Quantum Information Spring 2023 Problem Set 5

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.
Solution.
We model each one of the spin-$\frac{1}{2}$ systems by mapping them onto single qubits through the identification $|\uparrow\rangle \leftrightarrow |0\rangle, |\downarrow\rangle \leftrightarrow |1\rangle$ of the spin-up and spin-down states (in the z-direction) with the computational basis states of the qubit. By this identification, the Pauli operators of the spin systems correspond exactly to the Pauli operators of the qubits.

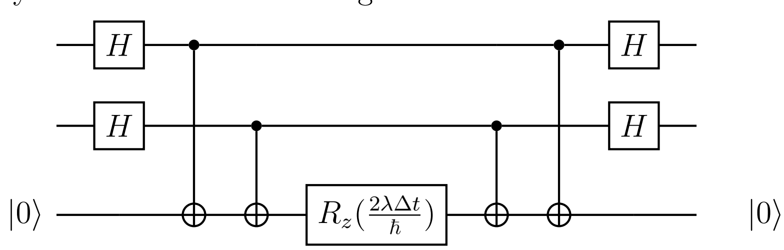
The time-evolution operator $U(\Delta t) = e^{-iH\Delta t/\hbar}$ for a small timestep Δt can be trotterized into

$$U(\Delta t) = e^{-iH\Delta t/\hbar} = \prod_k e^{-iH_k \Delta t/\hbar} + O(\Delta t^2) , \tag{2}$$

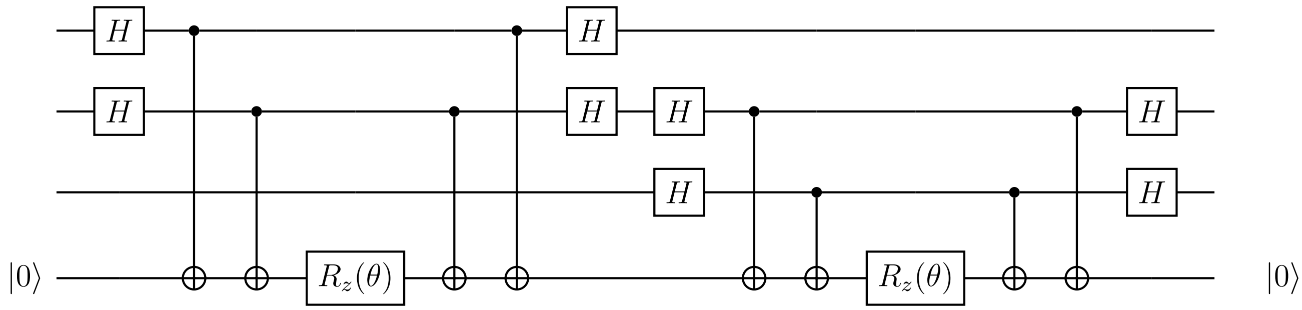
where the product is over all the different terms in the Hamiltonian. The terms acting only on single qubits can be implemented directly by single-qubit rotations:

$$e^{-i\mu\sigma_z\Delta t/\hbar} = e^{-\frac{i}{2}\left(\frac{2\mu\Delta t}{\hbar}\right)\sigma_z} = R_z\left(\frac{2\mu\Delta t}{\hbar}\right) . \tag{3}$$

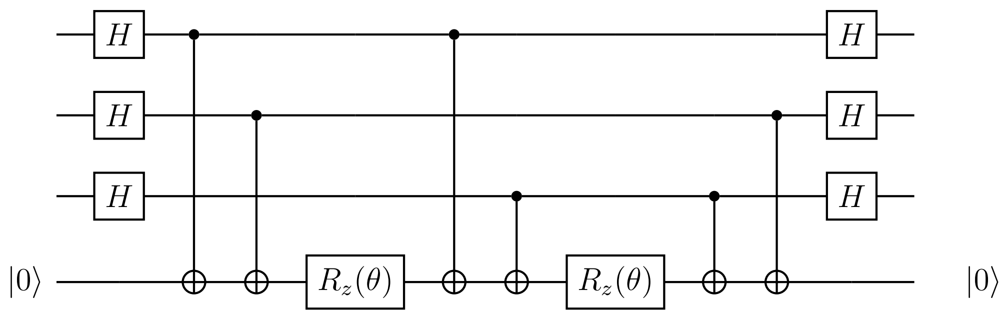
The terms $\exp\left(-i\lambda\sigma_x^{(i)}\sigma_x^{(i+1)}\Delta t/\hbar\right)$ acting on pairs of qubits can be implemented by a circuit of the following form:



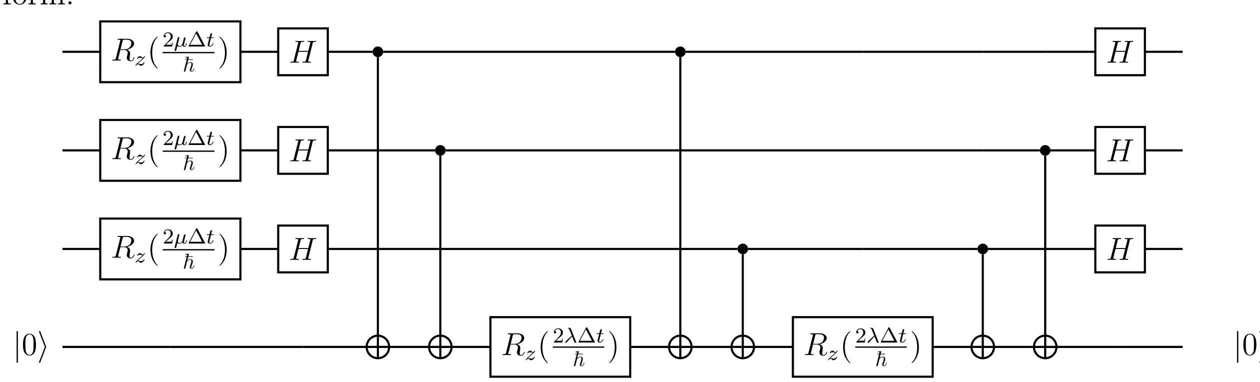
Check the first lecture of this week for the explanation of why this pattern of gates implements the interaction. Here, the first two qubits correspond to the two qubits acted on by the interaction term, and the third qubit is an ancilla used to implement the transformation. Since the ancilla is uncomputed back to the $|0\rangle$ state, it can be reused to implement another interaction. Thus, altogether for the circuit implementing the two interaction terms we have



where $\theta = \frac{2\lambda\Delta t}{\hbar}$. This can be further simplified by cancelling subsequent Hadamard gates and CNOT gates to



Thus, we get for the circuit implementing one time-step of the evolution the following form:



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).
Solution.
Replacing every CNOT gate by $2n+1$ CNOT gates keeps the logical operation the same but increases the error rate approximately by a factor of $2n+1$. Thus, we get for the extrapolation parameters in Richardson extrapolation $\alpha_0 = 1, \alpha_1 = 3, \alpha_2 = 5$. For the β-coefficients in the expansion we then find

$$\beta_0 = \frac{\alpha_1}{\alpha_1 - \alpha_0}\frac{\alpha_2}{\alpha_2 - \alpha_0} = \frac{3}{3-1}\frac{5}{5-1} = \frac{3}{2} \times \frac{5}{4} = \frac{15}{8}\,, \tag{4}$$

$$\beta_1 = \frac{\alpha_0}{\alpha_0 - \alpha_1}\frac{\alpha_2}{\alpha_2 - \alpha_1} = \frac{1}{1-3}\frac{5}{5-3} = -\frac{1}{2} \times \frac{5}{2} = -\frac{5}{4}\,, \tag{5}$$

$$\beta_2 = \frac{\alpha_0}{\alpha_0 - \alpha_2} = \frac{\alpha_1}{\alpha_1 - \alpha_2} = \frac{1}{1-5}\frac{3}{3-5} = \left(-\frac{1}{4}\right) \times \left(-\frac{3}{2}\right) = \frac{3}{8}\,. \tag{6}$$

For the noise-free estimate of the ground state energy up to an error of order $O(\epsilon^3)$ we then get from the Richardson extrapolation

$$\langle E\rangle_{est}(0) = \langle E\rangle(0) + O(\epsilon^3) = \sum_{k=0}^{2} \beta_k \langle E\rangle(\alpha_k \epsilon) \tag{7}$$

$$= \frac{15}{8} \times 3.314\text{ eV} - \frac{5}{4} \times 3.122\text{ eV} + \frac{3}{8} \times 3.423\text{ eV} \approx 3.595\text{ eV}\,. \tag{8}$$

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

$$f'(x) = af(x+b) + cf(x-b)\ , \tag{9}$$

for some explicit numbers a, b, and c.
Solution.
Elementary identities for quarter period shifts show that $\pm\cos x = \sin\left(x \pm \frac{\pi}{2}\right)$. Therefore,

$$f'(x) = \cos x = \frac{1}{2}(\cos x - (-\cos x)) \tag{10}$$

$$= \frac{1}{2}\left(\sin\left(x + \frac{\pi}{2}\right) - \sin\left(x - \frac{\pi}{2}\right)\right) \tag{11}$$

$$= \frac{1}{2}f\left(x + \frac{\pi}{2}\right) - \frac{1}{2}f\left(x - \frac{\pi}{2}\right)\,. \tag{12}$$

This form is the same as the parameter-shift rule for computing derivatives of Pauli rotation gates, which are related to trigonometric functions.

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

$$|\psi(\theta)\rangle = We^{-iP\theta/2}U\,|0\rangle\ , \tag{13}$$

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.
Solution.

$$f(\theta) = \langle 0| U^\dagger e^{iP\theta/2} W^\dagger O W e^{-iP\theta/2} U |0\rangle \ . \tag{14}$$

(b) Show that

$$f'(x) = \frac{1}{2}\Big(f\Big(x+\frac{\pi}{2}\Big) - f\Big(x-\frac{\pi}{2}\Big)\Big) \ . \tag{15}$$

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

$$[P,\rho] = i\big(e^{-iP\pi/4}\rho e^{iP\pi/4} - e^{iP\pi/4}\rho e^{-iP\pi/4}\big) \ , \tag{16}$$

for any operator ρ.
Solution.
Start by simply evaluating the derivative.

$$\begin{aligned} f'(\theta) &= \langle 0| U^\dagger \left(\frac{iP}{2} e^{iP\theta/2}\right) W^\dagger O W e^{-iP\theta/2} U |0\rangle \\ &+ \langle 0| U^\dagger e^{iP\theta/2} W^\dagger O W \left(\frac{-iP}{2} e^{-iP\theta/2}\right) U |0\rangle \ . \end{aligned} \tag{17}$$

Then rearrange in terms of the commutator of P.

$$f'(\theta) = \frac{i}{2} \langle 0| U^\dagger e^{iP\theta/2} \big(PW^\dagger O W - W^\dagger O W P\big) e^{-iP\theta/2} U |0\rangle \tag{18}$$

$$= \frac{i}{2} \langle 0| U^\dagger e^{iP\theta/2} \big[P, W^\dagger O W\big] e^{-iP\theta/2} U |0\rangle \ . \tag{19}$$

Then we can use the commutator identity from the hint.

$$f'(\theta) = -\frac{1}{2} \langle 0| U^\dagger e^{iP\theta/2} \big(e^{-iP\pi/4} W^\dagger O W e^{iP\pi/4} - e^{iP\pi/4} W^\dagger O W e^{-iP\pi/4}\big) e^{-iP\theta/2} U |0\rangle \tag{20}$$

$$\begin{aligned} &= -\frac{1}{2} \langle 0| U^\dagger e^{iP(\theta-\frac{\pi}{2})/2} W^\dagger O W e^{-iP(\theta-\frac{\pi}{2})/2} U |0\rangle \\ &+ \frac{1}{2} \langle 0| U^\dagger e^{iP(\theta+\frac{\pi}{2})/2} W^\dagger O W e^{-iP(\theta+\frac{\pi}{2})/2} U |0\rangle \end{aligned} \tag{21}$$

$$= \frac{1}{2} f\Big(\theta+\frac{\pi}{2}\Big) - \frac{1}{2} f\Big(\theta-\frac{\pi}{2}\Big) \tag{22}$$

This is what we wanted to show: $f'(\theta)$ can be exactly expressed as a linear combination of $f(\theta)$ (the same quantum circuit) with shifted parameter values.

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?

   Solution.
   See "vqe_solution.ipynb".