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Optimal Control of Landau-Zener Model

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Contents

1 Quantum Optimal Control Theory

The fundamental problem of Quantum Optimal Control Theory is to transfer the population from an initial state $|\psi_0\rangle$ to $|\psi_{\text{target}}\rangle$ by adjusting a set of control parameters within the Hamiltonian used to evolve the system. Consider the Hamiltonian

$$\hat{H}(\boldsymbol{u}(t)) = \hat{H}_0 + \sum_{i=1}^{m} f_i(u_i(t))\hat{H} \ , \tag{1}$$

where $\hat{H}_0$ is an uncontrollable drift of the Hamiltonian, $\boldsymbol{u}(t)$ is the control, and $f(\boldsymbol{u}(t))$ is some function. Thus, a control must be found such that

$$F = |\langle\psi_{\text{target}}|\psi(T)\rangle|^2 = 1 \ , \tag{2}$$

where F is the fidelity, and $\psi(T)$ is the solution at $t = T$ to the Schrödinger equation

$$i\frac{\partial\psi}{\partial t} = \hat{H}\left(\boldsymbol{u}(t), \psi(t)\right)\psi(t) \ . \tag{3}$$

Solutions to this problem are called optimal controls.[JJ del A]

1.1 Quantum Speed Limit

A subtlety of the above problem is that one is only searching for the control, $\boldsymbol{u}(t)$, which steers the initial state into the target-state at time $t = T$. It is often desirable to obtain the desired state in the shortest timespan possible, however, if a solution exists at $t = T_1 > T_2$, it might not exist at $t = T_2$. The shortest duration for which a solution can be found is called the *quantum speed limit* (QSL). This is due to the fact that quantum mechanics dictates that there is a limit of how many orthogonal states a system can pass through per unit time. A large energy difference to orthogonal states allows for fast oscillations within the system, however, as these differences cannot be arbitrarily large, a lower bound of how fast a system can evolve exists, which in turn leads to the QSL.
There are several ways of approximating the quantum speed limit, however, there is no known way to reliably estimate the QSL for a general state. Thus, the best option is often to just solve the problem at increasingly shorter durations until a solution no longer can be found [JJ]. If the initial state,$|\psi_0\rangle$, and the target-state, $|\psi_{\text{target}}\rangle$, are orthogonal, one can estimate the QSL from the orthogonalization time, which is how long it takes for a state to become orthogonal to itself. Consider $|\psi(0)\rangle = \sum_n^\infty c_n |\phi_n\rangle$, where $\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle$. Following [L. B. Levitin and T. Toffoli, "Fundamental limit on the rate of quantum dynamics: the unified bound is tight," Physical Review Letters, vol. 103, no. 16, p. 160502, 2009.] the norm squared of the survival probability is given as

$$\begin{aligned} |S(t)|^2 = |\langle\psi(0)|\psi(t)\rangle|^2 &= \sum_{n,m=0}^{\infty} |c_n|^2|c_m|^2\cos\left((E_n - E_m)t\right) \\ &\geq 1 + \frac{4t}{\pi^2}\frac{\mathrm{d}|S(t)|^2}{\mathrm{d}t} - \frac{4t^2}{\pi}\Delta E^2 \ , \end{aligned} \tag{4}$$

where the trigonometric inequality $\cos x \geq 1 - \left(4x\sin x - 2x^2\right)/\pi^2$ was used, and ΔE is the energy spread of the state. Since $|S(t)|^2 \geq 0$, then $\frac{\mathrm{d}|S(t)|^2}{\mathrm{d}t} = 0$ whenever $|S(t)| = 0$, which is the case at the orthogonalization time $t = \tau$. This leaves the inequality $0 \geq 1 - 4\tau^2\Delta E^2/\pi^2$, which yields the Mandelstram Tamm bound when solved

$$\tau_{\text{MT}} \geq \frac{\pi}{2\Delta E} \ . \tag{5}$$

This sets a lower bound of the orthogonalization time, however, the bound was derived using a constant Hamiltonian. In the case of optimal control the Hamiltonian is time dependent, which can be taken into account by using arguments from differential geometry [J. Anandan and Y. Aharonov, "Geometry of quantum evolution," Physical Review Letters, vol. 65, no. 14, p. 1697, 1990. [14] M. Gajdacz, K. K. Das, J. Arlt, J. F. Sherson, and T. Opatrny, "Time-limited optimal dynamics beyond the ' quantum speed limit," Physical Review A, vol. 92, no. 6, p. 062106, 2015.]

$$\tau_{\mathrm{MT}} \geq \frac{\pi}{2}\left(\int_0^T \Delta E \;\mathrm{d}t\right)^{-1} , \tag{6}$$

From this expression it is clear, that fast solutions require a large value of ΔE, as described earlier. Since 6 is dependent on the control $\boldsymbol{u}(t)$, one would have to take an infimum over all controls connecting the initial and target state in order to evaluate the lowest value of the bound. This in itself is a task just as difficult as solving the control problem.

1.2 GRAPE

A central part of optimal control is actually finding the solution to the control problem. One way of achieving this is through the method known as GRAPE, where the control in each iteration of the optimization process is updated using the gradient of a cost functional $\hat{J}$ [G. Jäger, D. M. Reich, M. H. Goerz, C. P. Koch, and U. Hohenester, "Optimal quantum control of boseeinstein condensates in magnetic microtraps: Comparison of gradient-ascent-pulse-engineering and krotov optimization schemes," Physical Review A, vol. 90, p. 033628, 2014.]. This cost functional is given by

$$J = \frac{1}{2}\left(1 - |\langle\psi_{\mathrm{target}}|\psi(T)\rangle|^2\right) + \frac{\gamma}{2}\sum_{n=1}^{m}\int_0^T \left(\frac{\partial u_n}{\partial t}\right)^2 \mathrm{d}t , \tag{7}$$

where m is the number of control parameters at each instance of time, and u_n is the n'th entry in $\boldsymbol{u}(t)$. The first term of the cost functional is half the fidelity, while the second term is a regularization, which penalizes large variations in the control. Thus, increasing γ will favor a very smooth control, while keeping it low allows the control to vary greatly.
In order to force the time evolution to satisfy the Schrödinger equation, one can introduce a Lagrange multiplier, $|\chi\rangle$, which yields the optimization Lagrangian

$$L = J + \mathrm{Re}\left[\int_0^T \langle\chi|\left(i\,|\dot{\psi}\rangle - \hat{H}\,|\psi\rangle\right)\mathrm{d}t\right] , \tag{8}$$

where $|\dot{\psi}\rangle$ is the time-derivative of the state $|\psi\rangle$. The optimal solutions are the stationary points of L, where

$$\frac{\delta L}{\delta\chi^*(t')} = \frac{\delta L}{\delta\psi^*(t')} = \frac{\delta L}{\delta u_n(t')} = 0 \quad \text{for} \quad n = 1,\ldots,m , \tag{9}$$

and $0 \leq t' \leq T$. Calculating the derivative with respect to the Lagrange multiplier, $\langle\chi(t')|$, yields

$$\frac{\delta L}{\delta\chi^*(t')} = \frac{1}{2}\left(i\,|\dot{\psi}\rangle - \hat{H}\,|\psi\rangle\right) , \tag{10}$$

or when rewritten

$$i\,|\dot{\psi}\rangle = \hat{H}\,|\psi\rangle , \tag{11}$$

which, as expected, is just the Schrödinger equation. Taking the derivative with respect to $\langle\psi(t')|$ yields

$$\begin{aligned}
\frac{\delta L}{\delta\psi^*(t')} &= \frac{\delta}{\delta\psi^*(t')}\left[\frac{1}{2}\int_0^T \left(i\,\langle\dot{\psi}|\chi\rangle - \langle\psi|\,\hat{H}\,|\psi\rangle\right)\mathrm{d}t\right] \\
&= -\frac{1}{2}H\,|\chi\rangle + \frac{\delta}{\delta\psi^*(t')}\left[\frac{i}{2}\left(\langle\psi|\chi\rangle\Big|_0^T - \int_0^T \langle\psi|\dot{\chi}\rangle\right)\right] \\
&= -\frac{1}{2}\left(H\,|\chi\rangle - i\,|\dot{\chi}\rangle\right) .
\end{aligned} \tag{12}$$

Furthermore, one also has to consider the derivative with respect to $\langle\psi(T)|$ due to explicit dependence in the fidelity. This yields

$$\frac{\delta L}{\delta\psi^*(T)} = -\frac{1}{2}\left(|\psi_{\text{target}}\rangle \langle\psi_{\text{target}}|\psi(T)\rangle - i\,|\chi(T)\rangle\right) \ . \tag{13}$$

Equation 12 takes the form of the Schrödinger equation for $|\chi(t')\rangle$,

$$i\,|\dot{\chi}\rangle = -\hat{H}\,|\chi\rangle \ , \tag{14}$$

however, the sign is flipped implying a backwards propagation in time. This is further enforced by equation 13, which states

$$|\chi(T)\rangle = -i\,|\psi_{\text{target}}\rangle \langle\psi_{\text{target}}|\psi(T)\rangle \ . \tag{15}$$

Thus, at $t = T$, $|\chi\rangle$ is given as the projection of the final state unto the target-state, which in case of a correct solution is simply the target-state. Hence, equations 12 and 13 can be interpreted as $|\chi\rangle$ being the target-state evolved backwards in time. Finally, the derivative with respect to the control parameters is

$$\begin{aligned}
\frac{\delta L}{\delta u_n(t')} &= -\operatorname{Re}\langle\chi|\,\frac{\partial\hat{H}}{\partial u_n(t')}\,|\psi\rangle + \frac{\gamma}{2}\frac{\delta}{\delta u_n(t')}\left[u_n\dot{u}_n\Big|_0^T - \int_0^T u_n\ddot{u}_n\mathrm{d}t\right] \\
&= \operatorname{Re}\langle\chi|\,\frac{\partial\hat{H}}{\partial u_n(t')}\,|\psi\rangle - \frac{\gamma}{2}\frac{\delta}{\delta u_n(t')}\left[\int_0^T u_n\ddot{u}_n\mathrm{d}t\right] \\
&= \operatorname{Re}\langle\chi|\,\frac{\partial\hat{H}}{\partial u_n(t')}\,|\psi\rangle - \frac{\gamma}{2}\frac{\delta}{\delta u_n(t')}\left[\int_0^T \left(\frac{\partial u_n}{\partial u_n(t')}\ddot{u}_n + u_n\frac{\partial\ddot{u}_n}{\partial u_n(t')}\right)\mathrm{d}t\right] \\
&= \operatorname{Re}\langle\chi|\,\frac{\partial\hat{H}}{\partial u_n(t')}\,|\psi\rangle - \gamma\ddot{u}_n \ .
\end{aligned} \tag{16}$$

A solution to the equations 12, 13 and 16 with the initial conditions

$$|\chi(T)\rangle = -i\,|\psi_{\text{target}}\rangle \langle\psi_{\text{target}}|\psi(T)\rangle \ , \tag{17}$$

$$|\psi(0)\rangle = |\psi_0\rangle \ , \tag{18}$$

$$\boldsymbol{u}(0) = \boldsymbol{u}_1 \ , \quad \boldsymbol{u}(T) = \boldsymbol{u}_2 \ , \tag{19}$$

will satisfy equation 9, but only for a stationary point of J, which is not necessarily the minimum. For small values of J however, it has been shown that the solution will be a minimum [A. Borzì and U. Hohenester, "Multigrid optimization schemes for solving bose-einstein condensate control problems," SIAM Journal on Scientific Computing, vol. 30, no. 1, pp. 441–462, 2008.]. This is very difficult though, due to the complexity of the equations. An alternative is to find the minimum of the reduced cost functional $\hat{J}(\boldsymbol{u}(t)) = J(\psi(\boldsymbol{u}(t))\ ,\ \boldsymbol{u}(t))$, where $\psi(\boldsymbol{u}(t))$ is a unique solution of the Schrödinger equation. This can be done by iteratively updating the control using the gradient of the reduced cost functional

$$\nabla\hat{J}_n = -\gamma\ddot{u}_n - \operatorname{Re}\langle\chi|\,\frac{\partial\hat{H}}{\partial u_n}\,|\psi\rangle \ , \tag{20}$$

which is method known as GRAPE.

2 Optimal Control of Two-Level System

In order to illustrate the use of quantum optimal control it was applied to the two-level Landau-Zener system with the goal of transferring the initial state $|\psi_0\rangle = |0\rangle_z$ into the target-state $|\psi_{\text{target}}\rangle = |1\rangle_z$. In this model the Hamiltonian in question is

$$\hat{H} = \Omega\hat{\sigma}_x + u\hat{\sigma}_z \ , \tag{21}$$

where σ_i's are Pauli matrices. Thus, the control adjusts the rotation around the z-axis in the Bloch sphere representation, while Ω represents a constant rotational speed around the x-axis giving rise to Rabi oscillations.

2.1 Analytical Approach

The two-state Landau-Zener problem is widely used in physics and was chosen because an analytical solution exists for arbitrary initial and final states, as detailed in [Gerhard C. Hegerfeldt. Driving at the quantum speed limit: Optimal control of a two-level system. Phys. Rev. Lett., 111:260501, Dec 2013]. In this article, however, the control $u(t)$ is allowed to change arbitrarily. Say we wanted to evolve an initial state,

$$|\psi_0\rangle = \cos\left(\frac{\theta_0}{2}\right)|0\rangle + e^{i\phi_0}\sin\left(\frac{\theta_0}{2}\right)|1\rangle, \tag{22}$$

to a final state,

$$|\psi_T\rangle = \cos\left(\frac{\theta_T}{2}\right)|0\rangle + e^{i\phi_T}\sin\left(\frac{\theta_T}{2}\right)|1\rangle, \tag{23}$$

at time T, seeking to find the lowest T for which such a transition is possible.

In [Gerhard C. Hegerfeldt. Driving at the quantum speed limit: Optimal control of a two-level system. Phys. Rev. Lett., 111:260501, Dec 2013], the optimal time-development operator is found to be,

$$\hat{U}_H(T,0) = e^{-i\phi_T\hat{\sigma}_z}e^{-i\Omega\hat{\sigma}_xT}e^{i\phi_0\hat{\sigma}_z}, \tag{24}$$

corresponding to a control consisting of two Dirac delta function pulses separated by a timespan T in which $u(T)=0$ and the QSL is $T_{\mathrm{QSL}} = |\frac{\theta_T-\theta_0}{2\Omega}|$. In our case, $|\psi_0\rangle = |0\rangle$, $|\psi_T\rangle = |0\rangle$, so $T_{\mathrm{QSL}} = \pi/2\Omega$ and $\phi_T = \phi_0 = 0$. Note that boundary conditions on $u(t)$ are irrelevant when $u(t)$ is allowed to consist of delta functions and, in particular, step functions.

2.2 Numerical Approach

For the optimization a steepest descent algorithm was used, such the control was updated at each iteration as

$$u(t)^{(i+1)} = u(t)^{(i)} - \alpha\nabla\hat{J}(u(t))\ , \tag{25}$$

where α was found at each iteration using a line search. In these calculations $\Omega = 1$ was chosen along with the boundary limits of the control $u(0) = 0$ and $u(T) = 2T$. Furthermore, $\gamma = 0$ was chosen, as the solutions were sufficiently smooth without requiring any penalizing.
Note, that for the most direct transfer of the initial state to the target state $u = 0$ would be the optimal solution, as described in the previous section. $\hat{\sigma}_x$ would rotate the initial state directly into the target state, however, due to the choice of boundaries of the control, this solution is not viable. Thus, by optimizing the control one is adjusting the rotation around the x-axis, such that $|\psi(T)\rangle = |\psi_{\mathrm{target}}\rangle$, while $u(T) = 2T$.

2.3 Optimization for $T = \frac{\pi}{2}$

An estimate for the QSL of this system can be made using the analytical solution of $u(t) = 0$. Expressing the initial and target state as a linear combination of eigenstates of the $\hat{\sigma}_x$ operator yields

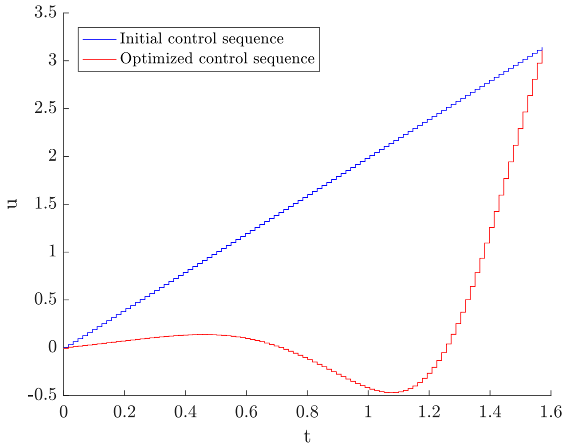
$$|0\rangle_z = \frac{1}{\sqrt{2}}\left(|1\rangle_x - |0\rangle_x\right) \tag{26}$$

$$|1\rangle_z = \frac{1}{\sqrt{2}}\left(|1\rangle_x + |0\rangle_x\right)\ . \tag{27}$$

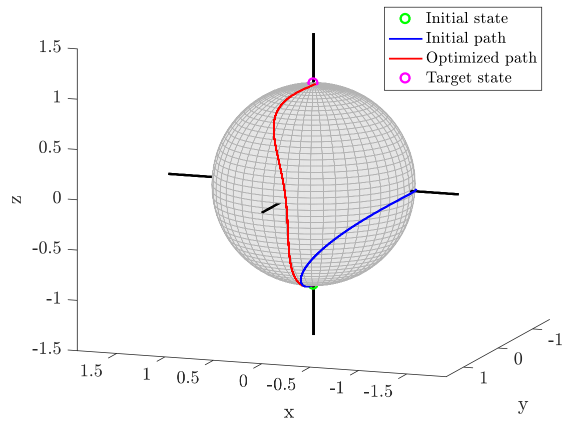
Thus, for $\Omega = 1$ and $u(t) = 0$ the Hamiltonian is constant, whereby time evolution can be performed easily

$$
\begin{aligned}
|\psi(t)\rangle &= e^{-i\hat{\sigma}_x t} |\psi_0\rangle \\
&= e^{-i\hat{\sigma}_x t} \frac{1}{\sqrt{2}} \left(|1\rangle_x - |0\rangle_x \right) \\
&= \frac{1}{\sqrt{2}} \left(e^{-it} |1\rangle_x - e^{it} |0\rangle_x \right) \\
&= e^{-it} \frac{1}{\sqrt{2}} \left(|1\rangle_x - e^{2it} |0\rangle_x \right) \ .
\end{aligned}
\tag{28}
$$

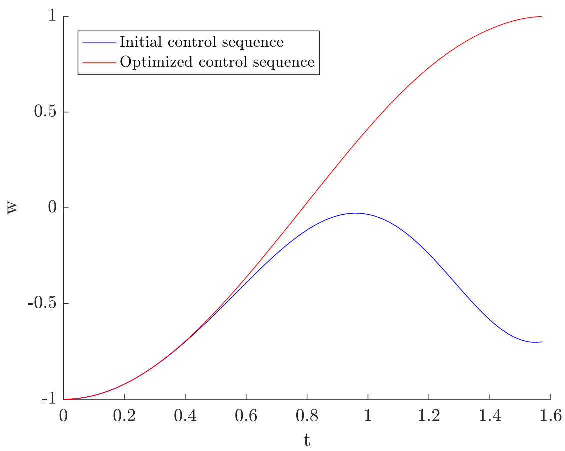
From equation 28 one sees that $|\psi(T)\rangle = |\psi_{\text{target}}\rangle$ for $T = \frac{\pi}{2}$. Of course in this model, $u(t) \neq 0$ for all times t, and solution times T must therefore be greater than or equal to $\pi/2$.



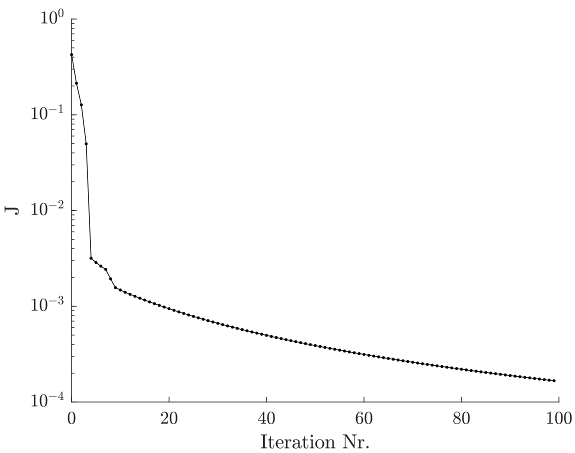
(a) *Control,* $\mathbf{u}(t)$*, before and after optimization for* $T = \frac{\pi}{2}$.



(b) *Path traced out by* $\psi(t)$ *on the Bloch sphere for* $T = \frac{\pi}{2}$.



(c) *Population inversion of the system as a function of time for* $T = \frac{\pi}{2}$.

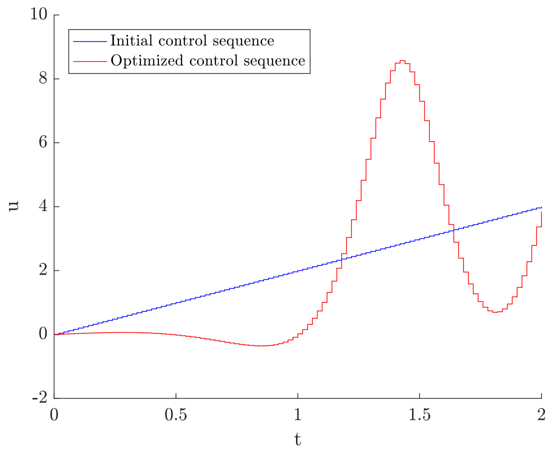


(d) *Reduced cost functional,* $\hat{J}$*, at each iteration of the optimization for* $T = \frac{\pi}{2}$.

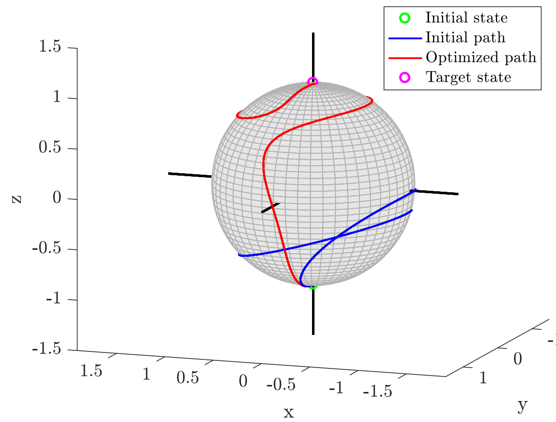
Indeed, performing the optimization for $T = \frac{\pi}{2}$ yields a complete transfer of the initial state into the target state, while $T_1 < T$ fails to converge. Starting with an initial control varying linearly, the optimized control is very different as seen in figure 1a: For the first third of the timespan it remains at zero, which, as described earlier, is the optimal solution when neglecting boundaries. But since it is required that $u(T) = 2T$ and that $u(t)$ be continuous, the control first decreases to compensate for the following sharp increase. The resulting path on the Bloch sphere is displayed in figure 1b. Had the control not decreased (resulting in a negative rotation around the z-axis) first, the large upswing in the end would have made the state miss its target. Consequently, the faster an increase in the control allowed, the lesser the need is for the preceeding negative rotation to correct the trajectory. The limit of this increase would be $u(t) = 0$ for all (arbitrarily small) timesteps except the last, where it jumps to $u(T) = 2T$, as is the analytical solution.

Just how smooth the transfer between the initial and target state is is made clear in figure 1c, where the population inversion, $w = |\langle 1|\psi\rangle|^2 - |\langle 0|\psi\rangle|^2$, is plotted. Although the path on the Bloch sphere is not completely straight, the population inversion is showing the same characteristics as the Rabi oscillations ($|\langle 1|\psi\rangle|^2 \propto \sin(\Omega t/2)$). However, as T is equal to half the period of the Rabi oscillation, the similarity between the solution and Rabi oscillations is to be expected. Finally, figure 1d illustrates, how the algorithm finds increasingly better solutions, as the reduced cost functional is gradually decreasing. Since $\gamma = 0$, one can read the fidelity directly of the figure as $F = 1 - 2J$. Thus, this solution yields a fidelity $F \sim 0.999$, however, since the cost has not yet converged on this figure, an even higher fidelity could be reached with more iterations of the algorithm.

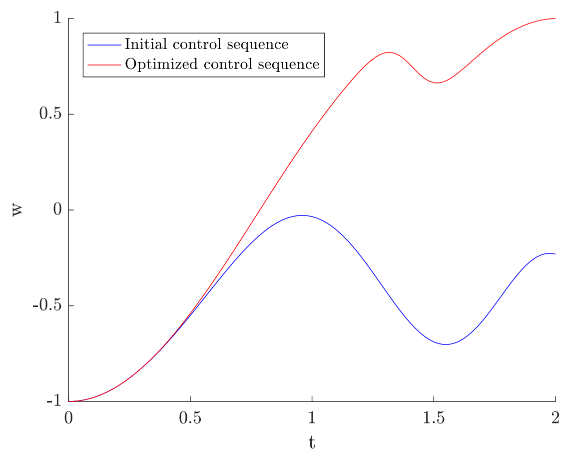
2.4 Optimization for $T = 2$



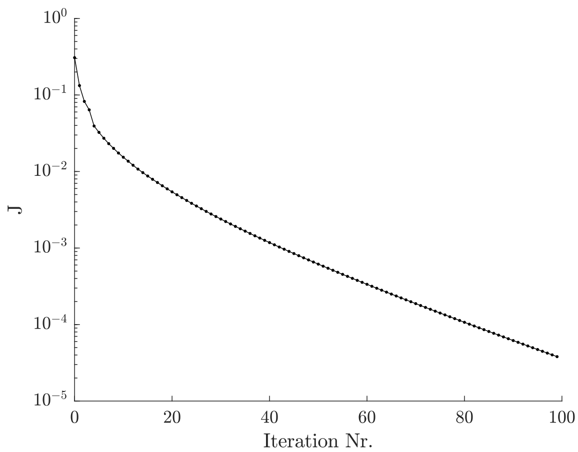
(a) *Control, $\mathbf{u}(t)$, before and after optimization for $T = 2$.*



(b) *Path traced out by $\psi(t)$ on the Bloch sphere for $T = 2$.*



(c) *Population inversion of the system as a function of time for $T = 2$.*



(d) *Reduced cost functional, $\hat{J}$, at each iteration of the optimization for $T = 2$.*

As described earlier, the GRAPE method will produce a solution, which steers the initial into the target state at $t = T$. Thus, running the algorithm for $T_2 > T_{\mathrm{QSL}}$ should produce a more indirect solution. This is indeed the case, as seen in figure 2a, where an Gaussian-like profile has been added on top of the previous solution in order to reach the target state at the desired time. This addition of course leads to a more indirect path, as illustrated in figure 2b. Hence, the population inversion of figure 2c is no longer similar to that of a Rabi oscillation.

Nevertheless, it should be noted that this is a completely valid solution, as it meets all the set requirements.

Bibliography