Simulating lattice spin models on today's quantum computers

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Quantum Computing

- Based on qubits: $|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$
- Utilise superposition and entanglement
- Promise of a ‘quantum advantage’
- Use-case: **quantum simulation** of spin systems, molecules...

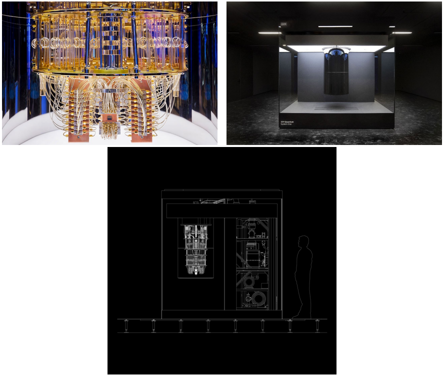


Figure: Superconducting quantum computers developed by IBM.
(Image sources: *https://www.nature.com/articles/d41586-021-03476-5; https://research.ibm.com/blog/fraunhofer-quantum-system-one; https://research.ibm.com/interactive/system-one)*

VQE - Variational Quantum Eigensolver

- Hybrid quantum-classical algorithm
- Finds the ground state by minimising the Hamiltonian expectation value using the **variational principle**:

$$\langle\psi(\theta)|H|\psi(\theta)\rangle \geq E_0$$

- Applications: chemistry, lattice models and many more

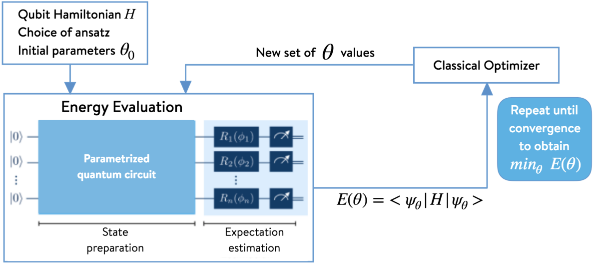


Figure: A schematic showing the steps of the VQE algorithm.
(Image source: *http://openqemist.1qbit.com/docs/vqe_microsoft_qsharp.html*)

Transverse-field Ising model

- **Hamiltonian of the model:**

$$H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x$$

- Non-commuting operators σ_x and σ_y $\Rightarrow$ quantum effects!
- Exhibits a quantum phase transition as the field h is varied
- Can measure magnetisation to find the transition point

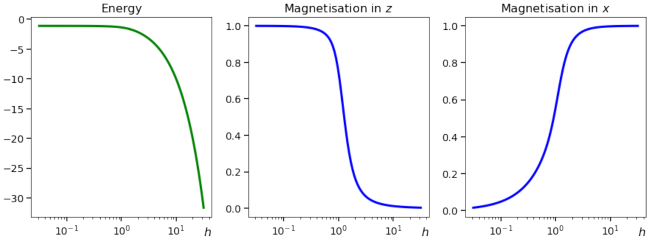


Figure: Solutions for various fields h found by 'exact' diagonalisation for a system of 4 spins in a chain.

Methods

- Choice of an **ansatz**
- Finding the right **optimiser** (COBYLA, SLSQP, SPSA, ...)
- Degenerate ground state for low h
  $\implies$ necessary to add a bias magnetic field in the z-direction:

$$-h_z \sum_i \sigma_i^z$$

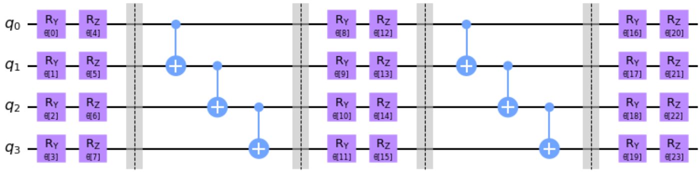
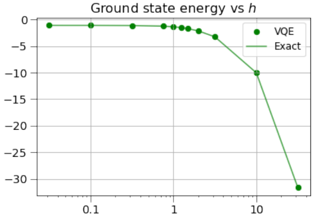


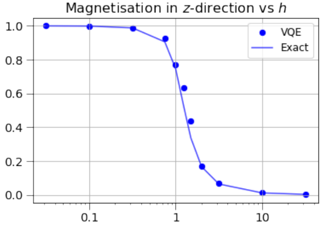
Figure: A standard ansatz of 'RyRz' type with layer depth equal to 2.

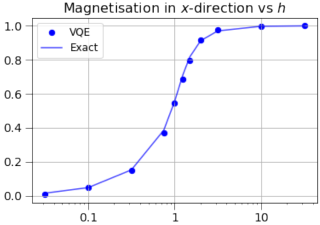
Ideal quantum computer simulation

Best set of results from an ideal simulation:

- 4 spins in a chain
- SLSQP, 1000 iterations
- Energy error: within 1-2%
- State fidelity: over 97%







Effects of noise and error mitigation

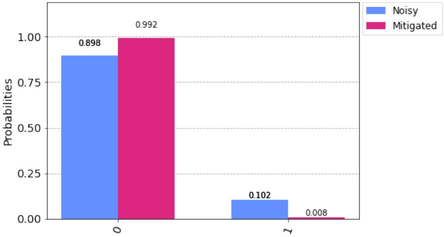
- In the near future only noisy and small devices available
- Full quantum error correction requires many qubits
- Measurement error mitigation:
  1. Perform measurements
  2. Measure basis states
  3. Construct calibration matrix M
  4. Apply inverted matrix to results

```
0 becomes {'0': 9022, '1': 978}
1 becomes {'1': 9049, '0': 951}
```

$$\Downarrow$$

$$M = \begin{bmatrix} 0.9022 & 0.0978 \\ 0.0951 & 0.9049 \end{bmatrix}$$

$$M^{-1} = \begin{bmatrix} 1.12117 & -0.12117 \\ -0.11783 & 1.11783 \end{bmatrix}$$

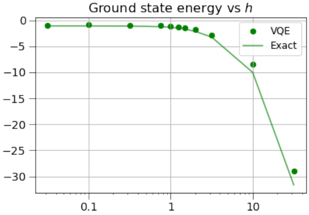


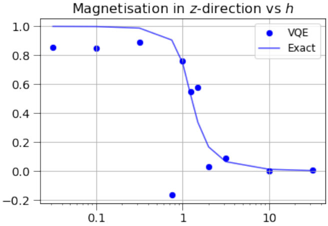
Question: Can today's noisy quantum computers be useful?

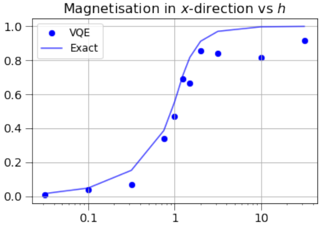
Real IBM hardware

Results from the IBMQ *Belem* device:

- 4 spins in a chain
- SPSA, 1000 iterations
- Energy error: within 10-20%
- State fidelity: mostly over 90%

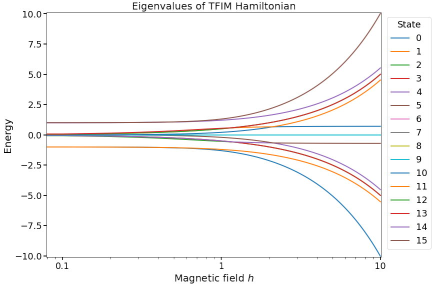






Excited states

- **Variational Quantum Deflation (VQD)** - extension to VQE for finding the excited states
- **Iterative method:** uses previously found ground state to get 1st excited state, which is then used for 2nd exited state, etc.
- Issue - difficult to deal with degenerate states



STATE	GROUND	1ST EXCITED
Energy *(Exact)*	-10.021 *-10.025*	-4.926 *-5.525*
Mag. in z *(Exact)*	0.000 *0.000*	-0.010 *0.000*
Mag. in x *(Exact)*	0.998 *0.997*	0.497 *0.498*
Fidelity	**0.993**	**0.001**

Table: An example set of results from VQD for field $h = 10$.

Conclusions and Outlook

What was achieved:

- Demonstrated a possibility to simulate lattice spin models on ideal quantum computers
- Analysed the effects of noise on the results
- Used real, noisy quantum computers to find ground states of a simple lattice Hamiltonian
- Attempted to find low-lying excited states with ideal quantum computer (partially successful)

Future work?

- Understand how to obtain excited states more reliably
- Attempt at using VQD on real hardware
- Scale up the number of qubits