Quantum Information Spring 2023 Problem Set 5

Solutions are due on Sunday May 28, 23:59.

1. **Spin chain simulation**
   Provide a quantum circuit for simulating one timestep of the dynamics of a chain of three interacting spin-$\frac{1}{2}$ particles (modelled by single qubits) with the Hamiltonian

$$H = \mu \sum_{i=1}^{3} \sigma_z^{(i)} + \lambda \sum_{i=1}^{2} \sigma_x^{(i)} \otimes \sigma_x^{(i+1)} , \tag{1}$$

   where $\sigma_k^{(i)}$ is the k'th Pauli matrix acting on the i'th particle.

2. **Richardson extrapolation**
   You have obtained the following expectation value $\langle E \rangle = 3.314$ eV for the ground state energy of some simulated system by preparing the (approximate) ground state on your NISQ computer. Now, by replacing every CNOT gate by three CNOT gates in your preparation circuit you instead measure the value $\langle E \rangle = 3.122$ eV for the ground state energy. Further, by replacing every CNOT gate by five CNOT gates in the original circuit you obtain $\langle E \rangle = 3.423$ eV. Use Richardson extrapolation to estimate the error-free expectation value for the ground state energy of the system.

   You can assume that the 1-qubit gate error rates are insignificant compared to the CNOT gate error rate (as they often are).

3. **Parameter-shift rule 1**
   Consider the function $f(x) = \sin x$. Write $f'(x)$ exactly in the form

$$f'(x) = af(x+b) + cf(x-b) , \tag{2}$$

   for some explicit numbers a, b, and c.

4. **Parameter-shift rule 2**
   Consider a quantum state produced by a parametrized quantum circuit

$$|\psi(\theta)\rangle = We^{-iP\theta/2}U|0\rangle , \tag{3}$$

   where W and U are arbitrary unitaries and $P = P^\dagger$ is a Pauli operator.

   (a) Let O be an observable. Write the expectation value of $f(\theta) = \langle\psi(\theta)|O|\psi(\theta)\rangle$ in the above state.

(b) Show that

$$f'(x) = \frac{1}{2}\left(f\left(x + \frac{\pi}{2}\right) - f\left(x - \frac{\pi}{2}\right)\right) . \tag{4}$$

Hint: use the fact that for any Pauli operator P the commutator satisfies

$$[P, \rho] = i\left(e^{-iP\pi/4}\rho e^{iP\pi/4} - e^{iP\pi/4}\rho e^{-iP\pi/4}\right) , \tag{5}$$

for any operator ρ.

5. **Variational quantum eigensolver (programming)**
In this problem you will use a variational quantum eigensolver to find the ground state of a Hamiltonian. Use the template notebook "vqe.ipynb" which you can find on the MyCourses page. I recommend using `jupyter.cs.aalto.fi`. Return your answer as a .ipynb-notebook (you can download the notebook from JupyterHub if you used the department cloud installation.)

- Implement the parameter-shift rule to make the "gradient"-function work.
- Run the VQE. Can you find the ground state?