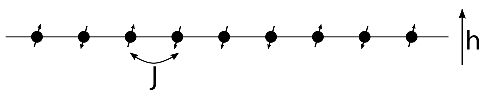
Hamiltonian Simulation Experiment - Technical Details

The vastly diverse physical properties of various materials have always played a crucial role in science and engineering. Since experiments are costly and classical simulation falls short, using quantum computers for simulations promises a huge potential. In this experiment we show how the Ion-Trap Quantum Computers of AQT can be used to simulate a magnetic system. Thus demonstrating the potential of quantum computers for material simulations.

The German IT service provider SVA System Vertrieb Alexander GmbH employs an AQT quantum computer to simulate macroscopic properties of a magnetic system, demonstrating the potential of quantum computers for material simulations. The material properties have always played a crucial role in science and engineering. Experiments in laboratories are costly and classical computers fall short in simulating quantum systems. These motivations led to the development of a new type of computer paradigm based on quantum physics: quantum computers. Their inherent utilization of quantum effects makes them the perfect candidates to simulate quantum systems efficiently. In the following paragraphs, we will show how the Ion-Trap Quantum Computers of AQT can be used to simulate magnetic systems. In our experiment, we want to measure the total magnetization of a simple Ising model after a certain amount of time has passed. We will discuss the formal system description, its formulation in the terms of a quantum circuit and finally the execution on a real quantum device.

Problem formulation

Magnetic systems are all-around us, but explanation of their behaviour (effects) requires sophisticated models due to their large sizes and the long-range nature of the magnetic force. One of the simplest models for magnetism is the one-dimensional transverse-field Ising model, which consists of spins located on a chain. The spins interact with their nearest neighbours and with an additional external field.



Two constants J, h represent the strength of the interaction between each two spins and between the external field and each spin, respectively. To describe the system from a mathematical point of view, we use a state-vector $|\psi(t)\rangle$ and a Hamiltonian which takes into account all interactions:

$$H = H_{zz} + H_x = \sum_{<j,k>} J\sigma_j^z\sigma_k^z + \sum_j h\sigma_j^x,$$

where σ_j^α with $\alpha \in \{x, y, z\}$ are Pauli-Operators describing the three distinct spin orientations. Both entities are related by the Schrödinger equation which describes the time evolution of the state-vector. As H is not time-dependent, the Schrödinger equation can be formally solved:

$$H|\psi(t)\rangle = -i\frac{\partial}{\partial t}|\psi(t)\rangle, \Rightarrow |\psi(t)\rangle = \exp(-itH)\,|\psi(t=0)\rangle.$$

As part of this formal solution, a new operator arises, called time evolution operator:

$$U_t = \exp(-itH).$$

With the help of this operator, we can calculate the state of our system after an evolution for time t given the current state of the system. In practice, it is crucial to find an efficient representation of this operator in terms of a quantum circuit. Since a direct implementation of the time evolution operator is usually not possible, we resort to two approximation schemes. The first idea is to break down the full evolution into smaller time steps with $t' = t/R$ which will allow us to use small time approximation schemes, called trotterization. The constant R determines the number of time-steps separating the total time t.

Additionally, we want to break up the sums in our Hamiltonian which will make the implementation with quantum circuit possible, while creating a small specific error.

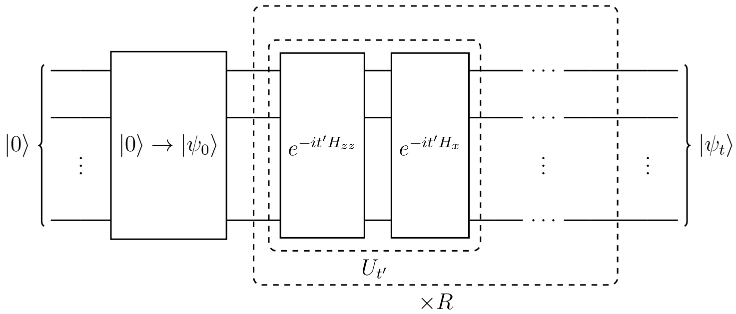
$$U_{t'} = \exp\left(-it'(H_{zz} + H_x)\right) \approx \exp\left(-it'H_{zz}\right)\exp\left(-it'H_x\right) \approx \prod_{<j,k>} \exp\left(-it'J\sigma_j^z\sigma_k^z\right) \prod_j \exp\left(-it'h\sigma_j^x\right).$$

These two terms can be implemented very easily since they relate to rotation gates on two and single qubit, respectively. As we can see in the following definition

$$\exp\left(-i\phi\sigma_j^x\right) = R_x(2\phi) \text{ and } \exp\left(-i\phi\sigma_j^z\sigma_k^z\right) = GMS(2\phi),$$

with some arbitrary real angle ϕ. The latter gate is called Mølmer–Sørensen gate.

The circuit for the calculation can now be composed as:



Magnetization of a magnetic system describes the measure of alignment of its individual parts with respect to some direction. The maximal magnetization is reached when the spin of each individual element aligns along the same direction. We talk about minimal magnetization when all spins are randomly oriented in such a way that their overall contribution cancels out. We are interested in the second power of the magnetization along the z-axis to avoid possible negative values

$$M^2 = |\langle\psi(t)| \sum_j \sigma_j^z |\psi(t)\rangle|^2$$

Experimental Execution

In our experiment, we want to measure the final magnetization of an Ising chain in an external transversal magnetic field and after a fixed amount of time. As the starting state we assume the Ising chain being fully magnetized along z-axis. To get an idea of how the system behaves, we calculate this property for various values of the exchange interaction of the spins J.

A quantum computer based on trapped ions seems to be the ideal candidate for such simulation. For example, the two-qubit rotation gates (called Mølmer–Sørensen gates) implementing the time evolution belong to the native gate set of the trapped ion quantum computer. In particular, we use the latest generation system from AQT called IBEX. Additionally, we can rely on an abundance of open-source software like Qiskit which allows a simple and straightforward implementation of our problem.

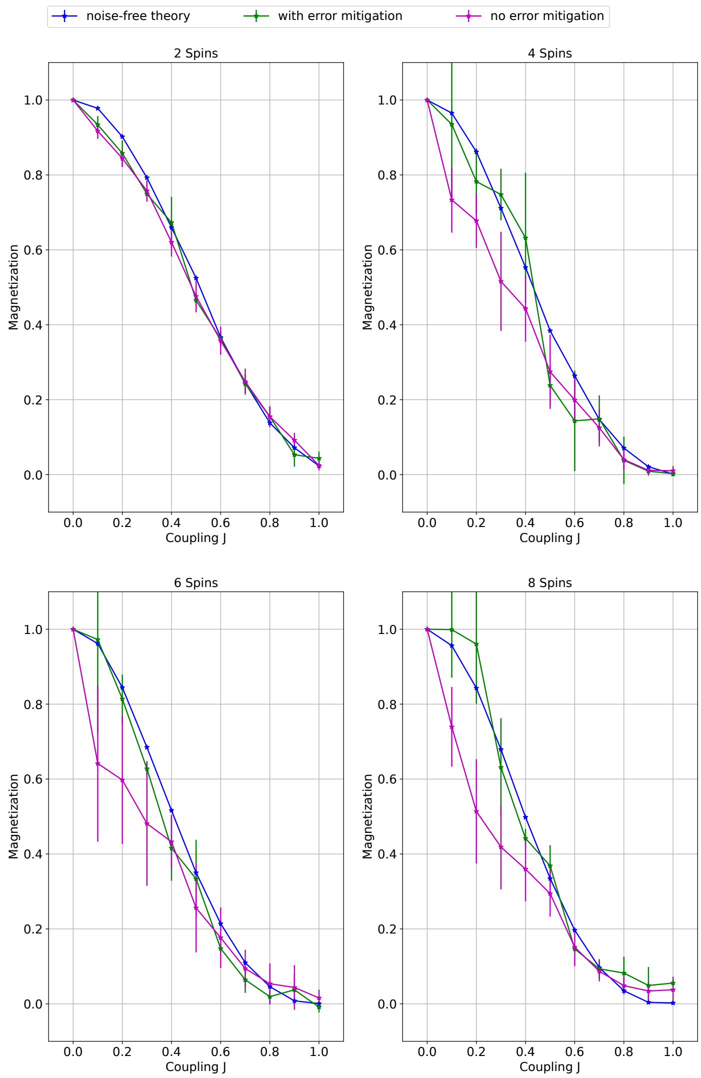
Unfortunately, the direct and unprocessed experimental results do not exhibit the expected features, since IBEX, as all other first generation quantum devices, performs with errors leading to noise. Nonetheless, such noise can be suppressed with error mitigation method called zero-noise extrapolation to such an extent that allows us to obtain improved and meaningful results. We do not have to implement the method ourselves, but we can rather utilize the well-known open-source error-mitigation software mitiq and apply it to our simulation. The results were obtained with zero-noise-extrapolation method with linear fit and scale factors of [1.25, 1.50, 1.75, 2.00].

Discussion

In the plots below we see the second power of magnetization for different number of qubits, i.e., spins, in dependence on the exchange interaction J. Let us note that we keep $h = 1$, $R = 20$ and $t = 1$ throughout our calculations. The blue line refers to a noise-free simulation of the trotterized problem which can be seen as the baseline. Furthermore, we see the red and green curves which correspond to the simulation on the quantum system with and without error mitigation, respectively. Comparing the results for different qubit numbers, we see a good performance when error-mitigation is used.

The negligible difference between mitigated and non-mitigated results for the 2-spin experiment reflects the high fidelity of the IBEX Q1 single- and double-qubit gates. The difference increases with the number of spins as the depth of the circuit grows with the qubit count. For deeper circuits the qubit coherence times start to play a role and affect the results as an additional source of error.

With the error-mitigation technique we were able to reproduce the expected behavior of the 8-spin system demonstrating small overall gate errors and great qubit control. The present results reveal great potential for the future development and applications.



References

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- **mitiq:** - https://github.com/unitaryfund/mitiq