Quantum Simulation of spin models on IBM Quantum Computers

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Molecular Nanomagnets

Each molecule contains a small number of exchange-coupled magnetic ions (spins). Molecules are arranged on a crystal lattice.

Prototypical systems to study quantum effects and promising for applications

\[
\text{Fe}_8\text{O}_2\text{(OH)}_{12}\text{(tacn)}_6\text{Br}_8
\]

\[
H_{\text{eff}}(S_1,...,S_N)
\]

\[
\text{Fe}^{3+}
\]
Molecular Nanomagnets as bits

Hysteresis and bistability at the single-molecule level → information storage in single molecules
Molecular Nanomagnets as qubits

Engineering the coupling between molecular spin qubits by coordination chemistry

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A modular design of molecular qubits to implement universal quantum gates
A lot of information can be obtained by studying how neutrons change their velocity when they are scattered by these materials.
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Inelastic Neutron Scattering

The pattern of maxima and minima reflects the spatial structure of the states involved in the transition.

A lot of information can be obtained by studying how neutrons change their velocity when they are scattered by these materials.
Challenge: interpretation of spectra of interesting molecules

- Experiments on rather small molecules can be interpreted by quantum simulations performed on classical computers.
- However, there is an exponential increase of the required computational resources and many molecules cannot be understood.


72Fe30

Europhys. Lett. 56, 863 (2001)
I can use a QUANTUM COMPUTER to simulate the dynamics and calculate neutron spectra!
Magnetic neutron cross-section

\[ S(Q, \omega) \propto \sum_{ij} \sum_{\alpha\beta} \sum_p F_i(Q) F_j(Q) \left( \delta_{\alpha\beta} - \frac{Q_\alpha Q_\beta}{Q^2} \right) \left\langle 0|s_i^\alpha|p\right\rangle \left\langle p|s_j^\beta|0\right\rangle e^{-iQ \cdot R_{ij}} \delta(\hbar\omega - E_p) \]

Atomic Form factors

Positions of magnetic ions

Can be extracted from dynamical correlations functions

1. Calculation of \( C_{ij}^{\alpha\beta}(t) \) by means of a QC (hard task for a classical device for large number of spins).

2. Obtain \( \left\langle 0|s_i^\alpha|p\right\rangle \left\langle p|s_j^\beta|0\right\rangle \) and \( E_p \) from a QC and easily compute \( S(Q, \omega) \) on a classical computer.

arXiv:1809.07974

Paper submitted
We experimentally test this method by computing the INS cross-section for prototypical spin clusters on IBM processors composed of transmon qubits (5- (ibmqx4), 16- (ibmqx5) and 20-qubits (ibmq20)).

\[ \mathcal{H} = \sum_{i=1}^{N-1} J_i^\alpha s_i^\alpha s_{i+1}^\alpha + B \sum_{i=1}^{N} g_i s_i^z \]

\(N = 2, 3, 4 \) (+ ancilla qubit).

e. g., for \(N=2\)

\[ \langle \sigma_2^x(t)\sigma_1^x \rangle_{00} = \langle \sigma_a^x \rangle + i\langle \sigma_a^y \rangle \]

arXiv:1809.07974
Very good agreement with exact calculation!
We computed the cross-section of spin dimers characterized by different degrees of entanglement: 1 Heisenberg model, 2 Heisenberg model with inequivalent ions, 3 Ising model.

By focusing on the $Q_x$-dependence of a single transition: amplitudes of the oscillations fingerprint the degree of entanglement (Nature Comm. 8, 14543 (2017)).

For a spin trimer:
Error assessment and scalability

We have studied the various errors and their propagation by comparing targeted experiments on the real hardware to numerical noisy simulations including all main errors: systematic-coherent, measurement and incoherent errors (including relaxation and dephasing).

1) elementary gates: $R_x(\vartheta)$ gate

We have quantified all errors and identified SCEs as the leading ones.
To test our error model, we compare the numerical simulation of dynamical correlation functions including errors to experimental results on 3, 4 and 5 qubits (e.g., involving a sequence of 105 noisy gates for N=4).

Different classes of errors can be distinguished:

- Incoherent Errors essentially yield to an overall attenuation
- Concatenation of SCEs can significantly alter the dynamics

MOSTLY CORRECTED BY OUR METHOD
Scalability and near-term perspectives

We can now quantitatively investigate the scalability of the method, by including a realistic propagation of errors:

• With current errors the maximum $N$ enabling a reliable computation is $\sim 6$

• Even a simple halving of SCEs (keeping fixed IEs) would enable a good simulation with $N = 12$

• by removing the main SCEs and keeping IEs (including $T_1$, $T_2$), the simulation for $N = 12$ is very good

SCEs are currently the main limiting factor and mitigating them is the key to scale to an interesting number of qubits.
Conclusions

- **Quantum simulation** of spin models of interest for physicists and chemists.

- By performing experiments on ibmqx4, ibmqx5, and ibmq20 chips, we show that state-of-the-art (non error-corrected) quantum computers can be used to efficiently calculate the neutron cross-section of finite-size spin systems.

This approach can be extended with forthcoming technological progresses to a number of spins that would make a quantum hardware much faster and efficient than a classical device for the practical interpretation of many experimental data.