Quantum Algorithms 2021/2022: Exercices 4

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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

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

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

   For instance, the operators σ_p and σ_q do commute. Therefore, $\{\sigma_p, \sigma_q\} = \sigma_p\sigma_q + \sigma_p\sigma_q = 2\sigma_q\sigma_q \neq 0$. 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.

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

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

$$\{a_p, a_p\} = 2\sigma_p^2 = 0. \tag{4}$$

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

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

   The second identity follows

$$\{a_p^\dagger, a_q^\dagger\} = a_p^\dagger a_q^\dagger + a_q^\dagger a_p^\dagger = \{a_q, a_p\}^\dagger = 0 \tag{6}$$

   Finally

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

   If $p = q$, we have

$$\{a_p, a_p^\dagger\} = \sigma_p\sigma_p^\dagger + \sigma_p^\dagger\sigma_p = 1. \tag{8}$$

   If $p < q$, we have

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

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

$$a_p^\dagger a_p = \sigma_p^\dagger \sigma_p = |1\rangle \langle 1| \tag{10}$$

   This is a standard local measurement.

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

   The expectation value of the hermitian operator is obtained as

$$a_p^\dagger a_{p+1} + hc = X_p X_{p+1} + Y_p Y_{p+1} \tag{12}$$

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

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

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

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

   Projecting

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

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

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

   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

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

   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

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

   which gives for $m \neq n$

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

   wich gives

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

   We obtain

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

   If

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

   the rates of diabatic transition is small compared to the energy differences. This means, using e.g. first-order perturbation theory, we can neglect this transition and obtain an adiabatic evolution.