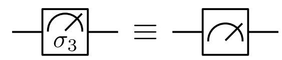
AQAlg: Advanced Quantum Algorithms **2024 - 2025**

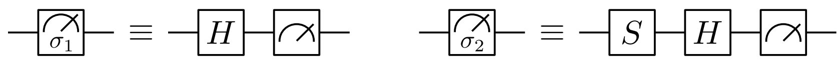
Exercises 4: Quantum chemistry and simulation

Lecturer: Simon Apers (apers@irif.fr)

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

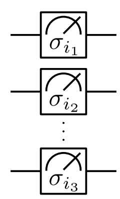


Show that the following correspond to measurements in the X- and Y-(eigen-)basis, respectively:



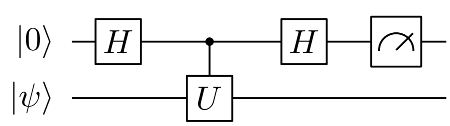
where $S = \begin{bmatrix} 1 & 0 \\ 0 & -i \end{bmatrix}$ is the phase gate. Based on this, give an algorithm for estimating the energy $\langle\psi|\sigma_i|\psi\rangle$ for a single Pauli σ_i, and $\langle\psi|H|\psi\rangle$ for a given single qubit Hamiltonian H.

Show that the following circuit represents a measurement in the $\sigma_{i_1} \otimes \cdots \otimes \sigma_{i_n}$-basis:



For an n-qubit state $|\psi\rangle$, show that we can use this circuit to estimate $\langle\psi|\sigma_{i_1} \otimes \cdots \otimes \sigma_{i_n}|\psi\rangle$ for a string of Pauli's, and $\langle\psi|H|\psi\rangle$ for a given n-qubit Hamiltonian.

Exercise 2 (Unitary Hamiltonian)**.** If a Hamiltonian H is also unitary (e.g., a product of Pauli matrices) then there is an alternative approach for estimating $\langle\psi|H|\psi\rangle$, which is simpler than quantum phase estimation and the Pauli approach from last section. 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 $(1 - \langle\psi|H|\psi\rangle)/2$.