33-658 Quantum Computing and Quantum Information Homework 11

1. (adapted from problem (9.8)) The Hamiltonian

$$H = \sum_n E_n |n\rangle\langle n|$$

is time-independent, and its interaction with its environment is given by Lindblad operators $\{L_n = \lambda_n |n\rangle\langle n|, \lambda_n \in \mathbb{R}\}$. Show that heat transfer and work rates both vanish. Derive and solve a differential equation for the evolution of the density matrix elements $\boldsymbol{\rho}_{mn}$. Under what condition do the coherences vanish?

2. Problem 19.5 (entropy of $\boldsymbol{\rho} = (\mathbf{1} + \vec{a} \cdot \vec{\boldsymbol{\sigma}})/2$)

3. Jordan-Wigner transformation of H_2 molecule

The H_2 molecule has two atoms, a and b, each of which has a $1s$ electron orbital that can be occupied spin $\sigma = \uparrow$ or $\downarrow$. Hence there are a total of 4 single-electron states that we label as $q = 1$ ($|a\uparrow\rangle$), $q = 2$ ($|b\uparrow\rangle$), $q = 3$ ($|a\downarrow\rangle$), $q = 4$ ($|b\downarrow\rangle$). The creation an anihilation operators for each single-particle state are

$$a_q = \left(\prod_{p=1}^{q-1} Z_p\right) \frac{1}{2}\left(X_q + iY_q\right), a_q^\dagger = \left(\prod_{p=1}^{q-1} Z_p\right) \frac{1}{2}\left(X_q - iY_q\right).$$

a) Starting from the empty state $|0000\rangle$ (no electrons), use creation and anihilation operators to create the three-electron state $|1011\rangle$. Be careful to obtain the correct sign.

b) Verify that the hopping (free fermion) Hamiltonian

$$H_{\mathrm{FF}} = -t \sum_\sigma \left(a_{a\sigma}^\dagger a_{b\sigma} + a_{b\sigma}^\dagger a_{a\sigma}\right)$$

can be expressed in terms of qubit operators as

$$H_{\mathrm{FF}} = -\frac{t}{2}\left(X_1 \otimes X_2 + Y_1 \otimes Y_2 + X_3 \otimes X_4 + Y_3 \otimes Y_4\right).$$

c) Verify that the number operator $n_q = a_q^\dagger a_q$ can be expressed as

$$n_q = \frac{1}{2}(1 - Z_q)$$

d) Verify that

$$a_1^\dagger a_3^\dagger a_3 a_1 = n_{a\uparrow} n_{a\downarrow}.$$

e) Verify that the Hubbard term

$$H_{\mathrm{H}} = U(a_1^\dagger a_3^\dagger a_3 a_1 + a_2^\dagger a_4^\dagger a_4 a_2)$$

can be expressed as

$$U\left(n_{a\uparrow} n_{a\downarrow} + n_{b\uparrow} n_{b\downarrow}\right) = \frac{U}{4}\left(2 + Z_1 \otimes Z_3 + Z_2 \otimes Z_4 - Z_1 - Z_2 - Z_3 - Z_4\right).$$