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DYNAMIC SYSTEMS AND OPTIMAL CONTROL

Research article

Krotov Type Optimization of Coherent and Incoherent Controls for Open Two-Qubit Systems

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Abstract.   This work considers two-qubit open quantum systems driven by coherent and incoherent controls. Incoherent control induces *time-dependent decoherence rates* via time-dependent spectral density of the environment which is used as a resource for controlling the system. The system evolves according to the Gorini–Kossakowski–Sudarshan–Lindblad master equation with time-dependent coefficients. For two types of interaction with coherent control, three types of objectives are considered: 1) maximizing the Hilbert–Schmidt overlap between the final and target density matrices; 2) minimizing the Hilbert–Schmidt distance between these matrices; 3) steering the overlap to a given value. For the first problem, we develop the Krotov type methods directly in terms of density matrices with or without regularization for piecewise continuous controls with constaints and find the cases where the methods produce (either exactly or with some precision) zero controls which satisfy the Pontryagin maximum principle and produce the overlap's values close to their upper bounds. For the problems 2) and 3), we find cases when the dual annealing method steers the objectives close to zero and produces a non-zero control.

Keywords: open quantum system, incoherent quantum control, nonlocal improvement, optimization

Научная статья

Оптимизация типа Кротова когерентного и некогерентного управлений для открытых двухкубитных систем

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Аннотация. Рассмотрены двухкубитные открытые квантовые системы с когерентным и некогерентным управлениями, где второе индуцирует *зависящие от времени скорости декогеренции* через зависящую от времени спектральную плотность окружения, используемую здесь как ресурс для управления системой. Система эволюционирует согласно мастер-уравнению Горини – Косаковского – Сударшана – Линдблада с зависящими от времени коэффициентами. Для двух типов взаимодействия с когерентным управлением рассмотрены три типа критериев: 1) максимизация перекрытия Гильберта – Шмидта между финальной и целевой матрицами плотности; 2) минимизация расстояния Гильберта – Шмидта между этими матрицами; 3) стремление перекрытия к заданному значению. Для первой задачи развиваем методы типа Кротова в терминах матриц плотности с регуляризацией и без для кусочно-непрерывных управлений с ограничениями и находим случаи, где методы дают (либо точно, либо с некоторой точностью) нулевые управления, которые удовлетворяют принципу максимума Понтрягина и дают значения перекрытия, близкие к верхним границам. Для задач 2) и 3) найдены случаи, когда метод двойного отжига делает критерии близкими к нулю и дает ненулевое управление.

Ключевые слова: открытая квантовая система, некогерентное квантовое управление, нелокальное улучшение, оптимизация

*Dedicated to the 90th anniversary of the birth and to the memory
of Vadim Fedorovich Krotov (1932–2015)*

1. Introduction

Optimal control of quantum systems attracts high interest due to various applications ranging from quantum computing to laser chemistry [18]. In many situations, controlled quantum systems are open, i.e., interacting with the environment. While in some situations the environment is treated as an obstacle, in other cases it can be a useful control resource, as for example was proposed to do via *incoherent control* in [30; 31], where spectral (generally time-dependent and non-equilibrium) density of incoherent photons is used as control function jointly with *coherent control* by lasers to manipulate the quantum system dynamics.

In the approach of [30], which is used in the present work, the incoherent control induces *time-dependent decoherence rates* $\gamma_k(t)$ via *time-dependent spectral density of the environment* $n(t)$, in addition to coherent control u, so that density matrix evolves according to the master equation

$$\dot{\rho}(t) = -i[H_0 + H_{c(t)}, \rho(t)] + \sum_k \gamma_k(t)\mathcal{D}_k(\rho(t)), \qquad (1.1)$$

where H_0 is the free Hamiltonian, $H_{c(t)}$ is the Hamiltonian induced by control $c = (u, n)$, $\mathcal{D}_k$ is a Gorini–Kossakowski–Sudarshan–Lindblad (GKSL) dissipator, and $[A, B] = AB - BA$ is the commutator of matrices A and B. In addition to general consideration, two physical classes of the environment were exploited — incoherent photons and quantum gas, with two explicit forms of $\mathcal{D}_k$ derived in the weak coupling limit (WCL) and low density limit, respectively. In [31], it was shown that for the master equation (1.1) with $\mathcal{D}_k$ derived in the WCL (describing atom interacting with photons) generic N-level quantum systems become approximately completely controllable in the set of density matrices. Following this general approach, various control problems for one- and two-qubit open systems controlled by simultaneous coherent and incoherent controls were considered [24; 27; 33].

Various tools are used in quantum optimal control such as Pontryagin maximum principle (PMP) [4], Krotov type methods [11; 13; 15; 21; 26; 37], [20, § 6.5]), Hamilton–Jacobi–Bellmann equation [12], Zhu–Rabitz [39] method, GRadient Ascent Pulse Engineering (GRAPE) [13;17;33], GRAPE with quasi-Newton optimizers [9], speed gradient method [32], gradient free Chopped RAndom Basis (CRAB) optimization [8], genetic algorithms [14;30], machine learning [10]. *Riemannian gradient optimization* approach over *complex Stiefel manifolds* for controlling open quantum systems for quantum technologies was developed in [29].

Theory of optimal control contains the approach based on deriving special *nonlocal exact increment formulas* and constructing the corresponding

tools for various problems (e.g., [2;3;5;6;25;35]). For the problems linear in real-valued states (including bilinear), e.g., the x- and ψ-procedures (ψ is co-state) ([35, Ch. 1], [38, § 5.4], [5, pp. 15–16, 31–32], [3, Sec. 3]) are known, where the x-procedure is an adaptation of the general Krotov method (see about this method, e.g., [19], [20, Ch. 6]) without regularization, while the ψ-procedure is symmetrical one.

This article considers two-qubit ($N = 4$) open quantum systems evolving according to the GKSL master equation with simultaneous coherent and incoherent controls, with two types of interaction with coherent control. Sec. 2 considers three types of objectives: 1) maximizing the overlap $\langle \rho(T), \rho_{\text{target}} \rangle$; 2) minimizing $\|\rho(T) - \rho_{\text{target}}\|$; 3) steering the overlap to a given $M \in (0, 1)$, i.e. minimizing $|\langle \rho(T), \rho_{\text{target}} \rangle - M|$. In Sec. 3, we develop for the problem 1) the Krotov type methods in terms of density matrices with or without regularization for piecewise continuous controls with constraints and find the cases where the methods produce (either exactly or with some precision) zero controls which satisfy the PMP and produce overlap's values which, for sufficiently large T, are close to $\max_{\rho} \langle \rho, \rho_{\text{target}} \rangle$.

In Sec. 4, for the problems 2) and 3), we use a parameterized class of controls and find cases when the dual annealing method steers objectives close to zero and produces non-zero control. Sec. 5 resumes the article.

2. Two-Qubit System and Objective Functionals

For two qubits, the Hilbert space is $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$. Consider the following GKSL master equation with coherent and incoherent controls:

$$\dot{\rho}(t) = -i\big[H_0 + H_{c(t)}, \rho(t)\big] + \varepsilon \mathcal{L}^D_{n(t)}(\rho(t)), \quad \rho(0) = \rho_0, \quad t \in [0, T], \quad (2.1)$$

where $\rho(t) : \mathcal{H} \to \mathcal{H}$ is density matrix (positive semi-definite, $\rho(t) \geq 0$, with unit trace, $\mathrm{Tr}\rho(t) = 1$); the parameter $\varepsilon > 0$ describes strength of the coupling between the system and its environment; the Hamiltonian $H_{c(t)} = \varepsilon H_{\text{eff},n(t)} + H_{u(t)}$, where scalar coherent control u and incoherent control $n = (n_1, n_2)$ are considered as piecewise continuous on $[0, T]$, control $c = (u, n)$; effective Hamiltonian $H_{\text{eff},n(t)}$ depends on $n(t)$ and describes the Lamb shift, Hamiltonian $H_{u(t)}$ describes interaction with $u(t)$, $\mathcal{L}^D_{n(t)}(\rho(t))$ is the controlled superoperator of dissipation, ρ_0 is the initial density matrix. The system of units is such that the Planck's constant $\hbar = 1$. Consider

$$H_0 := H_{0,1} + H_{0,2}, \quad H_{0,j} := \frac{\omega_j}{2} W_j, \quad W_1 := \sigma_z \otimes \mathbb{I}_2, \quad W_2 := \mathbb{I}_2 \otimes \sigma_z,$$

$$H_{\text{eff},n(t)} := \sum_{j=1}^{2} H_{\text{eff},n_j(t)}, \quad H_{\text{eff},n_j(t)} := \Lambda_j n_j(t) W_j, \quad H_{u(t)} := V u(t),$$

$$V = V_1 := Q_1 \otimes \mathbb{I}_2 + \mathbb{I}_2 \otimes Q_2 \quad \text{or} \quad V = V_2 := Q_1 \otimes Q_2,$$

$$Q_j := \sum_{\alpha=x,y,z} \lambda^j_\alpha \sigma_\alpha = \sin\theta_j \cos\varphi_j \sigma_x + \sin\theta_j \sin\varphi_j \sigma_y + \cos\theta_j \sigma_z,$$

where $j = 1, 2$, the parameters ω_j, $\Lambda_j > 0$, $\lambda^j := (\lambda^j_x, \lambda^j_y, \lambda^j_z) \in \mathbb{R}^3$ is a given unit vector, $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, and $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ are Pauli matrices. The work [28] considers the case $Q_1 = Q_2 = \sigma_x$, or, equivalently, $\theta_j = \pi/2$ and $\varphi_j = 0$.

The superoperator of dissipation acts on $\rho(t)$ as

$$\mathcal{L}^D_{n(t)}(\rho(t)) := \sum_{j=1}^{2} \left[\Omega_j \left(n_j(t) + 1 \right) \left(2\sigma^-_j \rho(t)\sigma^+_j - \left\{ \sigma^+_j \sigma^-_j, \rho(t) \right\} \right) \right.$$
$$\left. + \Omega_j n_j(t) \left(2\sigma^+_j \rho(t)\sigma^-_j - \left\{ \sigma^-_j \sigma^+_j, \rho(t) \right\} \right) \right],$$

where the parameters $\Omega_j > 0$, $j = 1, 2$; $\{A, B\} = AB + BA$ denotes anti-commutator of matrices A and B. The matrices $\sigma^\pm_1 = \sigma^\pm \otimes \mathbb{I}_2$, $\sigma^\pm_2 = \mathbb{I}_2 \otimes \sigma^\pm$ are obtained with $\sigma^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$, $\sigma^- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$, $\mathbb{I}_2$ is the 2×2 identity matrix.

Set the following constraints including the required $n_j(t) \geq 0$:

$$|u(t)| \leq \mu, \quad 0 \leq n_j(t) \leq n_{\max}, \quad j = 1, 2, \quad \mu,\, n_{\max} > 0,\; t \in [0, T]. \quad (2.2)$$

For the system (2.1), consider the control objectives

$$J_1(c) := \langle \rho(T), \rho_{\text{target}} \rangle = \text{Tr}(\rho(T)\rho_{\text{target}}) \to \sup \quad \text{(fixed } T > 0), \quad (2.3)$$
$$J_2(c, T) := T + P\|\rho(T) - \rho_{\text{target}}\| \to \inf, \quad (2.4)$$
$$J_3(c, T) := T + P|\langle \rho(T), \rho_{\text{target}} \rangle - M| \to \inf, \quad M \in (0, 1), \quad (2.5)$$

where the Hilbert–Schmidt distance is $\|\rho - \sigma\| = \left[\text{Tr}\left((\rho - \sigma)^2 \right) \right]^{1/2}$, $\rho(T)$ is the final state for given controls u, n; $P > 0$ is some penalty coefficient.

For (2.4) and (2.5), consider the following parameterized class of controls (inspired by CRAB [8] and (12) from [16]):

$$u(t) = \exp\left(-h_u \left(t - T/2 \right)^2 \right) \sum_{k=1}^{K} \left(A_k \sin(\nu_k t) + B_k \cos(\nu_k t) \right), \quad (2.6)$$
$$n_j(t) = C_j \exp\left(-h_{n_j} \left(t - T/2 \right)^2 \right), \quad j = 1, 2, \quad (2.7)$$

where K and $\nu_1, \ldots, \nu_K$ are given. The parameters h_u, h_{n_1}, h_{n_2}, $A_1, \ldots, A_K$, $B_1, \ldots, B_K$, and C_1, C_2 are bounded from above and below, where the zero lower bound for C_j is required and other bounds are arbitrary.

3. Krotov Type Methods for Maximizing the Overlap

For (2.3), introduce the auxiliary objective

$$I^\alpha(c; c^{(k)}) := I(c) + \frac{\widehat{\alpha}}{2\alpha}\|c - s\ c^{(k)}\|^2_{L^2[0,T]} \to \inf, \quad I(c) := b - J_1(c), \ (3.1)$$

where $b \in \{\max_\rho\langle\rho, \rho_{\text{target}}\rangle, 1\}$, $\alpha > 0$, $\widehat{\alpha} \in \{0, 1\}$ turns off and on the regularization; $c^{(k)} = (u^{(k)}, n_1^{(k)}, n_2^{(k)})$ is a given control, $s \in \{0, 1\}$ switches between the two regularization's types. The works [21], [20, § 6.5] for the Schrödinger equation consider both presence and absence of regularization (with $s = 0$ in our terms). The case $s = 0$ also reminds [37], where the Schrödinger equation is considered. The case $s = 1$ reminds the regularization in [35, p. 61] leading to the projection improvement procedures under constrained control; also this case reminds the regularized Krotov type methods used in [11; 13] for various quantum problems.

3.1. Pontryagin Function and Krotov Lagrangian

For (3.1), the corresponding Pontryagin function is

$$h^\alpha(t, \chi, \rho, c) = \left\langle\chi, -i[H_c, \rho] + \varepsilon\mathcal{L}_n^D(\rho)\right\rangle - \frac{\widehat{\alpha}}{2\alpha}\|c - sc^{(k)}(t)\|^2_2 =$$

$$= \left\langle\mathcal{K}^c(\chi, \rho), c\right\rangle - \frac{\widehat{\alpha}}{2\alpha}\|c - sc^{(k)}(t)\|^2_2 + \overline{h}(\chi, \rho),$$

where χ and ρ are 4×4 density matrices; $c = (u, n_1, n_2) \in \mathbb{R}^3$; the function $\mathcal{K}^c = (\mathcal{K}^u, \mathcal{K}^{n_1}, \mathcal{K}^{n_2})$ consists of $\mathcal{K}^u(\chi, \rho) = \langle\chi, -i[V, \rho]\rangle$ and

$$\mathcal{K}^{n_j}(\chi, \rho) = \left\langle\chi, -i[\Lambda_j W_j, \rho] + \varepsilon\Omega_j\left(2\sigma_j^- \rho\sigma_j^+ + 2\sigma_j^+ \rho\sigma_j^- - \{\mathbb{I}_4, \rho\}\right)\right\rangle$$

(the 4×4 identity matrix $\mathbb{I}_4$ appears in $\mathcal{K}^{n_j}$ since $\sigma_j^+ \sigma_j^- + \sigma_j^- \sigma_j^+ = \mathbb{I}_4$), $j = 1, 2$; the term

$$\overline{h}(\chi, \rho) = \left\langle\chi, -i[H_S, \rho] + \varepsilon\sum_{j=1}^2 \Omega_j\left(2\sigma_j^- \rho\sigma_j^+ - \{\sigma_j^+ \sigma_j^-, \rho\}\right)\right\rangle.$$

The Krotov Lagrangian for our problem is

$$L^\alpha(c, \rho) = G(\rho(T)) - \int_0^T R^\alpha(t, \rho(t), c(t))dt,$$

$$G(\rho(T)) = b - \langle\rho(T), \rho_{\text{target}}\rangle + \langle\chi(T), \rho(T)\rangle - \langle\chi(0), \rho_0\rangle,$$

$$R^\alpha(t, \rho, c) = \left\langle\chi(t), -i[H_c, \rho] + \varepsilon\mathcal{L}_n^D(\rho)\right\rangle + \langle\dot\chi(t), \rho\rangle - \frac{\widehat{\alpha}}{2\alpha}\|c - sc^{(k)}(t)\|^2_2.$$

The function χ is defined in Sec. 3.3. Note that $\int_0^T R^\alpha(t, \rho(t), c(t))dt$ is

$$\int_0^T \left(\frac{d}{dt}\langle \chi(t), \rho(t) \rangle - \frac{\widehat{\alpha}}{2\alpha}\|c(t) - sc^{(k)}(t)\|_2^2 \right) dt = \langle \chi(t), \rho(t) \rangle|_0^T -$$

$$- \frac{\widehat{\alpha}}{2\alpha}\|c - sc^{(k)}\|_{L^2[0,T]}^2 = G(\rho(T)) - b + \langle \rho(T), \rho_{\text{target}} \rangle -$$

$$- \frac{\widehat{\alpha}}{2\alpha}\|c - sc^{(k)}\|_{L^2[0,T]}^2, L^\alpha(c, \rho) = b - \langle \rho(T), \rho_{\text{target}} \rangle + \frac{\widehat{\alpha}}{2\alpha}\|c - sc^{(k)}\|_{L^2[0,T]}^2.$$

3.2. INCREMENT FORMULAS

Consider increment of L^α at (admissible) controls $c, c^{(k)}$:

$$L^\alpha(c, \rho) - L^\alpha(c^{(k)}, \rho^{(k)}) = G(\rho(T)) - G(\rho^{(k)}(T)) - \int_0^T (R^\alpha(t, \rho(t), c(t)) -$$

$$- R^\alpha(t, \rho^{(k)}(t), c^{(k)}(t)))dt, \tag{3.2}$$

where the process $(c^{(k)}, \rho^{(k)})$ is either given or obtained at the previous iteration. Following the idea of [19], set the conditions

$$G(\rho(T)) \leq G(\rho^{(k)}(T)) \quad \text{and} \quad R^\alpha(t, \rho(t), c(t)) \geq R^\alpha(t, \rho^{(k)}(t), c^{(k)}(t))$$

to make $L^\alpha(c, \rho) \leq L^\alpha(c^{(k)}, \rho^{(k)})$. To satisfy the inequality condition for G, we simply take $G(\rho(T)) = G(\rho^{(k)}(T))$ that gives

$$G(\rho(T)) - G(\rho^{(k)}(T)) = \langle \chi(T) - \rho_{\text{target}}, \rho(T) - \rho^{(k)}(T) \rangle = 0$$

and, as the result, implies *the transversality condition* $\chi(T) = \rho_{\text{target}}$.

We can represent the integrand in (3.2) as $\Delta_1 R^\alpha + \Delta_2 R$, where

$$\Delta_1 R^\alpha = R^\alpha(t, \rho(t), c(t)) - R^\alpha(t, \rho(t), c^{(k)}(t)),$$

$$\Delta_2 R = R^\alpha(t, \rho(t), c^{(k)}(t)) - R^\alpha(t, \rho^{(k)}(t), c^{(k)}(t)).$$

Here $\Delta_1 R^\alpha$ and $\Delta_2 R$ are constructed similarly to [19], [20, p. 243]. Then

$$\Delta_2 R = \langle \chi(t), -i[H_{c^{(k)}(t)}, \rho(t) - \rho^{(k)}(t)] + \varepsilon(\mathcal{L}_{n^{(k)}(t)}^D(\rho(t))$$

$$- \mathcal{L}_{n^{(k)}(t)}^D(\rho^{(k)}(t)))\rangle + \langle \dot\chi(t), \rho(t) - \rho^{(k)}(t) \rangle = \langle \rho(t) - \rho^{(k)}(t),$$

$$= i[H_{c^{(k)}(t)}, \chi(t)] + \dot\chi(t) \rangle + \varepsilon \langle \chi(t), \mathcal{L}_{n^{(k)}(t)}^D(\rho(t)) - \mathcal{L}_{n^{(k)}(t)}^D(\rho^{(k)}(t)) \rangle,$$

where the anticommutativity property of commutator and cyclic permutation of matrices under trace are used. To satisfy the condition $\Delta_2 R \geq 0$, let $\Delta_2 R = 0$. Transform the last term in $\Delta_2 R$, which is

$$\varepsilon \Big\langle \chi(t), \sum_{j=1}^2 \Big[\Big(\Omega_j(n_j^{(k)}(t) + 1)(2\sigma_j^- \rho(t)\sigma_j^+ - \{\sigma_j^+\sigma_j^-, \rho(t)\}) + \Omega_j n_j^{(k)}(t) \times$$

$$\times (2\sigma_j^+ \rho(t)\sigma_j^- - \{\sigma_j^-\sigma_j^+, \rho(t)\}) \Big) - \Big(\Omega_j(n_j^{(k)}(t) + 1)(2\sigma_j^- \rho^{(k)}(t)\sigma_j^+ -$$

$$- \{\sigma_j^+\sigma_j^-, \rho^{(k)}(t)\}) + \Omega_j n_j^{(k)}(t)(2\sigma_j^+ \rho^{(k)}(t)\sigma_j^- - \{\sigma_j^-\sigma_j^+, \rho^{(k)}(t)\}) \Big) \Big] \Big\rangle$$

to $\varepsilon\langle \mathcal{L}^{D,\dagger}_{n^{(k)}(t)}(\chi(t)), \rho(t) - \rho^{(k)}(t)\rangle$ with

$$\mathcal{L}^{D,\dagger}_{n^{(k)}(t)}(\chi(t)) := \sum_{j=1}^{2}\left[\Omega_j\left(n_j^{(k)}(t)+1\right)\left(2\sigma_j^+\chi(t)\sigma_j^- - \left\{\sigma_j^+\sigma_j^-, \chi(t)\right\}\right)+ \right.$$
$$\left. +\Omega_j n_j^{(k)}(t)\left(2\sigma_j^-\chi(t)\sigma_j^+ - \left\{\sigma_j^-\sigma_j^+, \chi(t)\right\}\right)\right],$$

here "$\dagger$" reflects that $\langle\chi(t), T_1(\rho(t)) - T_1(\rho^{(k)}(t))\rangle = \langle T_1^{\dagger}(\chi(t)), \rho(t) - \rho^{(k)}(t)\rangle$ and $\langle\chi(t), T_2(\rho(t)) - T_2(\rho^{(k)}(t))\rangle = \langle T_2^{\dagger}(\chi(t)), \rho(t) - \rho^{(k)}(t)\rangle$, where the operators $T_1 := 2\sigma_j^- \cdot \sigma_j^+$, $T_2 := 2\sigma_j^+ \cdot \sigma_j^-$ and $(\sigma_j^+)^{\top} = \sigma_j^-$, $(\sigma_j^-)^{\top} = \sigma_j^+$; note that $\sigma_j^+\sigma_j^-$, $\sigma_j^-\sigma_j^+$ are Hermitian. See also [11]. The condition $\Delta_2 R = 0$ leads to the *adjoint system*

$$\dot{\chi}^{(k)}(t) = -i[H_{c^{(k)}(t)}, \chi^{(k)}(t)] - \varepsilon\mathcal{L}^{D,\dagger}_{n^{(k)}(t)}(\chi(t)), \quad \chi^{(k)}(T) = \rho_{\text{target}}. \quad (3.3)$$

The system is solved backward in time. Further, we see that

$$\Delta_1 R^\alpha = h^\alpha(t, \chi^{(k)}(t), \rho(t), c(t)) - h^\alpha(t, \chi^{(k)}(t), \rho(t), c^{(k)}(t)) = \langle\mathcal{K}^c(\chi^{(k)}(t),$$
$$\rho(t)), c(t) - c^{(k)}(t)\rangle - \frac{\widehat{\alpha}}{2\alpha}\|c(t) - sc^{(k)}(t)\|_2^2 + \frac{\widehat{\alpha}}{2\alpha}\|c^{(k)}(t) - sc^{(k)}(t)\|_2^2.$$

The first increment formula (for I^α) is

$$I^\alpha(c; c^{(k)}) - I^\alpha(c^{(k)}; c^{(k)}) = -\int_0^T\left(\langle\mathcal{K}^c(\chi^{(k)}(t), \rho(t)), c(t) - c^{(k)}(t)\rangle - \right.$$
$$\left. -\frac{\widehat{\alpha}}{2\alpha}\|c(t) - sc^{(k)}(t)\|_2^2\right)dt - \frac{\widehat{\alpha}}{2\alpha}\int_0^T\|c^{(k)}(t) - sc^{(k)}(t)\|_2^2 dt. \quad (3.4)$$

Important that this exact and nonlocal formula does not contain any residual. If $\widehat{\alpha} = 0$, then $I^\alpha(c; c^{(k)}) = I(c)$ and $h(\chi, \rho, c) := h^\alpha(t, \chi, \rho, c)$.

Further, for deriving the second increment formula, we represent the integrand in (3.2) as the sum $\Delta_3 R + \Delta_4 R^\alpha$, where

$$\Delta_3 R = R(t, \rho(t), c(t)) - R(t, \rho^{(k)}(t), c(t)) =$$
$$= \langle i[H_{c(t)}, \chi(t)] + \dot{\chi}(t) + \varepsilon\mathcal{L}^{D,\dagger}_{n(t)}(\chi(t)), \rho(t) - \rho^{(k)}(t)\rangle,$$
$$\Delta_4 R^\alpha = R(t, \rho^{(k)}(t), c(t)) - R(t, \rho^{(k)}(t), c^{(k)}(t)) =$$
$$= h(\chi(t), \rho^{(k)}(t), c(t)) - h(\chi(t), \rho^{(k)}(t), c^{(k)}(t)) =$$
$$= \langle\mathcal{K}^c(\chi(t), \rho^{(k)}(t)), c(t) - c^{(k)}(t)\rangle + \frac{\widehat{\alpha}}{2\alpha}\|c(t) - sc^{(k)}(t)\|_2^2.$$

For $\Delta_3 R = 0$ we obtain

$$\dot{\chi}(t) = -i[H_{c(t)}, \chi(t)] - \varepsilon\mathcal{L}^{D,\dagger}_{n(t)}(\chi(t)), \qquad \chi(T) = \rho_{\text{target}}. \quad (3.5)$$

The second increment formula (for I^α) is

$$I^\alpha(c; c^{(k)}) - I^\alpha(c^{(k)}; c^{(k)}) = -\int_0^T \left(\langle \mathcal{K}^c(\chi(t), \rho^{(k)}(t)), c(t) - c^{(k)}(t) \rangle - \right.$$

$$\left. -\frac{\widehat{\alpha}}{2\alpha} \|c(t) - sc^{(k)}(t)\|_2^2 \right) dt - \frac{\widehat{\alpha}}{2\alpha} \int_0^T \|c^{(k)}(t) - sc^{(k)}(t)\|_2^2 dt. \quad (3.6)$$

3.3. WITHOUT REGULARIZATION: ρ- AND χ-METHODS

Here based on (3.4) for $\widehat{\alpha} = 0$, we construct the ρ-method. To obtain a control c such that $I(c) - I(c^{(k)}) \leq 0$ and using (3.4) for $\widehat{\alpha} = 0$, set the condition $\langle \mathcal{K}^c(\chi^{(k)}(t), \rho(t)), c(t) - c^{(k)}(t) \rangle \geq 0$, $t \in [0, T]$, for implementation of which we introduce the following mappings:

$$u^*(\rho, t) = \arg\max_{|u| \leq \mu} (\mathcal{K}^u(\chi^{(k)}(t), \rho)u) =$$

$$= \begin{cases} -\mu, & \mathcal{K}^u(\chi^{(k)}(t), \rho) < 0, \\ \mu, & \mathcal{K}^u(\chi^{(k)}(t), \rho) > 0, \\ u_{\text{sing}} \in [-\mu, \mu], & \mathcal{K}^u(\chi^{(k)}(t), \rho) = 0, \end{cases} \quad (3.7)$$

$$n_j^*(\rho, t) = \arg\max_{n_j \in [0, n_{\max}]} (\mathcal{K}^{n_j}(\chi^{(k)}(t), \rho)n_j) =$$

$$= \begin{cases} 0, & \mathcal{K}^{n_j}(\chi^{(k)}(t), \rho) < 0, \\ n_{\max}, & \mathcal{K}^{n_j}(\chi^{(k)}(t), \rho) > 0, \\ n_{j,\text{sing}} \in [0, n_{\max}], & \mathcal{K}^{n_j}(\chi^{(k)}(t), \rho) = 0, \end{cases} \quad j = 1, 2. \quad (3.8)$$

Define $n^*(\rho, t) := \left(n_1^*(\rho, t), n_2^*(\rho, t) \right)$ and $c^*(\rho, t) := \left(u^*(\rho, t), n^*(\rho, t) \right)$.

As the result, the system (2.1) is solved with $u^*(\rho(t), t)$ and $n^*(\rho(t), t)$:

$$\dot{\rho}(t) = -i\left[H_{c^*(\rho(t), t)}, \rho(t) \right] + \varepsilon \mathcal{L}_{n^*(\rho(t), t)}^D(\rho(t)), \quad \rho(0) = \rho_0. \quad (3.9)$$

The r.h.s. in (3.9) is, in general, discontinuous in ρ and t. As known from the x- and ψ-procedures's theory, solution of such a system can be non-unique. The works [36, Sec. 2], [22, Sec. 6], [23, App. 2] for the problems with scalar control and real-valued states explain, for the situation when the switching function becomes zero, how to construct control via differentiation of the equality of switching function to zero. Our case may include $\mathcal{K}^u(\chi^{(k)}(t), \rho(t)) = 0$, $\mathcal{K}^{n_1}(\chi^{(k)}(t), \rho(t)) = 0$, and $\mathcal{K}^{n_2}(\chi^{(k)}(t), \rho(t)) = 0$ whose differentiation gives the complicated expressions.

Define the sets $\Theta_1^u := \{t \in [0, T] : u^{(k+1)}(t) \neq u^{(k)}(t)\}$,

$$\Theta_1^{n_j} := \{t \in [0, T] : n_j^{(k+1)}(t) \neq n_j^{(k)}(t)\},$$

$$\Theta_{2,\rho}^u := \{t \in [0, T] : \mathcal{K}^u(\chi^{(k)}(t), \rho^{(k+1)}(t)) \neq 0\},$$

$$\Theta_{2,\rho}^{n_j} := \{t \in [0, T] : \mathcal{K}^{n_j}(\chi^{(k)}(t), \rho^{(k+1)}(t)) \neq 0\}, \quad j = 1, 2.$$

Algorithm of the ρ-method (no regularization). k-th $(k \geq 0)$ iteration (ρ-procedure) consists of the following steps.

1) If $k = 0$, then obtain $\rho^{(0)}$ from (2.1) and compute $I(c^{(0)})$; if $k > 0$ then for the known $c^{(k)}$ solve the adjoint system (3.3) to obtain $\chi^{(k)}$.

2) Form the mappings (3.7), (3.8).

3) Solve the system (3.9) and construct the set of pairs $\{(c, \rho)\}$, where each pair consists of a solution ρ of (3.9) and $c(t) = c^*(\rho(t), t)$.

4) Select the pair $(c^{(k+1)}, \rho^{(k+1)})$ which provides maximal decrease of $I(c)$; if there is no decrease then select any $(c^{(k+1)}, \rho^{(k+1)})$.

5) If the stopping criterion $|I(c^{(k+1)}) - I(c^{(k)})| < \epsilon \ll 1$ is not satisfied, then set $k := k + 1$ and go to step 1); otherwise stop.

Algorithm of the χ-method (no regularization). k-th $(k \geq 0)$ iteration (χ-procedure) consists of the following steps.

1) If $k = 0$, then obtain $\rho^{(0)}$ from (2.1) and compute $I(c^{(0)})$.

2) Form the mappings (3.10), (3.11).

3) Solve the system (3.12) and construct the set $\{(c, \chi)\}$, where, for each solution χ of (3.12), the corresponding control is $c(t) = c^*(\chi(t), t)$; construct the set of the corresponding pairs $\{(c, \rho)\}$ by solving (2.1).

4) Select the pair $(c^{(k+1)}, \rho^{(k+1)})$ which provides maximal decrease of $I(c)$; if there is no decrease then select any $(c^{(k+1)}, \rho^{(k+1)})$.

5) If the stopping criterion $|I(c^{(k+1)}) - I(c^{(k)})| < \epsilon \ll 1$ is not satisfied, then set $k := k + 1$ and go to the step 2); otherwise stop.

Proposition 1. *The ρ-procedure provides a resulting control $c^{(k+1)}$ such that the first integrand in (3.4) for $\widehat{\alpha} = 0$, $c(t) = c^{(k+1)}(t)$, $\rho(t) = \rho^{(k+1)}(t)$, $t \in [0, T]$ is non-negative and $I(c^{(k+1)}) \leq I(c^{(k)})$. The strong inequality $I(c^{(k+1)}) < I(c^{(k)})$ holds when at least one of the three sets $\Theta_1^u \cap \Theta_{2,\rho}^u$, $\Theta_1^{n_j} \cap \Theta_{2,\rho}^{n_j}$, $j = 1, 2$ has non-zero measure.*

Further, based on the second increment formula (3.6) for $\widehat{\alpha} = 0$, the *χ-method* is formulated. Introduce the mappings

$$u^*(\chi, t) = \arg \max_{|u| \leq \mu} (\mathcal{K}^u(\chi, \rho^{(k)}(t))u), \tag{3.10}$$

$$n_j^*(\chi, t) = \arg \max_{n_j \in [0, n_{\max}]} (\mathcal{K}^{n_j}(\chi, \rho^{(k)}(t))n_j), \quad j = 1, 2. \tag{3.11}$$

Form $n^*(\chi, t) := \big(n_1^*(\chi, t), n_2^*(\chi, t)\big)$ and $c^*(\chi, t) := \big(u^*(\chi, t), n^*(\chi, t)\big)$. Introduce the system (3.5) with $u^*(\chi(t), t)$ and $n^*(\chi(t), t)$:

$$\dot{\chi}(t) = -i\big[H_{c^*(\chi(t),t)}, \chi(t)\big] - \varepsilon \mathcal{L}_{n^*(\chi(t),t)}^{D,\dagger}(\chi(t)), \quad \chi(T) = \rho_{\text{target}}. \tag{3.12}$$

Introduce the sets $\Theta_{2,\chi}^u := \{t \in [0, T] : \mathcal{K}^u(\chi^{(k+1)}(t), \rho^{(k)}(t)) \neq 0\}$ and $\Theta_{2,\chi}^{n_j} := \{t \in [0, T] : \mathcal{K}^{n_j}(\chi^{(k+1)}(t), \rho^{(k)}(t)) \neq 0\}$, $j = 1, 2$.

Proposition 2. *The χ-procedure provides a resulting control $c^{(k+1)}$ such that the first integrand in (3.6) for $\widehat{\alpha} = 0$, $c(t) = c^{(k+1)}(t)$, $\chi(t) = \chi^{(k+1)}(t)$, $t \in [0,T]$ is non-negative and $I(c^{(k+1)}) \leq I(c^{(k)})$. The strong inequality $I(c^{(k+1)}) < I(c^{(k)})$ holds when at least one of the three sets $\Theta_1^u \cap \Theta_{2,\chi}^u$, $\Theta_1^{n_j} \cap \Theta_{2,\chi}^{n_j}$, $j = 1,2$ has non-zero measure.*

3.4. Regularized ρ- & χ-methods. Gradient Projection Method

Based on the increment formulas (3.4) and (3.6) for $\widehat{\alpha} = 1$, we briefly describe the corresponding regularized ρ- and χ-methods, which are called as ρ-method-reg(s,α) and χ-method-reg(s,α). In view of [35, p. 61] and (3.4), we construct the following mappings by deriving the stationary points of the corresponding quadratic concave functions under (2.2):

$$u^\alpha(\rho,t) = \arg\max_{|u|\leq\mu} \left(\mathcal{K}^u(\chi^{(k)}(t),\rho)u - \frac{1}{2\alpha}(u - su^{(k)}(t))^2 \right) =$$

$$= \begin{cases} -\mu, & u_{\text{st}}(\rho,t) < -\mu, \\ \mu, & u_{\text{st}}(\rho,t) > \mu, \\ u_{\text{st}}(\rho,t), & |u_{\text{st}}(\rho,t)| \leq \mu, \end{cases}$$

$$\text{where} \quad u_{\text{st}}(\rho,t) = su^{(k)}(t) + \alpha\mathcal{K}^u(\chi^{(k)}(t),\rho),$$

$$n_j^\alpha(\rho,t) = \arg\max_{n_j\in[0,n_{\max}]} \left(\mathcal{K}^{n_j}(\chi^{(k)}(t),\rho)n_j - \frac{1}{2\alpha}(n_j - sn_j^{(k)}(t))^2 \right) =$$

$$= \begin{cases} 0, & n_{\text{st},j}(\rho,t) < 0, \\ n_{\max}, & n_{\text{st},j}(\rho,t) > n_{\max}, \\ n_{\text{st},j}(\rho,t), & n_{\text{st},j}(\rho,t) \in [0,n_{\max}], \end{cases}$$

$$\text{where} \quad n_{\text{st},j}(\rho,t) = sn_j^{(k)}(t) + \alpha\mathcal{K}^{n_j}(\chi^{(k)}(t),\rho).$$

Consider $c^\alpha(\rho,t) = (c^\alpha(\rho,t), n_j^\alpha(\rho,t), j = 1,2)$ and substitute it into (3.9) instead of the mapping c^*. Note that the r.h.s. of this system is continuous in ρ by construction. This gives the ρ-*method-reg(s,α)*.

Consider ρ-method-reg(s,α) in the following projection form:

$$c^{(k+1)}(t) = c^\alpha(\rho^{(k+1)}(t),t) = \text{Pr}_Q\big(sc^{(k)}(t) + \alpha\mathcal{K}^c(\chi^{(k)}(t),\underline{\rho^{(k+1)}(t)})\big) \ (3.13)$$

where $Q = [-\mu,\mu] \times [0,n_{\max}]^2$ and Pr_Q is the orthogonal projection (in $\|\cdot\|_2$) which maps any point outside of Q to a closest point in Q, and leaves unchanged points in Q. The function $\rho^{(k+1)}$ is the unique solution of (2.1), where c^α is taken instead of c.

Consider the function $f(u) := \mathcal{K}^u(u - su^{(k)}(t)) - \frac{1}{2\alpha}(u - su^{(k)}(t))^2$. Its value at the stationary point is $f(u_{st}) = \frac{\alpha}{2}(\mathcal{K}^u)^2 \geq 0$. We analyze the cases $u_{\text{st}} > \mu$ and $u_{\text{st}} < -\mu$ using zeros $u_{0,1} = su^{(k)}(t) \in [-\mu,\mu]$ and

$u_{0,2} = su^{(k)}(t) + 2\alpha \mathcal{K}^u$ of $f(u)$. Omitting the details, the result is $f(\mu) \geq 0$ for $u_{\mathrm{st}} > \mu$ and $f(-\mu) \geq 0$ for $u_{\mathrm{st}} < -\mu$. Similarly for $n_{\mathrm{st},j}$, $j = 1, 2$. Thus, the increment (3.4) is ≤ 0 for c^α. Further, comparing (3.1) with (3.4) and using the basic property $\langle y - \mathrm{Pr}_X(y), \mathrm{Pr}_X(y) - x\rangle \geq 0$ of projection $\forall y \in \mathbb{R}^n$, $\forall x \in X \subset \mathbb{R}^n$, we obtain the following upper estimate (similar to (2.3) in [2]) for k-th iteration of ρ-method-reg(s,α) (regularized ρ-procedure):

$$I(c^{(k+1)}) - I(c^{(k)}) = -\int_0^T \langle \mathcal{K}^c(\chi^{(k)}(t), \rho(t)), c^{(k+1)}(t) - sc^{(k)}(t)\rangle dt =$$

$$= -\frac{1}{\alpha}\int_0^T \Big[\langle c^{(k+1)}(t) - sc^{(k)}(t), c^{(k+1)}(t) - sc^{(k)}(t)\rangle +$$

$$+ \langle (sc^{(k)}(t) + \alpha \mathcal{K}^c(\chi^{(k)}(t)) - c^{(k+1)}(t), c^{(k+1)}(t) - sc^{(k)}(t)\rangle \Big] dt \leq$$

$$\leq -\frac{1}{\alpha}\int_0^T \|c^{(k+1)}(t) - sc^{(k)}(t)\|_2^2 dt, \quad \alpha > 0, \quad c^{(k+1)}(t) = c^\alpha(\rho^{(k+1)}(t), t).$$

Taking into account the increment formula (3.6), we similarly construct χ-method-reg(s,α), where we consider the mapping

$$c^\alpha(\chi, t) = (c^\alpha(\chi, t), n_j^\alpha(\chi, t), j = 1, 2),$$

substitute it into (3.12) instead of c^*.

Proposition 3. *Each of the regularized ρ- and χ- procedures for any $\alpha > 0$ gives such $c^{(k+1)}(t) = c^\alpha(\rho^{(k+1)}(t), t)$ that $I(c^{(k+1)}) \leq I(c^{(k)})$, and if $c^{(k+1)}(t) \neq c^{(k)}(t)$ at a subset with non-zero measure on $[0, T]$ then $I(c^{(k+1)}) < I(c^{(k)})$.*

By analogy with [20, p. 239–240], for the increment (3.2) after differentiating the functions G, R one can obtain the gradient

$$\mathrm{grad}\, I(c^{(k)})(t) = -\mathcal{K}^c(\chi^{(k)}(t), \rho^{(k)}(t)), \quad t \in [0, T]. \tag{3.14}$$

The same system (3.3) as in ρ-method-reg(s,α) is used. For $s = 1$, the formula (3.13) reminds the following iterative formula of the one-step gradient projection method (GPM-1) based on (3.14) (see also [35, p. 59]):

$$c^{(k+1)}(t) = \mathrm{Pr}_Q\big(c^{(k)}(t) + \alpha^{(k)}\mathcal{K}^c(\chi^{(k)}(t), \underline{\rho^{(k)}(t)})\big), \quad t \in [0, T], \tag{3.15}$$

where α can be not only fixed but also chosen as dependent on k. The difference between (3.13) and (3.15) is that GPM-1 uses only the background, i.e. $(c^{(k)}, \rho^{(k)}, \chi^{(k)})$, while ρ-method-reg(s,α) uses both the background and the constructed control via c^α.

Consider the following functional to be minimized:

$$I^\beta(c) = 1 - J_1(c) + \int_0^T (\beta_1 u^2(t) + \beta_2(n_1(t) + n_2(t)))dt, \quad \beta_1, \beta_2 > 0.$$

Its gradient is

$$\operatorname{grad} I^\beta(c^{(k)})(t) = \Big(-\mathcal{K}^u(\chi^{(k)}(t), \rho^{(k)}(t)) + 2\beta_1 u^{(k)}(t),$$
$$- \mathcal{K}^{n_j}(\chi^{(k)}(t), \rho^{(k)}(t)) + \beta_2, \quad j = 1, 2 \Big). \qquad (3.16)$$

Using [1], [28, Sec. 5], we will consider in Subsec. 3.6 GPM-2 in the form

$$c^{(k+1)}(t) = \operatorname{Pr}_Q \big[c^{(k)}(t) - \alpha^{(k)} \operatorname{grad} I^\beta(c^{(k)})(t) +$$
$$+ \theta^{(k)}(c^{(k)}(t) - c^{(k+1)}(t)) \big], \quad t \in [0, T], \quad \theta^{(k)} \in (0, 1). \quad (3.17)$$

3.5. PMP. ZERO CONTROLS

By analogy with [7, Ch. 4], — where, for the problem of maximizing the same overlap with respect to the von Neumann equation with coherent control, the corresponding formulation of the PMP in terms of density matrices was done, — we, for our optimal control problem with (2.3) and a fixed final time T, formulate the corresponding PMP.

Proposition 4. *(PMP). For the system (2.1), where coherent and incoherent controls are in the class of piecewise continuous controls satisfying the constraints (2.2) for a fixed final time $T > 0$, if some admissible control $\widehat{c} = (\widehat{u}, \widehat{n}_1, \widehat{n}_2)$ is a strict local maximum point of $J_1(c)$ in the problem of maximizing J_1, then there exist solutions $\widehat{\rho}$ and $\widehat{\chi}$ of the systems (2.1), (3.3), where $\widehat{c} = (\widehat{u}, \widehat{n}_1, \widehat{n}_2)$, such that the pointwise condition $\max_{c \in Q} h(\widehat{\chi}(t), \widehat{\rho}(t), c) = h(\widehat{\chi}(t), \widehat{\rho}(t), \widehat{c}(t))$, $t \in [0, T]$ holds, where $Q := [-\mu, \mu] \times [0, n_{\max}]^2$. One has*

$$\max_{|u| \leq \mu} (\mathcal{K}^u(\widehat{\chi}(t), \widehat{\rho}(t)) u) = \mathcal{K}^u(\widehat{\chi}(t), \widehat{\rho}(t)) \widehat{u}(t), \quad t \in [0, T], \qquad (3.18)$$
$$\max_{n_j \in [0, n_{\max}]} (\mathcal{K}^{n_j}(\widehat{\chi}(t), \widehat{\rho}(t)) n_j) = \mathcal{K}^{n_j}(\widehat{\chi}(t), \widehat{\rho}(t)) \widehat{n}_j(t), \quad t \in [0, T]. \ (3.19)$$

Consider $\rho_0 = \operatorname{diag}(a_1, a_2, a_3, a_4)$ and $\rho_{\text{target}} = \operatorname{diag}(b_1, b_2, b_3, b_4)$ with a_j, $b_j \geq 0$ $(j = 1, 2, 3, 4)$, $\sum_{j=1}^4 a_j = 1$, and $\sum_{j=1}^4 b_j = 1$. One has $J_1(c) = \sum_{j=1}^4 d_j \rho_{jj}(T)$. As in [28], we parameterize ρ (using $x_j \in \mathbb{R}$, $j = \overline{1, 16}$ for ρ_{jj}, $j = 1, 2, 3, 4$ and $\operatorname{Re}\rho_{ij}$, $\operatorname{Im}\rho_{ij}$ with $i < j$, $i, j = 1, 2, 3, 4$) and χ (using $y_j \in \mathbb{R}$, $j = \overline{1, 16}$) and obtain bilinear systems in terms of x, y which correspond to (2.1) and (3.3). In these terms, $\mathcal{K}^u(\chi, \rho) = \langle \chi, -i[V, \rho] \rangle$ is realificated as $\mathcal{K}^u(y, x)$ (via Wolfram Mathematica), but the derived form is too complicated to present it here. For these ρ_0 and ρ_{target}, for the realifications of (2.1) and (3.3) with $c = \bar{c} = 0$ the corresponding exact analytical solutions are obtained (via Wolfram Mathematica) for any V including V_1, V_2 with any Q_1, Q_2 (since $H_{u(t)} = V u(t)$ becomes zero

for any t): $\overline{x}_i, \overline{y}_i$ have certain non-trivial forms if $i \in \{1, 8, 13, 16\}$, and $\overline{x}_i = \overline{y}_i = 0$ if $i \in \overline{1, 16} \setminus \{1, 8, 13, 16\}$. $\mathcal{K}^u(y, x)$ is a linear combination of terms $x_i y_j$ with $i, j = \overline{1, 16}$, $i \neq j$ such that if $i \in \{1, 8, 13, 16\}$ then $j \notin \{1, 8, 13, 16\}$. Thus, substituting $\overline{x}_j(t), \overline{y}_j(t)$ instead of x_j, y_j in $\mathcal{K}^u(y, x)$ gives $\mathcal{K}^u(\overline{y}(t), \overline{x}(t)) \equiv 0$ at the whole $[0, T]$ for any admissible values of the system's parameters. The condition (3.18) is satisfied. We set $\rho_0 = \frac{1}{4}\mathbb{I}_4$, $\rho_{\text{target}} = \text{diag}(1, 0, 0, 0)$ and obtain

$$\mathcal{K}^{n_1}(\overline{y}(t), \overline{x}(t)) = -e^{-2\varepsilon(\Omega_1 + \Omega_2)T} \left(e^{2\varepsilon\Omega_1 t} - 1\right)\left(2e^{2\varepsilon\Omega_2 T} - 1\right)\varepsilon\Omega_1 \leq 0,$$

$$\mathcal{K}^{n_2}(\overline{y}(t), \overline{x}(t)) = -e^{-2\varepsilon(\Omega_1 + \Omega_2)T} \left(e^{2\varepsilon\Omega_2 t} - 1\right)\left(2e^{2\varepsilon\Omega_1 T} - 1\right)\varepsilon\Omega_2 \leq 0,$$

where $\varepsilon, \Omega_1, \Omega_2 > 0$. Using (2.2), we obtain that (3.19) is satisfied for $j = 1, 2$. Thus, $c = \overline{c} = 0$ satisfies the PMP for any admissible values of the system's parameters and T. Similar result was obtained in [28].

3.6. NUMERICAL RESULTS

The Python programs for numerical simulations were written by the first author using such tools as `solve_ivp` from `SciPy`, etc. We consider (2.1) with $V = V_1$, $\varepsilon = 0.1$, $\omega_1 = 1$, $\omega_2 = \Omega_j = \Lambda_j = 0.5$ ($j = 1, 2$), $\rho_0 = \frac{1}{4}\mathbb{I}_4$. Set $\mu = 50$, $n_{\max} = 10$. Controls are interpolated as piecewise constant with 10^4 subintervals.

Case 1. Set $\rho_{\text{target}} = \text{diag}(1, 0, 0, 0)$ (pure quantum state), $T = 100$ and $V = V_1$ with $\theta_1 = \pi/3$, $\theta_2 = \pi/4$, $\varphi_1 = \pi/4$, $\varphi_2 = \pi/3$. Analytically solving (2.1) with $c = 0$, we have $b - J_1 \approx 4.54 \cdot 10^{-5}$ for any V, where $b = 1$ is the overlap's upper bound obtained [28] from $\langle \rho, \rho_{\text{target}} \rangle \to \max$ and is the largest eigenvalue of ρ_{target}. This gives a test optimal control problem.

Set the two initial guesses: 1) $c^{(0)} = (u^{(0)}, n_1^{(0)}, n_2^{(0)}) = (\mu, n_{\max}, n_{\max})$ being the furthest from $c = 0$ and giving $I(c^{(0)}) \approx 0.74$; 2) $u^{(0)} = (0, 0, 1)$ being not so far from $c = 0$ and giving $I(c^{(0)}) \approx 0.33$.

Set $c^{(0)} = (50, 10, 10)$. For the functional I^β, we use GPM-1, GPM-2 (3.17) with the gradient (3.16) (here is adapted for I^β). Take $\beta_1 = 0.01$, $\beta_2 = 0.1$. Fig. 1(a–d) show the following features of GPM and the dynamic control landscape of $I(c)$:

1) we observe that up to about 80th iterations of GPM-1, $I(c^{(k)})$ varies from 0.734 to 0.689 and hence *changes relatively slowly* (the dashed line in Fig. (a)) and the L^2-norms of $\mathcal{K}^u(\chi^{(k)}, \rho^{(k)})$, $\mathcal{K}^{n_j}(\chi^{(k)}, \rho^{(k)})$ ($j = 1, 2$) are *relatively small* (Fig. (d)), but the L^2-norms of $u^{(k)}$, $n_j^{(k)}$ ($j = 1, 2$) *change significantly* (Fig. (b));

2) after about 80th iterations of GPM-1 and up to $I(c^{(181)}) \approx 0.2$, the switching functions' L^2-norms become *larger* and I *decreases significantly*;

3) after $I(c^{(181)}) \approx 0.2$, GPM-1 becomes *drastically worse* (Fig. (a,d)) — now $\alpha^{(k)} = 1$ is *inappropriate* and GPM-1 is stopped when $k = 250$;
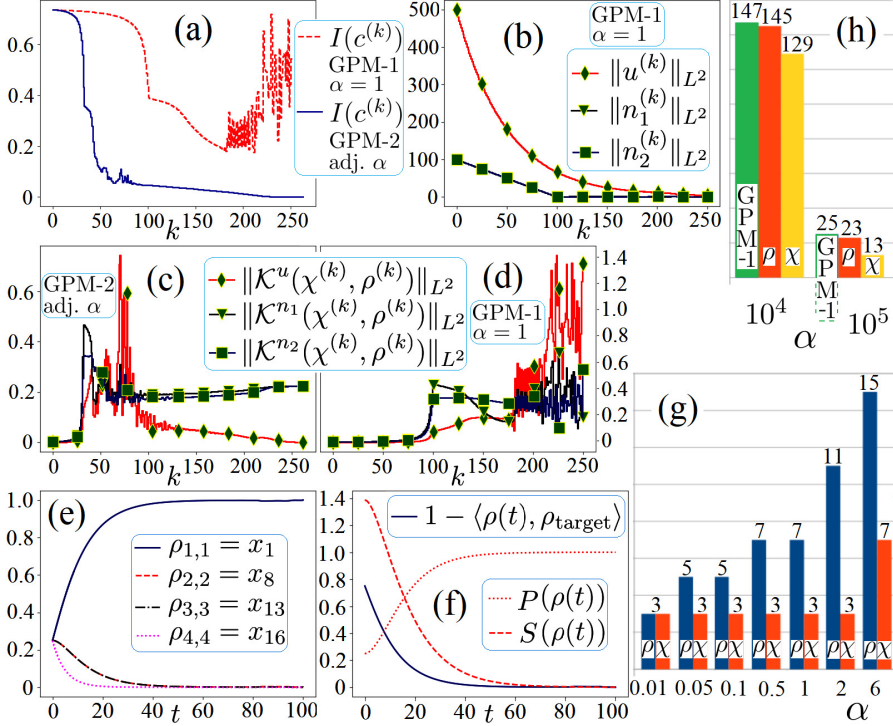
Figure 1. For Case 1. Subplots (a)–(d) show behavior vs iteration number k for $c^{(0)} = (50, 10, 10)$ for GPM-1 and GPM-2 of: (a) objective values; (b) L^2 norms of controls; (c) and (d) L^2 norms of switching functions; (g) shows numbers of the Cauchy problems solved in ρ-method-reg($s = 0$, α), χ-method-reg($s = 0$, α) for reaching $I \leq 5 \times 10^{-5}$ with the different fixed α. Subplot (h) for $c^{(0)} = (0, 0, 1)$ shows numbers the Cauchy problems solved in GPM-1, ρ-method-reg($s = 1$, α), and χ-method-reg($s = 1$, α) for reaching $I \leq 5 \times 10^{-5}$, where α is either 10^4 or 10^5 and is the same during a run. Subplots (e) and (f) show for both $c^{(0)}$ $\rho_{j,j}(t)$ ($j = \overline{1, 4}$), $1 - \langle \rho(t), \rho_{\text{target}} \rangle$, $S(\rho(t))$, and $P(\rho(t))$ at the numerically optimized c.

4) GPM-2 (initially $\alpha = 1$, $\theta^{(k)} = 0.7$, but $\alpha^{(k)} = 0.5$, $\theta^{(k)} = 0.85$, if $I \leq 0.1$, and $\alpha^{(k)} = 0.3$, $\theta^{(k)} = 0.9$, if $I \leq 0.05$) *provides* $c = 0$ with good precision and the stopping condition $I \leq 5 \cdot 10^{-5}$ (see the solid graph in Fig. (a)) at the cost of 523 Cauchy problems;

5) $c = 0$ *satisfying the PMP is not a stationary point* of $I(c)$ — in this case, Fig. (c) shows that $\|\mathcal{K}^u\|_{L^2}$ becomes zero while $\|\mathcal{K}^{n_1}\|_{L^2}$ and $\|\mathcal{K}^{n_2}\|_{L^2}$ do not.

Fig. 1(f) shows the von Neumann entropy $S(\rho(t)) = -\text{Tr}(\rho(t)) \log(\rho(t))$ and purity $P(\rho(t)) = \text{Tr}\rho^2(t)$ vs t at the whole $[0, T]$. Purification of quantum states leads to $P(\rho(T)) \approx 1$, $S(\rho(T)) \approx 0$, when $T = 100$, $c = 0$.

For the same $c^{(0)}$, Fig. 1(g) compares the numbers of the Cauchy problems for reaching $I \leq 5 \times 10^{-5}$ when we use ρ-method-reg($s = 0, \alpha^{(k)}$) and

χ-method-reg($s = 0, \alpha^{(k)}$) where $\alpha \in \{0.01, 0.05, 0.1, 0.5, 1, 2, 6\}$ is the same during a run. Both methods work sufficiently good, but the χ-method is faster than the ρ-method for the 2nd — 7th variants of α.

In contrast to $c^{(0)} = (\mu, n_{\max}, n_{\max}) = (50, 10, 10)$, consider $\underline{c^{(0)} = (0, 0, 1)}$, because it is interesting to analyze how the methods work starting in some proximity to $c = 0$. At the cost of solving only 3 Cauchy problems, ρ-method-reg($s = 0, \alpha = 1$) provides the zero controls and $I \leq 5 \times 10^{-5}$. The resulting $\mathcal{K}^u(y^{(0)}(t), x^{(1)}(t)) \equiv 0$, $\mathcal{K}^{n_j}(y^{(0)}(t), x^{(1)}(t)) \leq 0$, $j = 1, 2$ at $[0, T]$. Also at the same cost, the problem is solved via χ-method-reg($s = 0, \alpha = 1$). Further, 1000 iterations as of ρ-method-reg($s = 1, \alpha = 1$) and of GPM-1 with the unchanged $\alpha = 1$ gives only $I \approx 0.013$.

Each of ρ-method-reg($s = 1, \alpha$), χ-method-reg($s = 1, \alpha$), and GPM-1, where α is either 10^4 or 10^5 and is the same during a run, provides $I \leq 5 \times 10^{-5}$. Fig. 1(h) compares how many the Cauchy problems are solved in each run of these methods with the two variants for fixing α. The regularized χ-method is essentially faster here.

Consider the ρ-method without regularization. Knowing that $c = 0$ satisfies the PMP, we at the first iteration, — instead of differentiating the switching functions for deriving u_{sing}, etc., — try $u_{\text{sing}} = 0$ in (3.7), $n_{j,\text{sing}} = 0$ in (3.8) and obtain that $\mathcal{K}^u(y^{(0)}(t), x^{(1)}(t)) \equiv 0$, $\mathcal{K}^{n_j}(y^{(0)}(t), x^{(1)}(t)) \leq 0$, $t \in [0, T]$, $j = 1, 2$ and the condition given by Proposition 1 for $I(c^{(1)}) < I(c^{(0)})$ is realized.

Case 2. Set $I(c) = b - J_1(c)$, $\rho_{\text{target}} = \text{diag}(0.7, 0.1, 0.1, 0.1)$, and $T = 70$, where $b = 0.7$ is the overlap's upper bound obtained [28] as the largest eigenvalue of the ρ_{target}. If $c = 0$, then $I \approx 5.47 \cdot 10^{-4}$ for any V. Uniformly distributing $\{\lambda_m^j\}_{m=1}^{50}$ on the unit sphere [34] for $\lambda_m^1 = \lambda_m^2$, the corresponding set of Q_1, Q_2 is obtained. For these 50 problems, use ρ-method-reg($s = 0, \alpha = 1$), $c^{(0)} = (0.1, 1, 1)$. The condition $I \leq \varepsilon_{\text{stop}} = 5.6 \cdot 10^{-4}$ is reached for each problem, but numbers of the solved Cauchy problems vary from 3 to 23.

4. Steering States and the Overlap: Numerical Results

Consider the system (2.1) and J_2, J_3 to be minimized (see (2.4), (2.5)). Using the parameterized class of controls (2.6), (2.7) leads to the problems of minimizing the corresponding objective functions of T and $\mathbf{a} = (h_u, A_1, \ldots, A_K, B_1, \ldots, B_K, C_1, C_2, h_{n_1}, h_{n_2})$. SciPy implementation of the dual annealing method (DAM) is used. DAM realizes some zeroth-order and stochastic approach for finite-dimensional global optimization. DAM starts from some automatically generated point. In view of the stochastic nature of DAM, we perform more than one trial for each problem.

Case 1. Consider the problem of minimizing $J_2(c, T)$. Set $V = V_1$, where $\theta_1 = \theta_2 = \pi/2$, $\varphi_1 = \varphi_2 = 0$ (as considered in [28]). Also set $\rho_0 = \text{diag}(1, 0, 0, 0)$ corresponding to $x_0 = (1, \text{fifteen zeros})$ which is, as it

was shown in [28], singular, equilibrium state for the system $\dot{x}(t) = Ax(t)$, i.e. for any T the system's trajectory cannot leave x_0 without controls. Set $\rho_{\text{target}} = \text{diag}(0.1, 0.1, 0.3, 0.5)$. For (2.6), (2.7), consider $K = 3$, $\nu_1 = 0.5$, $\nu_2 = 1$, $\nu_3 = 2$, $h_u \in [0, 2]$, $|A_j| \leq 10$, $|B_j| \leq 10$ ($j = 1, 2, 3$), $C_j \in [0, 5]$ ($j = 1, 2$), $h_{n_j} \in [0, 2]$ ($j = 1, 2$), $T \in [0.5, 2]$. After 10 trials of DAM applied to (2.4) with $P = 10^3$, we stop with $\|\rho(T) - \rho_{\text{target}}\| \approx 0.03$ and see that, at each of these trials, the computed controls u, n_1, n_2 are not trivial. These 10 trials give such n_1, n_2 that the computed values of C_1 in (2.7) are from ≈ 0.08 to ≈ 2.09 and C_2 in (2.7) are from ≈ 3.57 to 5 under the constraints $C_j \in [0, 5]$, $j = 1, 2$. Fig. 2 visualizes the result of some trial, where the initial distance $\|\rho(T) - \rho_{\text{target}}\| \approx 0.57$, the largest occurred value is near 1. The resulting value $\|\rho(T) - \rho_{\text{target}}\| \approx 0.03$ is much closer to zero. Thus, using the class of controls (2.6), (2.7) and DAM is helpful.
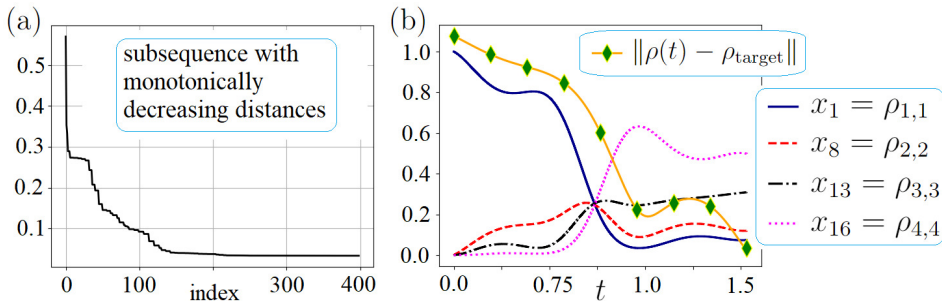

Figure 2. Steering states to $\rho_{\text{target}} = \text{diag}(0.1, 0.1, 0.3, 0.5)$ with $V = V_1$. 10 trials of DAM give non-trivial u, n_1, n_2. From a trial with $\|\rho(T) - \rho_{\text{target}}\| \approx 0.03$: (a) subsequence with monotonically decreasing values of $\|\rho(T) - \rho_{\text{target}}\|$ during the work of DAM; (b) the resulting $\rho_{j,j}$ and $\|\rho(t) - \rho_{\text{target}}\|$ vs t.

For $V = V_2$ with the same other settings, the best result from 10 trials of DAM also is $\|\rho(T) - \rho_{\text{target}}\| \approx 0.03$, and there are such the trials with $\|\rho(T) - \rho_{\text{target}}\| \approx 0.03$ that either n_1 is zero or not with non-trivial n_2.

Case 2. Consider the problem of minimizing $J_3(c, T)$. Set $V = V_1$, where $\theta_1 = \theta_2 = \pi/2$, $\varphi_1 = \varphi_2 = 0$. For the same other settings, after 10 trials of DAM, the best result for $|\langle \rho(T), \rho_{\text{target}} \rangle - M|$ is zero. All these 10 trials give that n_2 is zero with various precision.

5. Conclusions

This article considers two-qubit open quantum systems driven by coherent and incoherent controls, where the latter uses the environment as a resource and induces *time-dependent decoherence rates* so that the system evolves according to a GKSL master equation with time-dependent coefficients. For two types of interaction with coherent control, three types of objectives are considered: maximizing the overlap $\langle \rho(T), \rho_{\text{target}} \rangle$, minimizing $\|\rho(T) - \rho_{\text{target}}\|$, and steering the overlap to a given value. For the first

case we, based on [20; 35], etc., formulate in terms of density matrices the Krotov type methods based on the nonlocal exact increment formulas with or without regularization for piecewise continuous constrained controls, and also give PMP and GPM, find the cases where the methods produce (either exactly or with some precision) zero controls which satisfy the PMP and produce objectives close to $\max_{\rho}\langle\rho, \rho_{\text{target}}\rangle$ so that the system's free evolution itself achieves the goal. The Propositions 1–3 state that the Krotov type procedures do not produce worse controls, and provide conditions when the procedures give better controls. For the other problems, we use a parameterized class of controls and find cases when the dual annealing method steers objectives close to zero and produces non-zero control.

Comparing with the results beyond quantum control which are the basis for us (e.g., [20;35;38]), we develop the nonlocal improvement methods with or without regularization in terms of the GKSL master equation given in Sec 2 and density matrices. The work [11] develops such the Krotov type method in terms of the similar Markovian master equation and similar to ρ-method-reg(s, α), but only with coherent control and regularization. The difference from [13; 37] is that these works consider for the Schrödinger (linear in ψ and control) and Gross–Pitaevskii (not linear in ψ) equations the corresponding Krotov type methods with regularization (with $s = 0$ or $s = 1$ in our terms). The works [20, § 6.5], [21] consider the Schrödinger equation and the improvement methods with or without regularization (with $s = 0$ in our terms). Thus, we take into account and combine various known ideas and constructions to reflect the specifics (density matrices, two types of controls, two qubits, etc.) of the quantum problem and to develop the methodology of the nonlocal improvement methods to open quantum systems. Sec. 3.6 describes some interesting results of the formulated methods. Various aspects of solving the appearing equations whose r.h.s. are, in general, discontinuous in ρ, χ, and convergence of the methods should be carefully studied with numerical experiments in subsequent works. Using the dual annealing method, in Sec. 4 non-trivial incoherent controls were found for some objective functionals showing the appearance of the environment as a useful resource.

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