Exercises on Quantum-Computing Basics

Zohreh Davoudi, Vinay Vikramaditya

Nov 19, 2024

Problem 1:

(a) Prove the following equality for a two-qubit system:

$$\mathrm{CNOT}(1 \to 2) \cdot (I \otimes Z) \cdot \mathrm{CNOT}(1 \to 2) = Z \otimes Z, \tag{1}$$

where CNOT($1 \to 2$) is the Controlled-NOT gate with qubit 1 as the control and qubit 2 as the target.

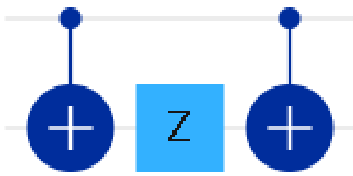

Figure 1: The gate representation of the ZZ operation.

Can you now express $e^{-i\theta ZZ/2}$ in terms of CNOT and RZ= $e^{-i\frac{\theta}{2}Z}$ gates?

(b) Use this to implement time evolution of the following Hamiltonian for L=4 sites

$$H = -J\sum_{i=1}^{L} Z_i Z_{i+1} - h\sum_{i=1}^{L} X_i, \tag{2}$$

with periodic boundary conditions and an appropriate number of Trotter steps on IBM's Quantum Circuit Composer. (Tip: Use the interface to create a circuit for one Trotter step, then copy and paste the code to create the full circuit.) Use the RZ, CNOT and RX gates for this.

(c) Use exact diagonalization with $J = 1, h = 1.5, T = 1$ to calculate the probabilities for the basis states and verify if the quantum circuit yields the same result.

Problem 2:

Consider a theory of non-relativistic fermions on a two-dimensional spatial lattice with N sites along each Cartesian coordinate with the Hamiltonian:

$$H = g \sum_{\boldsymbol{n}} \sum_{i=1}^{2} \left[\psi^\dagger(\boldsymbol{n})\psi(\boldsymbol{n}+\hat{i}) + \text{ H.c. } \right] + m \sum_{\boldsymbol{n}} \psi^\dagger(\boldsymbol{n})\psi(\boldsymbol{n}). \tag{3}$$

Here, g and m are positive constants, n is a site on the two-dimensional lattice, and $\hat{i}$ is a unit vector along the i^{th} Cartesian direction. Note that $\psi^\dagger(\boldsymbol{n})$ and $\psi(\boldsymbol{n})$ are two-component non-relativistic spinors at site $\boldsymbol{n}$ (they create and annihilate particle excitations only). The goal of this problem is to map the Hamiltonian in Eq. (3) to a spin Hamiltonian. Such a spin Hamiltonian can then be simulated on a qubit-based quantum computer.

a) One idea for mapping the non-relativistic fermions to spins is to consider the mapping:

$$\psi(\boldsymbol{n}) \to \sigma^+_{\boldsymbol{n}}, \quad \psi^\dagger(\boldsymbol{n}) \to \sigma^-_{\boldsymbol{n}}, \tag{4}$$

where $\sigma^\pm$are the raising and lowering Pauli matrices acting on the state of the system at site n. Show that this mapping will not work. [Consider the anticommutation relations that need to be satisfied for fermions.]

b) Now consider another mapping:

$$\psi(r) \to \left(\prod_{k=0}^{r-1} \sigma^z_k \right) \sigma^+_r, \quad \psi^\dagger(r) \to \left(\prod_{k=0}^{r-1} \sigma^z_k \right) \sigma^-_r, \tag{5}$$

where we have mapped each point n on the lattice to an index r where

$$r \in \left\{0, 1, 2, \cdots, N^2 - 1\right\}$$

with a chosen ordering (so that the number of Pauli-Z operations preceding each raising and lowering Pauli operator for a given site index r depends on the chosen ordering). Show that the spin operators representing ψ and $\psi^\dagger$ now satisfy the correct fermionic anticommutation relations.

c) Rewrite the Hamiltonian in Eq. (3) in terms of the spin operators using the mapping introduced in part b. To be explicit, write all the Hamiltonian terms for the simple case of a 4×4 lattice (i.e., 4 lattice sites along each Cartesian coordinate). Note that while your original fermionic Hamiltonian had only local terms and nearest-neighbor hoppings, the corresponding spin Hamiltonian involves both local and non-local spin interactions!

Problem 3:

Consider a Hamiltonian consisting of two non-commuting terms: $H = H_1 + H_2$.

(a) Derive the relation for the leading-order error of the first-order product formula:

$$e^{-it(H_1+H_2)} - (e^{-i\delta t H_1} e^{-i\delta t H_2})^{t/\delta t} = \frac{N_T}{2}[H_1, H_2](\delta t)^2 + (\delta t)^3, \tag{6}$$

where $N_T = t/\delta t$.

(b) [Bonus] Show that for the second-order product formula:

$$e^{-it(H_1+H_2)} - (e^{-i\delta t H_1/2} e^{-i\delta t H_2} e^{-i\delta t H_1/2})^{t/\delta t} = O(\delta t)^3. \tag{7}$$

(c) [Bonus] We can have an stronger stronger relation, that is a bound on the error of the product formula. Can you prove that:

$$\left\| e^{-i\delta t(H_1+H_2)} - e^{-i\delta t H_1} e^{-i\delta t H_2} \right\| \leq \frac{(\delta t)^2}{2} \left\| [H_1, H_2] \right\|. \tag{8}$$