Quantum Optimal Control of Atom Transport using Quantum Composer

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1.1 State Transfer and Quantum Optimal Control

Suppose we have a fixed initial state $\psi(0) = \psi_0 = \psi_{initial}$ and we want to evolve it into a fixed target state ψ_{target} in the fixed duration T. That is, we want to solve a *state transfer problem*

$$\psi_0 = \psi_{initial} \to \psi(T) = \psi_{\text{target}} \tag{1.1}$$

The states ψ_0 and $\psi(T)$ are connected by the Schrödinger equation

$$i\frac{\partial\psi(t)}{\partial t} = \hat{H}\psi(t), \quad \psi(0) = \psi_0 \tag{1.2}$$

where we have chosen units such that $\hbar = m = 1$. Often it is more convenient to express time evolution in terms of the time evolution operator $\hat{\mathcal{U}} = e^{-i\hat{H}\delta t}$ where δt is a suitable time interval. We can then propagate our state forward in time in by δt according to

$$\psi(t + \delta t) = \hat{\mathcal{U}}\psi(t) = e^{-i\hat{H}\delta t}\psi(t) \tag{1.3}$$

The two equations above are completely equivalent[1]. In both of these equations we see that the Hamiltonian $\hat{H}$ plays an important role in the time evolution of the state. In fact $\hat{H}$ is known as the *generator of time evolution* – it is very explicitly seen that $\hat{H}(t)$ decides what the state at $t + \delta t$ will be. Let us chop the time axis from $t = 0$ to $t = T$ into M smaller sub-intervals of length δt:

$$t_j \in [0 : \delta t : T], \quad j = 0, 1, 2, \ldots, M - 1 \tag{1.4}$$

By successively applying the time evolution operators $= \hat{\mathcal{U}}_j$ we can thus propagate the state from $t = 0$ to $t = T$ as

$$\psi(T) = \hat{\mathcal{U}}_{M-1} \ldots \hat{\mathcal{U}}_1\hat{\mathcal{U}}_0\psi(0) = \prod_j^{M-1} \hat{\mathcal{U}}_j\psi(0) = \prod_j^{M-1} e^{-i\hat{H}_j\delta t}\psi(0) \tag{1.5}$$

Suppose now that we could somehow *control* the Hamiltonian. In particular, suppose we had a *control function* $u(t)$ parametrizing the Hamiltonian such that $\hat{H} = \hat{H}(u(t))$. Let us write again the time evolution with explicit reference to the control function $u(t)$

$$\psi(T) = \prod_j^{M-1} \hat{\mathcal{U}}_j\psi(0) = \prod_j^{M-1} e^{-i\hat{H}(u(t_j))\delta t}\psi(0) \tag{1.6}$$

We can now explicitly see that to correctly steer the transfer defined by 1.1 we need to find a 'suitable' control function $u^*(t)$. But how exactly can we do that?

[1]Strictly speaking this is only exactly true if $\hat{H} \neq \hat{H}(t)$, but will still be approximately true in practice if we choose δt small enough

Solving this type of state transfer problem can be done within the framework of Quantum Optimal Control (QOC). To do this we recast the problem as an optimization task by maximizing the *fidelity*

$$\mathcal{F}[u(t)] \equiv \mathcal{F}(T) = |\langle \psi_{\text{target}} | \psi(T) \rangle|^2 \in [0;1] \tag{1.7}$$

$\mathcal{F}$ is a direct measure of the quality of the control $u(t)$ and maximizing it is equivalent to solving the original problem 1.1. If we can find $u^*(t)$ such that $\mathcal{F} \approx 1$, we call $u^*(t)$ an *optimal control*. The basic approach is then to start off with a guess $u^{(0)}(t)$ and then iteratively find a sequence of increasingly better control functions:

$$u^{(0)}(t) \to u^{(1)}(t) \to u^{(2)}(t) \to \cdots \to u^{(i)}(t) \tag{1.8}$$

$$\mathcal{F}[u^{(0)}(T)] \leq \mathcal{F}[u^{(1)}(T)] \leq \mathcal{F}[u^{(2)}(T)] \leq \cdots \leq \mathcal{F}[u^{(i)}(T)] \approx 1 \tag{1.9}$$

$$\Rightarrow u^{(i)}(t) = u^*(t) \tag{1.10}$$

Several standard algorithms for performing this type of iterative improvement exists, such as GRAPE, GROUP, and CRAB. The details of these algorithms will not be elaborated here.

The State Transfer Optimal Control Problem

starting from $u^0(t)$, iteratively find $u^{(i)}(t) = u^*(t)$ realizing

$$\psi(0) \xrightarrow{H(u^*(t))} \psi(T) \tag{1.11}$$

such that $\mathcal{F}[u^*(t)] = |\langle \psi_{\text{target}} | \psi(T) \rangle|^2 \approx 1$ is maximized

1.2 Transport problems

The previous section was generic in the sense that we did not decide on a particular quantum system. In the rest of this note we will consider a single particle in 1-D such that

$$\psi = \psi(x,t), \qquad \hat{H}(u(t)) = T + V(x, u(t)) \tag{1.12}$$

Let us consider the situation where V is a trapping potential on the form $V = V(x - u(t))$. In this case the control function $u(t)$ has dimensions of length and can usually be identified directly as a physical parameter of the system, for example the center position of a laser beam. Changing $u(t)$ then corresponds to moving the trapping potential in time. Suppose we let $u(0) = u_A$ and $u(T) = u_B$ with $u_A \neq u_B$, let the initial state ψ_0 be the ground state of $H(u(0))$, and let the target state ψ_{target} be the ground state of $H(u(T))$. Then we have defined a *Transport* problem, where we are trying to move an atom from position A to position B by manipulating the potential $V(x - u(t))$ through the control function $u(t)$. This type of Transport problem is an important ingredient in e.g. building a quantum computer based on arrays of trapped atoms.

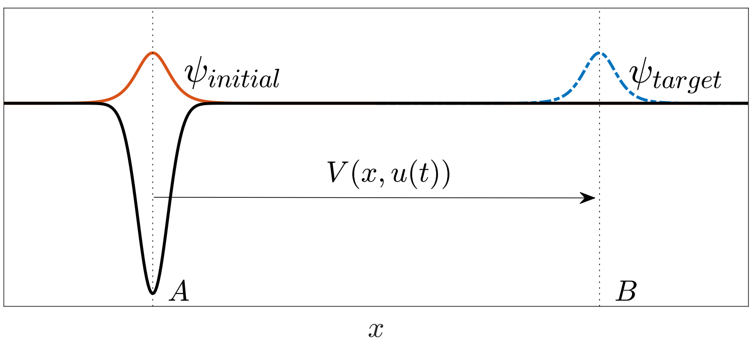
The Transport Problem

$$V(x, u(t)) = V(x - u(t)) \tag{1.13}$$

$$u(t): \text{ trap center position starting in } A \text{ and ending in } B \tag{1.14}$$

$$\psi_{initial}: \text{ ground state of corresponding to potential centered on } A \tag{1.15}$$

$$\psi_{\text{target}}: \text{ ground state of corresponding to potential centered on } B \tag{1.16}$$



1.3 Numerical exercises – Quantum Composer

In this section we explore how to use Quantum Composer to investigate, analyze, and solve the Transport problem above. Basic familiarity with Quantum Composer is assumed. Distributed with this note are complementary .flow files for the question below. The files cover two transport potentials $V(x - u(t))$:

$$\text{Harmonic oscillator :} \qquad V = \frac{1}{2}\omega^2 (x - u(t))^2 \tag{1.17}$$

$$\text{Gaussian tweezer :} \qquad V = -A \cdot \exp\left(-2\frac{(x - u(t))^2}{\sigma^2}\right) \tag{1.18}$$

Feel free to try your own trapping potentials!

Question 1 : Transport with a linear control function $u(t)$

files: Gaussian Transport - Linear Control.flow
Harmonic Transport - Linear Control.flow

The questions will refer to the *Gaussian Transport - Linear Control.flow* scene. The questions are the same for the *Harmonic* case, but with other parameter names.

(a) **Answer this question before opening the scene.**
The simplest thing that comes to mind when guessing for a control function is a linear one on the form

$$u(t) = a \cdot t + b \tag{1.19}$$

(1) Assuming $u_A = -x_c$ and $u_B = +x_c$, determine a and b such that $u(0) = u_A$ and $u(T) = u_B$.

(2) Insert a and b into the linear form such that u is given in terms of the process duration T and the seperation $2x_c$.

(3) **You can now open the scene**
Expand the collapsed 'Linear Control' block inside the 'Time evolution over linear control' block. Verify the expression you found in (1-2) us correct.

(b) Press the Play button to perform the time evolution of the state over the linear control function. The instantaneous state and the target state is plotted as well as the fidelity $\mathcal{F}$ as a function of time. Remember that the duration T is fixed!

(1) Keeping everything else the same, what do you think would happen with the final fidelity $\mathcal{F}(T)$ if you increase/decrease the center offset x_c? Formulate your answer in a short sentence or two, and then try adjusting the x_c value in the program. Describe in words the observed motion of the state for small/large values of seperation. You are welcome to adjust the parameters of the 'Spatial Dimension' node for this task if you feel it is necessary.

(2) Keeping everything else the same, what do you think would happen with the final fidelity $\mathcal{F}(T)$ if you increase/decrease the amplitude A? Formulate your answer in a short sentence or two, and then try adjusting the A value in the program. Describe in words the observed motion of the state for small/large values of A. You are welcome to adjust the parameters of the 'Spatial Dimension' node for this task if you feel it is necessary.

(3) Keeping everything else the same, what do you think would happen with the final fidelity $\mathcal{F}(T)$ if you increase/decrease the duration T? Formulate your answer in a short sentence or two, and then try adjusting the T value in the program. Describe in words the observed motion of the state for small/large values of T. You are welcome to adjust the time steps dt if you feel it is necessary.

(c) For any combination of the parameters[a] A, x_c, T, can you produce a perfect final fidelity $\mathcal{F}(T) = 1$? How hard/easy is it? Describe why.

[a] $x_c = 0$ does not count. . . :)

Question 2 : Transport with a linear control function $u(t)$ looping over T

files: Gaussian Transport - Linear Control for T.flow
Harmonic Transport - Linear Control for T.flow

The questions will refer to the *Gaussian Transport - Linear Control for T.flow* scene. The questions are the same for the *Harmonic* case, but with other parameter names.

(a) Now that you have played around with the linear control for a bit let us try doing a more systematic investigation.
Open the scene.
In this scene we have the exact same setup as before, except now we have added another loop over the duration T around the time evolution loop over t. This outer loop starts from a duration $T = T_{\text{min}}$ and progresses in steps of dT up to $T = T_{\text{max}}$. After each iteration of T the final fidelity $\mathcal{F}(T)$ and T is recorded in a 'Scalar Time Trace Plot', producing an $\mathcal{F}(T)$ curve. Be sure to position the screen such that you can see all the plots.

(1) Run the scene by pressing the Play button, and observe the motion of the state. After a while a trend can be seen on the $\mathcal{F}(T)$ curve (producing the entire curve will take a while). Explain what causes the pattern in the curve.

(2) Identify the shortest duration T^{linear} at which $\mathcal{F}(T) \approx 1$. This will be the to-beat duration in the next question.

(3) By having observed the time evolution for increasing values of T, what would you expect as $T \to \infty$?

Question 3 : Optimizing the Transport

files: Gaussian Transport - Grape optimization.flow
Harmonic Transport - Grape optimization.flow

The questions will refer to the *Gaussian Transport - Grape optimization.flow* scene. The questions are the same for the *Harmonic* case, but with other parameter names.

(a) By now you will have realized it is not particularly hard to obtain $\mathcal{F}(T) \approx 1$, even without doing any optimization. Just let $T \to \infty$! This is what is known as *adiabatic* transport. However, while this is practical for some purposes, it is in general not a good strategy – after all $T \to \infty$ is a fairly long time. If you are interested in building a quantum computer, you will be more interested in finding solutions that are as fast as possible. This is because a) the faster you can move your atoms around the faster your computer is b) quantum systems are extremely fragile and *decoheres* (loses its 'quantum-ness') on a characteristic time scale $\tau_{\text{decoherence}}$ through coupling to the external environment. These are a few reasons we are interested in producing $\mathcal{F}(T) \approx 1$ in the shortest duration T possible. The absolutely shortest duration at which the perfect transfer is possible is termed the Quantum Speed Limit and is denoted T_{QSL}. Finding T_{QSL} is extremely hard for pratically all problems. In this question, we are not concerned with finding the exact T_{QSL}, but you will try to get an estimate for it. We will also see how easy/hard it is to find better results than the linear control guess we had in the earlier questions.
Open the scene.
In this scene you will see two large blocks. The 'Playback time evolution over control' is almost exactly the same as the block from the previous questions, except that now the block is now a loop over a control (see boundary nodes). The control is now represented outside the block as a 'Control' node. Inside this node is the explicit values of the control function for each t, which can be manipulated by clicking and dragging the individual points. This means we can try all kinds of different control functions very easily.

(1) Untick the mark in the upper-left corner of the 'Optimization' block. The nodes inside will grey-out indicating they are disabled.

(2) Run the scene by pressing the Play button, and observe the 'Playback time evolution over control'. It should look just like before. Try adjusting the control away from a linear one by clicking and dragging the points in the 'Control' node. Can you find a good solution that is sufficiently non-linear? If you are unhappy with a point you fixed by dragging you can right click it to reset it.

(b) Now we are ready to perform actual state-of-the-art Quantum Optimal Control. The 'Optimization' block has a special 'Grape Optimization' boundary node that accepts a number of input parameters. The 'Problem' input encapsulates the potential $V(x, u(t))$, and the states ψ_0 and ψ_{target}. The second input is the 'Control' which acts as our initial guess $u^{(0)}(t)$ in the sequence 1.8. 'N' is the maximum number of iterations to be performed, i.e. the optimization terminates if $i = N$ in 1.8. 'TargetFidelity' is the fidelity threshold and the optimization will stop if $\mathcal{F}[u^{(i)}(T)]$ exceeds this value. Whatever the cause of the optimization termination, the control at iteration $u^{(i)}(t)$ is output through the right side boundary node. The rest of the parameters/options are not important for now.
Inside the node three plots are shown:

- The upper plot shows the intial control $u^{(0)}(t)$ and the current control $u^{(i)}(t)$.
- The middle plot shows $|\psi(x,t)|^2$ i.e. the probability density of the state as a function of x (second axis) *and* t (first axis, note the time is normalized to the duration T). You can think of this plot as 'looking down' on the state from above at it evolves in time.
- The bottom plot shows the final fidelity as a function of iteration, i.e. $\mathcal{F}[u^{(i)}(t)]$. This allows you to track the progress of the optimizer.

These three plots give you an indication of how the optimizer is 'steering' the contol (top), and how it affects the time evolution of the system (middle and bottom).

Question 4 : Optimizing the Transport (continued)

(b) (1) Tick the mark in the upper-left corner of the ’Optimization’ block. The nodes inside will re-activate.

(2) Connect the output ’Control’ of the ’Optimization’ block to the ’Control’ input of the ’Playback time evolution over control’ block. Now the optimized solution will be ’played back’ once the optmization has finished.

(3) Run the scene by pressing the Play button, and observe the plots in the ’Optimization’ block. You should now see great improvements to your initial guess, and the state being ’nudged’ into place!

(4) Try out different intial control functions by adjusting the ’Control’ node. Can you find some overall good strategies? Can you characterize them in a few words?

(5) Try to find optimal controls at a duration shorter than T^{linear} (the one you found in the previous question). How easy/hard is it?

(6) Given any linear guess with $T > T^{\text{linear}}$, argue why it should be probably easy to find optimal controls from that initial guess.

(7) Now the *real* challenge[a]: find the smallest time T at which $\mathcal{F}(T) \approx 1$ (a suitable threshold is 0.99-0.999). Do this by decreasing the duration slightly, finding a suitable control guess that will optimize to above fidelity threshold, and then repeat until you cannot cross the fidelity threshold. This will be $T_{\text{QSL}}^{\text{<your name>}}$ – your personal estimate for the Quantum Speed Limit!

[a]Obviously you should make a bet with your friend at this point – a piece of cake is often a suitable currency. Surely you are more clever physicist!