Quantum simulation of magnetic systems

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"Nature isn’t classical, dammit, and if you want to make a simulation of nature, you’d better make it quantum mechanical, and by golly it’s a wonderful problem, because it doesn’t look so easy”
The simulation of quantum systems by classical computers is intrinsically inefficient, because the required number of bits and operations grows \textit{exponentially} with the system size.
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A few dozens of controllable qubits could already outperform classical computers.

Digital Quantum Simulator

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\[
H = \sum_k H_k^{(1)} + \sum_k H_k^{(2)}
\]

\[
U(t,0) = e^{-iHt} \approx \left( \prod_k e^{-iH_k^{(1)}\tau} \prod_k e^{-iH_k^{(2)}\tau} \right)^n \quad \tau = \frac{t}{n}
\]

Optimizing the digitalization

Target: Pisa tower

Elementary “Trotter” brick in a discretized simulation of the target

\[ \tau' < \tau \Rightarrow n' > n \]

\[ \tau'' < \tau' \Rightarrow n'' > n' \]

\[ n\tau \gg T_2 \]

Coarse discretization

Good simulation

Simulator fails
Optimizing the digitalization

In the **NISQ** (noisy-intermediate scale quantum computing) era each operation is error-prone

By increasing the circuit depth we increase the error probability.

**Trade-off**

<table>
<thead>
<tr>
<th>Coarse discretization</th>
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Physical implementation: a few examples

- **State-of-the-art leading** technologies: superconducting *(transmon)* qubits
  - Existing chips with 5-53 qubits enable to implement non trivial quantum algorithms.
  - Other leading technology: trapped ions

- **Prospective** technologies: Molecular Nanomagnets
  - Other promising platforms: photons, quantum dots...
Superconducting qubits

The quantum dynamics of spin chains can be simulated by concatenating elementary gates.

Noisy results are corrected by exploiting symmetries of the extracted observables, thus recovering the correct dynamics.
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Extracting experimental observables

Quantum hardware simulating four-dimensional inelastic neutron scattering

Quantum simulations of the spin dynamics of prototypical spin systems are used to calculate the 4D inelastic neutron cross-section

In the near future, quantum computers will be used to interpret experiments which cannot be modeled by classical machines
Molecular Nanomagnets

- Long $T_2$
- MNMs
- Chemical tunability
- Multi-level structure

- $T_2 \approx 0.7$ ms!

References:
- Nat. Commun. 7, 11377 (2016)
Engineering the coupling between molecular qubits

- A **switchable** QQ interaction is mandatory to implement quantum simulations of interesting models, i.e. to implement both single- and two-qubit gates.

- Molecular qubits can be chemically tuned to effectively switch on/off the QQ coupling by **selectively exciting the switch**.

Engineering the coupling between molecular qubits

- A switchable QQ interaction is mandatory to implement quantum simulations of interesting models, i.e. to implement both single- and two-qubit gates.

- Molecular qubits can be chemically tuned to effectively switch on/off the QQ coupling by selectively exciting the switch.

- Numerical simulations show that these systems are a very promising platform for QS.

- A scalable arrays can be envisaged.

\[ \mathcal{H}_{\text{TIM}} = \lambda \sum_{k=1}^{N-1} s_{kz} s_{(k+1)z} + b \sum_{k=1}^{N} s_{kx} \]


Molecular qubits with embedded error-correction

The easily accessible multi-level structure of molecular qubits can embed quantum error correction at the single-molecule level: errors lead outside from the computational subspace and hence can be detected and corrected, without requiring additional qubits resources.

*Nature Nanotech. 9, 171–176 (2014)*
Molecular qubits with embedded error-correction

Molecular qubits with embedded error-correction


\[ S = \frac{1}{2}, \quad I = \frac{5}{2} \]

QEC embedded in a single molecule, without ancillae

\[ m_I \quad \frac{5}{2} \quad \frac{3}{2} \quad \frac{1}{2} \quad \frac{1}{2} \quad \frac{3}{2} \quad \frac{5}{2} \]
Collaborators

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Understanding → Design