Optimization of state transfer and exact dynamics for the open two-level quantum system.

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Quantum control

Master equation (GKSL) with control[a]

$$\frac{\partial\rho}{\partial t} = \mathcal{L}(\rho) = -i[H_0 + \sum_k u_k V_k, \rho] + \mathcal{L}_n(\rho),$$

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

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

[b] E.B. Davies. Quantum theory of open systems. *Academic Press* (1976).

[c] Luigi Accardi, Yun Gang Lu, Igor Volovich. Quantum Theory and Its Stochastic Limit. *Springer* (2002).

The control goal: optimizing the certain objective Mayer-type functional:

$$\mathcal{F}[u,n] = \mathcal{J}(\rho^{u,n}(T)).$$

Main objectives in quantum control:

- maximizing/minimizing observable mean value: $\mathcal{F}_O[u,n] = Tr(\rho^{u,n}(T)O) \to \sup/\inf$;
- state transfer[1]: $\mathcal{F}_{\rho_{target}}[u,n] = \|\rho^{u,n}(T) - \rho_{target}\|^2 \to \inf.$

In quantum control they use various numeric optimization methods, e.g. GRAPE[2], BFGS[3,], CRAB, etc. Many of this methods consider some finite-dimensional class of control, for instance piecewise constant functions, and utilize gradient for optimization by linear search.

Therefore we studied dynamics of the system with piecewise constant control.

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[1] Vadim N. Petruhanov, Alexander N. Pechen, "Optimal control for state preparation in two-qubit open quantum systems driven by coherent and incoherent controls via GRAPE approach", Int. J. Mod. Phys. A, 37:20-21 (2022), 2243017.

[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).

Consider the two-level open quantum system[4]:

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

where

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

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

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

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

[4] 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 $\mathbf{r} = (r_x, r_y, r_z)$, B, B^u, $B^n \in \mathbb{C}^{3\times 3}$, $b \in \mathbb{C}^3$.
Consider PConst control:

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

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

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

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

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

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

$$\frac{\partial}{\partial u_k} e^{A_k \Delta t_k} = \Delta t_k \int\limits_0^1 \exp(\alpha A_k \Delta t_k)\, B^u \exp((1-\alpha) A_k \Delta t_k) \mathrm{d}\alpha,$$

Diagonalization of the matrix exponentials

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:

$$\Delta = \frac{\hat{u}^6}{27} - \frac{\hat{u}^4\hat{n}^2}{108} + \frac{\hat{u}^4}{9} - \frac{5\hat{u}^2\hat{n}^2}{27} + \frac{\hat{n}^4}{27} + \frac{\hat{u}^2}{9} + \frac{2\hat{n}^2}{27} + \frac{1}{27}.$$

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

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

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

- **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.

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

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

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

Diagonalization of matrix exponential

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 (7) has roots $\lambda = -n \pm i$:

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

Proof

Then one real root is already factorized:

$$\det(A - \lambda\mathbb{I}) = -((\hat{n} + \lambda)^2 + 1)(2\hat{n} + \lambda) = 0.$$

Thus one root is $\lambda = -2\hat{n}$ and other two roots are complex conjugate $\lambda = -n \pm i$.

Conversely, let characteristic equation (7) have two complex conjugate roots $\lambda = -n \pm i$. Implementing Viet formula to the coefficient at λ^2:

$$-2\hat{n} + \lambda_3 = -4\hat{n}$$

we get that the third root is $\lambda = -2\hat{n}$. Now write Viet formula for the coefficient at λ:

$$5\hat{n}^2 + 1 = 5\hat{n}^2 + \hat{u}^2 + 1,$$

$$0 = \hat{u}^2.$$

Thus we get that $\hat{u} = 0$.

Exact solution for the case $u = 0$

Then 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:

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

Exact solution for the case $\gamma = 0$

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

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

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

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[5].

[5] 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

Conclusion

Optimization of quantum open dynamics often considered in piecewise constant control functional class. Thereby we studied gradient and dynamics for the open two-level quantum system with piecewise constant coherent and incoherent controls.

We derived the expressions for gradient and dynamics through matrix exponentials. Moreover, we diagonalized the matrix exponentials by finding eigenvalues and eigenvectors of the r.h.s matrix in Bloch parameterization. The low dimension ($\dim = 3$) of the system allows to right the exact expressions for the eigenvalues and the eigenvectors. We rigorously examined all possible root locations, constructed the Jordan normal forms, and checked the case of the absence of interaction with the environment.

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