AQAlg: Advanced Quantum Algorithms **2022 - 2023**

Exercises 4: Quantum chemistry and simulation

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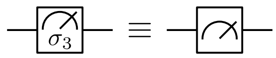
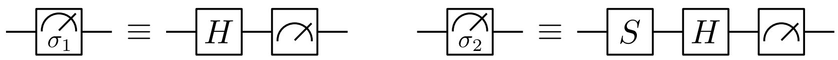
Exercise 1 (Pauli measurements)**.** The following corresponds to a qubit measurement in the standard (Z-)basis:

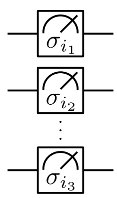


Show that the following correspond to measurements in the X- and Y-basis, respectively:



where $S = \begin{bmatrix} 1 & 0 \\ 0 & -i \end{bmatrix}$ is the phase gate. On the basis of this, give an algorithm for estimating the energy $\langle\psi|H|\psi\rangle$ for a qubit Hamiltonian H.

For an n-qubit state $|\psi\rangle$, show that we can estimate $\langle\psi|\sigma_{i_1} \otimes \cdots \otimes \sigma_{i_n}|\psi\rangle$ using the following circuit:



This implies that we can use this circuit to estimate $\langle\psi|H|\psi\rangle$ for a general n-qubit Hamiltonian.

Exercise 2 (#P-hard)**.** An independent set in a graph $G = (V, E)$ is a vertex subset $X \subseteq V$ such that no two vertices in X are adjacent (i.e., there exists no $(i, j) \in E$ such that $i, j \in X$). Counting the number of independent sets in G is a so-called #P-hard problem (i.e., it is *very* hard).

- Show that the ground states of the Ising Hamiltonian $H = \sum_{(i,j)\in E}(I - Z_i)(I - Z_j)$ correspond to independent sets in the graph.
- Conclude that evaluating the partition function $Z_T = \sum_i e^{-\lambda_i/T}$ of H for $T \to 0$ is #P-hard.

Exercise 3 (Metropolis algorithm)**.** The Metropolis algorithm for preparing a distribution π has transition probabilities

$$P(y|x) = \begin{cases} Q(y|x)\, A(y|x) & \text{if } y \neq x \\ 1 - \sum_y Q(y|x)\, A(y|x) & \text{if } y = x, \end{cases}$$

with $Q(y|x) = Q(x|y)$ a symmetric proposal distribution and $A(y|x) = \min\{1, \pi(y)/\pi(x)\}$ the acceptance probability.

- Show that this satisfies "detailed balance" with respect to the distribution π, i.e.,

$$\pi(x)P(y|x) = \pi(y)P(x|y).$$

- Show that this implies that π is a stationary distribution of the Markov chain.

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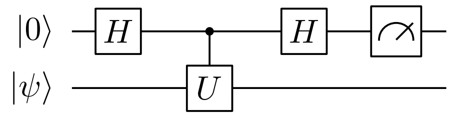
Exercise 4 (Unitary Hamiltonian)**.** If a Hamiltonian H is also unitary (e.g., product of Pauli matrices) then there is an alternative approach for estimating $\langle\psi|H|\psi\rangle$, which is still simpler than quantum phase estimation. Consider the following circuit:



Show that if $U = H$ (not to confuse with the Hadamard gate!) then the expected value of the measurement outcome is $\left(1 - \langle\psi|H|\psi\rangle\right)/2$.