

# PHYC90045 Introduction to Quantum Computing

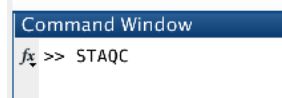
## Lab Session 11

### 11.1 Introduction

Welcome to Lab 11 of PHYC90045 Introduction to Quantum Computing. The purpose of this lab session is to get some experience with Adiabatic Quantum Computing (AQC) through the use of a Matlab based simulator STAQC (AQC simulator written by Sam Tonetto).

#### Instructions to access STAQC:

Download the files from the LMS. Open Matlab and navigate to directory with files. Type in “STAQC” in console. Refer to Appendix 1 in these lab notes for documentation.



### 11.2 Single-qubit system: eigenstates and eigenvalues

Before we embark on solving problems using the Adiabatic Quantum Computing (AQC) framework with STAQC, we need to review a few basics about eigenvalues and eigenvectors of operators. The eigensystem for a 2x2 Hermitian matrix  $M$  is defined as:  $M\chi = E\chi$  where  $\chi$  is a 1x2 column vector (the “eigenvector”, or “eigenstate” in QC parlance), and  $E$  is a number (eigenvalue), which is real when  $M$  is Hermitian (the case we consider here). In the case of a 2x2 matrix  $M$  there will be 2 eigenvectors  $\chi_{1,2}$  with corresponding eigenvalues  $E_{1,2}$ . When the eigenvalues are the same (distinct eigenvectors), the system is called “degenerate”. (NB. We use “E” for the eigenvalues because in terms of the physics, the eigenvalues of a Hamiltonian (energy) operator, which is what our  $M$  matrix will represent, are the allowed energies of the system).

Suppose, we have a single-qubit system described by a Hamiltonian operator involving the Z operation only, i.e. we write  $H_P = Z$  (we will use  $H_P$  to denote what will be the Hamiltonian operator encoding the “problem” to be solved (e.g. refer to how we encoded problems in QAOA of Lab10). Let’s solve the “eigensystem”  $H_P\chi = E\chi$ , i.e.  $Z\chi = E\chi$ . We already know the eigenvalues and eigenvectors from lectures – here they are using this notation.

$$\text{Hamiltonian: } H_P = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\text{Eigensystem: } Z\chi = E\chi$$

$$\chi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad Z\chi_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

i.e.  $Z\chi_1 = \chi_1 \rightarrow E_1 = +1$

$$\chi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad Z\chi_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$$

i.e.  $Z\chi_2 = -\chi_2 \rightarrow E_2 = -1$

In this example,  $\chi_2$  has the lowest eigenvalue (energy -1). We can re-cast into our ket notation which should look familiar:

$$|0\rangle \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$Z|0\rangle = +|0\rangle \quad Z|1\rangle = -|1\rangle$$

Let's look at another Hamiltonian operator that we will use in this lab,  $H_P = X$ . We have seen the eigensystem for this as well in lectures:

$$H_P|\pm\rangle \rightarrow X|\pm\rangle = \pm|\pm\rangle$$

where  $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$ . So the eigenvectors and eigenvalues of  $X$  are  $\chi_{1,2} \rightarrow |\pm\rangle$  and  $E_{1,2} \rightarrow \pm 1$ . Here, the state  $|-\rangle$  has the lowest energy.

Now we will make a Hamiltonian  $H(s)$ , depending on a parameter  $s$ , which is a simple linear combination of  $X$  and  $Z$ :

$$\begin{aligned} H(s) &= (1-s)H_X + s H_P \\ H_X &= X \\ H_P &= Z \end{aligned}$$

Clearly, at  $s=0$ , we have  $H(0) = H_X$  and at  $s=1$  we have  $H(1) = Z$ . Here,  $s$  is our “scaled” time, i.e.  $s = t/T$ , where  $T$  will be the total time of the AQC evolution (later) where we evolve from  $H(0) = H_X$  to our “problem” Hamiltonian  $H(1) = H_P$  (in this case  $H_P = Z$ ). Let's find the eigenstates of  $H(s)$  for any  $s$ , i.e. in ket notation we want to solve:

$$H(s)|\chi\rangle = E|\chi\rangle$$

Notes:

- The Energies will be dependent on  $s$ , i.e.  $E(s)$ , but we usually suppress that.
- For eigenvalues, we write  $E_i$  instead of the more customary  $\lambda_i$ , because the eigenvalues of a Hamiltonian are its energies.
- Hamiltonians are Hermitian, not unitary. They are not a quantum gate. (when we get to the QAOA lab we will see the difference more explicitly).

### Exercise 11.2.1

Generally, to solve an eigensystem we first calculate the eigenvalues through the characteristic equation, and then find the eigenvectors. To calculate the eigenvalues, we can re-arrange the above equation in matrix form as:

$$(H(s) - E)\chi = 0$$

and then solve the determinant (characteristic) equation  $\det((H(s) - E)) = 0$ .

$$\text{i.e. } \begin{vmatrix} [H(s)]_{11} - E & [H(s)]_{12} \\ [H(s)]_{21} & [H(s)]_{22} - E \end{vmatrix} = 0 \text{ where in matrix form we have } H(s) = \begin{bmatrix} [H(s)]_{11} & [H(s)]_{12} \\ [H(s)]_{21} & [H(s)]_{22} \end{bmatrix}.$$

This is a quadratic equation for  $E$  with two solutions,  $E_{1,2}$ . Using the fact that  $\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$ , find the eigenvalues of  $H(s)$  as a function of  $s$ .

$E_1$	
$E_2$	

(Here  $E_1$  is the defined as the lowest eigenvalue)

### Exercise 11.2.2

Hence, find  $\Delta = \min(E_2(s) - E_1(s))$ , the gap between the two eigenvalues of  $H(s)$ .

$$\Delta =$$

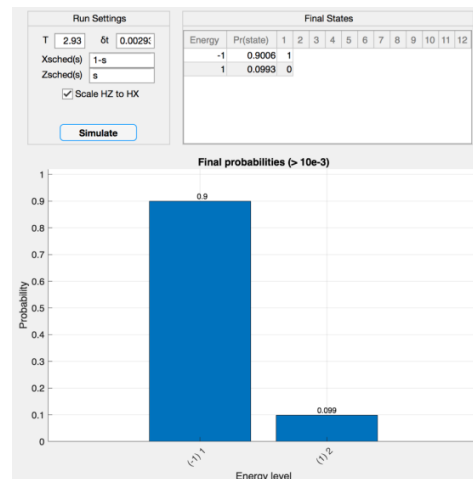
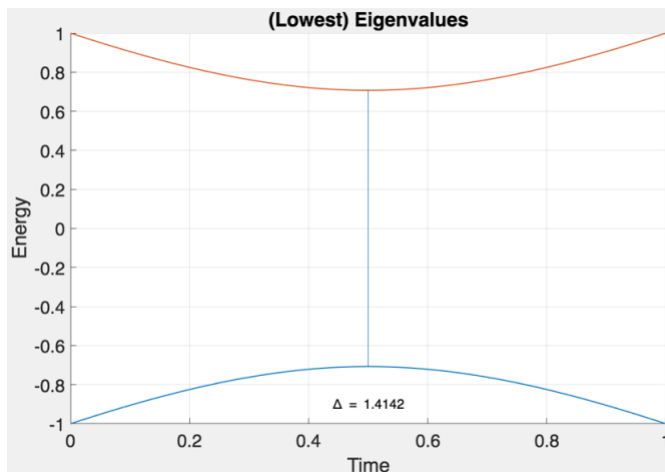
### Exercise 11.2.3

Using the eigenvalues  $E_{1,2}$  you have found, verify that the eigenstates of  $H(s)$  at  $s = \frac{1}{2}$  are:

$ \chi_1\rangle$	$\frac{1 - \sqrt{2}}{\sqrt{4 - 2\sqrt{2}}}  0\rangle + \frac{1}{\sqrt{4 - 2\sqrt{2}}}  1\rangle$
$ \chi_2\rangle$	$\frac{1 + \sqrt{2}}{\sqrt{4 + 2\sqrt{2}}}  0\rangle + \frac{1}{\sqrt{4 + 2\sqrt{2}}}  1\rangle$

### Exercise 11.2.4

STAQC assumes that the Hamiltonian is of the form  $H(s) = (1 - s)H_X + s H_P$  ( $H_P$  is synonymous with “HZ” in the STAQC definition), so we only need to specify  $H_P$  (refer to appendix). Program the problem Hamiltonian  $H_P = Z$  into the STAQC, run with default parameters ( $T=1$ ,  $\delta t = 0.001$ ) and verify the minimum gap you have calculated.



Using your solutions for the states, verify the probability distribution given by STAQC for the system at  $t=1$  (“Final” state, corresponding to  $s=1$ ).

## 11.3 Two-Qubit Hamiltonian

In AQC for multi-qubit systems we stick to the same basic form of the Hamiltonian,  $H(s) = (1 - s)H_X + s H_P$ . First we will extend to a simple example of two qubits, before we start contemplating a practical problem Hamiltonian case. For two qubits, our matrix representation will be  $4 \times 4$ , and there will be in general 4 eigenvalues, some of which may be degenerate (i.e. the same value).

### Exercise 11.3.1

Consider the two-qubit Hamiltonian:

$$H(s) = (1 - s)H_X + s H_P$$

$$H_X = X_1 + X_2$$

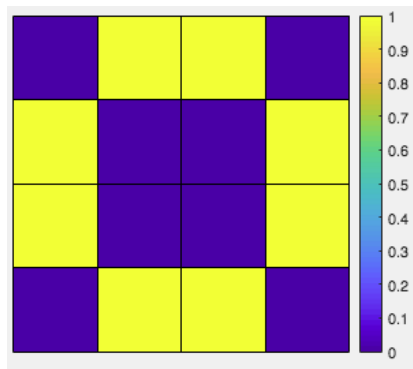
$$H_P = Z_1 + Z_2$$

Noting that  $H_X = X_1 + X_2$  is really  $H_X = X_1 \otimes I + I \otimes X_2$  etc, use the definition of outer products to get the matrices corresponding to  $H_X$  and  $H_P$  (here's some working space):

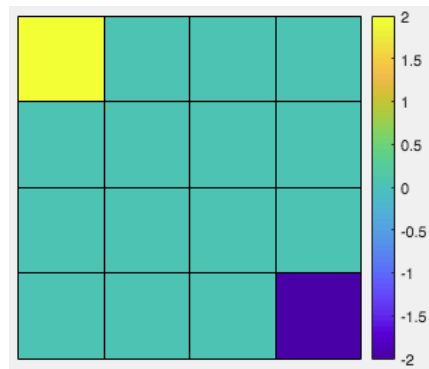
$$H_X = X_1 \otimes I + I \otimes X_2$$

$$H_P = Z_1 \otimes I + I \otimes Z_2$$

Program this  $H_P$  into STAQC and verify your matrices for  $H_X$  and  $H_P$  – you should obtain:



Left:  $H_X: H_X = X_1 \otimes I + I \otimes X_2$



Right:  $H_P: H_P = Z_1 \otimes I + I \otimes Z_2$

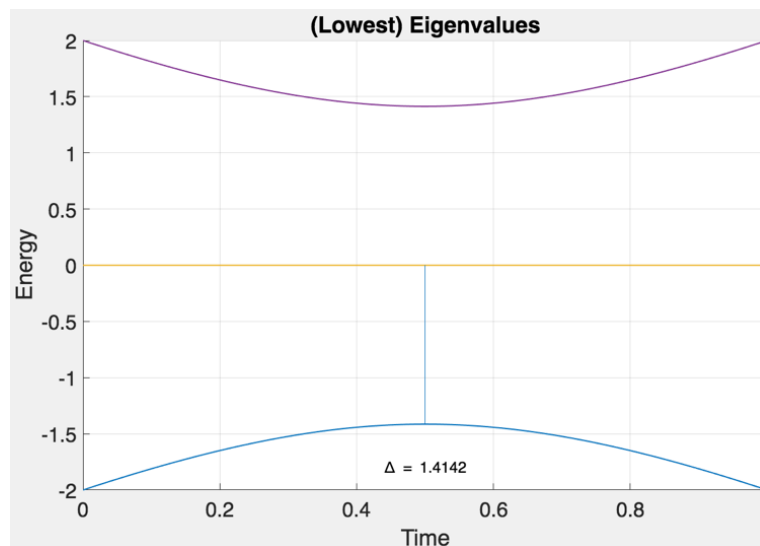
Compare with your matrices (NB pay attention to the colour scales).

### Exercise 11.3.2

The eigenvalues of  $H(s)$  are, in ascending order, given by:

$E_1$	
$E_2$	
$E_3$	
$E_4$	

(can you derive these?). Simulate the problem on STAQC with default parameters ( $T=1$ ,  $\delta t = 0.001$ ) to verify the eigenvalues. STAQC produces all the eigenvalues as function of  $s$ , from  $s = 0$  to  $s = 1$ , i.e.



Note again that “Time” is the actual time  $t = sT$ . This is important, as we will now see.

## 11.4 Introducing evolution

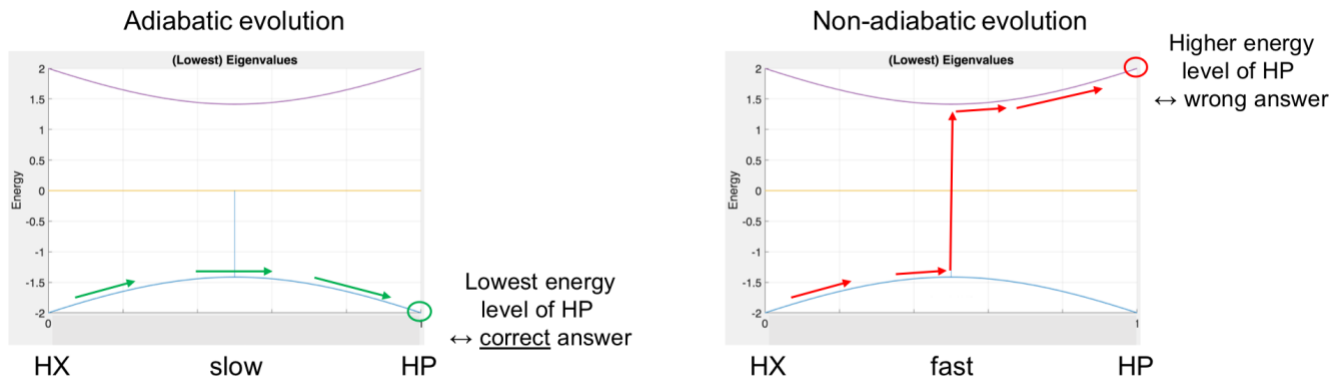
Now that you understand the eigenspectrum of energies (eigenvalues) as a function of the scaled “time” parameter  $s$ , we will look at the real magic of AQC – adiabatic evolution. The thing we are trying to do is evolve the Hamiltonian system from time  $t=0$  ( $s=0$ ), to the final time  $t=T$  ( $s=1$ ) so that:

$$H(s = 0) = H_X \rightarrow H(s = 1) = H_P$$

Generally we encode the answer to our original problem in the lowest eigenvalue (energy) state of  $H_P$ . While we can calculate that eigenvalue for small numbers of qubits (as we do in STAQC), for bigger systems that becomes impossible on a conventional computer (e.g.  $N \sim 40$  is about the limit), hence the promise of AQC as an alternative form of QC.

Remember from lectures: *adiabatic* means varying slowly. That is, if we vary the parameter  $s$  slowly enough the system will evolve staying in or close to the lowest eigenvalue (energy) state. *Hence, when we get to the end of the adiabatic evolution at  $s=1$  we should be in the lowest state of the  $H_P$  system and can read off the values of each qubit to get our problem solution (see figure below, left).*

But – how slow is slow enough? Basically, if the minimum gap is small it is easier it is to bump the system into the next highest (energy) eigenvalue state by going too fast...and hence when you get to the end of the evolution and read off the qubit values you won't be in the right solution state (see below, right). The gap is an important factor (but not the only one as we will see) in defining how slow the evolution needs to be in order to be in the adiabatic regime, and hence the value of  $T$  we must set.



### Exercise 11.4.1

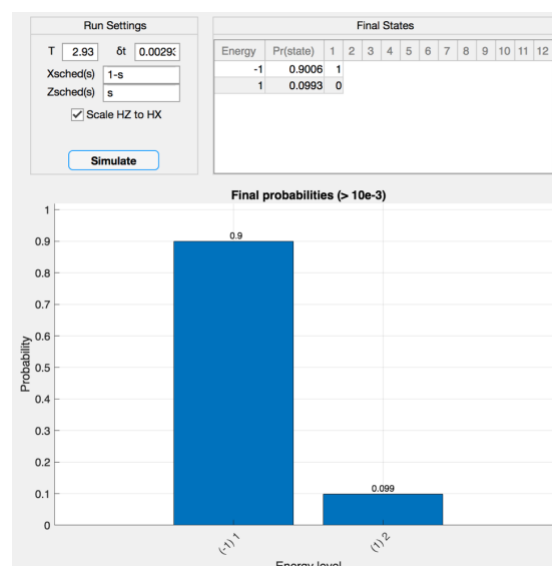
To see what happens when we evolve the system too quickly, or just slow enough, let's go back to the 1 qubit case:

$$H(s) = (1 - s)H_X + s H_P$$

$$H_X = X$$

$$H_P = Z$$

Program this system into STAQC and run the simulation for values of T from small to large. Inspect the results of the evolution by looking at the "Final Histogram" tab. How large must the timescale T be to get >90% probability of being in the ground-state of  $H_P$  at the end of the evolution ( $s=1$ )? i.e. the plot would look something like this:



### Exercise 11.4.2

Try this for the two qubit Hamiltonian in section 11.3.

## 11.5 Introducing couplings

Now that we can handle more than 1 qubit and evolved the system, we can introduce the next component that gets us closer to programming and solving real problems in the AQC framework.

### Exercise 11.5.1

In STAQC, program in the problem Hamiltonian

$$H_P = Z_1 + 2Z_2 + 2Z_1Z_2$$

(remember to think about this in the outer-product framework, which we suppress here for simplicity). STAQC will now run the eigensystem based on  $H(s) = (1 - s)H_X + s H_P$  with  $H_X = X_1 + X_2$  as the default. Run the simulation with default parameters and study the results. What is the minimum gap?

### Exercise 11.5.2

For the following Hamiltonians, with increasing numbers of qubits, program in STAQC and tabulate the minimum gap:

$$H_P = -Z_1 + Z_2 + Z_1 Z_2$$

$$H_P = -Z_1 + Z_2 - 2Z_3 + 2Z_4 + \sum_{i=1}^4 \sum_{j>i} Z_i Z_j$$

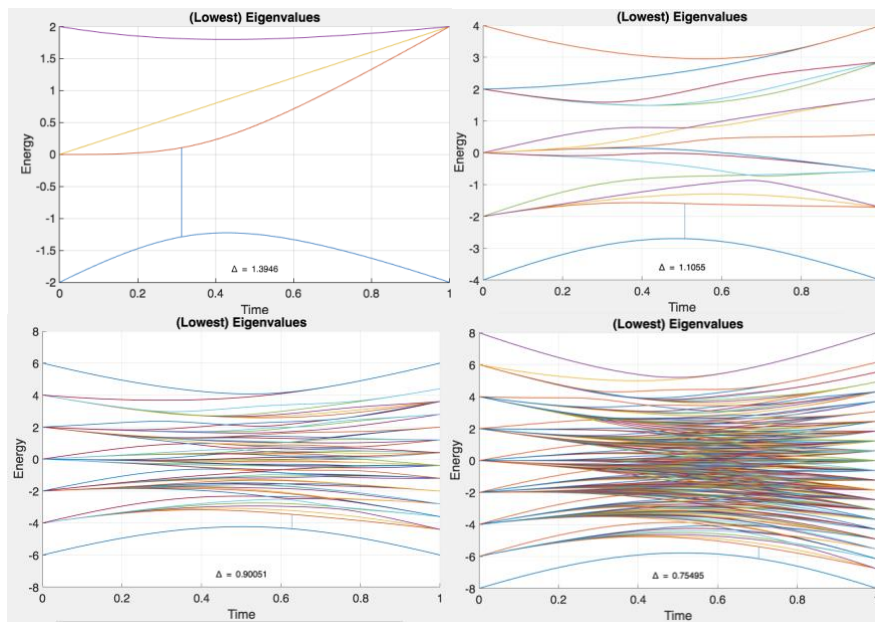
$$H_P = -Z_1 + Z_2 - 2Z_3 + 2Z_4 - 3Z_5 + 3Z_6 + \sum_{i=1}^6 \sum_{j>i} Z_i Z_j$$

$$H_P = -Z_1 + Z_2 - 2Z_3 + 2Z_4 - 3Z_5 + 3Z_6 - 4Z_7 + 4Z_8 + \sum_{i=1}^8 \sum_{j>i} Z_i Z_j$$

#Qubits	Min Gap	Timescale to achieve >90%
2	1.3946	
4	1.1055	
6	0.90051	
8	0.75495	

Marvel at how complicated the eigenvalue system becomes as the number of qubits grows (especially with couplings). Remember, STAQC only plots the lowest eigenvalues (energies) of the system as these are the relevant ones for the AQC computations. For N qubits, how many eigenvalues are there in total?

For the systems given above, you should see the following “eigen-spectra”:



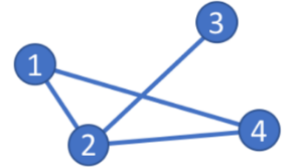
## 11.6 Graph problems in AQC

Luckily we have done a lot of the hard work in the QAOA lab. Recall from lectures that the Hamiltonian for the Graph Partitioning problem is:

$$H_P = A \left( \sum_i Z_i \right)^2 + B \left( \sum_{\langle ij \rangle} \frac{I - Z_i Z_j}{2} \right)$$

For  $A=1$ ,  $B=1$ , the problem Hamiltonian for the graph shown right is

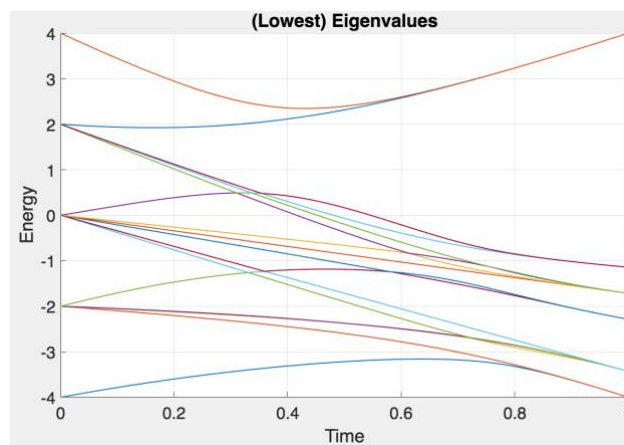
$$H_P = \frac{3}{2} (Z_1 Z_2 + Z_2 Z_4 + Z_1 Z_4 + Z_2 Z_3) + 2Z_1 Z_3 + 2Z_3 Z_4$$



### Exercise 11.6.1

Derive the problem Hamiltonian for the graph partitioning problem above, understand how the solution is represented. Program this into STAQC, run it with default parameters, inspect the outputs, compare with the solution.

NB. In the eigenspectrum, note that a higher eigenvalue curve starting at  $E = -2$  in  $H_X$  ends up in the ground-state of  $H_P$ , because the solution is doubly-degenerate. Although this might seem to imply that the minimum ground-excited gap is 0, it isn't that simple when  $H_P$  has degenerate ground-states (multiple valid solutions). It is usually the case that eigenvalue curves that end in degenerate ground-states of  $H_P$  are associated with eigenstates that do not couple to each other. So the minimum gap in this context would be between the ground-state eigenvalues and the lowest eigenvalue curve that doesn't end in the ground energy.



### Exercise 11.6.2

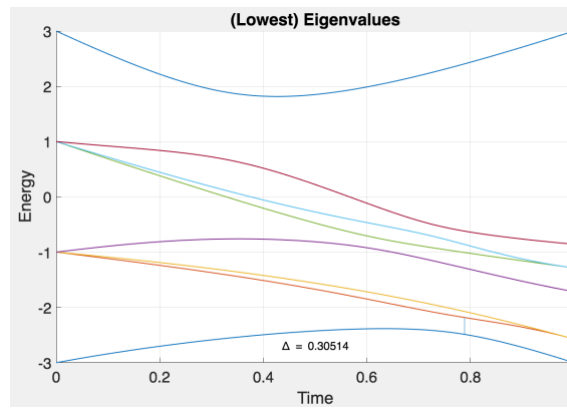
If you look in the “Final States” panel, note that for any given state, if you flip each bit in the state you end up with another state of the same energy. The solutions have *bit-flip symmetry*. In fact, this is true of any Hamiltonian with only  $Z_i Z_j$  terms.

This can be used to reduce the number of qubits needed to solve the graph partitioning problem. If we assume that in any solution, qubit 4 will be in the state  $|0\rangle$ , then the  $Z_4$  eigenvalue will be  $+1$  in  $H_P$ . This allows us to write a new Hamiltonian that involves only the first 3 qubits,

$$H'_P =$$

Program this into the STAQC and try running it for different sets of parameters.



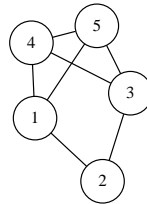


### Exercise 11.6.2

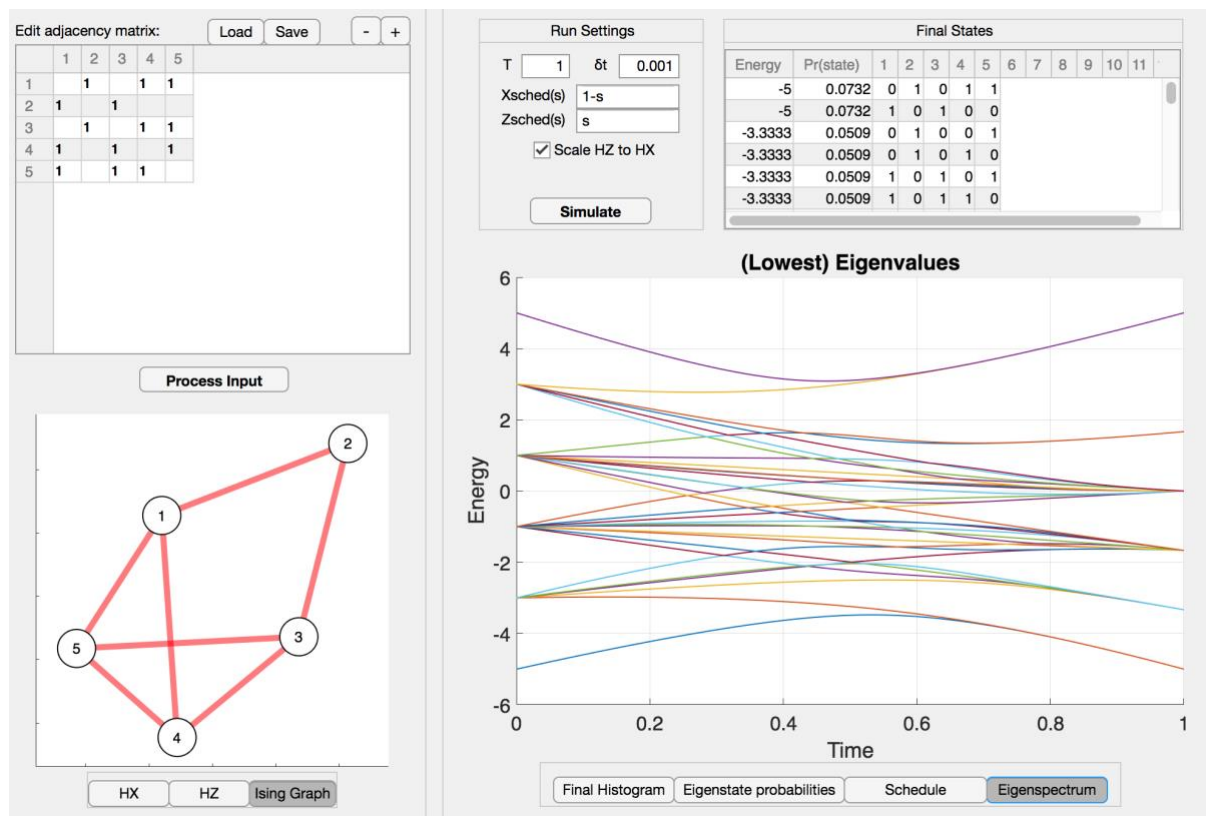
Recall from lectures that the Max-Cut Hamiltonian is

$$H_P = \sum_{\langle ij \rangle} Z_i Z_j$$

Program in the max-cut problem Hamiltonian for the graph shown below.



Run for different values of total timescale, T.



## Appendix 1: STAQC documentation

### Problem Input Panel

- In this panel you can specify your problem Hamiltonian. You don't have to worry about creating  $H_X$  – this is done automatically.
- Problem Hamiltonians can be specified through an *Adjacency Matrix*.
  - The off-diagonal  $(i,j)$  elements of the matrix represent coefficients of  $Z_i Z_j$
  - The on-diagonal elements represent coefficients of single-qubit  $Z$  terms.

For example,

	1	2	3
1		1	-2
2	1		-1
3	-2	-1	

represents the Hamiltonian  $H_Z = Z_1 Z_2 - 2Z_1 Z_3 - Z_2 + Z_3$

- You can also **load** or **save** adjacency matrices to text files. If you load your own adjacency matrix, keep in mind that it must be symmetric.
- After loading an adjacency matrix, click **Process Input** to construct the problem Hamiltonian. This also display outputs in the bottom-left:
  - **Ising Graph** shows the basic connectivity of the problem Hamiltonian specified. Anti-ferromagnetic (positive) couplings are shown in red, while Ferromagnetic (negative) couplings are shown in blue. You can use the scroll wheel to zoom if it is cut off.
  - **HX** shows a heat map of the initial transverse Hamiltonian, as a matrix.
  - **HZ** shows a heat map of the final problem Hamiltonian, as a matrix.

### Simulation Panel

- Once a problem Hamiltonian has been loaded, simulation parameters can be set in the “Run Settings” panel.

The Run Settings panel contains the following controls:

- T: Input field with value 1
- $\delta t$ : Input field with value 0.001
- Xsched(s): Input field with value 1-s
- Zsched(s): Input field with value s
- ☒ Scale HZ to HX
- Eigenvalues: Input field with value 12
- Simulate button

The settings are

- **T** is the timescale of Adiabatic Evolution. This determines the length of time over which the Adiabatic Quantum Computation occurs.
- **$\delta t$**  is the timestep of the numerical simulation. By default, whenever T is changed,  $\delta t$  will be adjusted to be  $T/1000$ . For larger simulations, you may want to increase the timestep to reduce simulation runtime.
- **Xsched(s)** and **Zsched(s)** are functions of the adiabatic parameter  $s \in [0,1]$ , which specify the factor multiplying the HX and HZ Hamiltonians for every value of s. Any valid matlab expression is allowable, so long as Xsched(1) = 0.

- **Scale HZ to HX** re-scales the problem Hamiltonian HZ during simulation, so that the maximum and minimum eigenvalues of HZ match the maximum and minimum eigenvalues of HX.
- For  $n \geq 9$  qubits, it is too inefficient to get every eigenvalue of  $H(s)$ , so **Eigenvalues** specifies how many lowest-lying eigenvalues to compute.
- Press **Simulate** to run the simulation. You can see the progress of the simulation and any error messages in the Matlab console.
- Outputs:
  - In the “Final States” panel, basis states are listed alongside their energies and probabilities of being measured. The basis states are ordered in energy from lowest-energy to highest.

Final States												
Energy	Pr(state)	1	2	3	4	5	6	7	8	9	10	11
-160	0.3261	1	0	1	0	0	1	1				
-158	0.3299	1	1	0	1	1	0	0				
-154	0.0138	0	1	0	1	1	0	0				
-152	0.0016	0	0	1	0	0	1	1				
-152	0.0127	1	0	0	1	1	0	0				
-152	0.0265	1	1	1	0	0	1	0				
-146	3.0000e-04	0	0	0	1	1	0	1				

- In the bottom-right window, you can toggle between
  - **Final Histogram** – The probabilities of measuring states of a certain energy at the end of the evolution.
  - **Eigenstate Probabilities** – This plots the probability of being in the lowest-lying eigenstates of  $H(s)$  during evolution.
  - **Schedule** – Plots the control schedules for HX and HZ.
  - **Eigenspectrum** – Plots the eigenvalues of  $H(s)$  throughout the evolution. If the ground state of  $H_Z$  is unique, this will also display the minimum gap between the ground and first excited levels.

### A note on units

The Matlab Simulator uses *atomic units*, which are suitable for describing the physics at very small scales. You don't need to worry too much about this, but if you're interested, and for a sense of perspective:

- If 1 unit of energy is  $1.65 \times 10^{-5}$  eV, then 1 unit of time will be 0.04 nanoseconds.
- Scaling the energy unit by a factor K will rescale the time unit by  $\hbar/K$ , where  $\hbar = 6.58 \times 10^{-16}$  eVs is Planck's reduced constant.