Quantum Algorithms: Exercices 5

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1 Quantum chemistry and the Jordan-Wigner transformation

We aim at implementing a quantum chemistry Hamiltonian

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s \tag{1}$$

with fermionic operators satisfying anti-commutation relations

$$\begin{aligned} \{a_p, a_q\} &= \{a_p^\dagger, a_q^\dagger\} = 0 \\ \{a_p, a_q^\dagger\} &= \delta_{p,q} \end{aligned} \tag{2}$$

1. A naive possibility to encode a fermion particle in terms of a qubit corresponds to $a_i = \sigma_i = |0\rangle\langle 1|$. Explain the problem with this method.
2. Show that $a_p = (\prod_{q=1}^{p-1} Z_q)\sigma_p$ is a fermionic operator (use the identity $\sigma_p Z_p = -Z_p \sigma_p$).
3. Express the operators $a_p^\dagger a_p$, $a_p^\dagger a_{p+1} + hc$, $a_q^\dagger a_l + hc$ in terms of pauli operators X, Y, Z. One can use the relations $\sigma_p^\dagger Z_p = \sigma_p^\dagger$. $\sigma_p \sigma_q^\dagger + \sigma_p^\dagger \sigma_q = (X_p X_q + Y_p Y_q)/2$.
4. Propose a circuit to measure these operator. One can use the relation to perform Y measurements $Y = SXS^\dagger$.

2 Quantum adiabatic theorem and quantum annealing

The quantum adiabatic theorem provides a key result to assess the performance of quantum optimization algorithms based on quantum annealing.

1. We consider an Hamiltonian evolution $H(t)$. We denote by $|E_n(t)\rangle, E_n(t)$ the sets of instantaneous eigenstates/eigenvalues of $H(t)$. We consider that the system is initialized in the eigenstate $|E_0(0)\rangle$. Write down the evolution of the wavefunction in the instantaneous eigenbasis.
2. Show that $\langle E_n(t)| \dot{E}_n(t)\rangle$ is purely imaginary.
3. Rewrite the equations of evolutions of $c_n(t)$ as a function of $\langle E_n(t)| \dot{H}(t) |E_m(t)\rangle$
4. Justify (without further calculations) the condition for an adiabatic evolution.

$$\left| \frac{\langle E_n(t)| \dot{H}(t) |E_m(t)\rangle}{E_m(t) - E_n(t)} \right| \ll |E_m(t) - E_n(t)| \tag{3}$$

5. Interpret the results in terms of requirements for performing quantum annealing.