers might perform better in the regime of few iterations. Due to time limitations, we only tested the SPSA and COBYLA, of which COBYLA performed significantly better.

To access excited states, the typical VQE needs to be modified, as it only allows for ground state calculations. For our approach, we choose the Variational Quantum Deflation algorithm (VQD), which can be used to iteratively estimate excited states. Here, at the first familiar VQE is used to compute the ground state. Higher excited states are generated by using a penalty term, which makes sure that the excited states do not overlap with lower states. In Fig. 6 - 8, we show our VQD results for the ground state, first excited state and second excited state. Here, due to issues with the reduced Hamiltonian, we had to refer to the more expensive full 12-qubit hamiltonian. For this reason, we could only perform very few iterations, explaining the strong discrepancy between the VQD data and the ideal results.

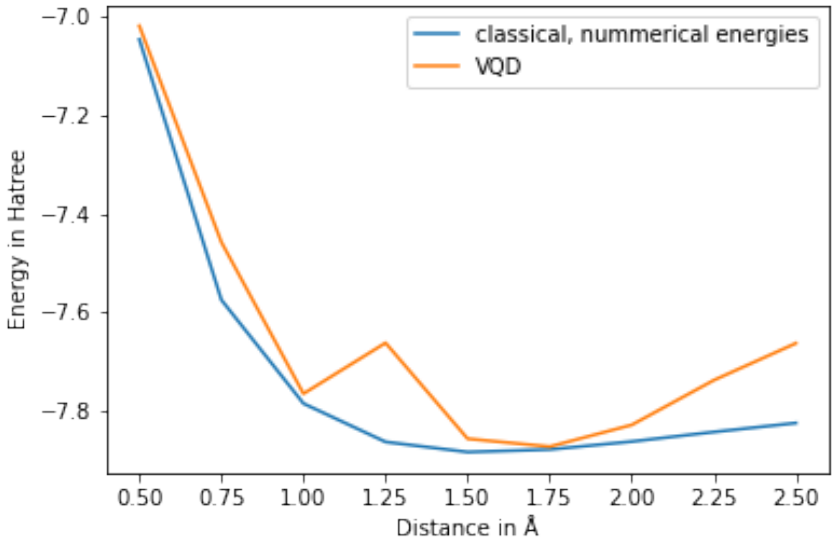

Figure 5: Ground state energy as a function of the interatomic distance.

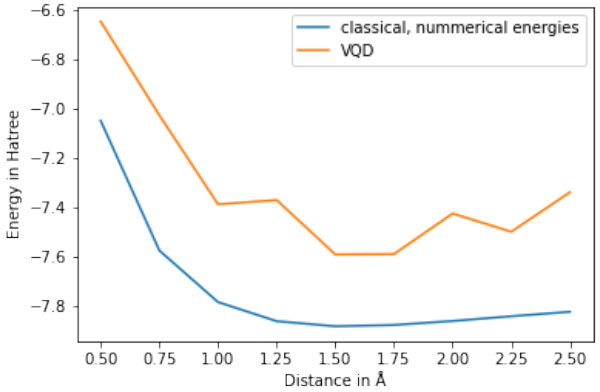

Figure 6: Ground state energy as a function of interatomic distance.

3 Acknowledgements

Last, we want to thank everybody involved in organising this exciting event! Also, we apologise for obvious mistakes, we are very tired... ;-)

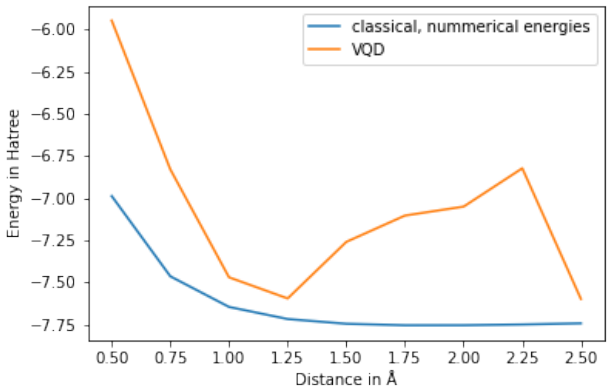

Figure 7: First excited state energy as a function of interatomic distance.

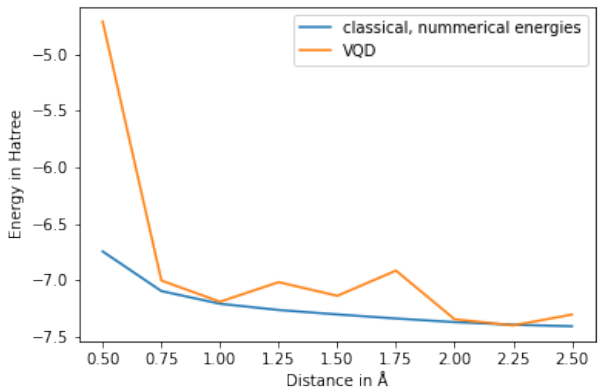

Figure 8: Second excited state energy as a function of interatomic distance.