# The final gate objective functional

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## 1 Introduction

Let the wave functions $\psi_j(t, ) \in [0,T] \times \mathbb{R}^D \to \mathbb{C}^N$ be governed by the Schrödinger equation,

$$\dot{\psi}_j + iH(t, )\psi_j = 0, \quad 0 \le t \le T, \quad \psi_j(0) = \mathbf{e}_j, \quad j = 1, 2, \ldots, N, \tag{1}$$

Here, $\mathbf{e}_j$ is the $j^{th}$ canonical unit vector (zero, except element number $j$ which is one). The Hamiltonian matrix satisfies

$$H(t, ) = H_0 + p(t, )H_c, \quad H(t, ) = H^\dagger(t, ),$$

where $p(t, )$ is a scalar function of time that depends on the parameter vector $= [\alpha_1, \alpha_2, \ldots, \alpha_D]^T \in \mathbb{R}^D$. We introduce

$$_{jk}(t, ) = \frac{\partial \psi_j(t, )}{\partial \alpha_k}, \quad k = 1, 2, \ldots, D.$$

By differentiating (1) with respect to $\alpha_k$,

$$\dot{}_{jk} + iH(t, )_{jk} = \mathbf{f}_{jk}(t, ), \quad 0 \le t \le T, \quad _{jk}(0) = 0, \tag{2}$$

$$\mathbf{f}_{jk}(t, ) = -i\frac{\partial p(t, )}{\partial \alpha_k} H_c \psi_j(t, ). \tag{3}$$

Let $U_g = [\mathbf{d}_1, \mathbf{d}_2, \ldots, \mathbf{d}_N] \in \mathbb{C}^{N\times N}$, represent the target unitary matrix ($U_g^{-1} = U_g^\dagger$) and collect the wave functions for the different initial data in the unitary matrix $U = U(T, \alpha) \in \mathbb{C}^{N\times N}$, where

$$U = [\psi_1, \psi_2, \ldots, \psi_N], \quad U^\dagger = U^{-1}.$$

An objective functional that measures the infidelity in the final unitary is given by

$$g(U(T, )) = 1 - \frac{1}{N^2}\left|S()\right|^2, \quad S() = \langle U(T, ), U_g \rangle_F. \tag{4}$$

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We define the Fröbenius matrix scalar product between square complex-valued matrices $A$ and $B$ by

$$\langle A, B\rangle_F = \mathrm{tr}\big(A^\dagger B\big) = \sum_{j=1}^{N} \langle \mathbf{a}_j, \mathbf{b}_j\rangle_2, \tag{5}$$

where $A = [\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_N]$ and $B = [\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_N]$. By differentiating (4) with respect to $\alpha_k$,

$$\frac{\partial g}{\partial \alpha_k} = -\frac{2}{N^2}\mathrm{Re}\left(\frac{\partial S}{\partial \alpha_k}\overline{S}\right). \tag{6}$$

From (4) and (5),

$$S() = \sum_{j=1}^{N} \langle \psi_j(T,), \mathbf{d}_j\rangle_2\,, \quad \frac{\partial S()}{\partial \alpha_k} = \sum_{j=1}^{N} \langle {}_{jk}(T,), \mathbf{d}_j\rangle_2\,. \tag{7}$$

## 2 The adjoint state equation

Define the adjoint state equation according to

$$-\dot{}_j - iH(t,)_j = \mathbf{g}_j(t), \quad T \geq t \geq 0, \quad {}_j(T) = \mathbf{d}_j, \quad j = 1, 2, \ldots, N. \tag{8}$$

Note that the adjoint equation is solved backwards in time and is subject to a terminal condition given by the $j^{th}$ column of the target unitary, $U_g$. The forcing function $\mathbf{g}_j(t)$ will be determined below.

The solutions of the state equation (2) and the adjoint state equation (8) are related. To establish this relation, let's consider

$$I := \int_0^T \langle {}_{jk}, \mathbf{g}_j\rangle_2\, d\tau = \int_0^T \langle {}_{jk}, -\dot{}_j - iH(t,)_j\rangle_2\, d\tau$$

$$= -\int_0^T \langle {}_{jk}, \dot{}_j\rangle_2\, d\tau + \int_0^T \langle iH(t,)_{jk}, {}_j\rangle_2\, d\tau. \tag{9}$$

By integration by parts,

$$\int_0^T \langle {}_{jk}, \dot{}_j\rangle_2\, d\tau = [\langle {}_{jk}, {}_j\rangle_2]_0^T - \int_0^T \langle \dot{}_{jk}, {}_j\rangle_2\, d\tau$$

$$= \langle {}_{jk}(T), \mathbf{d}_j\rangle_2 - \int_0^T \langle \dot{}_{jk}, {}_j\rangle_2\, d\tau,$$

because ${}_{jk}(0) = 0$ and ${}_j(T) = \mathbf{d}_j$. Thus,

$$I = -\langle {}_{jk}(T), \mathbf{d}_j\rangle_2 + \int_0^T \langle \dot{}_{jk} + iH(t,)_{jk}, {}_j\rangle_2\, d\tau$$

$$= -\langle {}_{jk}(T), \mathbf{d}_j\rangle_2 + \int_0^T \langle \mathbf{f}_{jk}, {}_j\rangle_2\, d\tau.$$

By choosing $\mathbf{g}_j(t) = 0$, we get $I = 0$. Therefore,

$$\langle {}_{jk}(T), \mathbf{d}_j \rangle_2 = \int_0^T \langle \mathbf{f}_{jk}, {}_j \rangle_2 \, d\tau. \tag{10}$$

Inserting (10) into (7) finally gives

$$\frac{\partial S()}{\partial \alpha_k} = \sum_{j=1}^{N} \int_0^T \langle \mathbf{f}_{jk}, {}_j \rangle_2 \, d\tau = \int_0^T \sum_{j=1}^{N} \langle \mathbf{f}_{jk}, {}_j \rangle_2 \, d\tau, \tag{11}$$

where $\mathbf{f}_{jk}(t)$ is given by (3). Similar to before, we can compute all components of the gradient of the objective function (6). We start by solving the Schrödinger equation forwards in time to obtain the terminal state $\psi_j(T) =: \mathbf{w}_j$ for $j = 1, 2, \ldots, N$. The time stepping is then reversed to integrate (1) backwards in time,

$$\dot{\psi}_j + iH(t, )\psi_j = 0, \quad T \geq t \geq 0, \quad \psi_j(T) = \mathbf{w}_j, \quad j = 1, 2, \ldots, N. \tag{12}$$

The adjoint wave equation (8) (with $\mathbf{g}_j = 0$) is simulataneously solved backwards in time to calculate ${}_j(t)$. At each time step, (3) is evaluated to calculate $\mathbf{f}_{jk}(t)$ and combined with ${}_j(t)$, accumulate the integral (11) to compute the gradient of the objective functional.