

ME 201/APh 250, Homework 5:

Assigned: Monday, May 20, 2019

Due: Friday, last day of class, May 31, 2019

- In class, we went through the circuits to obtain dynamical correlation functions. Such quantities are related to certain observables and can be used to predict the outcomes of experiments. They can be difficult to obtain classically and might actually be an interesting use case for NISQ devices.

A recent paper by a team from IBM[1] presented calculations on zero-temperature magnetic neutron cross-section obtained from dynamical spin-spin correlations $C_{ij}^{\alpha\beta}(t) = \langle s_i^\alpha(t) s_j^\beta \rangle_0$. The result for a two-spins system is presented and we will try to reproduce some of the figures.

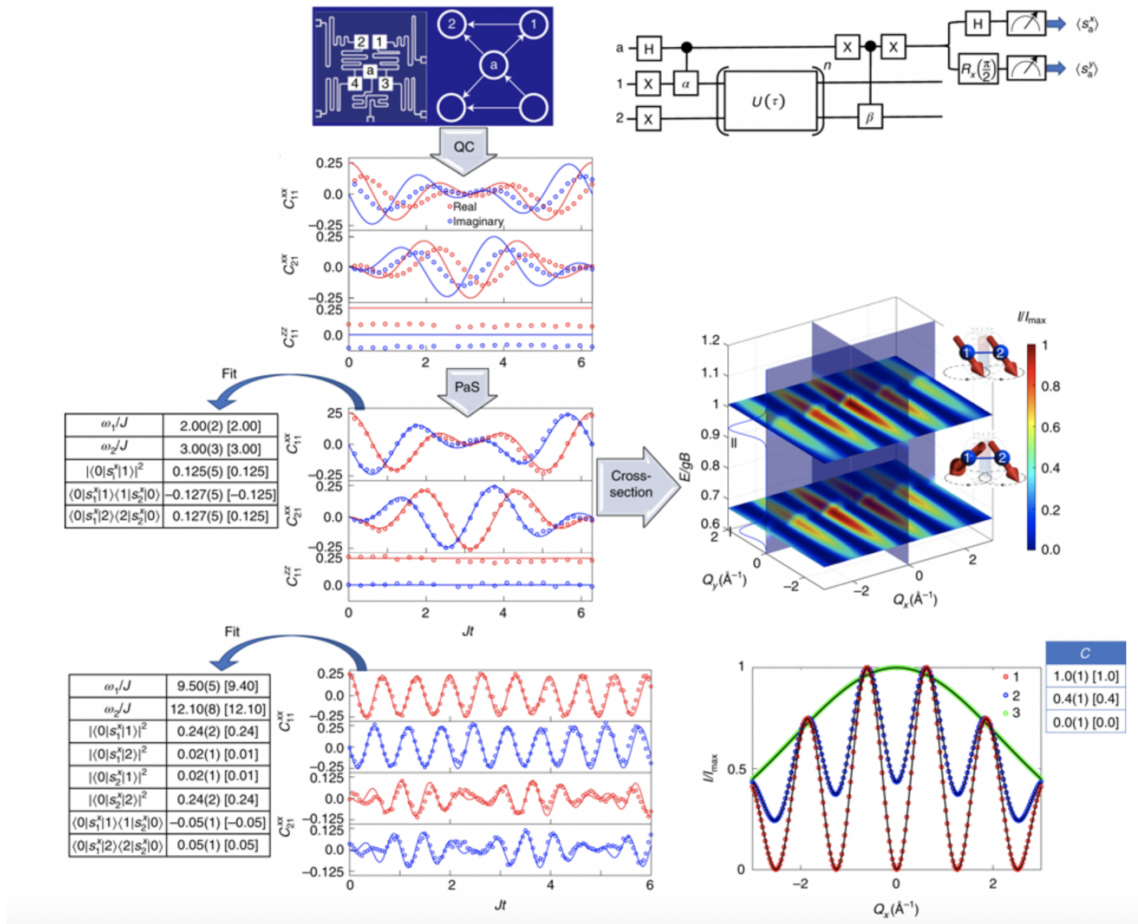


Figure 1: Adapted from [1]. Note the circuit to compute the dynamical spin-spin correlation function.

(a) Suppose the Hamiltonian is given by $H = J(s_1^x s_2^x + s_1^y s_2^y + s_1^z s_2^z) + 3J(s_1^z + s_2^z)$, we want to compute the imaginary and real part of C_{12}^{xx} at $Jt = 0.4$ for an initial state of $|11\rangle$. Implement

a 1st-order Trotter-Suzuki decomposition and ensure your results converged with the Trotter step. That is, plot the real and imaginary values of C_{12}^{xx} for different Trotter step sizes [7 marks]. Please attached a printed copy of your python script.

(b) Finally, plot the real and imaginary part of C_{12}^{xx} from the interval $Jt = 0.4$ to $Jt = 4.0$ at an interval step of 0.4 [3 marks].

[1]. A. Chiesa, F. Tacchino, M. Grossi, P. Santini, I. Tavernelli, D. Gerace and S. Carretta. *J. Nature Phys.* **15**, 455-459 (2019).

2. In the previous assignment, we obtain the ground state of H_2 molecule using VQE. We learned in class that we can implement a form of imaginary time evolution to obtain the ground state of Hamiltonians of interest. We will try to put to practice what we learned here.

(a) Let's consider a single spin system governed by the Hamiltonian $\hat{H} = \hat{Z}$ and suppose we start off in the initial state $|+\rangle$. Use the provided jupyter notebook to implement QITE protocol with a time step of $\tau = 0.1$ from $\beta = 0.0$ to $\beta = 2.5$. Please attached a printed copy of your jupyter notebook [10 marks].