Work Summary

Advancing the tight-binding model by adding site Hamiltonians and nearest-neighbor interaction. Simulate variational method in the context of GRAPE algorithm to find the ground state.

Main Work

1. Modified tight-binding model
2. Dynamics simulation
3. Variational method in the context of GRAPE alogrithm
4. Variational method results

1 Modified tight-binding model

In the modified tight-binding model, besides the hopping Hamiltonian, the site Hamiltonian and the nearest-neighbor interaction (Coulomb repulsion) are added. The Hamiltonians can be tranformed through the basis mapping from electron occupation states $\begin{pmatrix} |21\rangle \\ |41\rangle \\ |31\rangle \\ |42\rangle \\ |32\rangle \\ |43\rangle \end{pmatrix}$ to cavity energy levels $\begin{pmatrix} |0\rangle \\ |1\rangle \\ |2\rangle \\ |3\rangle \\ |4\rangle \\ |5\rangle \end{pmatrix}$. As a result, the hopping Hamiltonian

$$\hat{H}_{hop} = -J \begin{pmatrix} 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & -1 \\ -1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \end{pmatrix},$$

the nearest-neighbor Hamiltonian

$$\hat{H}_{NN} = K \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

and the site Hamilltonian

$$\hat{H}_{site} = - \begin{pmatrix} S_1 + S_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & S_1 + S_4 & 0 & 0 & 0 & 0 \\ 0 & 0 & S_1 + S_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & S_2 + S_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & S_2 + S_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & S_3 + S_4 \end{pmatrix},$$

where the site energies S_1, S_2, S_3, and S_4 represent the site Hamiltonian on the 4 sites respectively. Here, the negative sign is because each site and electrons should form bound states.

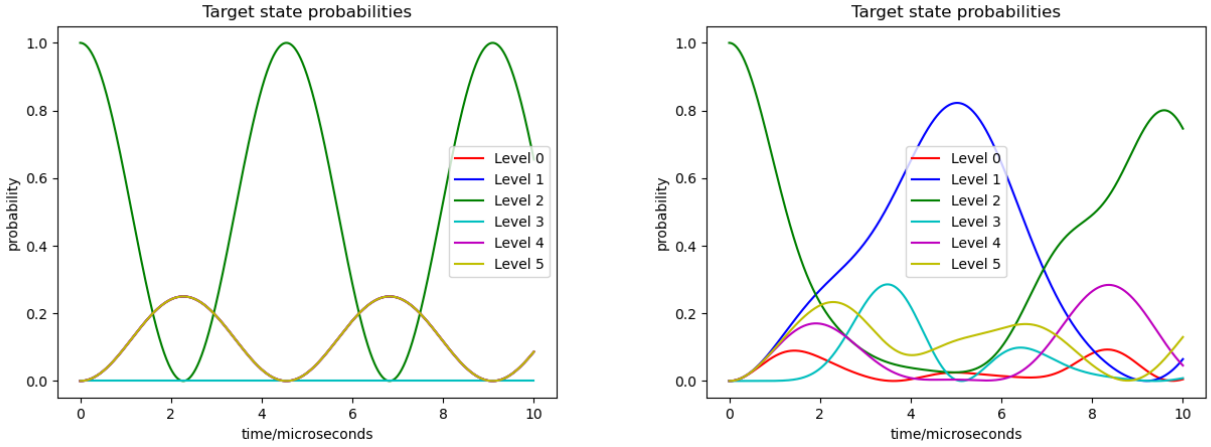
The introduction of the site energies are mainly to break the symmetries that causes destructive interference in the dynamics simulation. The site Hamiltonians can therefore be set individually or randomly only giving an overall scale. Note that all values of J, K, and S are in units of $\frac{1}{2\pi}$MHz, and as a comparison, the hopping Hamiltonian magnitude J is around 0.3.

2 Dynamics simulation

2.1 Including site Hamiltonian

2.1.1 Symmetry breaking

As discussion before, with random site Hamiltonians or indivually set site Hamiltonians, the symmetries in the 4 sites can be broken. A comparison of the dynamics is shown in Figure 1. Note that both starts with an initial state of $|2\rangle$ in the cavity, or equivalently $|13\rangle$ in the sites basis. Because of destructive interference, when there is no site Hamiltonian, the cavity level $|3\rangle$ should never be occupied as shown in left of Figure 1.



(a) Dynamincs without site Hamiltonian, i.e. $S = [0, 0, 0, 0]$ (b) Dynamincs with site Hamiltonian. Here, $S = [1, 2, 0, 0]$

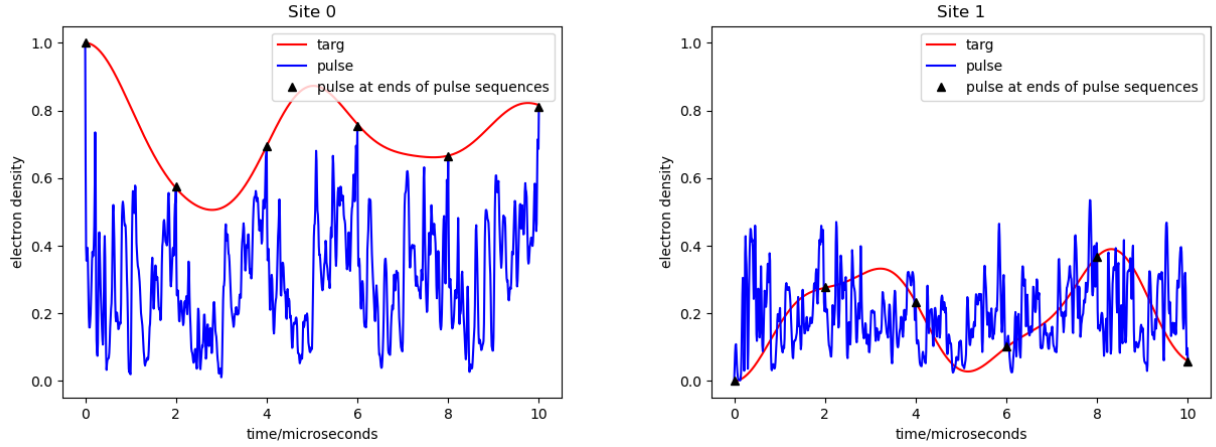
Figure 1: Dynamics showing symmetry breaking with the introduction of site Hamiltonian.

When the site Hamiltonian is introduced, the GRAPE-optimized pulse can drive the system to match the dynamics at the end of each pulse sequences. Similar to before, the electron densities resulting from Hamiltonian-driven and pulse-driven dynamics are shown in Figure 2.

2.1.2 GRAPE performance under different S/J

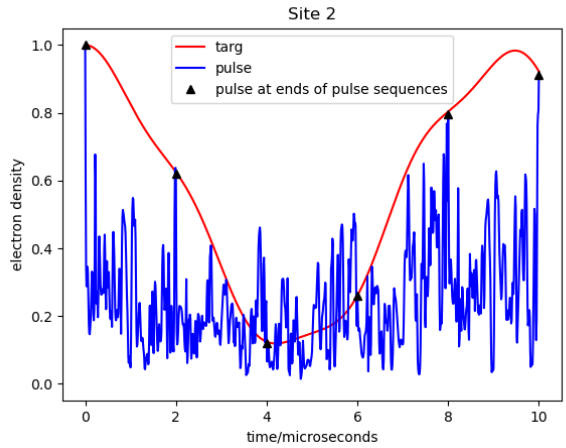
To examine the performance of GRAPE under a wide range of S/J, let S be generated randomly with a given scale. For example, if the scale is 5, then the 4 site Hamiltonian magnitudes are each generated randomly from a range of [0, 5] with uniform probability. To fairly simulate the effects of scaling, each result for a scaling is averaged over 5 different initial random seeding, i.e. average fidelity for 4 independently sampled magnitudes for $S_{1,2,3,4}$.

The graph of fidelity vs scaling/J is plotted in Figure 3. As expected, at small scaling, the performance tends to constant value, i.e. the value when there is no site Hamiltonian. At large scalings, the fidelity

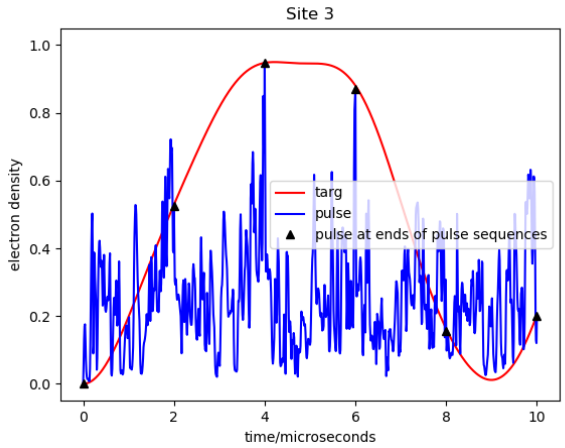


(a) Site 0

(b) Site 1



(c) Site 2



(d) Site 3

Figure 2: Site electron densities with site Hamiltonians. The pulse-driven dynamics are marked black at the end of each pulse sequence for clarity.

appears to be low. However, by examining the entries of the unitary, it can be shown that the unitary tends to identity at large scalings, which make it trivial to obtain a high fidelity for the pulse. The reason might be that when the site Hamiltonians are too large compared to the hopping Hamiltonians, the tunneling probabilities through the energy barriers are very low. Thus, the evolution unitary only approximates identity matrix for limited time scale. In intermediate scalings, the fidelity error fluctuates with no obvious pattern.

2.2 Including nearest-neighbor Hamiltonian

Similarly, when only including the nearest-neighbor and hopping Hamiltonian, the relation between the fidelity and K/J ratio is plotted in Figure 4.

The analysis is similar to the one in the previous section. The fidelity error tends to constant at low ratios, and tends to 0 at high ratios because the unitary tends to identity. The fidelity error fluctuates at intermediate ratios.

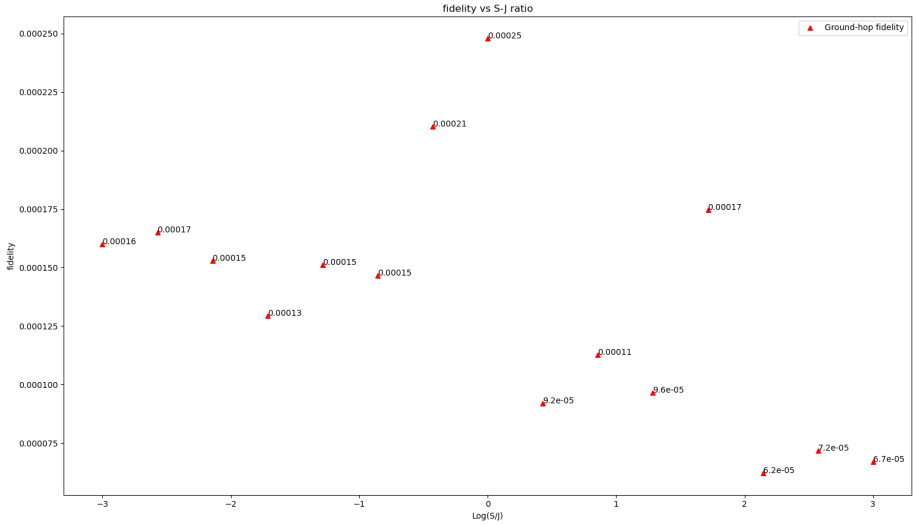


Figure 3: Semi-log plot of fidelity error vs $log\left(\frac{scaling}{J}\right)$.

3 Variational method in the context of GRAPE alogrithm

The variational method refers to methods that vary parameters of wave functions such that the expectation of Hamiltonian is minized. When the expected energy is close enough to ground state energy, the wave function well approximates the ground state wave function ignoring global phase.

In the context of GRAPE algorithm, the state parameters can be expressed to be $|\Psi\rangle = \hat{U}(\epsilon_n)|i\rangle$, where the unitary $\hat{U}(\epsilon_n)$ is driven by the pulse sequence for the controls and $|i\rangle$ is the initial state. Currently, there are 4 controls per time slice. Thus, the total number of parameters that determines $\hat{U}(\epsilon_n)$ is $4 \times n_{ts}$, where n_{ts} is the number of time slices. Normally the initial state is fixed, so the problem can then be expressed as

$$\min_{\epsilon_n} \langle\Psi|\hat{H}|\Psi\rangle$$

.

Therefore, within GRAPE algorithm, define

$$\text{fidelity} = \langle\Psi|\hat{H}|\Psi\rangle = \langle i|\hat{U}_1^\dagger \hat{U}_2^\dagger \cdots \hat{U}_{n_{ts}}^\dagger \hat{H} \hat{U}_{n_{ts}} \cdots \hat{U}_2 \hat{U}_1|i\rangle,$$

and the gradients

$$\frac{\partial \text{ fidelity}}{\partial \epsilon_i} = 2Re\left\{\langle i|\hat{U}_1^\dagger \hat{U}_2^\dagger \cdots \hat{U}_{n_{ts}}^\dagger \hat{H} \hat{U}_{n_{ts}} \cdots \frac{\partial \hat{U}_i}{\partial \epsilon_i} \cdots \hat{U}_1|i\rangle\right\},$$

where the gradients $\frac{\partial \hat{U}_i}{\partial \epsilon_i}$ have the same expressions as outlined in one of my previous reports.

4 Variational method results

Without specifications, the initial state $|i\rangle$ is set to be the ground state in the cavity $|0\rangle$.

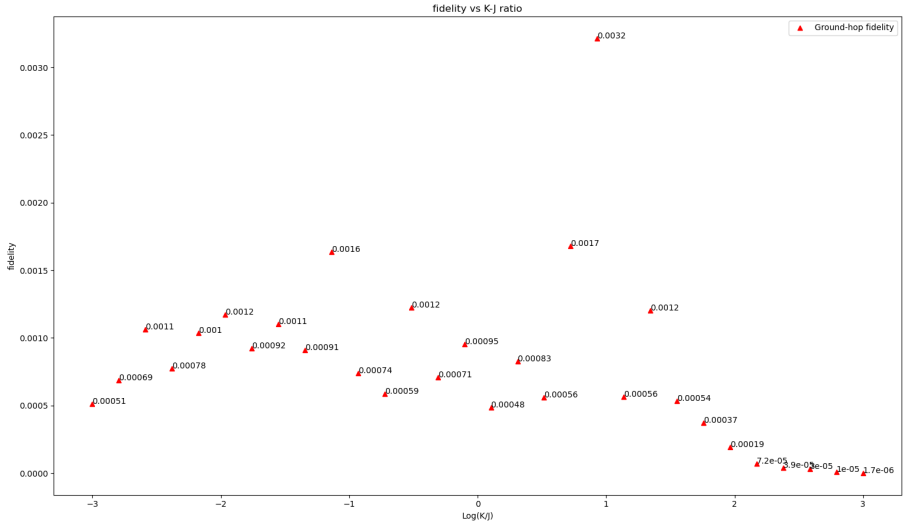


Figure 4: Semi-log plot of fidelity error vs $log\left(\frac{K}{J}\right)$.

4.1 Only hopping Hamiltonian

As analyzed before, the hopping Hamiltonian has degenerate eigenvalues at -2J, 0, and 2J. Therefore, the expected ground state energy should be around $E_0 = -2J \approx -0.691150$.

Figure 5 includes the plot of energy vs iterations and Figure 6 includes relative ennergy error vs iteration. Here the relative energy error is defined to be $\frac{E-E_0}{E_0}$.

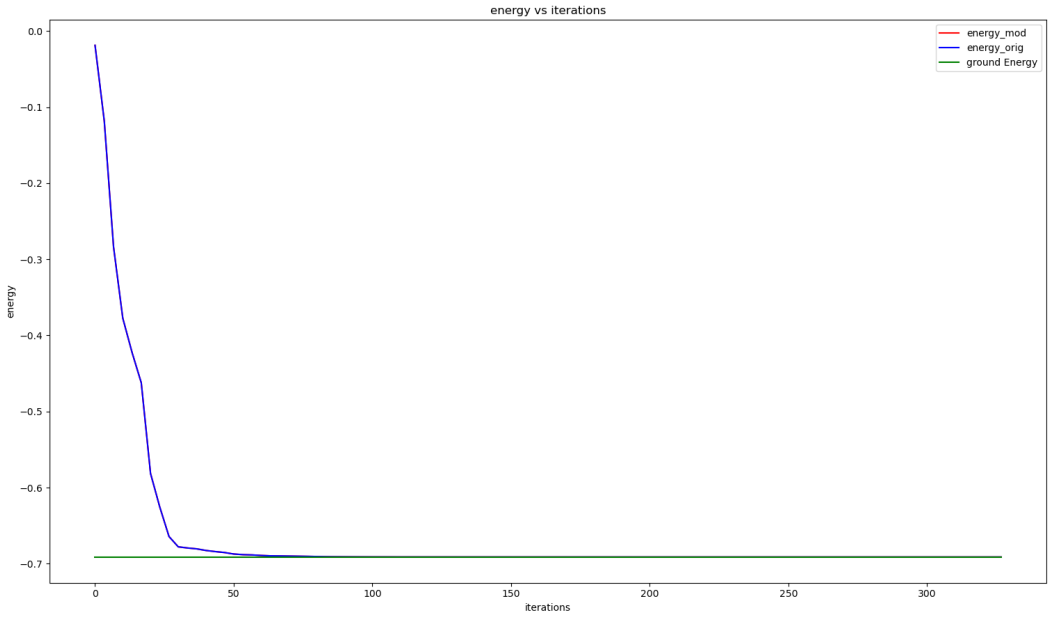


Figure 5: Energy vs number of iterations

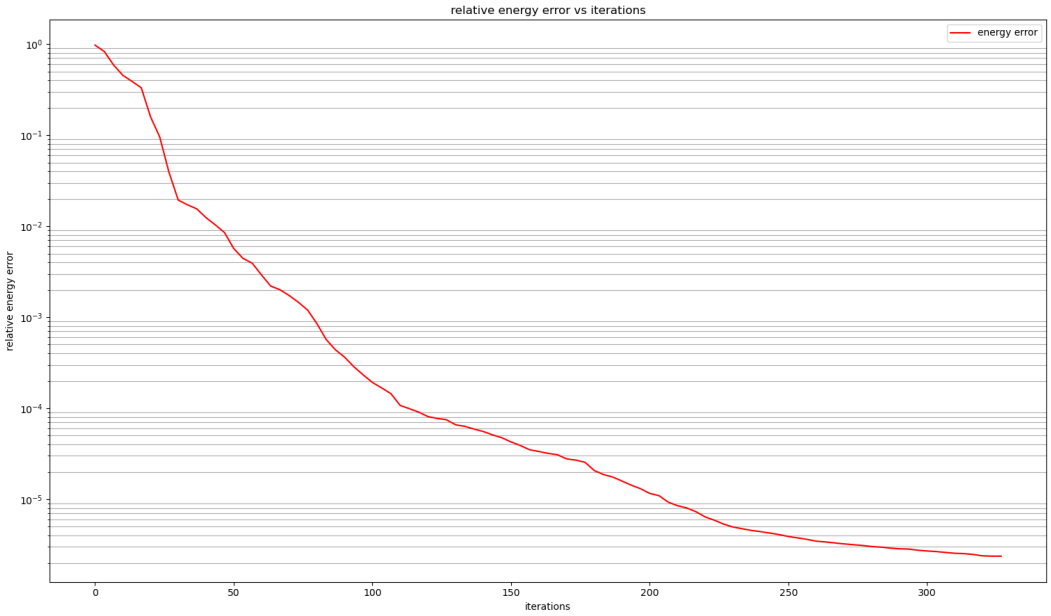


Figure 6: Semi-log plot of relative energy error vs number of iterations.

The above plots are plotted when the pulse sequence is of length 2μs and there are 100 time slices, i.e. 400 parameters to vary. Figure 7 shows the relative energy error at convergence for different number of time slices, and Figure 8 shows the number of iterations at which GRAPE converges for each number of time slices. It can be concluded that the variational method has an increase in performace after having more than around 30 time slices. However, no further obvious increase in performance is observed later.

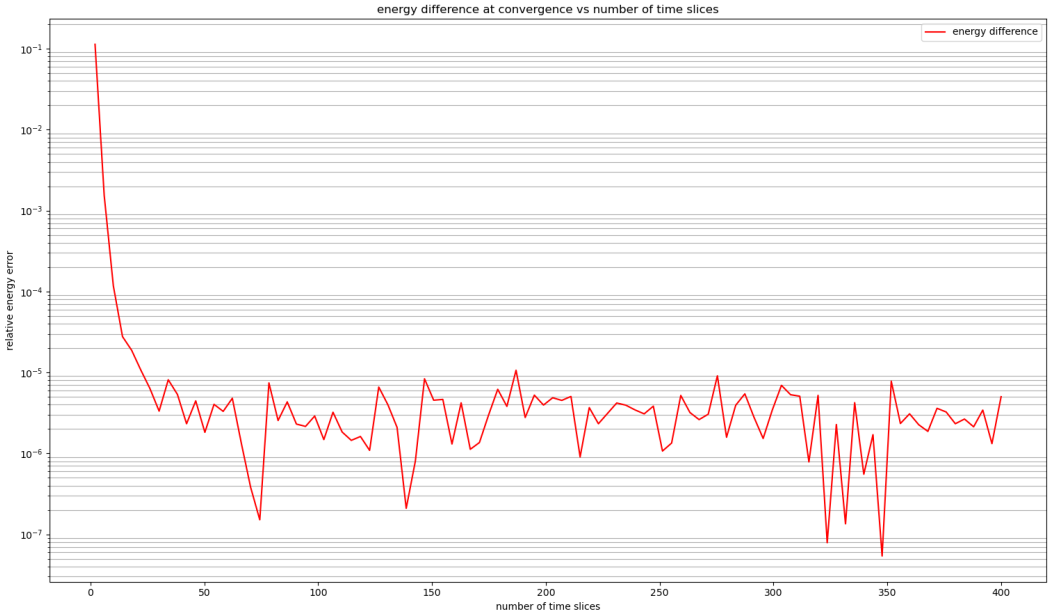


Figure 7: Semi-log plot of relative energy error vs number of time slices at convergence.

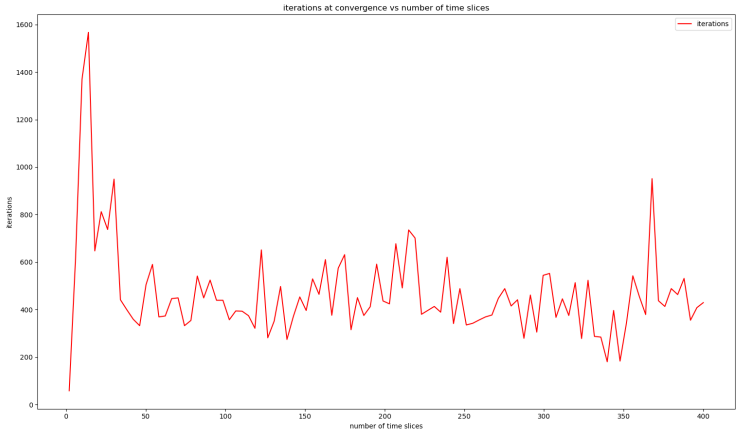


Figure 8: Iterations vs number of time slices at convergence

4.2 Including all Hamiltonians

Just to demonstrate the capability, the site Hamiltonian and nearest-neighbor Hamiltonian are both included in this section. As an example, set $K = 0.5$ and S randomly sampled from a scaling of 1.

The sampled S are [-0.5488, -0.7152, -0.6028, -0.5449]. These are all around same magnitude as J. The ground state energy of the resulting Hamiltonian should be around $E_0 = -1.85115$. Similar plots are shown in Figure 9 and Figure 10.

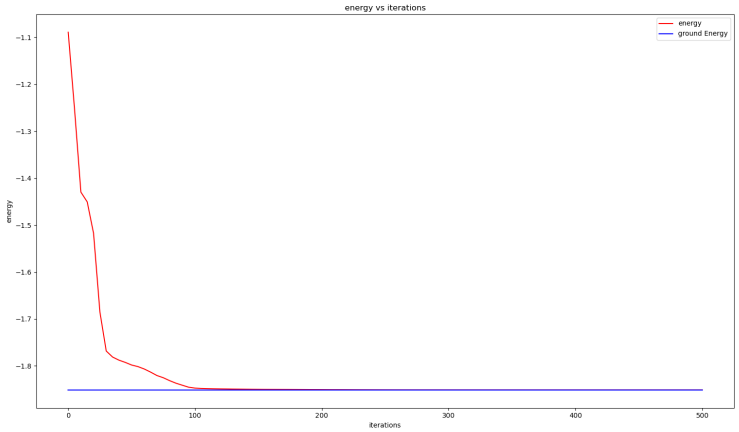


Figure 9: Energy vs number of iterations

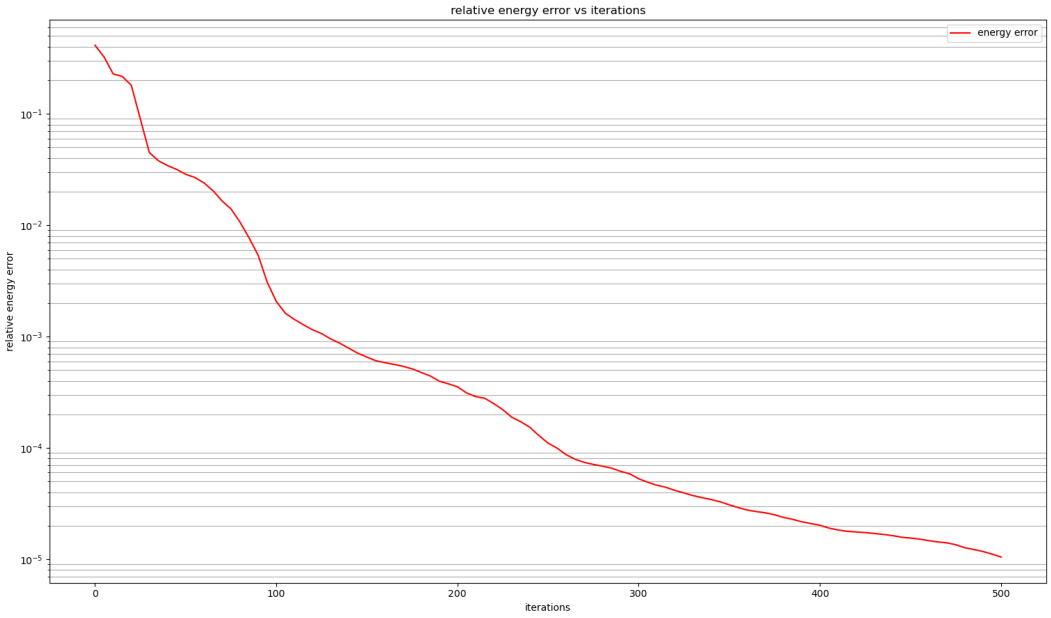


Figure 10: Semi-log plot of relative energy error vs number of iterations.

4.3 Adding possible penalties

One thought that I had was to add penalty Hamiltonians to the other undesired eigenstates. For example, when only hopping Hamiltonian is present, the ground state is degenerate with 2 eigenstates having -2J, and 2 degenerate states with 2J. The other $40 - 4 = 36$ eigenstates are degenerate with eigenenergy 0. However, 0 is not that big compared to $E_0 = -2J \approx -0.691150$. Therefore, one

solution can be adding penalty Hamiltonians to the other eigenstates so the 'gradient' from the other eigenstates to the ground states can be larger.

However, I tried but the results don't seem to improve significantly, so I haven't included the results here.