Work Summary

Further result for fock state transfer and some obvservations from literature review. Also, I have taken a more detailed look at the possibility of changing the definitions of fidelity in QuTip.

Main Work

1. State transfer to different fock states
2. QuTip implementation of GRAPE
3. Optimal expression of tight-binding model Hamiltonian
4. Target operator in tight binding model

1 State transfer to different fock states

As communicated last time in my email, when the initial state for cavity is vacuum, a few observation for the fidelity error is observed as below:

1. The fidelity error is in general lower when the target state is closer to the initial state.

2. When the initial guessed pulse has a larger amplitude, the fidelity error of target states that are further can improve.

3. Some initial pulse guess might lead to local minimum when they are too close to some special 'points,' for example identity operator.

There are many different terminating conditions. If the algorithm reports that function converged, then either the optimum is found or local minimum is reached. In other situations, the algorithm can report, for example, wall time exceeded. Then in that case increasing the wall time improves the performance. Normally for the problem of fock state transfer, when the initial pulse is reasonably set (sometimes need larger amplitude for the pulses), then the wall time is the limiting condition. Therefore, Figure 1 shows the relation between wall time, the target fock state, and fidelity error.

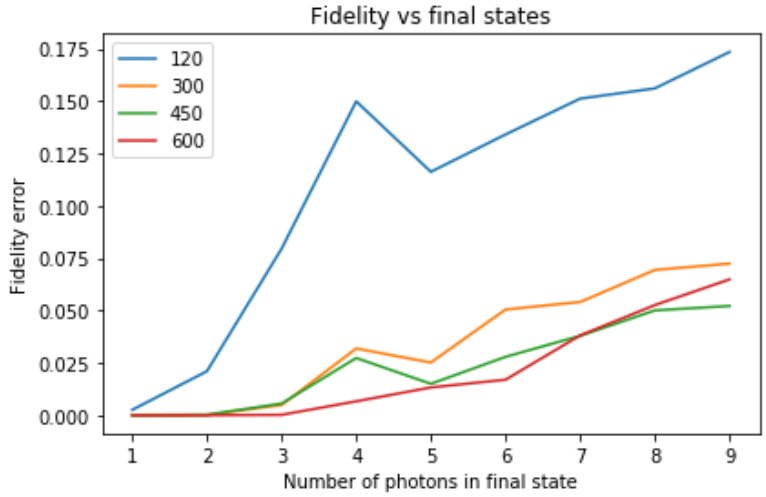


Figure 1: Fidelity error vs target fock states when different wall times are set. The labels are the wall time in seconds.

2 QuTip implementation of GRAPE

I have taken a much closer look at how QuTip implements GRAPE, and I have already set up a local version of QuTip which I can easily modify and test. Some details of the QuTip implementations are discussed below.

Here discuss the case when the target is an unitary operator, but it can be easily generalized to include target state. Assume the target operator is $\hat{U}_{targ}$. The control amplitudes remain constant in each time slot. Assume total n time slots and m controls, let the propagator, including both the drift and control Hamiltonians, be $\hat{A}_i$, where i range from 1 to n. The initial operator is $\hat{U}_i$, which is usually set to the identity operator. The resulting operator from the Hamiltonian is $\hat{U}_f = \hat{A}_n \cdots \hat{A}_2 \hat{A}_1 \hat{U}_i$. The default fidelity for unitary evolution is the Hilbert-Schmidt inner product $fid = Tr\left\{\hat{U}_{targ}^{-1}\hat{U}_f\right\}$. A normalization constant of N, the Hilbert space dimension, can be applied such that the maximum fidelity is 1.

QuTip calculates $\hat{A}_i$ through decomposition. Let the total Hamiltonian for time slot i be $\hat{H}_{tot}(t_i) = \hat{H}_{drift}(t_i) + \epsilon_i \hat{H}_{ctrl}$, where ϵ_i is the control pulse amplitude subject to optimization. Here only assumes one control. Let the eigen decomposition be $\hat{H}_{tot}(t_i) = \hat{V}\hat{D}\hat{V}^\dagger$, where $\hat{V}$ consists of the eigen vectors and $\hat{D}$ is the diagonal matrix consisting of the eigen values in the diagonal. Then, the propagator $\hat{A}_i = e^{-i\delta t \hat{H}_{tot}(t_i)} = \hat{V}e^{-i\delta t D}\hat{V}^\dagger$.

However, I am confused by how the propagator gradient is calculated, i.e. the calculation of $\frac{\partial \hat{A}_i}{\partial \epsilon_i}$. According to how it's implemented in QuTip, it seems to imply Equation 1. Here, λ_i is the eigenvalues of the total Hamiltonian $\hat{H}_{tot}(t_i)$.

$$\begin{aligned} \frac{\partial \hat{A}_i}{\partial \epsilon_i} &= \hat{V}\hat{B}\hat{V}^\dagger, \\ \text{where } B_{i,j} &= W_{i,j} * Q_{i,j}, \\ \hat{W} &= \hat{V}^\dagger \hat{H}_{ctrl} \hat{V}, \\ Q_{i,j} &= \frac{e^{-i\delta t\lambda_i} - e^{-i\delta t\lambda_j}}{(-i\delta t\lambda_i) - (-i\delta t\lambda_j)} \end{aligned} \tag{1}$$

After figuring out the source of these equations, it is worth finding the expression of the new 'weighted' fidelity definition, where it only counts parts of the operator that are relevant. Also, expressions for the propagator gradients need to be modified as well since they are based on the Hilbert-Schmidt inner product expression.

3 Optimal expression of tight-binding model Hamiltonian

Following the conventions set before for 2 electrons hopping between 4 sites, the total number of energy levels in harmonic oscillators is 6. Previously, I guessed the Hamiltonian basis mapping to be between the electron states $\begin{pmatrix} |21\rangle \\ |41\rangle \\ |31\rangle \\ |42\rangle \\ |32\rangle \\ |43\rangle \end{pmatrix}$ to the harmonic oscillator fock states $\begin{pmatrix} |0\rangle \\ |1\rangle \\ |2\rangle \\ |3\rangle \\ |4\rangle \\ |5\rangle \end{pmatrix}$. Then, the Hamiltonian can be written as Equation 2.

$$\hat{H} = -J_1 \begin{pmatrix} 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & -1 \\ -1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \end{pmatrix} \tag{2}$$

Since it is hard to cross large 'distances' in the harmonic oscillator fock states, it is desirable to minimize the distance between possible hopping. Any permutation of the basis is possible, and the corresponding Hamiltonian changes. Adopt the metric such that the score of a Hamiltonian is defined as

$$score = \sum_{i,j} |H_{i,j}| \times e^{|i-j|}$$

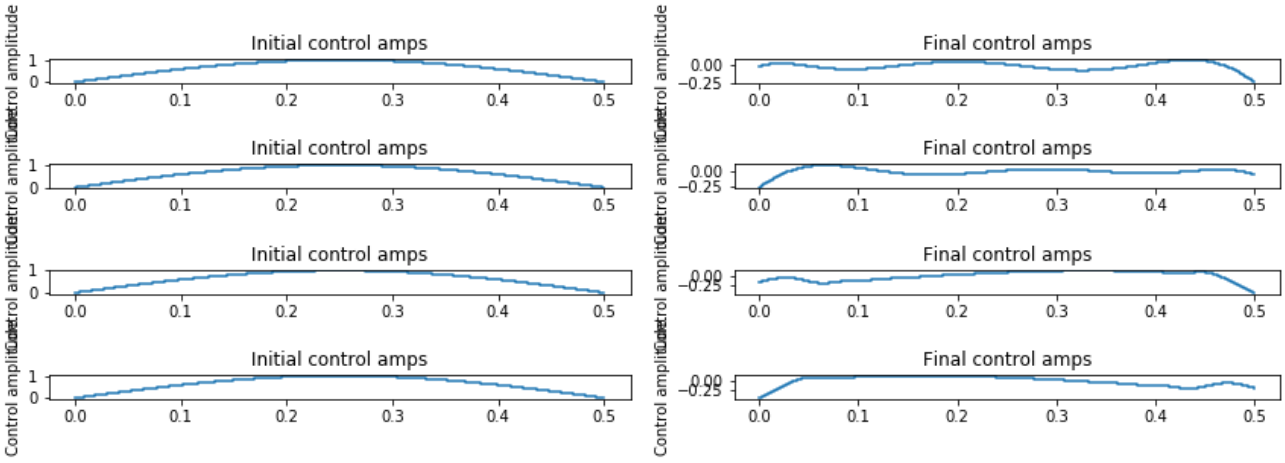
. When the score is minimized, the hopping Hamiltonian's non-zero entries are closest to the diagonal. After numerating through all possible permutations, it is observed that the score is the smallest when the Hamiltonian is in the form of 2. The possible permutations are the permutations between the -1 and 1 entries in the hopping Hamiltonian.

4 Target operator in tight binding model

As discussed last time, it seems desirable to have zero control pulse the analytical solution when the hopping Hamiltonian is set to 0. In this case, only the interaction Hamiltonian remains in the rotating frame. Let the projection operators be $\hat{P}_g = |g\rangle\langle g|$ and vice versa for the excited state. Then, the interaction Hamiltonian is $\hat{H}_{int} = \chi \hat{a}^\dagger \hat{a} \hat{P}_e$ and $\chi = 2\pi \times 2.2$MHz. Since the hopping Hamiltonian should only affect the harmonic oscillator when the qubit is in ground state, the hopping Hamiltonian can be written as $\hat{H}_{hop} = \hat{H}' \hat{P}_g$, where $\hat{H}'$ is defined by Equation 2. Thus, the target operator is shown in Equation 3.

$$
\begin{aligned}
\hat{U}_{targ} &= e^{-i\left(\hat{H}_{int}+\hat{H}_{hop}\right)t} \\
&= \sum_{n=0}^{\infty} \frac{\left(-i\left(\hat{H}_{int}+\hat{H}_{hop}\right)t\right)^n}{n!} \\
&= \hat{P}_g \sum_{n=0}^{\infty} \frac{\left(-i\hat{H}'t\right)^n}{n!} + \hat{P}_e \sum_{n=0}^{\infty} \frac{\left(-i\chi\hat{a}^\dagger\hat{a}t\right)^n}{n!} \\
&= \hat{P}_g e^{-i\hat{H}'t} + \hat{P}_e e^{-i\chi\hat{a}^\dagger\hat{a}t}
\end{aligned} \tag{3}
$$

As an example, set the evolution time to be 500ns as usual and the hopping magnitude to be J = 0.1MHz. Set the initial guessed pulse to be SINE function. The optimized pulse then gives a fidelity error of 0.000967, i.e. a fidelity of 99.90%. The initial and final pulse shapes are shown in Figure 2.



(a) Initial pulse shapes

(b) Final optimized pulse shapes

Figure 2: Initial and final pulse shapes for tight-binding Hamiltonian simulation.

However, a rough estimate for the phase change in this example is only on the order of $0.5 \times 0.1 \approx 0.02\pi$. When the amplitude of J is increased to 1.0, the fidelity error increases to 0.0457, giving a fidelity of 95.4%.