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

## Physics 213/113 Winter 2023 Assignment 2

## 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.

- 2. Classical circuits brain-warmer.
  - (a) Show that this circuit adds the input bits (at left) mod two:

Here  $XOR(a, b) \equiv (a + b) \bmod 2$ .

- (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.
- 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

$$\mathbf{H} = -J (2Z_1Z_2 + gX_1 + gX_2).$$

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

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

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

- (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 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

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

(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

$$\rho_1 \equiv \mathrm{tr}_{\mathcal{H}_2} |\Psi\rangle\langle\Psi|.$$

- (e) Find the eigenvalues  $\lambda_{\alpha}$  of  $\rho_1$ . Calculate the von Neumann entropy of  $\rho_1$ ,  $S(\rho_1) = -\sum_{\alpha} \lambda_{\alpha} \log \lambda_{\alpha}$  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):

$$\mathbf{H} = -J(Z_1Z_2 + Z_2Z_3 + Z_3Z_1 + gX_1 + gX_2 + gX_2).$$

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

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:

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

 $\sigma = \uparrow, \downarrow$  labels the electron spin. **c** and **c**<sup>†</sup> are fermion creation and annihilation operators,

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

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

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

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.

<sup>&</sup>lt;sup>1</sup>I got this problem from Tarun Grover.

- (a) Enumerate a basis of two-electron states (make sure they satisfy the Pauli exclusion principle).
- (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  $\mathbf{c}_{1\uparrow}^{\dagger}\mathbf{c}_{2\downarrow}^{\dagger}|0\rangle$  where  $|0\rangle$  is the state with no electrons,  $\mathbf{c}_{i\sigma}|0\rangle = 0$ . Find a basis for this subspace,  $\{\phi_a\}, a = 1..N$ .
- (c) Find the matrix elements of the Hamiltonian in this basis,

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

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

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

(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  $\mathcal{H}_i = \text{span}\{|0\rangle, \mathbf{c}_{i\uparrow}^{\dagger}|0\rangle, \mathbf{c}_{i\downarrow}^{\dagger}|0\rangle, \mathbf{c}_{i\uparrow}^{\dagger}\mathbf{c}_{i\downarrow}^{\dagger}|0\rangle\}$ . Using this bipartition, construct the reduced density matrix for the first site in the groundstate:

$$\rho_1 \equiv \operatorname{tr}_{\mathcal{H}_2} |\Psi\rangle \langle \Psi|$$
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- (f) Find the eigenvalues  $\lambda_{\alpha}$  of  $\rho_1$ . Calculate the von Neumann entropy of  $\rho_1$ ,  $S(\rho_1) = -\sum_{\alpha} \lambda_{\alpha} \log \lambda_{\alpha}$  as a function of U/t. What is the numerical value when  $U/t \to \infty$ ?
- (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?

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

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

The sign is important!

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

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