University of California at San Diego – Department of Physics – Prof. John McGreevy

Physics 213/113 Winter 2023
Assignment 2 – Solutions

Due 11:00am Tuesday, January 24, 2023

1. **Brain-warmer.** Consider a system of N qbits. Show (convince yourself) that the operator

$$\sum_{i=1}^{N} X_i$$

written in the eigenbasis of Z_i is the adjacency matrix of an N-dimensional hypercube.

First of all, the question makes sense since the number of vertices of the N-dimensional hypercube is 2^N, which is the dimension of the Hilbert space on N qbits. We can represent the vertices by their locations $s_1 \cdots s_N$, with each $s_i = \pm 1$. Two vertices of the hypercube share an edge if they differ in only one coordinate. To see the connection to $\sum_i X_i$, note that $|s_1 \cdots s_N\rangle$ provide a basis (of Z-eigenstates) for the Hilbert space of N qbits. In this basis the operator $\sum_i X_i$ has nonzero matrix elements only between states whose label differ in one coordinate (and those nonzero matrix elements are all one).

Alternatively, here's an inductive argument: The adjacency matrix for the 1-dimensional case is $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, which begins the induction. A d-dimensional hypercube is made by attaching 2 $(d-1)$-dimensional hypercubes, according to the rule

$$A_d = \begin{pmatrix} A_{d-1} & \mathbb{1}_{d-1} \\ \mathbb{1}_{d-1} & A_{d-1} \end{pmatrix}.$$

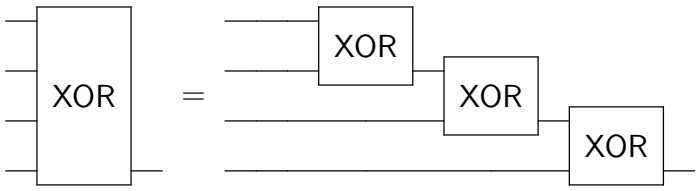
Compare this to the rule for adding an extra X:

$$\sum_i X_i = \mathbb{1}_2 \otimes \sum_{i=1}^{d-1} X_i + X_d \otimes \mathbb{1}_2^{\otimes(d-1)} = \begin{pmatrix} \sum_{i=1}^{d-1} X_i & \mathbb{1}_{d-1} \\ \mathbb{1}_{d-1} & \sum_{i=1}^{d-1} X_i \end{pmatrix}.$$

This fact plays a role in the recent proof of the Sensitivity Conjecture; see here.

2. **Classical circuits brain-warmer.**

(a) Show that this circuit adds the input bits (at left) mod two:

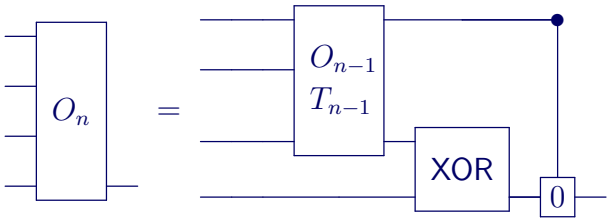


Here $\mathsf{XOR}(a,b) \equiv (a+b)\mathrm{mod}2$. We can proceed by induction on the number of input bits. The initial step with $n=2$ input bits is true since $\mathsf{XOR}(x,y) = (x+y)_2$. For induction step, the input to the $n+1$st XOR gate is $((\sum_{i=1}^{n} x_i)_2, x_{n+1})$, so the output is indeed $(\sum_{i=1}^{n+1} x_i)_2$.

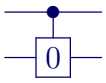
(b) [Optional] Construct a circuit with n input bits and one output bit that gives zero unless exactly one of the bits is one. The ingredients available are any gates that take two bits to at most two bits.

Here's a perhaps-overly-complicated solution I found, with some help from Hans Singh.

First, let's grant ourselves a gate T_n which takes n bits and outputs 1 if *greater* than one bit is 1 (we'll make it later). Then the following gives a recursive solution for the gate O_n which outputs 1 if exactly one bit is 1:



The gate with two labels O_{n-1}, T_{n-1} has two outputs – the top output is O_{n-1} and the bottom is T_{n-1}. The gate indicated by

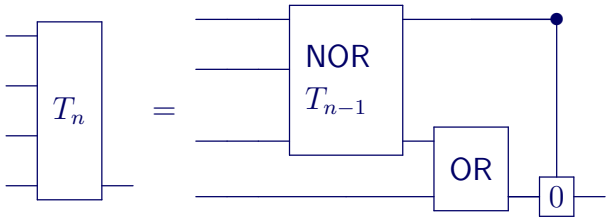


is a 'control-0' gate – if the top bit is 0, the output is the bottom bit, if the top bit is 1, the output is zero (and nothing happens to the top bit, which we can throw away). In quantum language, it is

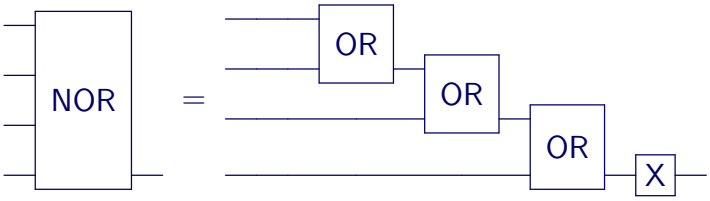
$$\mathsf{C0} \equiv |0\rangle\langle 0|_1 \otimes \mathbb{1}_2 + |1\rangle\langle 1|_1 \otimes |0\rangle\langle 0|_2.$$

The recursion starts by $O_2 = \mathsf{XOR}$.

Now we construct T_n. The construction is also recursive and very similar to the construction of O_n. The recursion starts by $T_2 = \mathsf{AND}$.

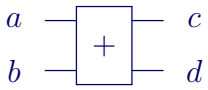


where OR is 1 if either or both of the inputs are 1 and NOR is OR followed by NOT (i.e. gives 1 only if all inputs are 0). The NOR on n bits can be accomplished by

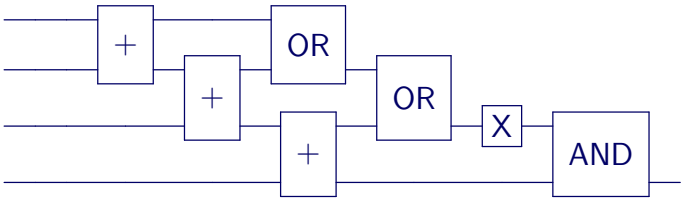


where X is the NOT gate.

Here's a more explicit representation. Define a two bit adder



by: $d = \mathsf{XOR}(a, b), c = \mathsf{AND}(a, b)$. Then the following will work:



The top part of the input to the final AND gate makes sure there is not more than one one being input, and the bottom input makes sure the number of ones being input is one mod two.

3. **Entanglement entropy in a quantum not-so-many-body system made from spins.**

   Consider the transverse-field Ising model on a lattice with only two ($L = 2$) sites, $i = 1, 2$, so that the Hilbert space is $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ where each of $\mathcal{H}_{1,2}$ is a two-state system, and the Hamiltonian is

$$\mathbf{H} = -J \left(2Z_1 Z_2 + gX_1 + gX_2\right).$$

(a) Find the matrix elements of the Hamiltonian in the eigenbasis of Z_1, Z_2

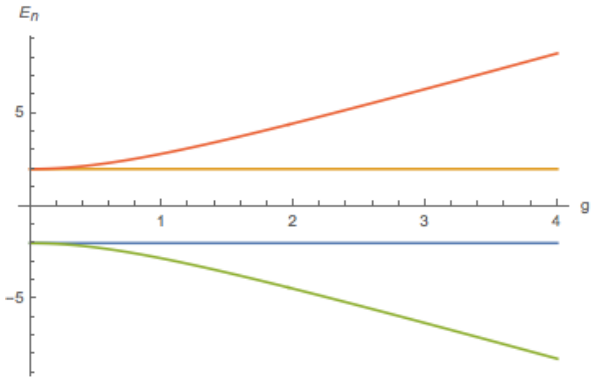
$$h_{ab} = \langle s_a | \mathbf{H} | s_b \rangle$$

where $a, b = 1..N$. What is N in terms of the system size L? Check that your matrix is hermitian.

$N = 2^L = 4$ here.

$$h_{ab} = \begin{pmatrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{pmatrix} \mathbf{H} \left(|00\rangle, |01\rangle, |10\rangle, |11\rangle \right) = \begin{pmatrix} -2 & g & g & 0 \\ g & 2 & 0 & g \\ g & 0 & 2 & g \\ 0 & g & g & -2 \end{pmatrix}.$$

(b) Find the eigenvalues of h and plot them as a function of g. (You may wish to use a computer for this and other parts of this problem.)



(c) Find the the groundstate of h – the eigenvector of the matrix h with the lowest eigenvalue; find the ground state energy (that lowest eigenvalue). Write the groundstate as

$$|\Psi\rangle = \sum_{a=1}^{N} \alpha_a |s_a\rangle .$$

For the 2-site case, we can do this by hand, but in preparation for the $L > 2$ case, let's just use this mathematica notebook.

(d) The Hilbert space is of the form $\mathcal{H}_1 \otimes \mathcal{H}_2$ where $\mathcal{H}_{1,2}$ are the Hilbert spaces of a single spin. Construct the reduced density matrix for the first site in the groundstate

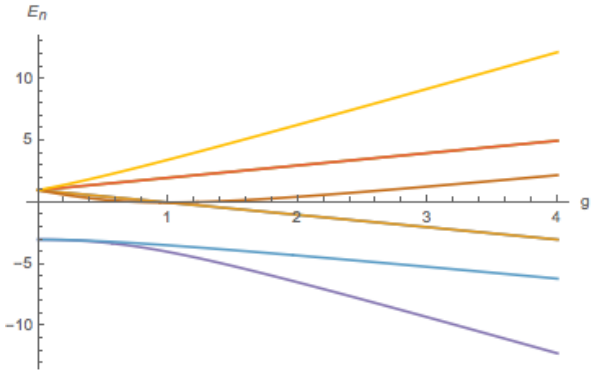
$$\boldsymbol{\rho}_1 \equiv \mathrm{tr}_{\mathcal{H}_2} |\Psi\rangle\langle\Psi|.$$

(e) Find the eigenvalues λ_α of $\boldsymbol{\rho}_1$. Calculate the von Neumann entropy of $\boldsymbol{\rho}_1$, $S(\boldsymbol{\rho}_1) = -\sum_\alpha \lambda_\alpha \log \lambda_\alpha$ as a function of g. What is the numerical value when $g \to \infty$? What about $g \to 0$? Do they agree with your expectations?

(f) [Bonus] Redo this problem with $L = 3$ sites (or more):

$$\mathbf{H} = -J\left(Z_1 Z_2 + Z_2 Z_3 + Z_3 Z_1 + g X_1 + g X_2 + g X_2\right).$$

Consider $L = 3$. There should be three gs in each row and column, since the X_i operators move the bit string $s_1 s_2 s_3$ by Hamming distance one, i.e. it changes exactly one of the bits. The diagonal entries are 3 (if the spins are all the same) and -1 for the other six entries. The spectrum looks like:



4. **Entanglement entropy in a quantum not-so-many-body system made from electrons.** [This problem is optional but strongly encouraged][1]

Consider a system consisting of two electrons, each with spin one-half, and each of which can occupy either of two sites labelled $i = 1, 2$. The dynamics is governed by the following (Hubbard) Hamiltonian:

$$\mathbf{H} = -t \sum_{\sigma=\uparrow,\downarrow} \left(\mathbf{c}^\dagger_{1\sigma}\mathbf{c}_{2\sigma} + \mathbf{c}^\dagger_{2\sigma}\mathbf{c}_{1\sigma}\right) + U \sum_i \mathbf{n}_{i\uparrow}\mathbf{n}_{i\downarrow}.$$

$\sigma = \uparrow, \downarrow$ labels the electron spin. $\mathbf{c}$ and $\mathbf{c}^\dagger$ are fermion creation and annihilation operators,

$$\{\mathbf{c}_{i\sigma}, \mathbf{c}^\dagger_{i'\sigma'}\} = \delta_{ii'}\delta_{\sigma\sigma'}$$

and $\mathbf{n}_{i\sigma} \equiv \mathbf{c}^\dagger_{i\sigma}\mathbf{c}_{i\sigma}$ is the number operator. The condition that there is a total of two electrons means we only consider states $|\psi\rangle$ with

$$\left(\sum_{i,\sigma} \mathbf{n}_{i\sigma} - 2\right)|\psi\rangle = 0.$$

[1] I got this problem from Tarun Grover.

The first term is a kinetic energy which allows the electrons to hop between the two sites. The second term is a potential energy which penalizes the states where two electrons sit at the same site, by an energy $U > 0$.

(a) Enumerate a basis of two-electron states (make sure they satisfy the Pauli exclusion principle).

States with two electrons on two sites are:

$$\{|\uparrow\downarrow, 0\rangle, |0, \uparrow\downarrow\rangle, |\uparrow, \uparrow\rangle, |\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle, |\downarrow, \downarrow\rangle\}$$

where I'll use the convention that the fermion creation operators are ordered as written, *e.g.*:

$$|\uparrow\downarrow, 0\rangle = c^\dagger_{1,\uparrow} c^\dagger_{1,\downarrow} |0\rangle .$$

(b) The Hamiltonian above has some symmetries. In particular, the total electron spin in the $\hat{z}$ direction is conserved. For simplicity, let's focus on the states where it is zero, such as $\mathbf{c}^\dagger_{1\uparrow}\mathbf{c}^\dagger_{2\downarrow}|0\rangle$ where $|0\rangle$ is the state with no electrons, $\mathbf{c}_{i\sigma}|0\rangle = 0$. Find a basis for this subspace, $\{\phi_a\}, a = 1..N$.

States with $S^z_1 + S^z_2 = 0$ are

$$\{|\uparrow\downarrow, 0\rangle, |0, \uparrow\downarrow\rangle, |\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle\}$$

(c) Find the matrix elements of the Hamiltonian in this basis,

$$h_{ab} \equiv \langle\phi_a|\mathbf{H}|\phi_b\rangle , \quad a, b = 1..N.$$

There are some signs we need to worry about in the hopping terms from the fermionic nature of the electron[2]. In particular, writing $H_t \equiv -t \sum_{\sigma=\uparrow,\downarrow} \left(\mathbf{c}^\dagger_{1\sigma}\mathbf{c}_{2\sigma} + \mathbf{c}^\dagger_{2\sigma}\mathbf{c}_{1\sigma}\right)$, we have *e.g.*

$$H_t |\uparrow\downarrow, 0\rangle = -t \left(\mathbf{c}^\dagger_{2\sigma}\mathbf{c}_{1\sigma}\right) \mathbf{c}^\dagger_{1\uparrow}\mathbf{c}^\dagger_{1\downarrow}|0\rangle \tag{1}$$

$$= -t \left(\mathbf{c}^\dagger_{2\uparrow}\mathbf{c}^\dagger_{1\downarrow} - \mathbf{c}^\dagger_{2\downarrow}\mathbf{c}^\dagger_{1\uparrow}\right)|0\rangle \tag{2}$$

$$= -t\left(-|\downarrow, \uparrow\rangle + |\uparrow\downarrow\rangle\right) = t\left(|\downarrow, \uparrow\rangle - |\uparrow\downarrow\rangle\right). \tag{3}$$

Since all the basis states have norm 1 (*e.g.* $\langle\downarrow, \uparrow | \downarrow, \uparrow\rangle = 1$), this gives the matrix elements

$$\langle\downarrow, \uparrow| H_t |\uparrow\downarrow, 0\rangle = +t, \quad \langle\uparrow, \downarrow| H_t |\uparrow\downarrow, 0\rangle = -t.$$

[2]Thanks to Hans Singh for an important correction here.

Similarly,

$$H_t \left|0, \uparrow\downarrow\right\rangle = -t \left(\mathbf{c}_{1\sigma}^\dagger \mathbf{c}_{2\sigma}\right) \mathbf{c}_{2\uparrow}^\dagger \mathbf{c}_{2\downarrow}^\dagger \left|0\right\rangle = -t \left(\left|\downarrow, \uparrow\right\rangle - \left|\uparrow\downarrow\right\rangle\right). \tag{4}$$

So in the given basis, we find:

$$h = \begin{pmatrix} U & 0 & t & -t \\ 0 & U & -t & t \\ t & -t & 0 & 0 \\ -t & t & 0 & 0 \end{pmatrix}$$

(d) Find the eigenstate and eigenvalue of the matrix h with the lowest eigenvalue. Write the groundstate as

$$\left|\Psi\right\rangle = \sum_{a=1}^{N} \alpha_a \left|\phi_a\right\rangle.$$

For $U > 0$, the lowest eigenvalue is

$$E_0 = \frac{U}{2}\left(1 - \sqrt{1 + \left(\frac{4t}{U}\right)^2}\right)$$

and the associated normalized eigenvector has

$$\alpha_a = \frac{1}{2 + \frac{32t^2}{\left(U + \sqrt{(4t)^2 + U^2}\right)^2}} \left(\frac{4t}{U + \sqrt{(4t)^2 + U^2}}, -\frac{4t}{U + \sqrt{(4t)^2 + U^2}}, -1, 1\right).$$

(e) Before imposing the global constraints on particle number and S^z, the Hilbert space can be factored (up to some signs because fermions are weird) by site: $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, where $\mathcal{H}_i = \text{span}\{\left|0\right\rangle, \mathbf{c}_{i\uparrow}^\dagger \left|0\right\rangle, \mathbf{c}_{i\downarrow}^\dagger \left|0\right\rangle, \mathbf{c}_{i\uparrow}^\dagger \mathbf{c}_{i\downarrow}^\dagger \left|0\right\rangle\}$. Using this bipartition, construct the reduced density matrix for the first site in the groundstate:

$$\boldsymbol{\rho}_1 \equiv \text{tr}_{\mathcal{H}_2} \left|\Psi\right\rangle \left\langle\Psi\right|.$$

$$\rho_1. = \left(\langle\uparrow\downarrow|_1, \langle 0|_1, \langle\uparrow|_1, \langle\downarrow|_1\right)\left(\alpha_1 |\uparrow\downarrow, 0\rangle + \alpha_2 |0, \uparrow\downarrow\rangle + \alpha_3 |\uparrow, \downarrow\rangle + \alpha_4 |\downarrow, \uparrow\rangle\right)$$
$$\cdot \left(\alpha_1^\star \langle\uparrow\downarrow, 0| + \alpha_2^\star \langle 0, \uparrow\downarrow| + \alpha_3^\star \langle\uparrow, \downarrow| + \alpha_4^\star \langle\downarrow, \uparrow|\right) \begin{pmatrix} |\uparrow\downarrow\rangle_1 \\ |0\rangle_1 \\ |\uparrow\rangle_1 \\ |\downarrow\rangle_1 \end{pmatrix}$$
$$= \left(\alpha_2 |0\rangle_1, |\alpha_1|^2 |\uparrow\downarrow\rangle_1, |\alpha_4|^2 |\downarrow\rangle_1, |\alpha_3|^2 |\uparrow\rangle_1\right) \begin{pmatrix} \alpha_2^\star \langle 0| \\ \alpha_2^\star \langle\uparrow\downarrow|_1 \\ \alpha_4^\star \langle\downarrow|_1 \\ \alpha_3^\star \langle\uparrow|_1 \end{pmatrix} \tag{5}$$
$$= |\alpha_2|^2 |0\rangle\langle 0| + |\alpha_1|^2 |\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\alpha_4|^2 |\downarrow\rangle\langle\downarrow| + |\alpha_3|^2 |\uparrow\rangle\langle\uparrow|. \tag{6}$$

(f) Find the eigenvalues λ_α of $\boldsymbol{\rho}_1$. Calculate the von Neumann entropy of $\boldsymbol{\rho}_1$, $S(\boldsymbol{\rho}_1) = -\sum_\alpha \lambda_\alpha \log \lambda_\alpha$ as a function of U/t. What is the numerical value when $U/t \to \infty$?

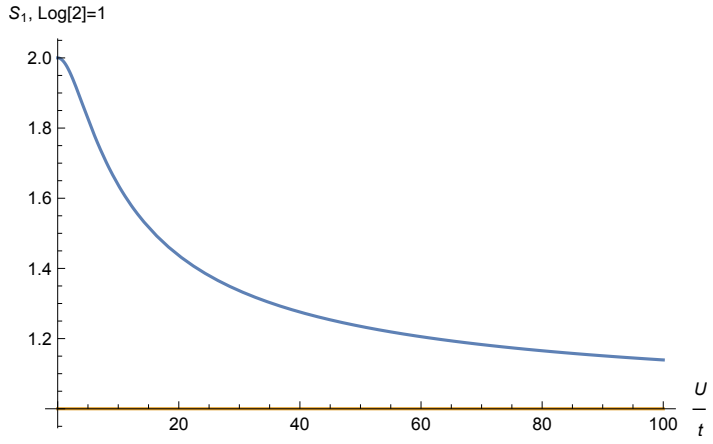
Using the form of α_a, the density matrix is of the form

$$\rho_1 = \mathcal{N} \mathrm{diag}\,(a, a, 1, 1)\,,$$

with $a = \frac{4t}{U + \sqrt{(4t)^2 + U^2}}$. $\mathrm{tr}\rho = 1$ then determines $\mathcal{N} = \frac{1}{2+2a}$. So the eigenvalues are $\frac{a}{2+2a}$ and $\frac{1}{2+2a}$. The von Neumann entropy is

$$S_1 = -\mathrm{tr}\rho_1 \log \rho_1 = 2\left(\frac{a}{2+2a} \log\left(\frac{a}{2+2a}\right) + \frac{1}{2+2a} \log\left(\frac{1}{2+2a}\right)\right).$$

It looks like this:



Since $a \to 0$ as $U/t \to \infty$, this approaches

$$S_1 \overset{U \gg t}{\to} \log 2 = 1.$$

This entropy reflects the fact that in this limit, the groundstate is degenerate between the two states with one particle per site: $|\uparrow,\downarrow\rangle$ and $|\downarrow,\uparrow\rangle$.

(g) **Super-Exchange.** Go back to the beginning and consider the limit $U \gg t$. What are the groundstates when $U/t \to \infty$, so that we may completely ignore the hopping term?

Let us consider the case where we have N sites and N electrons, instead of just $N = 2$. In the limit $U/t \to \infty$, we must have exactly one electron per site, since if we had no electrons at any site, we would have to have more than one at some other site, which would cost large energy U. So there is a single spin-half at each site.

At second order in degenerate perturbation theory, find the effective Hamiltonian which splits the degeneracy for small but nonzero t/U. Write the answer in terms of the spin operator

$$\vec{\mathbf{S}}_i \equiv \frac{1}{2}\mathbf{c}^\dagger_{i\sigma}\vec{\sigma}_{\sigma\sigma'}\mathbf{c}_{i\sigma'}.$$

The sign is important!

The effective Hamiltonian at second order acting on the degenerate subspace is

$$H = P\sum_i \frac{\mathbf{H}\,|i\rangle\,\langle i|\,\mathbf{H}}{E_0 - E_i}P$$

where P is a projector onto the degenerate subspace with energy E_0 and i runs over 'virtual' states outside the subspace (note that $\sum_i |i\rangle\langle i| = 1 - P$). The most important (lowest energy) virtual intermediate state comes from hopping a single electron to a neighboring site. This virtual state has energy $E_i - E_0 = U$ above the groundstate space. The hopping matrix elements are each $(-t)$. The tricky bit is that if the neighboring electrons are in the *same* spin state then the hopping matrix element vanishes by the Pauli principle, since the hopping term doesn't change the spin. Since the perturbation by finite hopping term respects the $\mathsf{SU}(2)$ spin rotation symmetry generated by $\sum_i \mathbf{S}_i \equiv \sum_i \mathbf{c}^\dagger_i\vec{\sigma}\mathbf{c}_i$, we must be able to write the effective hamiltonian in terms of $\mathsf{SU}(2)$ invariant combinations of these operators Therefore

$$H = -c\frac{t^2}{U}\sum_{\langle ij\rangle}\vec{\mathbf{S}}_i \cdot \vec{\mathbf{S}}_j \tag{7}$$

for some constant c. The minus sign is ubiquitous in second-order perturbation theory (since the excited state has *higher* energy than the ground state).

But actually $c < 0$! To see this we can compute just a few of the terms in the case of $L = 2$.

$$H_{eff} = \frac{1}{-U} H_t \left(|\uparrow\downarrow, 0\rangle\langle\uparrow\downarrow, 0| + |0, \uparrow\downarrow\rangle\langle 0, \uparrow\downarrow| \right) H_t \tag{8}$$

$$\overset{(3),(4)}{=} -\frac{t^2}{U} \left[(|\downarrow, \uparrow\rangle - |\uparrow, \downarrow\rangle) (\langle\downarrow, \uparrow| - \langle\uparrow, \downarrow|) + (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) (\langle\uparrow, \downarrow| - \langle\downarrow, \uparrow|) \right] \tag{9}$$

$$= -\frac{2t^2}{U} \left(|\uparrow, \downarrow\rangle\langle\downarrow, \uparrow| + h.c. - |\uparrow, \downarrow\rangle\langle\uparrow, \downarrow| - |\downarrow, \uparrow\rangle\langle\downarrow, \uparrow| \right). \tag{10}$$

Now let's compare to (7).

$$S_1^z S_2^z = |\uparrow, \uparrow\rangle\langle\uparrow, \uparrow| + |\downarrow, \downarrow\rangle\langle\downarrow, \downarrow| - |\uparrow, \downarrow\rangle\langle\uparrow, \downarrow| - |\downarrow, \uparrow\rangle\langle\downarrow, \uparrow| = \mathbb{1} - 2 \left(|\uparrow, \downarrow\rangle\langle\uparrow, \downarrow| + |\downarrow, \uparrow\rangle\langle\downarrow, \uparrow| \right).$$

And the off-diagonal terms are

$$S_1^x S_2^x + S_1^y S_2^y = 2 S_1^+ S_2^- + h.c. = 2 \left(|\uparrow, \downarrow\rangle\langle\downarrow, \uparrow| + |\downarrow, \uparrow\rangle\langle\uparrow, \downarrow| \right).$$

Comparing these expressions, we find $c = -4$.

Therefore the groundstate for two sites at $U \gg t$ is a singlet, *i.e.* a Bell pair $\frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ which is maximally entangled, in the sense that $\mathrm{tr}_1 |\psi\rangle\langle\psi| = \frac{1}{2}\mathbb{1}$, and hence the entanglement entropy is $S = 1$.

(h) Redo all the previous parts for the case where the two particles are spin-half bosons,

$$\mathbf{c}_{i\sigma} \rightsquigarrow \mathbf{b}_{i\sigma}, \quad [\mathbf{b}_{i\sigma}, \mathbf{b}_{i'\sigma'}^\dagger] = \delta_{ii'}\delta_{\sigma\sigma'}.$$

Nearly everything is the same, except the wavefunctions are symmetric, so the signs in the hopping matrix elements are missing. The missing relative sign in the hopping matrix elements means that the spin-spin interaction will be ferromagnetic. If we had $L > 2$, it would matter that it is no longer true that hopping is blocked when the neighboring spins are in the same state; this adds an extra term to the effective hamiltonian proportional to the identity operator. Also, the calculation would be different if we left the $m_z = 0$ sector, since then states like $\frac{b_{\uparrow 1}^{\dagger 2}}{\sqrt{2}} |0\rangle$ would contribute.