1 $|0\rangle \to |2\rangle$ State Evolution

In this simulation, the optimization was run to realise the state evolution $|0\rangle \to |1\rangle$ and then $|0\rangle \to |2\rangle$. The first pulse shape should be close to the ideal solution of a π-pulse: a gaussian pulse which performs a bit flip on a qubit, while the second is non-trivial. Therefore they are suitable goals to test the method and package.

Hamiltonian

The anharmonic resonator (qubit) in **??** was chosen as it is a simple model for a physical qubit. As stated earlier such a system will be referred to as a qubit even though it has more than two energy levels. To induce transitions between the states of the qubit, control pulse terms were added to **??**, resulting in

$$\hat{H} = \omega_q \hat{a}^\dagger \hat{a} + \frac{K_q}{2}(\hat{a}^\dagger)^2\hat{a}^2 + \Omega(t)\mathrm{e}^{-i\omega_q t}\hat{a} + \Omega^*(t)\mathrm{e}^{i\omega_q t}\hat{a}^\dagger, \tag{1.1}$$

where $\Omega(t)$ is the complex amplitude of the control pulse. Looking at the Hamiltonian above, it can be argued that it can be written in the form in **??**, which is needed by `krotov`, with $u_0(t) = \Omega(t)\mathrm{e}^{i\omega_q t}$ and $u_1(t) = \Omega^*(t)\mathrm{e}^{-i\omega_q t}$. However, there are two problems that need to be adressed. Firstly, the oscillating factors require an unnecessarily fine time discretization of the pulses. Secondly, the Krotov package expects real-valued pulse amplitudes $\{u_i(t)\}$ as inputs. The first problem was avoided by transforming the Hamiltonian into the interaction picture with respect to $\omega_q \hat{a}^\dagger \hat{a}$, also known as the rotating frame. That is the Hamiltonian is transformed with

$$\hat{U}\hat{H}\hat{U}^\dagger + i\frac{\mathrm{d}\hat{U}}{\mathrm{d}t}\hat{U}^\dagger, \tag{1.2}$$

where $\hat{U} = \mathrm{e}^{-i\omega_q \hat{a}^\dagger \hat{a} t}$ which results in

$$\hat{H} \to \frac{K_q}{2}(\hat{a}^\dagger)^2\hat{a}^2 + \Omega(t)\hat{a} + \Omega^*(t)\hat{a}^\dagger. \tag{1.3}$$

Now the pulse amplitudes $u_0(t) = \Omega(t)$ and $u_1(t) = \Omega^*(t)$, i.e. the envelope of the physical control pulse which varies significantly slower than the actual pulse. The second problem was easily fixed with a rearrangment of the terms

$$\Omega(t)\hat{a} + \Omega^*(t)\hat{a}^\dagger = \Big[\mathrm{Re}[\Omega(t)] + i\mathrm{Im}[\Omega(t)]\Big]\hat{a} + \Big[\mathrm{Re}[\Omega(t)] - i\mathrm{Im}[\Omega(t)]\Big]\hat{a}^\dagger =$$
$$= \mathrm{Re}[\Omega(t)]\big(\hat{a} + \hat{a}^\dagger\big) + \mathrm{Im}[\Omega(t)]i\big(\hat{a} - \hat{a}^\dagger\big).$$

For intuition, $\big(\hat{a} + \hat{a}^\dagger\big)$ and $i\big(\hat{a} - \hat{a}^\dagger\big)$ correspond to rotations around the Bloch sphere[1] along the x-axis and y-axis respectively. Thus the final Hamiltonian became

$$\hat{H} = \underbrace{K_q/2(\hat{a}^\dagger)^2\hat{a}^2}_{\hat{H}_d} + \underbrace{\mathrm{Re}[\Omega(t)]}_{u_0(t)}\underbrace{(\hat{a} + \hat{a}^\dagger)}_{\hat{H}_0} + \underbrace{\mathrm{Im}[\Omega(t)]}_{u_1(t)}\underbrace{i(\hat{a} - \hat{a}^\dagger)}_{\hat{H}_1}. \tag{1.4}$$

The parameters of the qubit were chosen to model real superconducting qubits with $K_q = 2\pi \times 297\,\mathrm{MHz}$ (and $\omega_q = 2\pi \times 6.2815\,\mathrm{GHz}$). The system Hamiltonian in Equation (1.4) was simulated with a truncated Hilbert space size conveniently chosen to be $N_q = 3$. A smaller truncated Hilbert space, and consequently smaller matrices, requires less computations but could possibly yield a poor approximation of the Hamiltonian. Thus the solutions of the optimization were analysed with this in mind.

Optimization Setup

As the long-term goal is to use this method in physical systems some constraints were added. To simulate the constraints of physical arbitrary waveform generators (AWG) a maximum sample rate of $4\,\mathrm{GSa\,s^{-1}}$ was chosen. Recall that the physcal pulses oscillate at $\omega_q = 6.2815\,\mathrm{GHz}$, a rate which $4\,\mathrm{GSa\,s^{-1}}$ can impossibly resolve. Although AWGs with higher sample rates than $4\,\mathrm{GSa\,s^{-1}}$ exist, they are expensive. However, rotating frame transformation permits the use of a relatively low rate AWG to generate the pulse envelopes $\Omega(t)$ and a high rate tone generator to create a carrier signal at ω_q, with these signals later combined in a mixer. Further,

[1] A quick explanation of how the Bloch sphere is used for visualization is given in **??**.

due to the noise sensitivity of superconducting systems an amplitude constraint is needed to keep the system cool enough. To set a realistic maximum amplitude A_m some derivation was required. First the maximum amplitude was chosen with the assumption that a gaussian pulse

$$g(t) = \frac{\pi/2}{\sigma\sqrt{2\pi}} \mathrm{e}^{-\frac{1}{2}\left(\frac{t}{\sigma}\right)^2} \tag{1.5}$$

with $\sigma = 3\,\mathrm{ns}$ can physically realise a π-rotation $|0\rangle \to |1\rangle$ in a planar transmon qubit. The problem with gaussian pulses however is that they do not go to zero at the edges. To fix this `krotov` provides a function for generating Blackman pulses. A Blackman pulse with a total length of 6σ is a good approximation of a Gaussian pulse, with the added benefit of going to zero at the edges. However, due to the approximation, the integral of the Blackman pulse will not exactly be equal to the integral of the corresponding gaussian pulse, which is needed to realise the π-rotation. This can be fixed by using a prefactor C which can be calculated by solving

$$C \int_0^{6\sigma} \frac{1}{\sqrt{2\pi}\sigma} B(t) = \int_0^{6\sigma} g(t - 3\sigma)\,\mathrm{d}t \tag{1.6}$$

where $B(t)$ is the Blackman pulse. This is now used to determine the maximum amplitude

$$A(\sigma) = \frac{C}{\max(\sigma, 3)\sqrt{2\pi}} \tag{1.7}$$

with $A_m = A(\sigma = 3)$. This amplitude constraint is enforced by calling a function after every iteration which limits all pulse shape values $|\Omega| < A_m$. Conveniently, the Blackman pulse was also used as the initial guess pulse with $u_0(t) = A(T/6)B(t)$, $u_1(t) = 0$.

Another constraint was added so that the edges of the pulses were always zero. This was done with a switch-on/switch-off of 2 ns. This ramp shape is half a Blackman pulse and is provided by `krotov`'s `flattop` function.

For the $|0\rangle \to |1\rangle$ state evolution, pulse shapes were optimized with varying lengths from 4.25 ns to 30 ns with convergence criteria $F > 0.99999$ or $\Delta F < 10^{-7}$. The step size was chosen as $\lambda = \frac{1}{\frac{1}{2}A_m}$. The reason for optimizing for various pulse lengths was that faster pulse changes gives a broader support in the frequency spectrum which can ultimately induce transitions in other levels. Therefore the optimization needs to find a solution which circumvents this problem.

Lastly, for the $|0\rangle \to |2\rangle$ state evolution, pulse shapes were optimized with varying lengths from 22 ns to 30 ns with convergence criteria $F > 0.99999$ or $\Delta F < 10^{-9}$. The low ΔF was needed because the changes were very small in the beginning of the optimization. The step size was chosen as $\lambda = \frac{1}{2A_m}$ due to slow convergence. In contrast to the $|0\rangle \to |1\rangle$ state evolution both initial guess pulses were chosen to be Blackman pulses $u_0(t) = u_1(t) = A(T/6)B(T)$.