Digital quantum simulation of spin models

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Main article's results

- *"Quantum computers as universal quantum simulators: state-of-art and perspectives"* by Francesco Tacchino, Alessandro Chiesa, Stefano Carretta, and Dario Gerace
- Theoretical background: mapping spin-type hamiltonian $\longrightarrow$ unitary time evolution operator $\longrightarrow$ quantum circuit
- Main architectural UQS: ion traps and superconducting qubits
  - Experimental achievements
  - Compare their performances
  - Challenges to achieve simulation of many body problem
- Goal project: Simulate the evolution of spins in a 2 and 3 spin Heisenberg model

Step 1. The Heisenberg Hamiltonian model

Heisenberg Hamiltonian of N spins 1/2 immerged in a magnetic field

$$\mathcal{H} = -g\mu_b \sum_{i=1}^{N} \vec{B}\vec{S_i} - \sum_{<i,j>} J_{ij}\vec{S_i}\vec{S_j}$$

- Homogenous magnetic field $\vec{B} = B\vec{e_z}$
- Redefine coupling Constant $J < 0$
- Suppose equivalent spins $\implies$ g-factor $g < 0$

Step 2 and 3. Map the Hamiltonian into a set of Pauli matrices in the form of a sum of local interactions

- Spin operator $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$

Isotropic Heisenberg Hamiltonian of 3 spins 1/2

$$
\begin{aligned}
\mathcal{H}_3 &= H_B + H_{int}^{1,2} + H_{int}^{2,3} \\
&= \frac{Bg}{2}\left(\sigma_z^{(1)} + \sigma_z^{(2)} + \sigma_z^{(3)}\right) \\
&+ J\left(\sigma_x^{(1)}\sigma_x^{(2)} + \sigma_y^{(1)}\sigma_y^{(2)} + \sigma_z^{(1)}\sigma_z^{(2)}\right) \\
&+ J\left(\sigma_x^{(2)}\sigma_x^{(3)} + \sigma_y^{(2)}\sigma_y^{(3)} + \sigma_z^{(2)}\sigma_z^{(3)}\right)
\end{aligned}
$$

- Already in the form $\mathcal{H} = \sum_l H_l$

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Step 4. Write the unitary operator of the time evolution

- Properties of Pauli's operators :
  1. $[\sigma_\alpha^{(j)}, \sigma_\beta^{(j)}] = 2i\epsilon_{\alpha\beta\gamma}\sigma_\gamma^{(j)}$
  2. $[\sigma_\alpha^{(j)}, \sigma_\beta^{(k)}] = 0$
- Then easy computation gives:
  1. $[H_B, H_{int}^{1,2} + H_{int}^{2,3}] = 0$
  2. $[H_{int}^{1,2}, H_{int}^{2,3}] \neq 0$
- The unitary operators to implement are
  1. 2-spin model : $e^{-i\mathcal{H}_2 t} = e^{-iH_B t} e^{-iH_{int}^{1,2} t}$
  2. 3-spin model : $e^{-i\mathcal{H}_3 t} \approx e^{-iH_B t} \left(e^{-iH_{int}^{1,2} t/n} e^{H_{int}^{2,3} t/n} \right)^n$
     $\Longrightarrow$ Trotterization

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Step 5. The time evolution as quantum gates

Example : the non interacting 2-spin Hamiltonian H_B

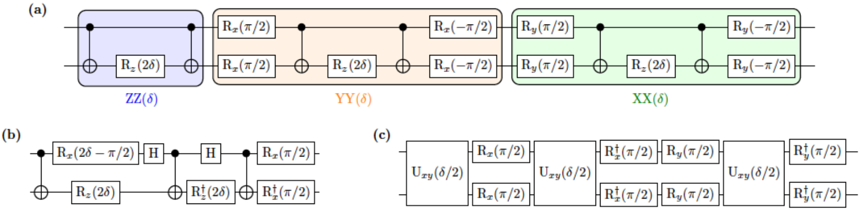
- $$H_B = \frac{Bg}{2}(\sigma_z^{(1)} + \sigma_z^{(2)}) = H_B^1 + H_B^2 \quad \longrightarrow \quad [H_B^1, H_B^2] = 0$$

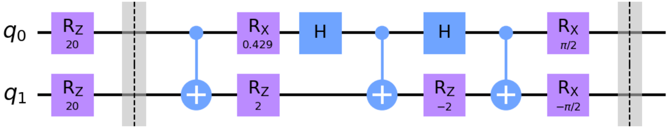
$\Longrightarrow$ Can only consider $H_B^1 = Bg \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

- $$e^{-iH_B^1 t} = \exp \begin{pmatrix} -i\frac{Bg}{2}t & 0 \\ 0 & i\frac{Bg}{2}t \end{pmatrix} = \begin{pmatrix} e^{-i\frac{Bg}{2}t} & 0 \\ 0 & e^{i\frac{Bg}{2}t} \end{pmatrix}$$

$= R_z(Bgt)$ gate on the first qubit

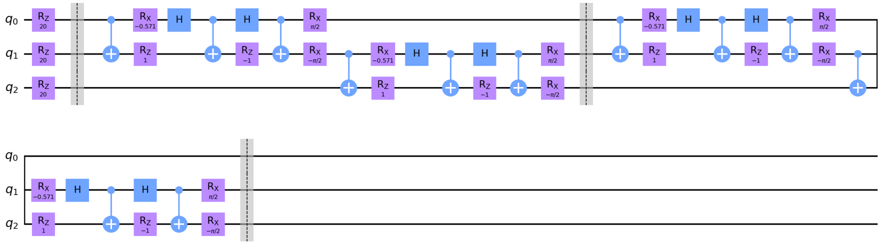
The implemented time evolution for 2 spins



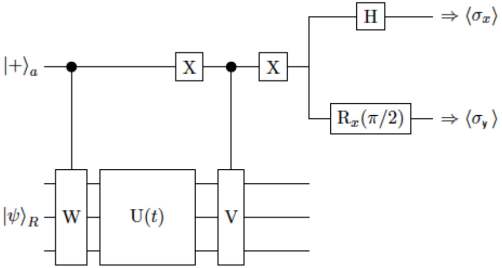


The implemented time evolution for 3 spins

- Trotterization steps $n = 2$



QASM simulations: Correlation function implementation



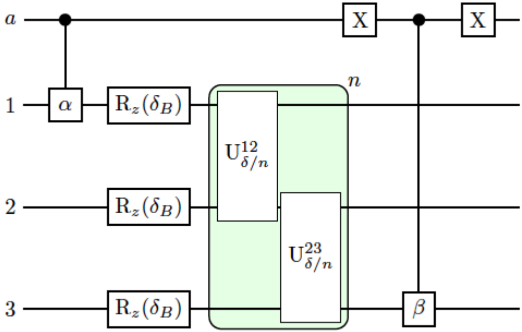
$$\begin{cases} X = HZH \\ Y = R_z^{\dagger}(\frac{\pi}{2}) Z R_z(\frac{\pi}{2}) \end{cases}$$

$C_{VW}(t) =< V^{\dagger}(t) W >=< \psi | e^{iHtV} e^{-iHt} W | \psi >$

$$|\phi_{out}\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle_a VU(t) |\psi\rangle_R + \langle 1|_a U(t) W |\psi\rangle_R \right)$$

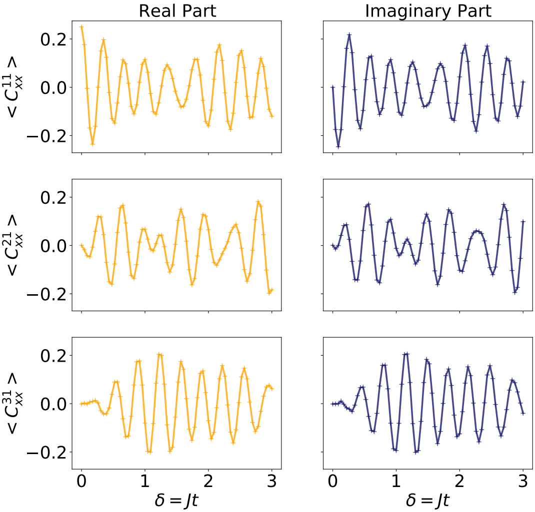
$$\langle \sigma_x^a \rangle = \langle \phi_{out} | \sigma_x^a \otimes \mathbb{I} | \phi_{out} \rangle = \tfrac{1}{2} \left(C_{VW}(t) + C_{VW}^{\dagger}(t) \right) = \mathrm{Re}\left(C_{VW}(t) \right)$$

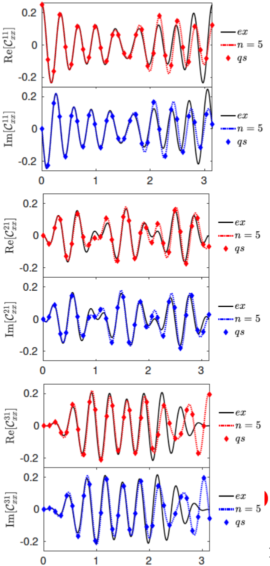
Correlation function of spin operators



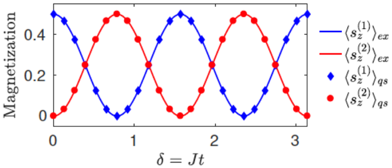
- Retrieve the spin-spin dynamical correlation $C_{ij}^{\alpha\beta} = \langle s_\alpha^i(t) s_\beta^{(j)} \rangle = \frac{1}{4} \langle \sigma_\alpha^i(t) \sigma_\beta^{(j)} \rangle$
- Describes how spins at different positions are related across space and time.

QASM simulations: 3-spin correlations results for $|\psi_0\rangle = |111\rangle$



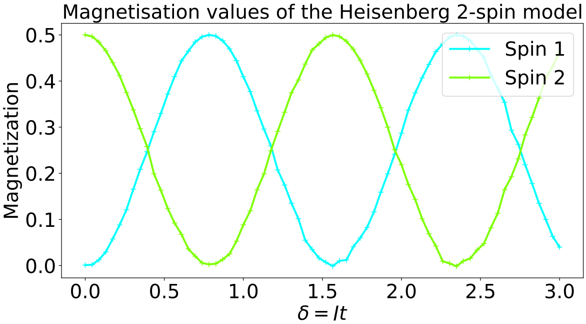


QASM simulations: the magnetization of the 2 spin model

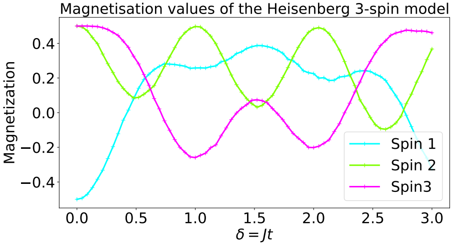


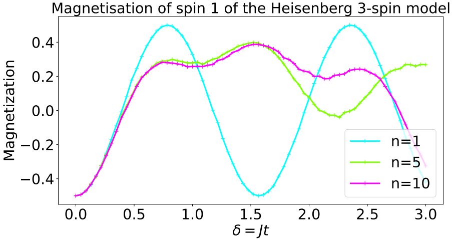
$$\langle s_z^{(i)} \rangle = \frac{1}{2} \langle \sigma_z^{(i)} \rangle$$

$$\begin{cases} Bg = 20J \\ |\psi_0\rangle = \frac{1}{\sqrt{2}} |0\rangle \left(|0\rangle + |1\rangle \right) \end{cases}$$

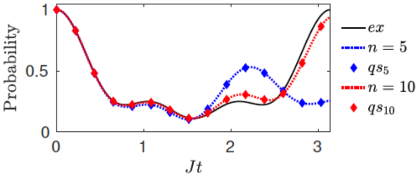


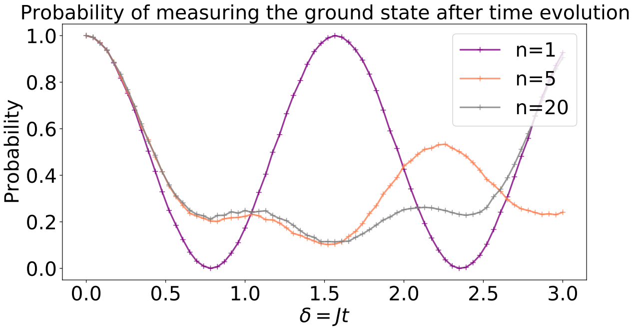
QASM simulations: the magnetization of the 3 spin model for $|\psi_0\rangle = |100\rangle$





QASM simulations: the probability of retrieving the ground state $|\psi_0\rangle = |100\rangle$





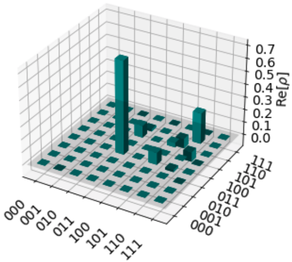
QASM simulation with noise: computation of the fidelity

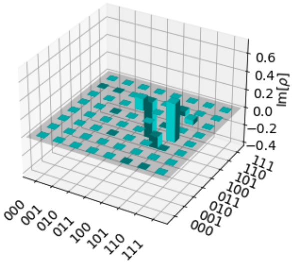
- The fidelity measures the closeness of two quantum states
- For two density matrices ρ and ρ', $F(\rho, \rho') = \left(\mathrm{Tr}\left\{\sqrt{\sqrt{\rho}\rho'\sqrt{\rho}}\right\}\right)^2$

Let's compute the exact, the simulated, and the simulated with noise density matrix of the quantum state after its evolution by a time t

The exact density matrix

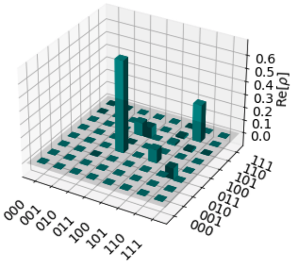
$$\rho_{exact} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.72478 & 0 & 0.09337 - 0.12819i & -0.01735 + 0.41716i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.09337 + 0.12819i & 0 & 0.0347 & -0.07602 + 0.05067i & 0 \\ 0 & 0 & 0 & -0.01735 - 0.41716i & 0 & -0.07602 - 0.05067i & 0.24052 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

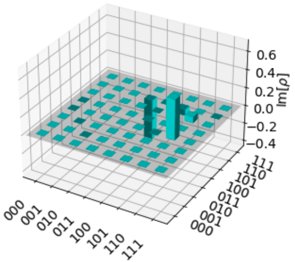




The density matrix after n=10 trotterization steps computed by the QASM simulator

$$\rho_{trot} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.69914 & 0 & 0.10106 - 0.00209i & -0.08715 + 0.43878i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.10106 + 0.00209i & 0 & 0.01462 & -0.01391 + 0.06317i & 0 \\ 0 & 0 & 0 & -0.08715 - 0.43878i & 0 & -0.01391 - 0.06317i & 0.28625 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

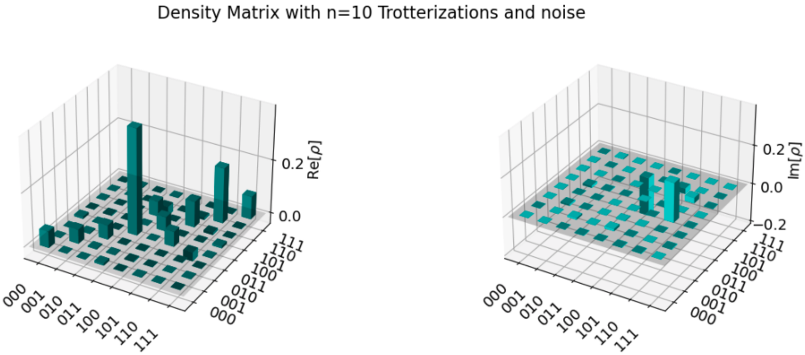




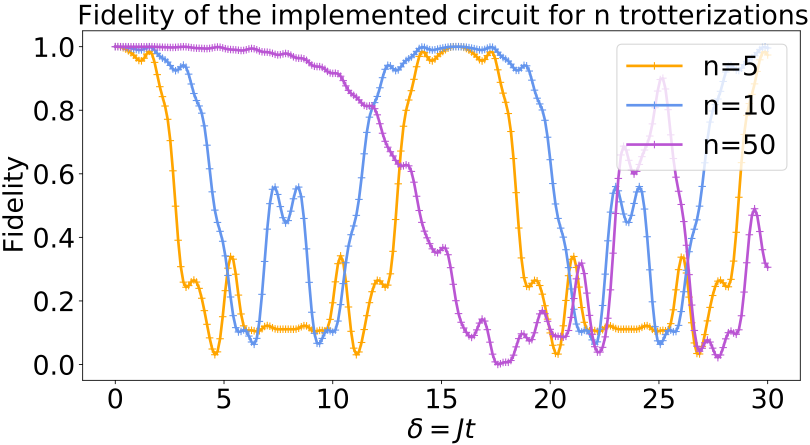
The density matrix after n=10 trotterization steps computed by the noisy QASM simulator

$$\rho_{noise} = \begin{bmatrix}
0.06076 & 0.00031 + 0.00024i & 0.00006 - 0.00009i & 0.00769 - 0.00135i & -0.00045 - 0.00037i & 0.00178 - 0.00248i & 0.00054 - 0.002i & -0.00004 + 0.00008i \\
0.00031 - 0.00024i & 0.05292 & 0.00278 + 0.00734i & 0.00169 + 0.00054i & -0.00365 + 0.01067i & -0.00042 - 0.00066i & 0.00001 + 0.00017i & 0.00162 - 0.00348i \\
0.00006 + 0.00009i & 0.00278 - 0.00734i & 0.05327 & -0.00009 + 0.00023i & -0.00145 + 0.00238i & -0.00029 + 0.0008i & -0.00052 - 0.0006i & -0.00034 - 0.00122i \\
0.00769 + 0.00135i & 0.00169 - 0.00054i & -0.00009 - 0.00023i & 0.39248 & 0.00032 + 0.00045i & 0.05602 - 0.00015i & -0.03311 + 0.2016i & 0.00179 - 0.00117i \\
-0.00045 + 0.00037i & -0.00365 - 0.01067i & -0.00145 - 0.00238i & 0.00032 - 0.00045i & 0.05303 & -0.00017 - 0.00016i & -0.00073 + 0.0003i & 0.00805 + 0.00026i \\
0.00178 + 0.00248i & -0.00042 + 0.00066i & -0.00029 - 0.0008i & 0.05602 + 0.00015i & -0.00017 + 0.00016i & 0.09626 & -0.00824 + 0.02752i & -0.00037 - 0.00079i \\
0.00054 + 0.002i & 0.00001 - 0.00017i & -0.00052 + 0.0006i & -0.03311 - 0.2016i & -0.00073 - 0.0003i & -0.00824 - 0.02752i & 0.2061 & -0.00165 - 0.00055i \\
-0.00004 - 0.00008i & 0.00162 + 0.00348i & -0.00034 + 0.00122i & 0.00179 + 0.00117i & 0.00805 - 0.00026i & -0.00037 + 0.00079i & -0.00165 + 0.00055i & 0.08517
\end{bmatrix}$$

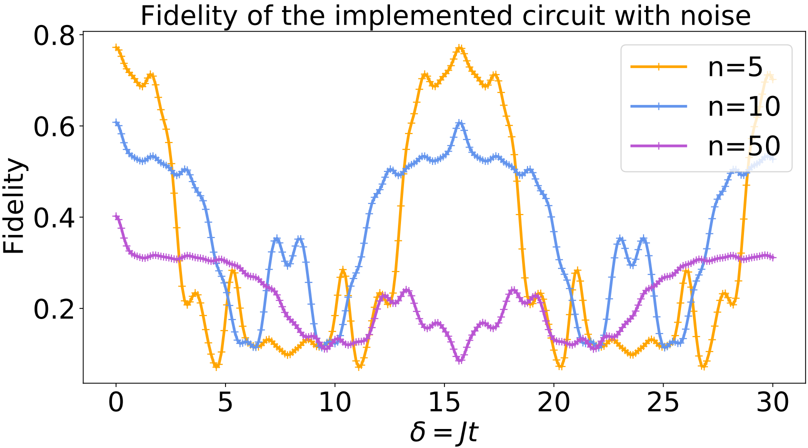
The density matrix after n=10 trotterization steps computed by the noisy QASM simulator



Fidelity of the simulation without noise for $|\psi_0\rangle = |011\rangle$



Fidelity of the simulation with noise for $|\psi_0\rangle = |011\rangle$



Conclusion

- Errors come from the trotterization:
  1. QASM simulation: $n \longrightarrow \infty \implies F \longrightarrow 1$
  2. QASM simulation with noise : $n \longrightarrow \infty \implies F \longrightarrow 0$
- Necessity to improve the real quantum hardwares to simulate faithfully the evolution of quantum states in time
- Still a very promising area as it has many applications in fermionic systems (Solid State physics, quantum chemistry, material sciences), and many new quantum hardware development (magnetic molecules, ions in silicone, semi-conductor)

References

Francesco Tacchino, Alessandro Chiesa, Stefano Carretta, and Dario Gerace, *Quantum computers as universal quantum simulators: state-of-art and perspectives*. Available on https://arxiv.org/abs/1907.03505

A. Chiesa, F. Tacchino, M. Grossi, P. Santini, I. Tavernelli, D. Gerace, and S. Carretta, , *Quantum hardware simulating four-dimensional inelastic neutron scattering*. Available on https://arxiv.org/abs/1809.07974