1.) ENTANGLEMENT IN A 2-SITE QUANTUM ISING MODEL IN A TRANSVERSE FIELD

Consider a two-site version of the quantum Ising model in a transverse field with Hamiltonian,
\[ \hat{H} = -J \hat{\sigma}_1^z \hat{\sigma}_2^z - h \hat{\sigma}_1^x - h \hat{\sigma}_2^x, \]  
(1)
where the two spin-1/2 operators are given by \( \hat{S}_j^\mu = \frac{1}{2} \hat{\sigma}_j^\mu \) with \( j = 1, 2 \) the site-label and \( \mu = x, y, z \) labeling the components of spin.

A convenient orthonormal basis of states which spans the full Hilbert space for this model consists of a direct product of eigenstates of \( \hat{\sigma}_z \) denoted, for example,
\[ |\phi_1\rangle = |\uparrow\rangle_1 \otimes |\uparrow\rangle_2; \quad |\phi_2\rangle = |\downarrow\rangle_1 \otimes |\downarrow\rangle_2 \quad |\phi_3\rangle = |\uparrow\rangle_1 \otimes |\downarrow\rangle_2 \quad |\phi_4\rangle = |\downarrow\rangle_1 \otimes |\uparrow\rangle_2, \]  
(2)
where \( \hat{\sigma}_z^1 \uparrow\rangle_1 = +| \uparrow\rangle_1, \hat{\sigma}_z^1 \downarrow\rangle_1 = -| \downarrow\rangle_1 \), and so on.

(a) Find the matrix elements for this Hamiltonian, \( h_{\alpha\beta} = \langle \phi_\alpha | \hat{H} | \phi_\beta \rangle \), with \( \alpha, \beta = 1, 2, 3, 4 \).

(b) Find the eigenstate and eigenvalue of the matrix \( h \) with the lowest eigenvalue. If one denotes this (normalized) eigenstate as \( |\Psi\rangle \), you should be now able to express it as \( |\Psi\rangle = \sum_{\alpha=1}^4 A_\alpha |\phi_\alpha\rangle \) with known values of the coefficients \( A_\alpha \).

(c) We are interested in the entanglement entropy of the state \( |\Psi\rangle \) for a bipartition that divides sites 1 and 2. Consider first the full system density matrix of the system which for a pure state is simply the projection operator on to the state \( |\Psi\rangle \),
\[ \hat{\rho} = |\Psi\rangle\langle\Psi|. \]  
(3)
To calculate the entanglement entropy between the 2-sites we first need to find the reduced density matrix, which we denote by \( \hat{\rho}_1 \), for this bipartition. Therefore, calculate
\[ \hat{\rho}_1 = Tr_2(\hat{\rho}) \]  
(4)
where \( Tr_2 \) denotes a trace over the Hilbert space of site 2, that is over the 2-states \( |\uparrow\rangle_2, |\downarrow\rangle_2 \). This gives the reduced density matrix \( \hat{\rho}_1 \) for the subsystem consisting of site 1.

(d) Re-express the density-matrix operator, \( \hat{\rho}_1 \) as a \( 2 \times 2 \) matrix in the basis \( |\uparrow\rangle_1, |\downarrow\rangle_1 \), with matrix elements, for example, \( 1 \langle \uparrow | \hat{\rho}_1 | \uparrow \rangle_1 \) and so on.

(e) Diagonalize your \( 2 \times 2 \) matrix representation of \( \hat{\rho}_1 \) to obtain its eigenvalues \( \lambda_i \).

(f) The von Neumann (bi-partite entanglement) entropy is defined as,
\[ S_1^{vN} = -Tr_1[\hat{\rho}_1 \ln(\hat{\rho}_1)] = - \sum_i \lambda_i \ln(\lambda_i). \]  
(5)
Calculate \( S_1^{vN} \) as a function of \( h/J \) and make a sketch of \( S_1^{vN} \) versus \( h/J \).

(g) What is the value of \( S_1^{vN} \) as \( h/J \to \infty \)? As \( h/J \to 0 \)? Explain the physics behind these two limits.
2.) 2-SITE HUBBARD MODEL AND ENTANGLEMENT ENTROPY

The Hubbard model refers to one of the simplest Hamiltonians for electrons moving through a crystal which are interacting with one another. The Hubbard model is a tight-binding model where the electrons sit on the “sites” of a lattice, hop between the sites with a kinetic energy (hopping amplitude denoted $t$) and have an onsite repulsion of strength $U$ whenever 2 electrons (of opposite spin) occupy the same site.

Here we consider a “baby” 2-site model with Hubbard Hamiltonian,

$$\hat{H} = -t \sum_{\sigma = \uparrow, \downarrow} (\hat{c}_{1\sigma}^\dagger \hat{c}_{2\sigma} + \hat{c}_{2\sigma}^\dagger \hat{c}_{1\sigma}) + U (\hat{n}_{1\uparrow} \hat{n}_{1\downarrow} + \hat{n}_{2\uparrow} \hat{n}_{2\downarrow}), \tag{6}$$

where 1 and 2 are site labels and $\sigma = \uparrow, \downarrow$ denotes the electron spin. The electron creation/destruction operators, $\hat{c}_{i\sigma}^\dagger$, $\hat{c}_{i\sigma}$, with site label $i = 1, 2$ satisfy the canonical Fermion anti-commutation relations,

$$[\hat{c}_{i\sigma}, \hat{c}_{j\sigma'}^\dagger]_+ = \delta_{ij} \delta_{\sigma\sigma'}; \quad [\hat{c}_{i\sigma}, \hat{c}_{j\sigma'}]_+ = [\hat{c}_{i\sigma}^\dagger, \hat{c}_{j\sigma'}^\dagger]_+ = 0, \tag{7}$$

where we’ve used the anticommutation notation, $\{\hat{A}, \hat{B}\}_+ = \hat{A}\hat{B} + \hat{B}\hat{A}$. Here, $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$ is the electron number operator, denoting the number of spin $\sigma$ electrons on site $i$.

The kinetic energy term hops an electron from one site to the other, while the potential energy penalizes the electrons an energy cost $U$ for being on the same site. Recall that the Pauli exclusion principle implies that the two electrons cannot have the same spin, if they sit on the same site. In this problem, we will calculate the entanglement entropy of this system for a partition that divides sites 1 from 2.

(a) We will start by assuming that there are two electrons present in the system. Given this, how many configurations (states) can you write down that satisfy the Pauli exclusion?

(b) Let us further assume that the total electron spin along the $\hat{z}$ direction is zero. The allowed set of configurations with this constraint is smaller than that in part (a) above. For example, one of them is given by $|\phi_1\rangle = \hat{c}_{1\uparrow}^\dagger \hat{c}_{2\downarrow}^\dagger |0\rangle$, where $|0\rangle$ denotes a state with no electrons; this state $|\phi_1\rangle$ has an up spin electron on site 1 and a down spin electron on site 2. Write down the allowed configurations $|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_N\rangle$ where $N$ is the total number of allowed configurations with this constraint.

(c) As in problem (1), find the matrix elements $h_{\alpha\beta} = \langle \phi_\alpha | \hat{H} | \phi_\beta \rangle$ of the Hamiltonian $\hat{H}$ for $\alpha, \beta = 1$ to $N$.

(d) Find the eigenstate $|\Psi\rangle$ and eigenvalue of the matrix $h$ with the lowest eigenvalue, and express the state as $|\Psi\rangle = \sum_{\alpha = 1}^N A_\alpha |\phi_\alpha\rangle$ with known value of the coefficients $A_\alpha$.

(e) We are again interested in the entanglement entropy of the state $|\Psi\rangle$ for a bipartition that divides sites 1 and 2. Calculate the reduced density matrix,

$$\hat{\rho}_1 = \text{Tr}_2 (\hat{\rho}) = \text{Tr}_2 [|\Psi\rangle \langle \Psi|], \tag{8}$$

by tracing over the 4-states on site 2 (no electron on site 2, an up-spin electron present on site 2, a down-spin electron present on site 2, both an up and a down spin electron present on site 2).

(f) Diagonalize $\hat{\rho}_1$ to obtain its eigenvalues $\lambda_i$ and calculate the von Neumann entropy $S_1^N = -\sum \lambda_i \ln(\lambda_i)$ as a function of $U/t$. What is the value of $S_1^N$ as $U/t \to \infty$? Could you have guessed this answer without a calculation?

3.) MAJORANA ZERO MODES IN 1D SUPERCONDUCTING WIRES

Decoherence is a major impediment in building a scalable quantum computer. Quantum computing requires two seemingly contradictory requirements. Firstly, one needs to engineer a quantum system with q-bits (quantum degrees of freedom) which can be readily and reliably manipulated (i.e. controlled) by the (classical) experimenter. But “external” degrees of freedom which can be used for controlling the quantum state in a quantum computer will invariably entangle with the state, causing decoherence of the quantum state in the computer. With too much decoherence a quantum computer will cease to operate, and will not be able to outperform a classical computer.

“Topological quantum computing” provides one possible way to avoid such decoherence. In certain two-dimensional systems of interacting quantum particles (say electrons), the quantum particles “condense” into a topologically ordered...
state. These topologically ordered states can support gapped “quasi-particle” excitations - excitations which behave like particles but can have fractional anyon statistics (neither bosonic nor fermionic) or even “non-Abelian” statistics. Quantum computation can then in principle be performed by braiding such quasiparticles around one another. Since the quantum statistics of these quasiparticles is encoded “non-locally” in terms of the original electrons, their braiding properties are protected from (local) disturbances which would otherwise lead to decoherence.

During the past 3-4 years it has been realized that one should be able to engineer one-dimensional “wires” which can support non-Abelian quasiparticles at the two ends of the wire - or at the boundary between two segments of a wire which are in a different state. Building wire networks out of such wires would enable one to move and braid these non-Abelian quasiparticles and implement topological quantum computing.

A semiconducting quantum wire with strong spin-orbit scattering which is resting on top of a superconductor, when placed in an external magnetic field, can enter a topological-state which supports Majorana-zero mode at the two ends of the wire. Here we consider a toy model for such a 1d wire system which will enable us to demonstrate that there are Majorana zero-modes bound to each end. A recent journal article that discusses the physics of such wires can be found at: http://www.kitp.ucsb.edu/sites/default/files/users/mpaf/p152.pdf

The appropriate Hamiltonian for such a wire takes the form,

$$\hat{H} = -\sum_{j=1}^{N-1} (t \hat{c}_j^\dagger \hat{c}_{j+1} + t \hat{c}_{j+1}^\dagger \hat{c}_j + \Delta \hat{c}_j \hat{c}_{j+1} + \Delta c_{j+1}^\dagger c_j) - \mu \sum_{j=1}^{N} (\hat{c}_j^\dagger \hat{c}_j)$$

where the electron creation/destruction operators at site $j$, denoted $\hat{c}_j^\dagger$, $\hat{c}_j$ satisfy canonical Fermion anti-commutation relations,

$$[\hat{c}_i, \hat{c}_j^\dagger]_+ = \delta_{ij}; \quad [\hat{c}_i, \hat{c}_j]_+ = [\hat{c}_i^\dagger, \hat{c}_j^\dagger]_+ = 0.$$

Notice that these electron operators do not have a spin-label (due to the spin-orbit interaction and the external magnetic field the electron spin is not conserved, and the spin can be ignored).

The first 2 terms in the Hamiltonian describe the hopping motion of electrons along the wire, the third and fourth terms represent the coupling of the wire to a (bulk) superconductor ($\Delta$ represents the amplitude for tunneling Cooper pairs between the superconductor and the wire) and the last term controls the number of electrons on the wire ($\mu$ is the chemical potential). We will now explore 2 special cases for the parameters, $t, \Delta, \mu$, for which the Hamiltonian can be easily solved.

First consider the case with $t = \Delta = 0$ and $\mu < 0$,

$$\hat{H}_\mu \equiv \hat{H}(t = \Delta = 0, \mu < 0) = +|\mu| \sum_{j=1}^{N} \hat{c}_j^\dagger \hat{c}_j.$$

Let $|\text{vac}\rangle_c$ denote a state with no electrons present, that satisfies, $\hat{c}_j |\text{vac}\rangle_c = 0$ for all $j$. Consider a set of states of the form,

$$|n_1, n_2, ..., n_N\rangle_c = \prod_{j=1}^{N} (\hat{c}_j^\dagger)^{n_j} |\text{vac}\rangle_c,$$

where $n_j = 0, 1$ denotes the number of electrons present on each site $j$.

(a) Using the anticommutation relations of the $\hat{c}_j^\dagger$, $\hat{c}_j$ show that these states form an orthonormal set,

$$\langle n_1, n_2, ..., n_N| n_1', n_2', ..., n_N'\rangle_c = \prod_{j=1}^{N} \delta_{n_j, n_j'}.$$

There are $2^N$ such states, so that this orthonormal set spans the full Hilbert space.

(b) Moreover, show that the states $|n_1, n_2, ..., n_N\rangle_c$ are eigenstates of $\hat{H}_\mu$, and obtain an expression for the eigenvalues, $E\{n_j\}$.

(c) Show that the ground state of $\hat{H}_\mu$ is non-degenerate. What is the energy gap between the ground state and the lowest energy excited state(s)? What is the degeneracy of this lowest energy excited state multiplet? Since the ground state is unique, there are no zero-energy quasiparticles living at the ends of the wires (cf to discussion below).
Next consider the special case with $t = \Delta > 0, \mu = 0$,
\[
\hat{H}_t \equiv \hat{H}(t = \Delta, \mu = 0) = -t \sum_{j=1}^{N-1} (\hat{c}^\dagger_j \hat{c}_{j+1} + \hat{c}^\dagger_{j+1} \hat{c}_j + \hat{c}_j \hat{c}_{j+1} + \hat{c}^\dagger_j \hat{c}^\dagger_{j+1} \hat{c}^\dagger_{j+1} \hat{c}_j).
\] (14)

In order to solve this Hamiltonian it is useful to define two sets of Majorana (real) Fermion operators,
\[
\gamma_{A,j} = i(\hat{c}^\dagger_j - \hat{c}_j); \quad \gamma_{B,j} = (\hat{c}^\dagger_j + \hat{c}_j).
\] (15)

Notice that these Majorana operators are self-adjoint (real), satisfying $\gamma_{A,j}^\dagger = \gamma_{A,j}$ and $\gamma_{B,j}^\dagger = \gamma_{B,j}$.

(d) Show that these Majorana operators satisfy the following anti-commutation relations,
\[
[\gamma_{A,j}, \gamma_{A,j'}]_+ = [\gamma_{B,j}, \gamma_{B,j'}]_+ = 2\delta_{jj'}; \quad [\gamma_{A,j}, \gamma_{B,j'}]_+ = 0.
\] (16)

(e) Re-express the Hamiltonian $\hat{H}_t$ in terms of the Majorana operators, $\gamma_{A,j}$ and $\gamma_{B,j}$.

It is convenient to define a new set of (complex) Fermion operators, $\hat{d}^\dagger_j, \hat{d}_j$, via,
\[
\hat{d}_j = (\gamma_{A,j+1} + i\gamma_{B,j})/2
\] (17) for $j = 1, 2, ..., N - 1$ and
\[
\hat{d}_{\text{end}} = (\gamma_{A,1} + i\gamma_{B,N})/2.
\] (18)

Notice that the complex Fermion operator $\hat{d}_{\text{end}}$ is very “non-local”, being defined as a linear combination of two real operators on opposite ends of the wire.

(f) Verify that these new complex $d$-Fermion operators satisfy the same canonical anticommutation relations as the complex $c$-Fermions, ie
\[
[\hat{d}_j, \hat{d}^\dagger_{j'}]_+ = \delta_{jj'}; \quad [\hat{d}_{\text{end}}, \hat{d}^\dagger_{\text{end}}]_+ = 1; \quad [\hat{d}_{\text{end}}, \hat{d}_j]_+ = 0; \quad \text{etc}
\] (19)

(g) Show that the Hamiltonian $\hat{H}_t$, when re-expressed in terms of the $d$–Fermion operators, takes a simple “site-local” form,
\[
\hat{H}_t = t \sum_{j=1}^{N-1} \hat{d}^\dagger_j \hat{d}_j,
\] (20)

and is independent of the operator $\hat{d}_{\text{end}}$.

(h) Next consider an orthonormal complete set of states built from the $d$–operators,
\[
|0; n_1, n_2, ..., n_{N-1}\rangle_d = \prod_{j=1}^{N-1} (\hat{d}^\dagger_j)^{n_j} |\text{vac}\rangle_d; \quad |1; n_1, n_2, ..., n_{N-1}\rangle_d = \hat{d}^\dagger_{\text{end}} |0; n_1, n_2, ..., n_{N-1}\rangle_d,
\] (21)

where $n_j = 0, 1$ for each $j = 1, 2, ..., N - 1$. The state $|\text{vac}\rangle_d$, which corresponds to a vacuum of $d$–Fermions (no $d$–Fermions present), is annihilated by the destruction operators $\hat{d}_j |\text{vac}\rangle_d = \hat{d}_{\text{end}} |\text{vac}\rangle_d = 0$. Show that these states are eigenstates of $\hat{H}_t$, and find the corresponding eigenvalues, $E(0; \{n_j\}), E(1; \{n_j\})$.

(i) For $t > 0$, show that the ground state of $\hat{H}_t$ is 2-fold degenerate, and that the 2-states, denoted $|0_g\rangle, |1_g\rangle$ satisfy,
\[
|1_g\rangle = \hat{d}^\dagger_{\text{end}} |0_g\rangle; \quad \hat{d}_{\text{end}} |0_g\rangle = 0.
\] (22)

What is the energy gap between these 2-degenerate ground states and the lowest energy excited states?

Remarkably, the complex Fermion operator that toggles between the 2-ground states, $\hat{d}_{\text{end}}$, is built from two Majorana operators that are on opposite ends of the wire, since $\hat{d}_{\text{end}} = (\gamma_{A,1} + i\gamma_{B,N})/2$. [The operators $\gamma_{A,1}$ and $\gamma_{B,N}$ are sometimes referred to as “Majorana zero modes.”] The robustness of the 2-fold degenerate ground state
manifold against decoherence can be understood by considering the set of “local” operators, denoted $\hat{O}_j$, which are operators that can be built from electron operators $\hat{c}_{j'}$, with $j' \approx j$. One can show that any local operator, when projected into the 2-fold degenerate ground state manifold, is proportional to the identity,

$$\langle 0_g | \hat{O}_j | 0_g \rangle = \langle 1_g | \hat{O}_j | 1_g \rangle; \quad \langle 0_g | \hat{O}_j | 1_g \rangle = \langle 1_g | \hat{O}_j | 0_g \rangle = 0. \quad (23)$$

This implies that the two ground states cannot be distinguished by making local measurements and that local measurements cannot cause transitions between the two states. The 2-fold degenerate ground state manifold is robust against local decoherence.