

Quantum Algorithms: Exercices 5

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1 Quantum chemistry and the Jordan-Wigner transformation

We aim at implementing a quantum chemistry Hamiltonian

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

with

1. A naive possibility to encode a fermion particle in terms of a qubit corresponds to $a_p = \sigma_p = |0\rangle_p \langle 1|$. We must ensure that fermionic operators satisfy anti-commutation relations

$$\begin{aligned} \{a_p, a_q\} &= \{a_p^\dagger, a_q^\dagger\} = 0 \\ \{a_p, a_q^\dagger\} &= \delta_{p,q}. \end{aligned} \quad (2)$$

For instance, the operators σ_p and σ_q do commute. Therefore, $\{\sigma_p, \sigma_q\} = \sigma_p \sigma_q + \sigma_p \sigma_q = 2\sigma_p \sigma_q \neq 0$. This means that the operators σ_p are not valid fermionic operators.

2. Show that $a_p = (\prod_{i=1}^{p-1} Z_i) \sigma_p$ does the job.

$$\begin{aligned} \{a_p, a_q\} &= a_p a_q + a_q a_p = \left(\prod_{i=1}^{p-1} Z_i \right) \sigma_p \left(\prod_{j=1}^{q-1} Z_j \right) \sigma_q + \left(\prod_{j=1}^{p-1} Z_j \right) \sigma_q \left(\prod_{i=1}^{p-1} Z_i \right) \sigma_p \\ &= \sigma_p \left(\prod_{i=p}^{q-1} Z_i \right) \sigma_q + \sigma_q \left(\prod_{i=p}^{q-1} Z_i \right) \sigma_p, \end{aligned} \quad (3)$$

where we assumed without loss of generality $p \leq q$. If $p = q$, we obtain

$$\{a_p, a_p\} = 2\sigma_p^2 = 0. \quad (4)$$

If $p < q$, we use the identity $\sigma_p Z_p = -Z_p \sigma_p$ to write

$$\{a_p, a_q\} = -\left(\prod_{i=p}^{q-1} Z_i \right) \sigma_q \sigma_p + \left(\prod_{i=p}^{q-1} Z_i \right) \sigma_q \sigma_p = 0, \quad (5)$$

The second identity follows

$$\{a_p^\dagger, a_q^\dagger\} = a_p^\dagger a_q^\dagger + a_q^\dagger a_p^\dagger = \{a_q, a_p\}^\dagger = 0 \quad (6)$$

Finally

$$\begin{aligned} \{a_p, a_q^\dagger\} &= a_p a_q^\dagger + a_q^\dagger a_p = \left(\prod_{i=1}^{p-1} Z_i \right) \sigma_p \sigma_q^\dagger \left(\prod_{j=1}^{q-1} Z_j \right) + \sigma_q^\dagger \left(\prod_{j=1}^{q-1} Z_j \right) \left(\prod_{i=1}^{p-1} Z_i \right) \sigma_p \\ &= \sigma_p \sigma_q^\dagger \left(\prod_{i=p}^{q-1} Z_i \right) + \sigma_q^\dagger \left(\prod_{i=p}^{q-1} Z_i \right) \sigma_p, \end{aligned} \quad (7)$$

If $p = q$, we have

$$\{a_p, a_p^\dagger\} = \sigma_p \sigma_p^\dagger + \sigma_p^\dagger \sigma_p = 1. \quad (8)$$

If $p < q$, we have

$$\{a_p, a_p^\dagger\} = (\sigma_p \sigma_q^\dagger - \sigma_q^\dagger \sigma_p) \left(\prod_{i=p}^{q-1} Z_i \right) = 0 \quad (9)$$

3. Propose a circuit to measure the operator $\langle a_p^\dagger a_p \rangle$, $\langle a_p^\dagger a_{p+1} + hc \rangle$, $\langle a_p^\dagger a_{q>p+1} + hc \rangle$.

$$a_p^\dagger a_p = \sigma_p^\dagger \sigma_p = |1\rangle \langle 1| \quad (10)$$

This is a standard local measurement.

$$a_p^\dagger a_{p+1} = \sigma_p^\dagger Z_p \sigma_{p+1} = \sigma_p^\dagger \sigma_{p+1} \quad (11)$$

The expectation value of the hermitian operator is obtained as

$$a_p^\dagger a_{p+1} + hc = (X_p X_{p+1} + Y_p Y_{p+1})/2 \quad (12)$$

This can be measured by first measuring $X_p X_{p+1}$, then $Y_p Y_{p+1}$, and adding the two outcomes.

The second term can be measured using the relation $Y = SXS^\dagger$.

$$a_p^\dagger a_q = \sigma_p^\dagger \left(\prod_{i=p}^{q-1} Z_i \right) \sigma_q \quad (13)$$

Consequence: we will have to measure operators of the type $X_p (\prod_{i=p}^{q-1} Z_i) X_q$.

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 write $|\psi(t)\rangle = \sum_n c_n(t) |E_n(t)\rangle$. The Schrödinger equation gives

$$\begin{aligned} i\hbar \partial_t |\psi(t)\rangle &= H(t) |\psi(t)\rangle \\ i\hbar \sum_n \dot{c}_n(t) |E_n(t)\rangle + c_n(t) |\dot{E}_n(t)\rangle &= \sum_n H(t) |E_n(t)\rangle = \sum_n E_n(t) |E_n(t)\rangle \end{aligned} \quad (14)$$

Projecting

$$i\hbar \dot{c}_n(t) = -i\hbar \sum_m c_m(t) \langle E_n(t) | \dot{E}_m(t) \rangle + E_n(t) c_n(t) \quad (15)$$

2. $\langle E_n(t) | E_n(t) \rangle = 1$. Therefore

$$\langle E_n(t) | \dot{E}_n(t) \rangle + \langle \dot{E}_n(t) | E_n(t) \rangle = 0 \quad (16)$$

This means that we have an imaginary term, which we write as $\hbar \langle E_n(t) | \dot{E}_n(t) \rangle = i\epsilon_n(t)$. The equation of motion become

$$i\hbar \dot{c}_n(t) + \epsilon_n(t) c_n(t) = E'_n(t) c_n(t) - i\hbar \sum_{m \neq n} \langle E_n(t) | \dot{E}_m(t) \rangle c_m(t) \quad (17)$$

with $E'_n(t) = E_n + \epsilon_n(t)$. We have $H(t) |E_n(t)\rangle = E_n(t) |E_n(t)\rangle$. Therefore

$$H(t) |\dot{E}_n(t)\rangle + H(t) |\dot{E}_n(t)\rangle = \dot{E}_n(t) |E_n(t)\rangle + E_n(t) |\dot{E}_n(t)\rangle \quad (18)$$

which gives for $m \neq n$

$$\langle E_m(t) | \dot{H}(t) | E_n(t) \rangle + E_m(t) \langle E_m(t) | \dot{E}_n(t) \rangle = E_n(t) \langle E_m(t) | \dot{E}_n(t) \rangle \quad (19)$$

wich gives

$$\langle E_m(t) | \dot{E}_n(t) \rangle = \frac{\langle E_m(t) | \dot{H}(t) | E_n(t) \rangle}{E_n(t) - E_m(t)} \quad (20)$$

We obtain

$$i\hbar \dot{c}_n(t) = E'_n(t) c_n(t) - i\hbar \sum_{m \neq n} \frac{\langle E_n(t) | \dot{H}(t) | E_m(t) \rangle}{E_m(t) - E_n(t)} c_m(t) \quad (21)$$

If

$$\left| \frac{\langle E_n(t) | \dot{H}(t) | E_m(t) \rangle}{E_m(t) - E_n(t)} \right| \ll |E_m(t) - E_n(t)| \quad (22)$$

the rates of diabatic transition is small compared to the energy differences. This means we can neglect this transition and obtain an adiabatic evolution.