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Gradient Projection Method and Stochastic Search for Some Optimal Control Models with Spin Chains. I

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Abstract: This article (I) considers optimal control models for both transferring an excitation from the first spin to the last spin in a chain of N spins and keeping an excitation initially given at the last spin. Each model employs an external controlled parabolic magnetic field represented by two control functions. For these models, the corresponding infinite-dimensional gradients and the projection-type linearized Pontryagin maximum principle are given along with their finite-dimensional analogues. The finite-dimensional gradient projection method in its one-, two-, and three-step forms is represented. A special class of controls for the transfer model is introduced for a genetic algorithm, and the corresponding transfer example for the case of $N = 30$ spins is given.

Keywords: quantum optimal control, gradient projection method, genetic algorithm, spin chains

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Научная статья

Метод проекции градиента и стохастический поиск для некоторых моделей оптимального управления со спиновыми цепочками. I

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Аннотация: В данной статье (I) рассматриваются модели оптимального управления как по передаче возбуждения с первого спина на последний спин в цепочке из N спинов, так и по удержанию возбуждения, данного на последнем спине. Каждая модель использует внешнее параболическое магнитное поле, представленное двумя управляющими функциями. Для этих моделей представлены соответствующие бесконечномерные градиенты и проекционного типа линеаризованный принцип максимума Понтрягина вместе с их конечномерными аналогами. Приведен конечномерный метод проекции градиента в его одно-, двух- и трехшаговых формах. Введен специальный класс управлений для модели о передаче, ориентируясь на генетический алгоритм, и дан соответствующий пример передачи для случая $N = 30$ спинов.

Ключевые слова: квантовое оптимальное управление, метод проекции градиента, генетический алгоритм, спиновые цепочки

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Dedicated to the memory of Prof. V.A. Dykhta[1]
whose contribution to the mathematical theory of optimal control and its applications is impressive and relates, in particular, to quantum control

1. Introduction

Quantum optimal control (QOC) is an actual scientific direction, which is important, e.g., for quantum chemistry, quantum computations and quantum information processing, etc. This direction uses various results from mathematics, e.g., from the theory of optimal control (TOC), the theory of Lie groups and algebras, etc. For numerical solution of various quantum optimization problems, as is known, various adaptations of op-

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`http://ait.mtas.ru/en/archive/volume86issue10/ARC10-007Morzhin.pdf`.

timization methods and approaches before known beyond QOC are used with taking into account various specific quantum properties.

From the points of view of mathematics, the article [18] (2009) is the first article where the first-order gradient projection method (GPM) was developed for minimizing just on a complex finite-dimensional Stiefel manifold under an equality-type constraint, while before in mathematics the first-order GPM was known [1] for minimizing in $\mathbb{R}^n$ under an equality-type constraint. Second, [18] is pioneering also in the meaning that there the method was developed with such the complex Stiefel matrices that represent the notion of finite-dimensional Kraus operators being important for various quantum technologies.

In QOC, the direction of developing quantum multi-step — mainly two-step — GPM forms for various optimal control problems (OCPs) [13–15] is important. This article adjoins those works and adapts the one- and two- and three-step GPM forms (GPM-jS, $j = 1, 2, 3$) for some OCPs devoted to transfer and keeping (in the sense of the probability invariant) at a spin chain driven by an external parabolic magnetic field. As far as the author knows, Article I is the first article which adapts GPM for the considered here spin chains' OCPs. The Pontryagin maximum principle (PMP) (e.g., [15]), genetic algorithm (GA) (stochastic zeroth-order global search, e.g., in [19]) are traditionally used in QOC.

The transfer model given in [6; 7; 16] is modified here using a certain type of pointwise constraints on controls (adjustment of the admissible set). Moreover, the article considers such the problem that initially has an excitation at the last spin and requires to keep the excitation at the last spin. While [7; 16] use the regularized first-order iterative Krotov method (about this method in TOC and QOC, one can see, e.g., in [11]), the article [6] uses the CRAB (Chopped RAndom-Basis) method described in that article. The works [10; 23], etc. consider another objective functional and [10], etc. use the Gurman method of derived OCPs, which is long known in TOC. In general for the direction devoted to transferring quantum information along a spin chain, consider also the pioneering article [3] (2003) and, e.g., [9].

For each of the considered OCPs, this article obtains, first, the corresponding adjoint system, infinite-dimensional gradient under piecewise continuous (PCont.) controls and, second, obtains the finite-dimensional gradient under piecewise constant (PConst.) controls from the infinite-dimensional gradient. This way relates to the approach known both in TOC [2; 5] and QOC [13, slides 16, 17]. Using PConst. controls in QOC is a popular approach integrated, e.g., into the GRAPE (GRadient Ascent Pulse Engineering) method and GPM in [20], etc. so that gradients under PConst. controls are obtained directly in comparison to the approach of [2; 5; 13] and the current article. In QOC, the direction to use some parameterization (e.g., PConst.) of controls together with a zeroth-order stochastic optimization tool, e.g., GA, is important. Separately from GPM, this article orienting to GA considers some special classes of controls for the transfer and keeping problems (Example 3 below is given in this regard).

As is known in the mathematical optimization theory, GPM-1S in its various forms is long known and traditional both for finite- and infinite-dimensional optimization (e.g., [4; 8; 24]). The articles [1; 17], etc. give such the GPM-2S, GPM-3S and the two- and three-order GPM forms that were constructed for minimizing a function in $\mathbb{R}^n$ in the frames of convex smooth optimization beyond quantum physics. These methods remind the Polyak heavy-ball method [21] long known for unconstrained optimization. Thus, this paper is relevant to the direction of accelerating gradient-based optimization through the quantum applications. For this direction, and without citing a large number of the relevant mathematical articles known to the author, note also, e.g., the Nesterov accelerated gradient method. In mathematics, the direction of two- and three-step GPM forms for a *non-convex* continuously differentiable objective function, even with a *convex* compact feasible set in $\mathbb{R}^n$, is still *open for development*, as far as the author knows, including for automatic adaptive adjustment of the step-size and inertial parameters. Article I does not aimed to construct such an automatic adaptive scheme for adjusting the GPM parameters and to give a rigorous theoretical study of the iterative behavior of GPM-2S, GPM-3S for the considered nonlinear OCPs. The article notes this open direction and contributes to it through considering the spin chains' problems.

This article is devoted to obtaining new results that extend those presented in [7; 16; 23], etc. First, Article I suggests a certain pointwise time-dependent constraint on controls for the transfer problem and introduces the problem of keeping an excitation initially given at the last spin under this constraint. Second, Article I adapts the projection-type linearized PMP and GPM (in its noted above forms and frames) for the considered OCPs. Third, for the transfer problem, Article I shows numerically (for the case of 30 spins) the effectiveness of combining GA with the simple parameterized class of controls suggested below.

2. Optimal Control Models with Spin Chains

Based on [7; 16; 23], etc., this article considers a one-dimensional spin chain of $N > 1$ sites coupled via nearest-neighbor interactions on some time range $[0, T]$, as determined by

$$\frac{d\psi^u(t)}{dt} = -i\big(H_0 + H_1(t, u(t))\big)\psi^u(t), \quad \psi^u(0) = \psi_0, \quad u = (u_1, u_2), \tag{2.1}$$

$$H_0 = -2JI_N + J\begin{pmatrix} 1 & 1 & 0 & \dots & 0 & 0 \\ 1 & 0 & 1 & \dots & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & 0 & \dots & 1 & 1 \end{pmatrix} = \begin{pmatrix} -1 & 1 & 0 & \dots & 0 & 0 \\ 1 & -2 & 1 & \dots & 0 & 0 \\ 0 & 1 & -2 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & -2 & 1 \\ 0 & 0 & 0 & \dots & 1 & -1 \end{pmatrix} \text{ at } J = 1, \tag{2.2}$$

$$H_1(t, u) = \mathrm{diag}(g_m(t, u))_{m=1}^N, \quad g_m(t, u) = u_1(m - 1 - \sigma(t) - u_2)^2. \tag{2.3}$$

This vector ordinary differential equation (ODE) with complex-valued state $\psi^u(t)$ satisfies the invariant $\|\psi^u(t)\|_{\mathbb{C}^N} = 1$, i.e. $\psi^u(t) \in S^{2N-1}(1) \subset \mathbb{C}^N$. In this regard, note the known Hopf fibration $S^1 \hookrightarrow S^{2N-1} \xrightarrow{p} \mathbb{C}P^{N-1}$ which has the total space S^{2N-1}, base $\mathbb{C}P^{N-1}$ (complex projection space being a Köhler manifold and representing physical states modulo $e^{i\varphi}$), and fiber S^1. Here u_1 and $u_2 = d - \sigma$ are real-valued program controls, describe correspondingly the *intensity* and shifted *position* of an external magnetic parabolic field (in [7; 16], $d(t)$ represents the position). Here H_0, H_1 are correspondingly the time-independent free Hamiltonian, time-dependent controlling Hamiltonian (constant real sparse matrices), the interspin coupling J in the Heisenberg-type H_0 and the Planck constant are already conditionally set to 1. As described in [16], the dimension of the effective Hilbert space is simply N, i.e. not 2^N, in this case.

First, we consider *PCont.* u, the shift $\sigma(t) = w\,t$, $w = (N-1)/T$ and introduce the following pointwise constraint for regulating the admissible ranges of values of the intensity and shifted position:

$$u(t) = (u_1(t), u_2(t)) \in Q_u(t) := [-b_1(t),\, b_1(t)] \times [-b_2(t),\, b_2(t)] \tag{2.4}$$

where $t \in [0, T]$ and, by analogy with [15, Eq. (4)] considering some another OCPs, we take the concave functions

$$b_l = \bar{b}_l \operatorname{sinc}\left(2^{q_l} \pi (t/T - 1/2)^{q_l}\right), \quad l = 1, 2$$

with $\bar{b}_l > 0$, $q_l \in [3, 8] \subset \mathbb{N}$. This means $b_l(0) = b_l(T) = 0$, $l = 1, 2$ and represents the considered here requirement of calm switching on and off of u_1, u_2 with $u_l(0) = u_l(T) = 0$, $l = 1, 2$.

As a variant, consider *PConst.* u, the shift

$$\sigma(t) = w \sum\nolimits_{j=0}^{M-1} \theta_{[t_j, t_{j+1})}(t)(t_j + t_{j+1})/2, \quad w = (N-1)/T \tag{2.5}$$

($\theta_{[t_j, t_{j+1})}$ is the characteristic function), a given time grid

$$\Theta_M = \{t_0 = 0,\ t_1 = (\Delta t)_1, \ldots,\ t_{M-1} = T - (\Delta t)_M,\ t_M = T\} \tag{2.6}$$

(as a variant, the grid can be uniform with $\Delta t = T/M$), vector

$$\mathbf{a} = (a_1, \ldots, a_s, \ldots, a_{2M}) = \big(c_{1,1}, \ldots,\ c_{1,M},\ c_{2,1}, \ldots,\ c_{2,M}\big) \tag{2.7}$$

with $c_j = (c_{l,j})_{l=1}^2 = u(t_{j-1})$ ($j \in \overline{1, M}$) (i.e. the values of u along all the partial ranges at $[0, T]$), and the constraint

$$\mathbf{a} \in Q_{\mathbf{a}} = (\bigtimes\nolimits_{j=1}^{M} [-\nu_{1,j}, \nu_{1,j}]) \bigtimes (\bigtimes\nolimits_{j=1}^{M} [-\nu_{2,j}, \nu_{2,j}]) \subset \mathbb{R}^{2M}. \tag{2.8}$$

Here we define $\nu_{l,j}$ from b_l. If $\Delta t = T/M$ is sufficiently small, then one can simply define $\nu_{l,j} = b_l(t_j + \Delta/2)$ for (2.8). Let $r \in \overline{1, M}$ to show which particular range is taken. For some sth element of $\mathbf{a}$, we have

$$r = \begin{cases} s \bmod M, & s \bmod M \neq 0, \\ M, & s \bmod M = 0, \end{cases} \qquad l = \begin{cases} \lfloor s/M \rfloor + 1, & s \bmod\ \neq 0, \\ \lfloor s/M \rfloor, & s \bmod M = 0. \end{cases}$$

Under some class $\mathcal{U}$ of admissible controls, consider the problem of *transfer* $\psi^u(0) = \psi_0 = (1, 0, \dots, 0)^{\mathrm{T}}$ to $\psi_{\mathrm{g}} = (0, \dots, 0, 1)^{\mathrm{T}}$ in the meaning to obtain the final probability (invariant) $\big|\langle \psi^u(T), \psi_{\mathrm{g}} \rangle\big|^2_{\mathbb{C}^N} = 1$ (with a good precision). A possible way is, as in [7; 16; 23], to consider a fixed T and the corresponding problem to maximize the final probability, i.e.

$$\begin{aligned} I_1(u) = F(\psi^u(T); \psi_{\mathrm{g}}) = 1 - \big|\langle \psi^u(T), \psi_{\mathrm{g}} \rangle\big|^2 = \\ = 1 - \langle \psi_{\mathrm{g}}, \psi^u(T) \rangle \langle \psi^u(T), \psi_{\mathrm{g}} \rangle = 1 - |\psi^u_N(T)|^2 \to \min_{u \in \mathcal{U}} \end{aligned} \tag{2.9}$$

and T is changed, if needed. Here $F(\psi; \psi_{\mathrm{g}})$ is continuously differentiable in ψ. The geometry of $I_1(u)$ depends on several factors, including $F(\psi; \psi_{\mathrm{g}})$. In the view of $\|\psi\| = 1$, one has $F(\psi; \psi_{\mathrm{g}}) \in [0, 1]$. The minimal value of $F(\psi; \psi_{\mathrm{g}})$, i.e. 0, is reached at $\psi = (0, ..., 0, \psi_N)^{\mathrm{T}}$ with ψ_N being on the complex unit circle $S^1(1)$. If one takes $\psi = \widehat{\psi} e^{i\varphi}$ with $\varphi \in [0, 2\pi)$, then $|\psi_N|^2 = |\widehat{\psi}_N|^2 |e^{i\varphi}|^2 = |\widehat{\psi}_N|^2$, i.e. F is invariant under the phase factor. At $t = 0$, one has the largest value $F(\psi_0; \psi_{\mathrm{g}}) = 1 - |\langle \psi_0, \psi_{\mathrm{g}} \rangle|^2 = 1$. Moreover, $F(\psi; \psi_{\mathrm{g}}) = \sin^2(g_{\mathrm{FS}}(\psi, \psi_{\mathrm{g}}))$, where $g_{\mathrm{FS}}(\psi, \psi_{\mathrm{g}}) = \arccos |\langle \psi, \psi_{\mathrm{g}} \rangle| = \arcsin \sqrt{F(\psi; \psi_{\mathrm{g}})} \in [0, \pi/2]$ is the Fubini–Study distance on $\mathbb{C}P^{N-1}$.

Of course, one can expect such a case that, under some given T, etc., there is such a control process $(\widehat{u}, \psi^{\widehat{u}})$ that is *globally optimal* in this OCP from the point of view of TOC, — i.e. the objective functional I_1 cannot be decreased more via any way, — but $F(\psi^{\widehat{u}}(T); \psi_{\mathrm{g}})$ is *significantly larger* than 0. One can formulate the problem to obtain such a pair (u, T) that $\big|\langle \psi^u(T), \psi_{\mathrm{g}} \rangle|^2 = 1$ and $\Upsilon(u, T) = T \to \min$ under variable T. In practice, one can look for a finite set of such values of T that $I_1 \approx 0$ with a good precision for each of these cases; then, one can take the minimal T over this finite set. Below GPM is considered only under a fixed T.

For the transfer problem and orienting to GA, this article introduces the following *special parameterized class of continuous controls* representing possible non-instantaneous pulses near $t = 0, T$:

$$Q_u(t) \ni u_l(t) = \begin{cases} \theta^{\mathrm{L}}_l b_l(t), & t \in [0, \widehat{t}_1), \\ \frac{y_l - \theta^{\mathrm{L}}_l b_l(\widehat{t}_1)}{(\widehat{t}_2 - \widehat{t}_1)^2} (t - \widehat{t}_1)^2 + \theta^{\mathrm{L}}_l b_l(\widehat{t}_1), & t \in [\widehat{t}_1, \widehat{t}_2), \\ y_l, & t \in [\widehat{t}_2, \widehat{t}_3), \\ \frac{y_l - \theta^{\mathrm{R}}_l b_l(\widehat{t}_4)}{(\widehat{t}_4 - \widehat{t}_3)^2} (t - \widehat{t}_4)^2 + \theta^{\mathrm{R}}_l b_l(\widehat{t}_4), & t \in [\widehat{t}_3, \widehat{t}_4), \\ \theta^{\mathrm{R}}_l b_l(t), & t \in [\widehat{t}_4, T], \end{cases} \tag{2.10}$$

where "L" and "R" mean "left" and "right", $l = 1, 2$, $0 < \widehat{t}_1 < \widehat{t}_2 < \widehat{t}_3 < \widehat{t}_4 < T$. For this class, we take its controlling parameters together as

$$\mathbf{x} = \big(\theta^{\mathrm{L}}_1, \theta^{\mathrm{R}}_1,\ \theta^{\mathrm{L}}_2, \theta^{\mathrm{R}}_2,\ y_1, y_2,\ \widehat{t}_1, \widehat{t}_2, \widehat{t}_3, \widehat{t}_4\big) \in Q_{\mathbf{x}} \tag{2.11}$$

with $Q_{\mathbf{x}}$ representing $\theta_l^{\mathrm{L}}, \theta_l^{\mathrm{R}} \in [-1,1]$, $y_l \in [-0.1\bar{b}_l, 0.1\bar{b}_l]$, $l = 1,2$, $\widehat{t_1} \in [\xi_1, \xi_2]$, $\widehat{t_2} \in [\xi_3, \xi_4]$, $\widehat{t_3} \in [\xi_5, \xi_6]$, $\widehat{t_4} \in [\xi_7, \xi_8]$ with such given $\{\xi_s\}_{s=1}^{8}$ that $0 < \xi_1 < \xi_2 < \xi_3 < \xi_4 \le 0.2T$, $0.8T \le \xi_5 < \xi_6 < \xi_7 < \xi_8 < T$. This class is inspired, e.g., by Fig. (a),(b) in [12]. Such u is below approximated via its PConst. version at a given grid Θ_M via taking $u_l(t_j)$ at each $[t_j, t_{j+1})$.

In the case of PConst. u (arbitrary PConst. u or as an approximation for (2.10)) and PConst. σ (2.5), the dynamic system is discrete-continuous and exactly is solved, as Lemma 2 shows, simply via a chronological product of ψ_0 and certain unitary propagators corresponding to Θ_M. Since the coefficients of the considered ODE are constant, then, e.g., the theory of the Magnus expansion is not needed here. In contrast, [12] reduces the complex-valued ODE to its real-valued form, then uses a piecewise linear representation for PCont. controls together with the Radau method. Moreover, by analogy with the keeping problem given in [15, Subsect. 4.8] for some another quantum dynamics, this article considers such the problem that considers an excitation given at the last spin at $t = 0$ and requires to keep the excitation at the last spin at a given $[0,T]$. Here we have $\psi_{\mathrm{g}} = (0,0,\dots,1)^{\mathrm{T}}$, i.e. as in the transfer problem, and, in contrast to the transfer problem, we can take $\psi^u(0) = \psi_{\mathrm{g}}$ in the keeping problem (this case relates to the phase factor $\varphi = 0$). In contrast to the transfer problem, here the goal is to obtain such u that the invariant $|\langle \psi^u(t), \psi_0 \rangle|^2 \equiv 1$ at $[0,T]$ is hold. For the keeping problem, consider

$$I_2(u) = F(\psi^u(T); \psi_{\mathrm{g}}) + P_\psi \int_0^T F(\psi^u(t); \psi_{\mathrm{g}}) dt \to \min_{u \in \mathcal{U}}, \quad P_\psi > 0. \quad (2.12)$$

Both for the transfer and keeping problems under PCont. u and in addition to the time-dependent constraint (2.4), consider the following composite objective functionals containing $I_p(u)$, $p \in \{1,2\}$:

$$\Phi_p(u) = I_p(u) + \int_0^T \sum\nolimits_{l=1}^{2} P_{u_l} S_l(t) u_l^2(t) dt \to \min_{u \in \mathcal{U}}. \quad (2.13)$$

Here $P_{u_l} \ge 0$, $l = 1,2$, the functions $S_l(t) = \exp[C_{S_l}(t/T - 1/2)^2]$ are taken with sufficiently large $C_{S_l} > 0$, $l = 1,2$. In order to adjust u_1, u_2 near $t = 0, T$, this tool is in addition to (2.4) and is by analogy with [15, Eq. (5)] considering some another quantum OCPs. The choice $S_l(t) \equiv 1$ yields the classical Tikhonov regularization.

With respect to the finite-dimensional GPM developed below, we consider PConst. controls and the corresponding objective functions $f_p(\mathbf{a}) = \Phi_p(u)$ ($p \in \{1,2\}$) to be minimized in view of (2.5)–(2.9), (2.13), where we take certain PConst. S_l, $l = 1,2$ at a certain grid Θ_M, as well as σ.

Beyond GPM, when the special class of controls (2.10) for the transfer problem is used via some PConst. approximation for this class, consider:

1) $2M$-dimensional vector $\mathbf{a}$ defined in (2.7) and representing u in order to solve (2.1) via the way given below in Lemma 2; 2) 10-dimensional vector $\mathbf{x}$ defined in (2.11) and consisting of the parameters of (2.10) in order to optimize u under a given T and

$$f_3(\mathbf{x}) = I_1(u(\cdot;\mathbf{x})) + P_{\mathbf{x}} \sum\nolimits_{j=0}^{M-1} \sum\nolimits_{l=1}^{2} |u_l(t_j;\mathbf{x})| \to \min_{\mathbf{x}\in Q_{\mathbf{x}}}, \quad P_{\mathbf{x}} \geq 0. \quad (2.14)$$

Further, also for the transfer problem, but under T being free at a given range $[T_1, T_2]$, $T_1 > 0$, we consider $t = T\,\tau$, $\tau \in [0,1]$, introduce $v = (\breve{u}, T)$, $\breve{u}(\tau) = u(T\tau)$, $\breve{\sigma}(\tau) = \sigma(T\tau)$, etc., and

$$\frac{d\breve{\psi}^{\,v}(\tau)}{d\tau} = -i\,T\left(H_0 + \breve{H}_1(\tau, \breve{u}(\tau))\breve{\psi}^{\,v}(\tau), \quad \tau \in [0,1], \quad \breve{\psi}^{\,v}(0) = \psi_0 \quad (2.15)$$

for an arbitrary N. Consider the corresponding analogue for the special class (2.10), approximate this analogue at the grid

$$\{\tau_0 = 0 < \ldots < \tau_j < \ldots < \tau_M = 1\} \quad (2.16)$$

and then instead of (2.14) consider

$$\breve{f}_3(\mathbf{x}, T) = 1 - \left|\langle \breve{\psi}^{\,v}(\tau = 1), \psi_{\mathrm{g}}\rangle\right|^2 + P_{\mathbf{x}} \sum\nolimits_{j=1}^{M-1} \sum\nolimits_{l=1}^{2} |\breve{u}_l(\tau_j;\mathbf{x}, T)| +$$
$$+ P_T\,T \to \min_{(\mathbf{x},T)}, \quad P_{\mathbf{x}},\ P_T \geq 0. \quad (2.17)$$

For the keeping problem and orienting to GA, consider the following special parameterized continuous class of controls:

$$u(t) = \left(\mathrm{Pr}_{Q_{u}(t)}\Big(\sum\nolimits_{i=1}^{M_{\sin}} \kappa_{l,i} \sin\left(\lceil \omega_{l,i} \rceil \pi t/T\right)\Big),\ l = 1,2\right), \quad t \in [0,T],$$

where $\mathrm{Pr}_{Q_u(t)}$ means the orthogonal projection onto $Q_{u(t)}$ at each t. Consider the corresponding $4M_{\sin}$-dimensional vector

$$\mathbf{y} = (\kappa_{1,1},\ \kappa_{1,1},\ \ldots,\ \kappa_{2,M_{\sin}},\ \omega_{2,M_{\sin}}) \in Q_{\mathbf{y}}$$

($Q_{\mathbf{y}}$ is a given convex compact set), approximate u at Θ_M for obtaining its PConst. version, introduce $P_{\mathbf{y}} \geq 0$ and consider the following objective function to be minimized under a given T:

$$f_4(\mathbf{y}) = \max_{j\in\overline{1,M}} F(\psi^u(t_j);\psi_{\mathrm{g}}) + P_{\mathbf{y}} \sum\nolimits_{j=0}^{M-1} \sum\nolimits_{l=1}^{2} |u_l(t_j;\mathbf{y})| \to \min_{y\in Q_{\mathbf{y}}}.$$

Here, as a variant, one can consider directly $m_{l,i} \in [1, \overline{N}] \in \mathbb{N}$ instead of $\lceil \omega_{l,i} \rceil$, because, e.g., the GA implementation [22] allows to use mixed types of variables to be optimized.

3. Infinite-Dimensional Gradients, Projection-Type Linearized PMP, Zero Control

Lemma 1. *With a given final time T, PCont. control $u = (u_1, u_2)$, consider the transfer problem (2.1)–(2.4), (2.9), (2.13), i.e. in the terms of $\Phi_1(u)$, or the keeping problem (2.1)–(2.4), (2.12), (2.13), i.e. in the terms* *of* $\Phi_2(u)$. *For these problems, the following constructions with a given admissible control* $u^{(k)}$ *are hold (the index "p" for the quantum and adjoint systems' solutions is omitted): 1) the adjoint equation*

$$\frac{d\eta^{u^{(k)}}(t)}{dt} = -i\left(H_0 + H_1(t, u^{(k)}(t))\right)\eta^{u^{(k)}}(t) + \\ + \begin{cases} 0, & \Phi = \Phi_1, \\ 2P_\psi\langle\psi_{\rm g}, \psi^{u^{(k)}}(t)\rangle\psi_{\rm g} = (0, \ldots, 0, 2P_\psi(\psi_N^{u^{(k)}}(t))^*)^{\rm T}, & \Phi = \Phi_2; \end{cases} \quad (3.1)$$

2) the final-time condition

$$\eta^{u^{(k)}}(T) = \eta^{u^{(k)}}_{\rm Transv.} = 2\langle\psi_{\rm g}, \psi^{u^{(k)}}(T)\rangle\psi_{\rm g} = (0, \ldots, 0, 2(\psi_N^{u^{(k)}}(T))^*)^{\rm T}; \quad (3.2)$$

3) the infinite-dimensional gradients ($p \in \{1,2\}$)

$$\nabla\Phi_p(u^{(k)})(t) = \Big(-\,{\rm Im}\Big\langle \eta^{u^{(k)}}(t), \frac{\partial H_1(t,u)}{\partial u_l}\Big|_{u=u^{(k)}(t)} \psi^{u^{(k)}}(t) \Big\rangle_{\mathbb{C}^N} + \\ + 2P_{u_l}S_l(t)u_l^{(k)}(t),\ l = 1,2\Big), \quad t \in [0,T], \quad (3.3)$$

where
$$\frac{\partial H_1}{\partial u_1} = {\rm diag}\{(m-1-\sigma(t)-u_2)^2\}_{m=1}^N, \\ \frac{\partial H_1}{\partial u_2} = -2u_1{\rm diag}\{(m-1-\sigma(t)-u_2)\}_{m=1}^N;$$

4) the gradient increment formula

$$\Phi_p(u) - \Phi_p(u^{(k)}) = \langle\nabla\Phi_p(u^{(k)}), u - u^{(k)}\rangle_{L_2([0,T],\mathbb{R}^2)} - \\ - |\langle\psi_{\rm g}, \psi^u(T) - \psi^{u^{(k)}}(T)\rangle|^2 + r_p,\ p \in \{1,2\}. \quad (3.4)$$

Proof. By analogy with [11, §6.5], [15, Sect. 2], Krotov Lagrangian long known in TOC is adapted here. We take it at an admissible (u, ψ^u) and with a solving linear function $\varphi(t,\psi) = {\rm Re}\langle\eta(t),\psi\rangle = \frac{1}{2}\big(\langle\eta(t),\psi\rangle + \langle\psi,\eta(t)\rangle\big)$ (this form of φ is taken as in [11, p. 256]):

$$KL_p(u) = G(\psi^u(T)) - \int_0^T R(t, \eta(t), \psi^u(t), u(t))dt \equiv \Phi_p(u), \\ G(\psi^u(T)) = F(\psi^u(T); \psi_{\rm g}) + {\rm Re}\langle\eta(T), \psi^u(T)\rangle - {\rm Re}\langle\eta(0), \psi^u(0)\rangle, \\ R(t, \eta(t), \psi^u(t), u(t)) = {\rm Re}\Big[\langle\eta(t), -i(H_0 + H_1(t,u(t)))\psi^u(t)\rangle + \\ + \Big\langle\frac{d\eta(t)}{dt}, \psi^u(t)\Big\rangle\Big] - P_\psi F(\psi^u(t); \psi_{\rm g}) - \sum_{l=1}^2 P_{u_l}S_l(t)u_l^2(t)$$

with $P_\psi = 0$, if $p = 1$, and $\eta(t)$ to be defined. At an arbitrary admissible u and a given admissible $u^{(k)}$, consider

$$KL_p(u) - KL_p(u^{(k)}) = G(\psi^u(T)) - G(\psi^{u^{(k)}}(T)) - \\ - \int_0^T [R(t, \eta(t), \psi^u(t), u(t)) - R(t, \eta(t), \psi^{u^{(k)}}(t), u^{(k)}(t))]dt$$

where $\psi^{u^{(k)}}$ is the solution of (2.1) with $u = u^{(k)}$, while η is determined below. For $p \in \{1, 2\}$, the quadratic increment $G(\psi^u(T)) - G(\psi^{u^{(k)}}(T))$ is equally represented by the finite Taylor expansion

$$\mathrm{Re}\big\langle \eta(T) + \nabla_\psi F(\psi; \psi_{\mathrm{g}})\big|_{\psi = \psi^{u^{(k)}}(T)}, \psi^u(T) - \psi^{u^{(k)}}(T)\big\rangle - |\langle \psi_{\mathrm{g}}, \psi^u(T) - \psi^{u^{(k)}}(T)\rangle|^2.$$

Here the Wirtinger-type gradient

$$\nabla_\psi F(\psi^{u^{(k)}}(T); \psi_{\mathrm{g}}) = -2\langle \psi_{\mathrm{g}}, \psi^{u^{(k)}}(T)\rangle \psi_{\mathrm{g}} \in T_\psi \mathbb{C}^N$$

and Hessian matrix $H_F = -2\psi_{\mathrm{g}}\psi_{\mathrm{g}}^*$ are used. In this expansion, the first-order term is taken to be zero for obtaining (3.2), whereas the second-order term is taken for (3.4). Consider how the increment for R is used for deriving (3.1), (3.3), (3.4). This increment is linear (for $p = 1$) or quadratic (for $p = 2$) in $\psi^u(t)$. Depending on p, we derive the corresponding finite Taylor expansion. Its first-order part related to $\psi^u(t) - \psi^{u^{(k)}}(t)$ provides (3.1), the rest gives (3.3), (3.4) with some r_p. □

Corollary 1. *In the transfer problem, consider the control $u = 0$. Then the solution of (2.1) is $\psi^{u=0}(t) = e^{-iH_0 t}\psi_0$, the solution of (3.1), (3.2) is $\eta^{u=0}(t) = e^{iH_0(T-t)}\eta^{u=0}_{\mathrm{Transv.}}$, and the gradient (3.3) becomes*

$$\nabla\Phi_1(0)(t) = \Big(-\,\mathrm{Im}\,\Big\langle e^{iH_0(T-t)}\eta^{u=0}_{\mathrm{Transv.}}, \frac{\partial H_1(t,u)}{\partial u_l}\Big|_{u=0} e^{-iH_0 t}\psi_0\Big\rangle,\ l = 1, 2\Big)$$

with $\frac{\partial H_1(t,u)}{\partial u_1}\Big|_{u=0} = \mathrm{diag}\{(m - 1 - \sigma(t))^2\}_{m=1}^N$ *and* $\frac{\partial H_1(t,u)}{\partial u_2}\Big|_{u=0} = 0_N$.

Proof. For obtaining

$$\eta^{u=0}(t) = e^{iH_0(T-t)}\eta^{u=0}_{\mathrm{Transv.}}, \text{ one has } e^{-iH_0 T}c = \eta^{u=0}_{\mathrm{Transv.}},$$

multiples it by $e^{iH_0 T}$, obtains $e^{iH_0 T}e^{-iH_0 T}c = I_N c$ using that the matrices $iH_0 T$, $-iH_0 T$ commute and matrix exponentials are invertible matrices. Taking $\psi^{u=0}(t)$, $\eta^{u=0}(t)$, $u = 0$ in (3.3) gives the gradient formula for the case $u = 0$. □

By analogy with the projection-type linearized PMP known in TOC and used for QOC, e.g., in [15], the following theorem is considered.

Theorem 1. *(Projection-type linearized PMP). With PCont. u, consider the transfer problem (2.1)–(2.4), (2.9), (2.13), i.e. in the terms of $\Phi_1(u)$, and the keeping problem (2.1)–(2.4), (2.12), (2.13), i.e. in the terms of $\Phi_2(u)$. For any OCP among these problems, if an admissible control $\widetilde{u}$ is a local minimum point for the corresponding $\Phi_p(u)$, $p \in \{1, 2\}$, then for $\widetilde{u}$ there exist such the solutions $\psi^{\widetilde{u}}, \eta^{\widetilde{u}}$ of (2.1), (3.1), (3.2) that the following pointwise condition is hold:*

$$\widetilde{u}(t) = \mathrm{Pr}_{Q_u(t)}\left(\widetilde{u}(t) - \alpha\nabla\Phi_p(\widetilde{u})(t)\right) \quad \forall\ \alpha > 0,\ t \in [0, T]. \qquad (3.5)$$

An extremal control $\widetilde{u}$ is determined by (3.5) for any $\alpha > 0$.

Example 1. Consider the transfer problem with $\Phi_1(u) = I_1(u)$, $N = 3$. Here, following (2.2), (2.3), take $H_0 = \begin{pmatrix} -1 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{pmatrix}$, $H_1 = u_1 \operatorname{diag}\big((\sigma(t) + u_2)^2, (1-\sigma(t)-u_2)^2, (2-\sigma(t)-u_2)^2\big)$. Following Corollary 1, one analytically obtains $\nabla\Phi_1(0)(t) = \big(\text{non-zero large expression}, 0\big)$, i.e. $u \equiv 0$ at the whole $[0, T]$ for any $T > 0$. The second component of the vector condition (3.5) is $0 = 0$ at the whole $[0, T]$. Substituting the solution $\psi^{u=0}(t) = e^{-iH_0 t}\psi_0$ into the function $F(\psi; \psi_{\rm g})$ instead of ψ gives $F_1 = \frac{1}{18}\big(6\cos t + 3\cos(2t) - 2\cos(3t) + 11\big)$ which is shown in Fig. 1(a) for $t \in [0, 4\pi]$. Here we see that $u = 0$ *cannot* provide the transfer. $\square$

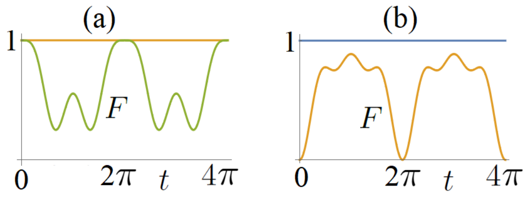

Figure 1. $F(\psi^{u=0}(t); \psi_{\rm g})$ vs t: (a) in the transfer problem (Example 1, $\psi_0 \neq \psi_{\rm g}$); (b) in the keeping problem (Example 2, $\psi_0 = \psi_{\rm g}$).

Example 2. For the keeping problem, the quantum system with the condition $\psi^{u=0}(0) = \psi_{\rm g}$ has the solution $\psi^{u=0}(t) = e^{-iH_0 t}\psi_{\rm g}$ whose substitution into $F(\psi; \psi_{\rm g})$ gives $F = 1 - |\langle \psi^{u=0}(t); \psi_{\rm g}\rangle|^2 = \frac{2}{9}(7\cos t + 2\cos(2t) + 9)\sin^2\frac{t}{2}$ reaching 0 at $t = 2\pi n$, $n = 1, 2, \ldots$ This is shown in Fig. 1(b) for $t \in [0, 4\pi]$. Here we see that $u = 0$ *cannot* provide the keeping. $\square$

4. System's States Representation via Matrix Exponentials, Condition for Optimality, Finite-Dimensional GPM

Lemma 2. *Consider the system (2.1)–(2.3). With a given grid Θ_M defined in (2.6), consider correspondingly PConst. σ in the form (2.5) and PConst. u with its representation as* $\mathbf{a}$ *at Θ_M. For a given admissible PConst. u, consider the exact formulas*

$$\psi^u(t_{j+1}) = e^{A(c_{j+1})(t_{j+1}-t_j)}\psi^u(t_j), \quad j \in \overline{0, M-1}, \quad \psi^u(t_0) = \psi_0, \tag{4.1}$$

$$A(c_{j+1}) = -i\Big(H_0 + c_{1,j+1}\operatorname{diag}\big(\big(m - 1 - \frac{t_j + t_{j+1}}{2}w - c_{2,j+1}\big)^2\big)_{m=1}^{N}\Big) \tag{4.2}$$

where $\psi^u(t_j)$ ($j \in \overline{1, M}$) depends continuously on $\mathbf{a}$. *Consider the transfer problem (2.1)–(2.4), (2.9), (2.13) and the keeping problem (2.1)–(2.4),* *(2.12), (2.13) on the grid Θ_M, in the terms of the corresponding objective functions $f_p(\mathbf{a})$, $p = 1, 2$. Here we have the increment formula*

$$\Phi_p(u) - \Phi_p(u^{(k)}) = f_p(\mathbf{a}) - f_p(\mathbf{a}^{(k)}) = \langle \nabla f_p(\mathbf{a}^{(k)}), \mathbf{a} - \mathbf{a}^{(k)} \rangle + R_p \qquad (4.3)$$

where the gradient consists of

$$(\nabla f_p(\mathbf{a}^{(k)}))_s = \int_{t_j}^{t_{j+1}} d_l^{(k)}(t; \mathbf{a}^{(k)}) dt, \quad d_l^{(k)} = (\nabla \Phi_p(u^{(k)})(t))_l \qquad (4.4)$$

with the indices $p \in \{1, 2\}$, $s \in \overline{1, 2M}$, $j \in \overline{0, M-1}$, $l \in \{1, 2\}$.

Proof. The formulas (4.1), (4.2) describe the construction of the continuous function ψ^u on $[0, T]$ by sequentially deriving the function's parts along all the particular time ranges, where each subsequent part continues the previous one without a jump. The sequential Cauchy problems

$$\frac{d\psi^{c_{j+1}}(t)}{dt} = A(c_{j+1}) \psi^{c_{j+1}}(t), \quad \psi^{c_{j+1}}(t_j) = \begin{cases} \psi^{c_j}(t_j), & j \neq 0, \\ \psi_0, & j = 0, \end{cases}$$

are solved under $j = \overline{0, M-1}$ with $\psi^{c_j}(t_j)$ taken to connect the neighboring parts of the composite trajectory. The continuity of $\psi^u(t_j)$ in $\{\mathbf{a}_s\}$ is based on considering all these matrix exponentials as uniformly converging series and on the preservation of the continuous dependence under the matrices' product. The formulas (4.3), (4.4) are derived basing on (2.3), (2.4). Here we take $c_{j+1}^{(k)}$ during a half of $[t_j, t_{j+1}]$. Under PConst. u, $u^{(k)}$, one has

$$\begin{aligned} & f_p(\mathbf{a}) - f_p(\mathbf{a}^{(k)}) = \Phi_p(u) - \Phi_p(u^{(k)}) = \\ & = \sum_{j=0}^{M-1} \sum_{l=1}^{2} \Big(\int_{t_j}^{t_{j+1}} G_l^{(k)}(t; \mathbf{a}) dt \Big)_l \big(u_l(t_j) - u_l^{(k)}(t_j) \big) + R_p = \\ & = \sum_{s=1}^{2M} (\nabla f_p(\mathbf{a}^{(k)}))_s \, (\mathbf{a}_s - \mathbf{a}_s^{(k)}) + R_p = \langle \nabla f_p(\mathbf{a}^{(k)}), \, \mathbf{a} - \mathbf{a}^{(k)} \rangle + R_p. \ \Box \end{aligned}$$

As N increases, the complexity of computing the matrix exponentials of order N increases. For the transfer / keeping problem with PConst. u, etc., one can solve (3.1), (3.2) simply by operating with the matrix exponentials that were previously computed for solving (2.1) and with the known algebraic fact that $e^{-B} = (e^B)^*$ for any anti-Hermitian matrix B (the corresponding details are omitted in Article I for brevity).

The next theorem takes into account the projection-type first-order necessary condition for optimality known (e.g., [24, part 2, p. 99]) in mathematics and does not require convexity/ strong convexity for $f_p(\mathbf{a})$ on the whole $Q_{\mathbf{a}}$.

Theorem 2. *(Necessary first-order condition for local optimality). For the transfer problem (2.1)–(2.4), (2.9), (2.13) and the keeping problem (2.1)–(2.4), (2.12), (2.13) both considered on the grid Θ_M and in the terms of the corresponding objective functions $f_p(\mathbf{a})$, $p = 1, 2$, and taking into account the gradient* $\operatorname{grad} f_p(\mathbf{a}_*)$ *using Lemma 1, one has that if*

$\mathbf{a}_*$ *is a local minimum point of* $f_p(\mathbf{a})$*, then the following equality is hold:* $\mathbf{a}_* = \mathrm{Pr}_{Q_{\mathbf{a}}}\big(\mathbf{a}_* - \alpha\,\nabla f_p(\mathbf{a}_*)\big)\ \forall\ \alpha > 0.$

Using the obtained finite-dimensional gradients, consider

$$\begin{aligned}
&\text{GPM-1S:}\quad \mathbf{a}^{(k+1)} = \mathrm{Pr}_{Q_{\mathbf{a}}}\big(\mathbf{a}^{(k)} - \alpha_k\,\nabla f_p(\mathbf{a}^{(k)})\big), \quad k \ge 0,\\
&\text{GPM-2S:}\quad \mathbf{a}^{(k+1)} = \mathrm{Pr}_{Q_{\mathbf{a}}}\big(\mathbf{a}^{(k)} - \alpha_k\,\nabla f_p(\mathbf{a}^{(k)}) +\\
&\qquad\qquad\qquad + \beta_k(\mathbf{a}^{(k)} - \mathbf{a}^{(k-1)})\big), \quad k \ge 1,\\
&\text{GPM-3S:}\quad \mathbf{a}^{(k+1)} = \mathrm{Pr}_{Q_{\mathbf{a}}}\big(\mathbf{a}^{(k)} - \alpha_k\,\nabla f_p(\mathbf{a}^{(k)}) + \beta_k(\mathbf{a}^{(k)} - \mathbf{a}^{(k-1)}) +\\
&\qquad\qquad\qquad + \gamma_k(\mathbf{a}^{(k-1)} - \mathbf{a}^{(k-2)})\big), \quad k \ge 2.
\end{aligned}$$

Here the projections are easily and uniquely and exactly analytically obtained. This article suggests to look for significant improvements of $\mathbf{a}^{(0)}$ with respect to $f_p(\mathbf{a})$ over a series of iterations, not necessarily in a monotonous manner, with trying to manually adjust the GPM coefficients by setting them equal to some fixed values for the series of iterations, e.g., $\alpha > 0,\ \beta \in (0,1), \gamma \in (0,\beta)$ in GPM-3S. Thus, after performing the series of iterations, we are interested in the corresponding last improving control and monotonically decreasing subsequence for f_p. For stopping GPM-2S and GPM-3S, one can consider, e.g., the following indicators (along with a simple upper limit on GPM iterations): 1) reaching a predefined lower threshold for the objective function's values; 2) absence of significant improvement for a predefined number of GPM iterations after good improvements or without them. The GPM quality depends on $\mathbf{a}^{(0)}$, on how precisely the integrals in (4.4) are approximated. Solving one Cauchy problem (2.1) can be considered as a unit of computational complexity for GPM.

5. GA for the Transfer Problem with $N = 30$ Spins

Example 3. Under $N = 30$, consider the transformed system (2.15), which evolves at $[0,1]$ with respect to τ, contains T as a controlling parameter. Consider a certain non-uniform grid (2.16) with $M = 300$. The objective function $\smile{f}_3(\mathbf{x}, T)$ defined in (2.17) should be minimized. Take $\bar{b}_1 = 2,\ \bar{b}_2 = 1,\ q_1 = q_2 = 8,\ \theta_1^{\mathrm{L}}, \theta_2^{\mathrm{L}}, \theta_1^{\mathrm{R}}, \theta_2^{\mathrm{R}} \in [-1,1]$, also $y_1 \in [-0.4, 0.4]$, $y_2 \in [-0.2, 0.2]$, $\widehat{\tau_1} \in [0.03, 0.07]$, $\widehat{\tau_2} \in [0.1, 0.14]$, $\widehat{\tau_3} \in [0.86, 0.9]$, $\widehat{\tau_4} \in [0.93, 0.97]$, $T \in [33, 39]$, $P_T = 0$, $P_{\mathbf{x}} = 0$. The corresponding program written by the author in Python uses `scipy.linalg.expm` representing the Padé approximation with a variable order for computing matrix exponentials given in (4.1), (4.2), also uses, e.g., the GA implementation [22] for which the parameters `max_num_iteration` $= 10^3$, `population_size` $= 50$, etc. were used. For the same problem, 16 trial runs of GA were performed. Over these runs, such the values $\{\smile{F}_s\}_{s=1}^{16}$, $\{T_s\}_{s=1}^{16}$ of $\smile{F} = 1 - \big|\langle\smile{\psi}^{\,v}(\tau =$

$1), \psi_{\rm g}\rangle\big|^2$, T were computed that $\mathrm{mean}\{\breve{F}_s\}_{s=1}^{16} \approx 0.011$, i.e. $\approx 1.1\,\%$ of the upper bound 1 for $\breve{F}$, $\min\{\breve{F}_s\}_{s=1}^{16} \approx 0.0026$, $\max\{\breve{F}_s\}_{s=1}^{16} \approx 0.020$, $\mathrm{mean}\{T_s\}_{s=1}^{16} \approx 36.6$. Here the best result is $(\breve{F} \approx 2.62 \cdot 10^{-3},\ T \approx 36.28)$. Although the special class of controls is simple, the final infidelity $\breve{F}$ is near $0.3\,\%$ of 1. Fig. 2 visualizes the best obtained result.

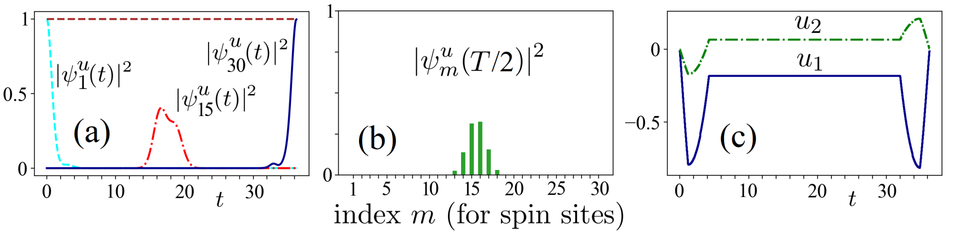

Figure 2. For Example 3 with $N = 30$, the GA results (before adding normally distributed noises): (a), (b) transfer in the terms of $|\psi_m^u(t)|^2$; (c) resulting controls.

Table 1.

For Example 3. The statistical results over a lot of cases of noised controls.

σ in $\mathcal{N}$	$\min Y$	$\max Y$	$\min W$	$\max W$	$\mathrm{mean}\, W$	$\mathrm{median}\, W$
0.05	≈ -0.29	≈ 0.26	≈ 0.008	≈ 0.236	≈ 0.052	≈ 0.046
0.1	≈ -0.54	≈ 0.52	≈ 0.023	≈ 0.655	≈ 0.181	≈ 0.165
0.15	≈ -0.76	≈ 0.84	≈ 0.040	≈ 0.907	≈ 0.354	≈ 0.334
0.2	≈ -1.10	≈ 1.05	≈ 0.056	≈ 0.977	≈ 0.526	≈ 0.520

Further, the following sensitivity analysis was performed. First, the best computed values of T, $\theta_1^{\rm L}$, etc. were rounded with six digits after the decimal point. Second, at each pth run among 10^4 independent runs, random values $\{n_{l,j,p}\}_{j=0}^{M-1}$ ($M = 300$, $l = 1,2$) were generated with the normal distribution $\mathcal{N}(\sigma = 0.05, \mu = 0)$ and added to the PConst. u_1, u_2 obtained above, i.e. we have $2M \cdot 10^4$ values $\{u_l(\tau_j) + n_{l,j,p}\}$ of $2 \cdot 10^4$ such *noised* controls and compute the corresponding 10^4 values $W = \{1 - \big|\langle \breve{\psi}^{\,v}(1), \psi_{\rm g}\rangle\big|^2\}$. The size of the corresponding $Y = \{n_{l,j,p}\}$ is $2M \cdot 10^4$. The value T is taken the same. Such the computations were performed also for $\sigma = 0.1,\ 0.15,\ 0.2$ in $\mathcal{N}$. Thus, the quantum ODE was solved $4 \cdot 10^4$ times using (4.1), (4.2) and $1.2 \cdot 10^7$ matrix exponentials (of order 30) were computed here. Table 3 shows the obtained min, max of Y (tailed values) and min, max, arithmetic mean, median of W for each $\sigma \in \{0.05, 0.1, 0.15, 0.2\}$. We see that some mild noise does not much change the final infidelity obtained via the GA approach.

6. Conclusion

This article (I) considers two optimal control models, one of which is devoted to transfer an excitation given at the first spin along a chain of N spins to the last spin — the other to keeping an excitation given at the last spin. Each model employs an external controlled parabolic magnetic field represented by two control functions. For these models, the corresponding infinite-dimensional gradients (Lemma 1) and the projection-type linearized PMP (Theorem 1) are given along with their finite-dimensional analogues (Lemma 1, Theorem 2). The finite-dimensional GPM in its one- and two- and three-step forms is represented in the planned frames. A special class of controls for the transfer model is introduced (2.10) for a genetic algorithm, and the corresponding transfer example (No. 3) for the case of $N = 30$ spins is given.

References

1. Antipin A.S. Minimization of convex functions on convex sets by means of differential equations. *Differ. Equat.*, 1994, vol. 30, pp. 1365–1375. https://www.mathnet.ru/eng/de9433
2. Arguchintsev A.V., Srochko V.A. Solution of a linear-quadratic problem on a set of piecewise constant controls with parameterization of the functional. *Proc. Steklov Inst. Math.*, 2022, vol. 319, pp. S43–S53. https://doi.org/10.1134/S0081543822060050
3. Bose S. Quantum communication through an unmodulated spin chain. *Phys. Rev. Lett.*, 2003, vol. 91, art. no. 207901. https://doi.org/10.1103/PhysRevLett.91.207901
4. Buldaev A.S. Perturbation methods in optimal control problems. *Optimization and Optimal Control*. New York, Springer, 2010, pp. 325–373. https://doi.org/10.1007/978-0-387-89496-6_17
5. Buldaev A. On one approach to the optimization of discrete-continuous controlled systems. *20th Intern. Conf. MOTOR: Rev. Sel. Papers*. Cham, Springer, 2021, pp. 463–477. https://doi.org/10.1007/978-3-030-86433-0_32
6. Caneva T., Calarco T., Montangero S. Chopped random-basis quantum optimization. *Phys. Rev. A*, 2011, vol. 84, art. no. 022326. https://doi.org/10.1103/PhysRevA.84.022326
7. Caneva T., Murphy M., Calarco T., Fazio R., Montangero S., Giovannetti V., Santoro G.E. Optimal control at the quantum speed limit. *Phys. Rev. Lett.*, 2009, vol. 103, art. no. 240501. https://doi.org/10.1103/PhysRevLett.103.240501
8. Demyanov V.F., Rubinov A.M. *Approximate Methods in Optimization Problems*. Leningrad, Leningrad Univ. Press, 1968. https://search.rsl.ru/en/record/01006108423 (in Russian)
9. Fel'dman E.B., Pechen A.N., Zenchuk A.I. Complete structural restoring of transferred multi-qubit quantum state. *Phys. Lett. A*, 2021, vol. 413, art. no. 127605. https://doi.org/10.1016/j.physleta.2021.127605
10. Gurman V.I., Rasina I.V. Optimization of processes in a spin chain. *Autom. Remote Control*, 2014, vol. 75, pp. 2212–2216. https://doi.org/10.1134/S0005117914120108
11. Krotov V.F. *Global Methods in Optimal Control Theory*. New York, Marcel Dekker Inc., 1996.

12. Morzhin O.V. About one approach to the optimal control problem of signal transfer along a spin chain. *Proc. 7th Int. Conf. DYSC*. Irkutsk, 2025. P. 81–84. Available at: https://math.isu.ru/ru/conference/2025/ (in Russian)
13. Morzhin O.V. Talk at the *3rd workshop MMPQT*. Moscow, 2019. Availablet: https://www.mathnet.ru/eng/present25886 (accessed on 27 April, 2026). (in Russian)
14. Morzhin O.V., Pechen A.N. Optimal state manipulation for a two-qubit system driven by coherent and incoherent controls. *Quantum Inf. Process.*, 2023, vol. 22, art. no. 241. https://doi.org/10.1007/s11128-023-03946-x
15. Morzhin O.V., Pechen A.N. Gradient projection method for constrained quantum control. *J. Phys. A: Math. Theor.*, 2025, vol. 58, art. no. 135303. https://doi.org/10.1088/1751-8121/adbe1a
16. Murphy M., Montangero S., Giovannetti V., Calarco T. Communication at the quantum speed limit along a spin chain. *Phys. Rev. Lett.*, 2010, vol. 82, art. no. 022318. https://doi.org/10.1103/PhysRevA.82.022318
17. Nedich A. The three-step gradient projection method for minimization problems. *Russian Math. (Iz. VUZ)*, 1993, vol. 37, no. 10, pp. 30–36. https://www.mathnet.ru/eng/ivm4551 (in Russian)
18. Oza A., Pechen A., Dominy J., Beltrani V., Moore K., Rabitz H. Optimization search effort over the control landscapes for open quantum systems with Kraus-map evolution. *J. Phys. A: Math. Theor.*, 2009, vol. 42, art. no. 205305. https://doi.org/10.1088/1751-8113/42/20/205305
19. Pechen A., Rabitz H. Teaching the environment to control quantum systems. *Phys. Rev. A*, 2006, vol. 73, art. no. 062102. https://doi.org/10.1103/PhysRevA.73.062102
20. Pechen A.N., Volkov B.O. Diverse efficiency of observable optimization for four-level quantum systems with higher-order traps. *Phys. Scr.*, 2026, vol. 101, art. no. 025101.
21. Polyak B.T. Some methods of speeding up the convergence of iteration methods. *USSR Comput. Math. Math. Phys.*, 1964, vol. 4, no. 5, pp. 1–17.
22. Solgi R. Genetic algorithm: Python implementation. Available online: `https://github.com/rmsolgi/geneticalgorithm` (accessed on 27 April, 2026).
23. Trushkova E.A. On one class of optimal control problems for quantum systems. *Autom. Remote Control*, 2013, vol. 74, no. 1, pp. 26–35.
24. Zhadan V.G. *Optimization Methods.* 2nd ed. URSS, Moscow, 2024. https://search.rsl.ru/en/record/01013035489 (in Russian)

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