1 Optimization Problem

let S be set of feasible Hamiltonians, $|\phi_0\rangle$ the ground state and $|\psi\rangle$ the target state.

formally, problem can be formulated by these equations

$$H^*, t^* = \underset{H \in S, t \in \mathbb{R}}{\arg\max} \mathcal{F}(e^{iHt} |\phi_0\rangle, |\psi\rangle) \tag{1}$$

where $\mathcal{F}$ is fidelity.

1.1 Numerical Optimization

to be completed

1.2 Continuous Analytical Optimization

in a continuous framework, let $\vec{v} \in \mathbb{R}^m$ degrees of freedom for the whole evolution (Hamiltonian and time).

$$\tilde{H} = Ht = f(\vec{v})$$

$$\tilde{H} = \sum_{i,j} H_{ij} |i\rangle\langle j| = \sum_{i,j} f_{ij}(\vec{v}) |i\rangle\langle j|$$

then

$$\vec{\boldsymbol{\nabla}} \mathcal{F}(e^{\tilde{H}(\vec{v})} |\phi_0\rangle, |\psi\rangle)\Big|_{\vec{v}=\vec{v}^*} = \vec{0}$$

$$\forall k \qquad \sum_{i,j} \frac{\partial \mathcal{F}(e^{iHt} |\phi_0\rangle, |\psi\rangle)}{\partial \tilde{H}_{ij}} \frac{\partial \tilde{H}_{ij}}{\partial v_k}\Big|_{\vec{v}=\vec{v}^*} = 0$$

now we are going to compute $\frac{\partial \mathcal{F}}{\partial \tilde{H}_{ij}}$

Lemma 1.

$$\frac{\partial H^k}{\partial H_{mn}} = \sum_l H^l_{mi} H^{k-l-1}_{jn}$$

Lemma 2. *if* $H = U^\dagger D U$

$$\frac{\partial H^k}{\partial H_{mn}} = \sum_{i,j,\alpha,\beta} U^\dagger_{m\alpha} U^\dagger_{i\beta} U_{\alpha j} U_{\beta n} \frac{D^k_{\alpha\alpha} - D^k_{\beta\beta}}{D_{\alpha\alpha} - D_{\beta\beta}} |i\rangle\langle j|$$

without loosing generalization, we can assume $|\phi_0\rangle = |1\rangle$

by using two aformentioned lemma, we can show

$$\frac{\partial \mathcal{F}}{\partial \tilde{H}_{ij}} = \sum_{p,q,\alpha,\beta,\gamma} \langle\psi|p\rangle \langle q|\psi\rangle U^\dagger_{i\alpha} U^\dagger_{2\beta} U_{\alpha 1} U_{\beta j} U^\dagger_{1\gamma} U_{\gamma p} \frac{(e^{iD_{\alpha\alpha}} - e^{iD_{\beta\beta}})e^{-iD_{\gamma\gamma}} + (e^{-iD_{\alpha\alpha}} - e^{-iD_{\beta\beta}})e^{iD_{\gamma\gamma}}}{D_{\alpha\alpha} - D_{\beta\beta}}$$