Optimal control of open quantum systems

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Master equation (GKSL) with control

$$\frac{\partial \rho_t}{\partial t} = \mathcal{L}_t(\rho_t) = -i[H_0 + \sum_k u_k(t)V_k, \rho_t] + \mathcal{L}_{n(t)}(\rho_t),$$

$\mathcal{H}$ — Hilbert space of pure states $|\psi\rangle \in \mathcal{H}$, e.g. $\mathcal{H} = \mathbb{C}^N$;
ρ_t — density matrix, describes mixed states,
$\rho_t \in \mathcal{B}(\mathcal{H})$, $\rho_t \geq 0$, $\mathrm{Tr}\rho_t = 1$;
$H_0 = H_0^\dagger$ — free Hamiltonian of the system,
$V_k = V_k^\dagger$ — interaction Hamiltonian;
$u_k(t)$ — coherent control, e.g. a laser pulse;
$n(t) = n_{ij}(t)$ — incoherent control, $n_{ij}(t) \geqslant 0$, *e.g. spectral density.*
$\mathcal{L}(.)_{n(t)} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ - dissipative (linear) operator, given by two different limits: *weak coupling limit*[a,b] and *low density limit*.

[a] E.B. Davies. Quantum theory of open systems. *Academic Press* (1976).
[b] Luigi Accardi, Yun Gang Lu, Igor Volovich. Quantum Theory and Its Stochastic Limit. *Springer* (2002).

Weak coupling limit[1], environment — incoherent radiation:

$$\mathcal{L} = \mathcal{L}_0 + \sum_k u_k(t)\mathcal{L}_k + \sum_{i<j} n_{ij}(t)\mathcal{L}_{ij},$$

where

$$\begin{aligned}
\mathcal{L}_k &= -i[V_k, \cdot\,], \\
\mathcal{L}_0 &= -i[H_0, \cdot] + \sum_{i<j} A_{ij}\mathcal{M}_{ij}, \\
\mathcal{L}_{ij} &= A_{ij}(\mathcal{M}_{ij} + \mathcal{M}_{ji}), \\
\mathcal{M}_{ij}(\rho) &= 2|i\rangle\langle j|\rho|j\rangle\langle i| - |i\rangle\langle i|\rho - \rho|i\rangle\langle i|,
\end{aligned}$$

$|i\rangle = e_i$ — orthonormal basis, $A_{ij} \geq 0$ are Einstein coefficients.

[1] A. Pechen and H. Rabitz. Teaching the environment to control quantum systems. *Phys. Rev. A*, **73**, 062102, (2006).

Control objectives

- Control goal — optimizing certain objective functional;
- Mayer-type functional:

$$\mathcal{J}_0(\rho_T) = \mathcal{J}_0(\rho_T[u,n]) = \mathcal{F}[u,n].$$

Main objectives:

- observable mean value: $\mathcal{F}_O[u,n] = Tr[\rho_T O] \to \sup/\inf;$
- state-to-state transition: $\mathcal{F}_{\rho_{target}}[u,n] = \|\rho_T^{u,n} - \rho_{target}\| \to \inf.$

GRadient Ascent Pulse Engineering (GRAPE) method was proposed[2] before for generating NMR pulses, and is widely used for coherently controlled quantum systems with assumption of piecewise constant control.
Gradient is widely used in other gradient-based algorithms[3,4]. Algorithms using gradient are general local, therefore should be applied to *trap-free* functional landscapes[5].

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[2] N. Khaneja, T. Reiss, C. Kehlet, T. Schulte-Herbrüggen, and S.J. Glaser. Optimal control of coupled spin dynamics: design of nmr pulse sequences by gradient ascent algorithms. *J. Magn. Reson.,* **172(2)**, 296–305, (2005).

[3] M. Dalgaard, F. Motzoi, J.H.M. Jensen, and J. Sherson. Hessian-based optimization of constrained quantum control *Phys. Rev. A*, **102**, 042612, (2020).

[4] R. Eitan, M. Mundt, and D.J. Tannor. Optimal control with accelerated convergence: Combining the Krotov and quasi-Newton methods. *Phys. Rev. A*, **83**, 053426, (2011).

[5] A.N. Pechen and D.J. Tannor. Are there traps in quantum control landscapes? Phys. Rev. Lett. **106**, 120402, (2011).

Generally, gradient of objective functional with respect to control is needed:

$$\frac{\delta \mathcal{F}}{\delta [u, n]} = \frac{\delta \mathcal{J}}{\delta \rho_T} \frac{\delta \rho_T}{\delta [u, n]}.$$

Finite-dimensional approximation — step functions:

$$u_k(t) = \sum_{m=1}^{M} u_k^m \chi_{[t_{m-1}, t_m)}(t), \quad n_{ij}(t) = \sum_{m=1}^{M} n_{ij}^m \chi_{[t_{m-1}, t_m)}(t),$$

$$0 < t_0 < t_1 < \cdots < t_M = T,$$

$$\rho_T = e^{\Delta t_M \mathcal{L}^M} \ldots e^{\Delta t_1 \mathcal{L}^1} \rho_0,$$

$$\mathcal{L}^m \equiv \mathcal{L}(t_m), \quad \Delta t_m = t_m - t_{m-1}, \quad m = 1, \ldots, M.$$

General case. N-level system

Theorem

Gradient of final state ρ_T with respect to control equals[a]:

$$\frac{\partial}{\partial u_k^m}\rho_T = e^{\Delta t_M \mathcal{L}^M}\dots\left(\frac{\partial}{\partial u_k^m}e^{\Delta t_m \mathcal{L}^m}\right)\dots e^{\Delta t_1 \mathcal{L}^1}\rho_0,$$

$$\frac{\partial}{\partial n_{ij}^m}\rho_T = e^{\Delta t_M \mathcal{L}^M}\dots\left(\frac{\partial}{\partial n_{ij}^m}e^{\Delta t_m \mathcal{L}^m}\right)\dots e^{\Delta t_1 \mathcal{L}^1}\rho_0,$$

$$\frac{\partial}{\partial u_k^m}e^{\Delta t_m \mathcal{L}^m} = \Delta t_m \int_0^1 \exp(\alpha \Delta t_m \mathcal{L}^m)\mathcal{L}_k^m \exp((1-\alpha)\Delta t_m \mathcal{L}^m)\,\mathrm{d}\alpha,$$

$$\frac{\partial}{\partial n_{ij}^m}e^{\Delta t_m \mathcal{L}^m} = \Delta t_m \int_0^1 \exp(\alpha \Delta t_m \mathcal{L}^m)\mathcal{L}_{ij}^m \exp((1-\alpha)\Delta t_m \mathcal{L}^m)\,\mathrm{d}\alpha.$$

[a] V.N. Petruhanov, A.N. Pechen. Gradient ascent pulse engineering for open quantum systems driven by coherent and incoherent controls (in preparation).

Example: controlled qubit

Consider a two-level open quantum system[6]:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_t = -i[H_0 + Vu(t), \rho_t] + \gamma \mathcal{L}_{n(t)}(\rho_t), \quad \rho(0) = \rho_0,$$

where

$$H_0 = \omega \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad V = \mu\sigma_x = \mu \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\mathcal{L}_{n(t)}(\rho_t) = n(t)\left(\sigma^+\rho_t\sigma^- + \sigma^-\rho_t\sigma^+ - \frac{1}{2}\{\sigma^-\sigma^+ + \sigma^+\sigma^-, \rho_t\}\right) +$$

$$+\left(\sigma^+\rho_t\sigma^- - \frac{1}{2}\{\sigma^-\sigma^+, \rho_t\}\right), \quad n(t) \geqslant 0,$$

$$\sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}; \quad \mu \in \mathbb{R},\, \mu \neq 0,\, \omega > 0,\, \gamma > 0.$$

[6] O.V. Morzhin, A.N. Pechen. Minimal time generation of density matrices for a two-level quantum system driven by coherent and incoherent controls. *Int. J. Theor. Phys.* **60**, 576–584 (2021).

$$u(t) = \sum_{k=1}^{M} u_k \chi_{[t_{k-1},t_k)}(t), \quad n(t) = \sum_{k=1}^{M} n_k \chi_{[t_{k-1},t_k)}(t),$$

$$0 = t_0 < t_1 < \cdots < t_N = T,$$

Equation in Bloch representation:

$$\frac{\mathrm{d}\mathbf{r}(t)}{\mathrm{d}t} = (B + u(t)B^u + n(t)B^n)\mathbf{r}(t) + b,$$

where $\mathbf{r} = (r_x, r_y, r_z)$.

$$\mathbf{r}^k \equiv \mathbf{r}(t_k) = F_k \mathbf{r}^{k-1} + g_k,$$

$$A_k = B + B^u u_k + B^n n_k$$

$$F_k = e^{A_k \Delta t_k}, \quad g_k = (e^{A_k \Delta t_k} - \mathbb{I})A_k^{-1} b, \quad \Delta t_k = t_k - t_{k-1},$$

$$\mathbf{r}_T = \mathbf{r}^M = F_M F_{M-1} \dots F_1 \mathbf{r}_0 + F_M \dots F_2 g_1 + \ldots + F_M g_{M-1} + g_M$$

Gradient of final state

Theorem

Derivatives of final state $\mathbf{r}_T$ with respect to control:

$$\frac{\partial \mathbf{r}_T}{\partial u_j} = F_N \dots F_{j+1} \left[\frac{\partial F_j}{\partial u_j} \mathbf{r}^j + \frac{\partial g_j}{\partial u_j} \right],$$

$$\frac{\partial \mathbf{r}_T}{\partial n_j} = F_N \dots F_{j+1} \left[\frac{\partial F_j}{\partial n_j} \mathbf{r}^j + \frac{\partial g_j}{\partial n_j} \right].$$

$$\frac{\partial g_k}{\partial u_k} = \left(\frac{\partial F_k}{\partial u_k} - (e^{A_k \Delta t_k} - I) A_k^{-1} B^u \right) A_k^{-1} b,$$

$$\frac{\partial F_k}{\partial u_k} = \Delta t_k \int_0^1 \exp(\alpha A_k \Delta t_k)\, B^u \exp((1-\alpha) A_k \Delta t_k) d\alpha.$$

Consider the two-level open quantum system[7]:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = -i[H_0 + Vu, \rho] + \gamma\mathcal{L}_n(\rho), \quad \rho(0) = \rho_0,$$

where

$$H_0 = \omega\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad V = \mu\sigma_x = \mu\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\mathcal{L}_n(\rho) = n\left(\sigma^+\rho\sigma^- + \sigma^-\rho\sigma^+ - \frac{1}{2}\{\sigma^-\sigma^+ + \sigma^+\sigma^-, \rho\}\right) +$$

$$+\left(\sigma^+\rho\sigma^- - \frac{1}{2}\{\sigma^-\sigma^+, \rho\}\right), \quad n \geqslant 0,$$

$$\sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}; \quad \mu \in \mathbb{R},\, \mu \neq 0,\, \omega > 0,\, \gamma > 0.$$

[7] O.V. Morzhin, A.N. Pechen. Minimal time generation of density matrices for a two-level quantum system driven by coherent and incoherent controls. *Int. J. Theor. Phys.* **60**, 576–584 (2021).

Evolution in Bloch ball. Piecewise constant control

Change from density matrix to Bloch vector:

$$r_i = \mathrm{Tr}\rho\sigma_i, \quad i \in \{x, y, z\}, \quad \rho = \frac{1}{2}(I + (\mathbf{r}, \boldsymbol{\sigma})).$$

Then we have dynamics for Bloch vector:

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = (B + uB^u + nB^n)\mathbf{r} + b,$$

where $\mathbf{r} = (r_x, r_y, r_z)$, $\|\mathbf{r}\| \leq 1$, $\quad B,\ B^u,\ B^n \in \mathbb{C}^{3\times 3}$, $b \in \mathbb{C}^3$.
Consider PConst control:

$$u(t) = \sum_{k=1}^{M} u_k \chi_{[t_{k-1}, t_k)}(t), \quad n(t) = \sum_{k=1}^{M} n_k \chi_{[t_{k-1}, t_k)}(t),$$

$$0 = t_0 < t_1 < \cdots < t_N = T,$$

The sequence of states $\{\mathbf{r}^k\}_{k=0}^{M}$:

$$\begin{aligned}\mathbf{r}^k \equiv \mathbf{r}(t_k) &= e^{A_k \Delta t_k}\mathbf{r}^{k-1} + \mathbf{g}_k \\ &= e^{A_k \Delta t_k} \ldots e^{A_1 \Delta t_1}\mathbf{r}_0 + e^{A_k \Delta t_k} \ldots e^{A_2 \Delta t_2}\mathbf{g}_1 + \ldots + e^{A_k \Delta t_k}\mathbf{g}_{k-1} + \mathbf{g}_k,\end{aligned}$$

where

$$\mathbf{g}_k = (e^{A_k \Delta t_k} - \mathbb{I})A_k^{-1}\mathbf{b}, \quad \Delta t_k = t_k - t_{k-1},$$
$$A_k = B + B^u u_k + B^n n_k.$$

Gradient of the final state

Gradient of the objective functional is founded by the chain rule:

$$\frac{\delta \mathcal{F}}{\delta [u,n]} = \frac{\delta \mathcal{J}}{\delta \rho} \circ \frac{\delta \rho}{\delta \mathbf{r}} \circ \frac{\delta \mathbf{r}(T)}{\delta [u,n]}.$$

Theorem

If control is piecewise constant then the derivatives of the final state $\mathbf{r}(T) = \mathbf{r}^M$ with respect to the components of control u are

$$\frac{\partial \mathbf{r}(T)}{\partial u_j} = e^{A_N \Delta t_N} \dots e^{A_{j+1}\Delta t_{j+1}} \left[\frac{\partial}{\partial u_j} \left(e^{A_j \Delta t_j} \right) \mathbf{r}_{j-1} + \frac{\partial \mathbf{g}_j}{\partial u_j} \right],$$

Here the derivatives are given by

$$\frac{\partial \mathbf{g}_k}{\partial u_k} = \left(\frac{\partial}{\partial u_k} e^{A_k \Delta t_k} - (e^{A_k \Delta t_k} - \mathbb{I}) A_k^{-1} B^u \right) A_k^{-1} \mathbf{b},$$

$$\frac{\partial}{\partial u_k} e^{A_k \Delta t_k} = \Delta t_k \int_0^1 \exp(\alpha A_k \Delta t_k)\, B^u \exp((1-\alpha) A_k \Delta t_k) \mathrm{d}\alpha,$$

To diagonalize the matrix exponentials $e^{A_k \Delta t_k}$ consider the characteristic equation for $\frac{1}{\omega}A[u, n]$, which is a 3rd order algebraic equation with the known solution by the Cardano formula:

$$\lambda^3 + 4\hat{n}\lambda^2 + (5\hat{n}^2 + \hat{u}^2 + 1)\lambda + \hat{u}^2\hat{n} + 2\hat{n}^3 + 2\hat{n} = 0,$$

where

$$\hat{u} = \frac{2\mu u}{\omega}, \quad \hat{n} = \frac{\gamma}{\omega}\left(n + \frac{1}{2}\right).$$

The discriminant:

$$p = \frac{\hat{u}^2}{3} - \frac{\hat{n}^2}{9} + \frac{1}{3}, \quad q = -\frac{\hat{u}^2\hat{n}}{6} + \frac{\hat{n}^3}{27} + \frac{\hat{n}}{3},$$
$$\Delta = p^3 + q^2.$$

If $p \neq 0$:

$$\lambda_k = -\frac{4\hat{n}}{3} + \xi_k - \frac{p}{\xi_k}, \quad \xi_k = \sqrt[3]{-q + \sqrt{\Delta}}, \quad k = 1, 2, 3.$$

If $p = 0$:

$$\lambda_k = -\frac{4\hat{n}}{3} + \xi_k, \quad \xi_k = \sqrt[3]{-2q}, \quad k = 1, 2, 3. \tag{1}$$

Diagonalization of the matrix exponentials

If $\lambda \neq -\hat{n} \pm i \Leftrightarrow \hat{u} \neq 0$ then the eigenvector for the eigenvalue λ:

$$h_\lambda = \begin{pmatrix} \dfrac{\hat{u}}{1+(\hat{n}+\lambda)^2} \\ \dfrac{\hat{u}(\hat{n}+\lambda)}{1+(\hat{n}+\lambda)^2} \\ -1 \end{pmatrix},$$

For the Jordan chain:

$$h'_\lambda = \frac{\hat{u}}{[1+(\hat{n}+\lambda)^2]^2} \begin{pmatrix} -2(\hat{n}+\lambda) \\ 1-(\hat{n}+\lambda)^2 \\ 0 \end{pmatrix}, \tag{2}$$

$$h''_\lambda = \frac{\hat{u}}{[1+(\hat{n}+\lambda)^2]^3} \begin{pmatrix} 3(\hat{n}+\lambda)^2-1 \\ ((\hat{n}+\lambda)^2-3)(\hat{n}+\lambda) \\ 0 \end{pmatrix}. \tag{3}$$

The diagonalized matrix exponential:

$$e^{A\Delta t} = Se^{\Lambda\omega\Delta t}S^{-1}.$$

- **The case $\Delta \neq 0$.** Three different eigenvalues

$$\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3), \quad e^{\Lambda\omega\Delta t} = \mathrm{diag}(e^{\lambda_1\omega\Delta t}, e^{\lambda_2\omega\Delta t}, e^{\lambda_3\omega\Delta t}), \\ S = (h_{\lambda_1}, h_{\lambda_2}, h_{\lambda_3}).$$

- **The case $\Delta = 0$ ($|p|^2 + |q|^2 \neq 0$).** One root λ_1 with multiplicity 1 and one double root λ_2, thereby we construct the Jordan normal form.

$$\lambda_1 = -\frac{4\hat{n}}{3}, \quad \lambda_2 = -\frac{4\hat{n}}{3} + p.$$

$$h_{\lambda_1} = \begin{pmatrix} \dfrac{4}{1+\frac{\hat{n}^2}{9}} \\ -\dfrac{\hat{u}\hat{n}}{3(1+\frac{\hat{n}^2}{9})} \\ -1 \end{pmatrix}, \quad h_{\lambda_2} = \begin{pmatrix} \dfrac{\hat{u}}{1+\left(\frac{\hat{n}}{3}-p\right)^2} \\ \dfrac{\hat{u}\left(\frac{\hat{n}}{3}-p\right)}{1+\left(\frac{\hat{n}}{3}-p\right)^2} \\ -1 \end{pmatrix},$$

$$h'_{\lambda_2} = \frac{1}{\left[1+\left(\frac{\hat{n}}{3}-p\right)^2\right]^2} \begin{pmatrix} 2\left(\frac{\hat{n}}{3}-p\right) \\ 1-\left(\frac{\hat{n}}{3}-p\right)^2 \\ 0 \end{pmatrix}.$$

Thus

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 1 \\ 0 & 0 & \lambda_2 \end{pmatrix}, \quad e^{\Lambda\omega\Delta t} = \begin{pmatrix} e^{\lambda_1\omega\Delta t} & 0 & 0 \\ 0 & e^{\lambda_2\omega\Delta t} & \omega\Delta t\, e^{\lambda_2\omega\Delta t} \\ 0 & 0 & e^{\lambda_2\omega\Delta t} \end{pmatrix},$$

$$S = (h_{\lambda_1}, h_{\lambda_2}, h'_{\lambda_2}).$$

- **The case $p = q = 0$.** Triple root λ, in this case $\hat{u} = 2\sqrt{2}$, $\hat{n} = 3\sqrt{3}$ and

$$\lambda = -\frac{4\hat{n}}{3} = -4\sqrt{3}.$$

$$h_\lambda = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{\sqrt{3}}{\sqrt{2}} \\ -1 \end{pmatrix}, \quad h'_\lambda = \begin{pmatrix} \frac{\sqrt{3}}{2\sqrt{2}} \\ \frac{1}{2\sqrt{2}} \\ 0 \end{pmatrix}, \quad h''_\lambda = \begin{pmatrix} \frac{1}{2\sqrt{2}} \\ 0 \\ 0 \end{pmatrix}.$$

Then

$$\Lambda = \begin{pmatrix} \lambda & 1 & 0 \\ 0 & \lambda & 1 \\ 0 & 0 & \lambda \end{pmatrix}, \quad e^{\Lambda\omega\Delta t} = e^{\lambda\omega\Delta t} \begin{pmatrix} 1 & \omega\Delta t & \frac{(\omega\Delta t)^2}{2} \\ 0 & 1 & \omega\Delta t \\ 0 & 0 & 1 \end{pmatrix}, \quad S = (h_\lambda, h'_\lambda, h''_\lambda).$$

Exact solution for the case $u = 0$

Proposition

Coherent control equals zero $\hat{u} = 0$ if and only if the characteristic equation (14) has roots $\lambda = -\hat{n} \pm i$:

$$\hat{u} = 0 \Longleftrightarrow \lambda = -\hat{n} \pm i.$$

If $\hat{u} = 0$ the matrix exponential takes the comprehensible form:

$$e^{A\Delta t} = \begin{pmatrix} e^{-\hat{n}\omega\Delta t}\cos(\hat{n}\omega\Delta t) & e^{-\hat{n}\omega\Delta t}\sin(\hat{n}\omega\Delta t) & 0 \\ -e^{-\hat{n}\omega\Delta t}\sin(\hat{n}\omega\Delta t) & e^{-\hat{n}\omega\Delta t}\cos(\hat{n}\omega\Delta t) & 0 \\ 0 & 0 & e^{-2\hat{n}\omega\Delta t}. \end{pmatrix}$$

Thus it simply describes an exponentially decaying rotation in the xy-plane and exponential decay along z-axis in case $\hat{n} > 0$.
Then the exact evolution is as follows:

$$\mathbf{r} = \begin{pmatrix} e^{-\hat{n}\omega\Delta t}\cos(\hat{n}\omega\Delta t) & e^{-\hat{n}\omega\Delta t}\sin(\hat{n}\omega\Delta t) & 0 \\ -e^{-\hat{n}\omega\Delta t}\sin(\hat{n}\omega\Delta t) & e^{-\hat{n}\omega\Delta t}\cos(\hat{n}\omega\Delta t) & 0 \\ 0 & 0 & e^{-2\hat{n}\omega\Delta t} \end{pmatrix} \mathbf{r}_0 + \begin{pmatrix} 0 \\ 0 \\ \dfrac{1 - e^{-2\hat{n}\omega\Delta t}}{2\hat{n} + 1} \end{pmatrix}.$$

The condition $\hat{\gamma} = 0$ corresponds to the case when the system is isolated from the environment. In this case $\hat{n} = 0$ and

$$\lambda = 0,\ \pm i\sqrt{1+u^2}.$$

$$e^{A\Delta t} = \begin{pmatrix} \dfrac{\hat{u}^2 + \cos(\bar{\omega}\Delta t)}{1+\hat{u}^2} & \dfrac{\sin(\bar{\omega}\Delta t)}{\sqrt{1+\hat{u}^2}} & \dfrac{\hat{u}}{1+\hat{u}^2}(-1+\cos(\bar{\omega}\Delta t)) \\ -\dfrac{\sin(\bar{\omega}\Delta t)}{\sqrt{1+\hat{u}^2}} & \cos(\bar{\omega}\Delta t) & -\dfrac{\hat{u}}{\sqrt{1+\hat{u}^2}}\sin(\bar{\omega}\Delta t) \\ \dfrac{\hat{u}}{1+\hat{u}^2}(-1+\cos(\bar{\omega}\Delta t)) & \dfrac{\hat{u}}{\sqrt{1+\hat{u}^2}}\sin(\bar{\omega}\Delta t) & \dfrac{1+\hat{u}^2\cos(\bar{\omega}\Delta t)}{1+\hat{u}^2}, \end{pmatrix}$$

where $\bar{\omega} = \omega\sqrt{1+\hat{u}^2}$. The corresponding evolution of the Bloch vector is

$$\mathbf{r} = e^{A\Delta t}\mathbf{r}_0.$$

This result coincides with the known result for closed dynamics[8].

[8] B. O. Volkov, O. V. Morzhin, A. N. Pechen, "Quantum control landscape for ultrafast generation of single-qubit phase shift quantum gates", J. Phys. A: Math. Theor., **54**:21 (2021), 215303

Objective – state-to-state control (controllability):

$$\mathcal{F}[u,n] = \mathcal{J}(\rho_T^{u,n}) = \|\rho_T^{u,n} - \rho_{target}\|_{\mathrm{HS}} = |\mathbf{r}_T^{u,n} - \mathbf{r}_{target}| \to \inf$$

Constraint: $n \geq 0$ Unconstrained control: $n = w^2$
Gradient descent method:

$$(u^{(k+1)}, w^{(k+1)}) = (u^{(k)}, w^{(k)}) - h_k \mathrm{grad}_{u,w} \mathcal{F}[u^{(k)}, {w^{(k)}}^2].$$

Stopping criterion: $\mathcal{F}_k = \mathcal{F}[u^{(k)}, {w^{(k)}}^2] < \varepsilon.$
$\omega = 1$, $\mu = 0.1$, $\gamma = 0.01$, $T = 5$;
$\varepsilon = 10^{-3}$,
N $= 10$

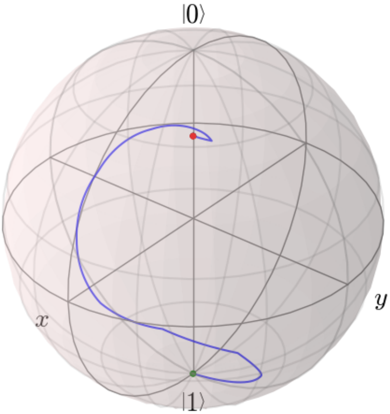
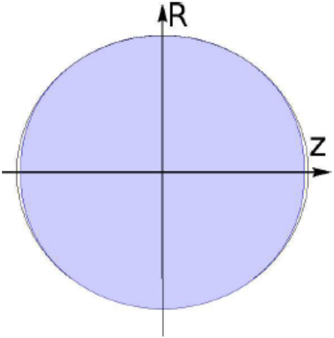
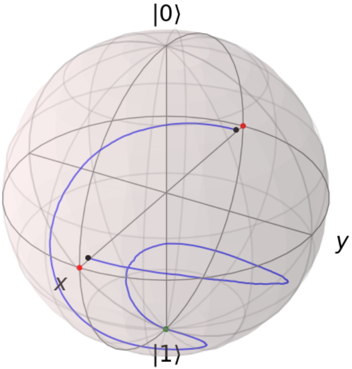


Рис.: Steering from $\mathbf{r}_0 = (0, 0, -1)$ (green point) to $\mathbf{r}_{\text{target}} = (0, 0, 0.5)$ (red point). Dynamics of Bloch vector $\mathbf{r}$ under optimal control.

Set of attainability[9]: there are some "lacunes" — regions with size of $\sim \frac{\gamma}{\omega}$ close to $(\pm 1, 0, 0)$ which cannot be attained. $\mathbf{r}_0 = (0, 0, -1)$, $\mathbf{r}_{\mathrm{target}_{1,2}} = (\pm 1, 0, 0)$.





[9] L. Lokutsievskiy and A. Pechen. Reachable sets for two-level open quantum systems driven by coherent and incoherent controls. Journal of Physics A: Mathematical and Theoretical, 54(39):395304, sep 2021.

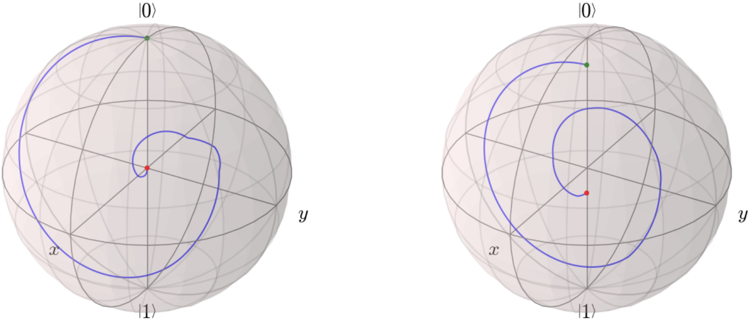
Master-equation for the two-qubit system[10,11]:

$$\frac{d\rho(t)}{dt} = -i\left[H_S + \varepsilon H_{\mathrm{eff},n(t)} + Vu(t), \rho(t)\right] + \varepsilon \mathcal{L}_{n(t)}(\rho(t)),$$

$$\begin{aligned}
H_S &= \frac{\omega_1}{2}\left(\sigma^z \otimes \mathbb{I}_2\right) + \frac{\omega_2}{2}\left(\mathbb{I}_2 \otimes \sigma^z\right), \\
H_{\mathrm{eff},n(t)} &= \Lambda_1 n_{\omega_1}(t)\left(\sigma^z \otimes \mathbb{I}_2\right) + \Lambda_2 n_{\omega_2}(t)\left(\mathbb{I}_2 \otimes \sigma^z\right), \\
V &= \sigma^x \otimes \mathbb{I}_2 + \mathbb{I}_2 \otimes \sigma^x, \\
\mathcal{L}_{n(t)}(\rho(t)) &= \mathcal{L}_{n(t),1}(\rho(t)) + \mathcal{L}_{n(t),2}(\rho(t)), \\
\mathcal{L}_{n(t),j}(\rho(t)) &= \Omega_j(n_{\omega_j}(t)+1)\left(2\sigma_j^- \rho \sigma_j^+ - \sigma_j^+\sigma_j^-\rho - \rho\sigma_j^+\sigma_j^-\right) \\
&\quad + \Omega_j n_{\omega_j}(t)\left(2\sigma_j^+ \rho \sigma_j^- - \sigma_j^-\sigma_j^+\rho - \rho\sigma_j^-\sigma_j^+\right), \; j = 1, 2.
\end{aligned}$$

[10] O.V. Morzhin, A.N. Pechen. Maximization of the overlap between density matrices for a two-level open quantum system driven by coherent and incoherent controls. *Lobachevskii J. Math.* **40** (10), 1532–1548 (2019).

[11] Petruhanov V.N., Pechen A.N. Optimal control for state preparation in two-qubit open quantum systems driven by coherent and incoherent controls via GRAPE approach (submitted).



(a) (b)

Рис.: Two qubit system: steering from $\rho_0 = \mathrm{diag}(0.9, 0.1, 0, 0)$ to $\rho_{\mathrm{target}} = \mathrm{diag}(0.2, 0.3, 0.2, 0.3)$. First (a) and second qubit (b).

Gradient and Hessian in L^2 control space

Consider the general case of system driven by a control $f(t) \in L^2$:

$$\dot{\rho}_t^f = \mathcal{L}_t^f \rho_t = [\mathcal{K}_t + f(t)\mathcal{N}_t]\rho_t^f.$$

Solution:

$$\rho_t^f = V_t^f \rho_0.$$

Functional of the final state dependent on control:

$$\mathcal{F}^f = \mathcal{J}(\rho_T^f) = \mathcal{J}(V_T^f \rho_0). \tag{4}$$

Theorem

Gradient and Hessian of functional (4) equal

$$\frac{\delta \mathcal{F}^f}{\delta f(t)} = \frac{\delta \mathcal{J}}{\delta \rho}\left(\rho_T^f\right) \circ V_T^f \mathcal{N}_t^f \rho_0,$$

$$\frac{\delta^2 \mathcal{F}^f}{\delta f(t_1)\,\delta f(t_2)} = \frac{\delta \mathcal{J}}{\delta \rho}\left(\rho_T^f\right) \circ V_T^f \hat{T}\{\mathcal{N}_{t_1}^f \mathcal{N}_{t_2}^f\}\rho_0 + \frac{\delta^2 \mathcal{J}}{\delta \rho^2}\left(V_T^f \mathcal{N}_{t_1}^f \rho_0, V_T^f \mathcal{N}_{t_2}^f \rho_0\right),$$

where $\mathcal{N}_t^f = {V_t^f}^{-1} \mathcal{N}_t V_t^f$.

Thank you!