A small quantum control problem

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A 2-qubit gate

We want to design a gate that transforms

$$|\mathbf{u}\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$$

into

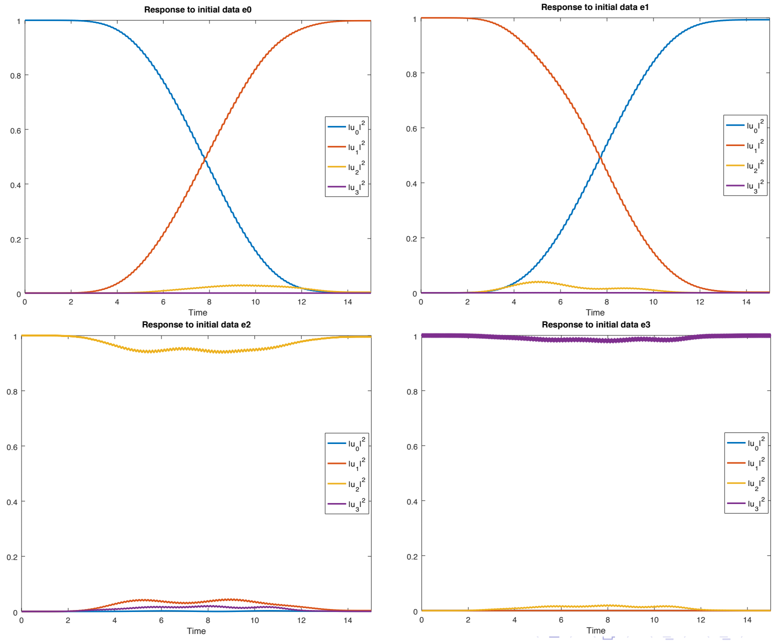
$$|\mathbf{v}\rangle = b|00\rangle + a|01\rangle + c|10\rangle + d|11\rangle$$

This operation can be described in matrix notation as

$$\mathbf{v} = G\mathbf{u}, \quad G = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Note that G is unitary.

An example


Response to initial data e0
Response to initial data e1
Response to initial data e2
Response to initial data e3
Time
$|u_0|^2$
$|u_1|^2$
$|u_2|^2$
$|u_3|^2$

The control problem

The quantum state is governed by the ODE

$$\dot{\Psi}_k = i(H_0 + p(t)H_c)\Psi_k, \quad t \in [0, T], \quad \Psi_k(0) = \mathbf{e}_k,$$

for $k = 0, 1, 2, 3$, where $\mathbf{e}_k$ is the k^{th} unit vector, $\Psi_k \in \mathbb{C}^4$, and

$$H_0 = \mathrm{diag}(0, \omega_1, \omega_2, \omega_3), \quad H_c = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & \sqrt{2} & 0 \\ 0 & \sqrt{2} & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$

The (unitary) solution operator is formally

$$U = \exp\left(i \int_0^T (H_0 + p(\tau)H_c)\, d\tau \right), \quad \Psi_k(T) = U\,\mathbf{e}_k.$$

Challenge: Determine the control function $p(t)$ such that $U = G$.

Optimization problem

Expand the control function in a basis $p_q(t)$,

$$p(t) = \sum_{q=1}^{M} \alpha_q p_q(t)$$

Let $\mathbf{d}_k = G\mathbf{e}_k$ be the target state.
Minimize the functional

$$g(\Psi) = \sum_{k=0}^{3} \int_0^T w_k(\tau) \left(|\Psi_k(\tau)|^2 - |\mathbf{d}_k|^2 \right)^2 \, d\tau,$$

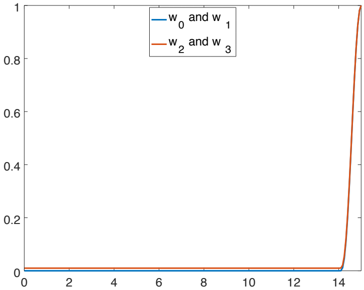
under the constraint that Ψ_k satisfies the above ODE.

Designing the control and weight functions

The basis functions (induce resonance),

$$p_{2q-1}(t) = \cos(\omega_1 t) f_q(t),$$
$$p_{2q}(t) = \sin(\omega_1 t) f_q(t).$$

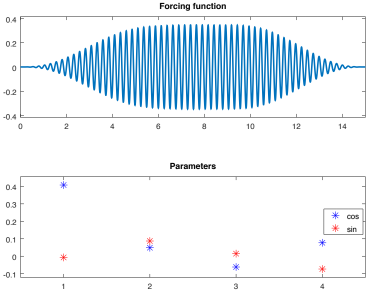
The first 4 functions $f_q(t)$ and the weight functions $w_k(t)$:



Numerical solution approach

- Discretize the ODE by Leap-Frog (2nd order accurate, energy stable)
- Evaluate cost functional $g(\Psi)$ by solving the ODE for 4 initial conditions
- Evaluate gradient $\nabla_\alpha g$ by solving the ODE forwards and then backwards, together with the adjoint ODE
- Start with 1 parameter and do a line search for optima: α_{10}
- For 2 parameters, start from $(\alpha_{10}, 0)$ and call **sqp** (sequential quadratic programming) in octave. New optima: $(\alpha 11, \alpha 21)$.
- Add next level polynomials, repeat optimization starting from previous optima.
- Keep adding polynomials until cost function is sufficiently small.

Control function with 4 polynomials



Resulting numerical "solution operator"

$$\widetilde{U} \approx \begin{pmatrix} 4.12_{-2} + 2.31_{-2} i & -4.20_{-1} + 9.03_{-1} i & 2.14_{-2} - 1.61_{-2} i & -5.96_{-6} + 9.45_{-5} i \\ 5.73_{-1} + 8.18_{-1} i & 3.76_{-2} - 3.10_{-2} i & 5.38_{-2} - 1.70_{-2} i & -5.78_{-4} + 2.95_{-4} i \\ -5.38_{-2} - 2.28_{-2} i & 5.00_{-3} - 2.38_{-2} i & 6.49_{-1} - 7.58_{-1} i & -8.88_{-3} + 1.33_{-2} i \\ 1.63_{-4} - 2.35_{-4} i & 3.41_{-4} + 1.27_{-4} i & 8.42_{-3} + 1.40_{-2} i & 6.16_{-1} + 7.87_{-1} i \end{pmatrix}$$

Only approximately unitary (time-integration errors).