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G. Ciaramella[a], J. Salomon[b] & A. Borzì[c]
[a] Institut für Mathematik, Universität Würzburg, Emil-Fischer-Strasse 31, 97074 Würzburg, Germany
[b] Universite Paris-Dauphine, Ceremade, Place du Marechal Lattre de Tassigny, 75775 Paris, France
[c] Institut für Mathematik, Universität Würzburg, Emil-Fischer-Strasse 30, 97074 Würzburg, Germany
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A method for solving exact-controllability problems governed by closed quantum spin systems

G. Ciaramella[a], J. Salomon[b,*] and A. Borzì[c]

[a]*Institut für Mathematik, Universität Würzburg, Emil-Fischer-Strasse 31, 97074 Würzburg, Germany;* [b]*Universite Paris-Dauphine, Ceremade, Place du Marechal Lattre de Tassigny, 75775 Paris, France;* [c]*Institut für Mathematik, Universität Würzburg, Emil-Fischer-Strasse 30, 97074 Würzburg, Germany*

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The Liouville–von Neumann master equation models closed quantum spin systems that arise in nuclear magnetic resonance applications. In this paper, an efficient and robust computational framework to solve exact-controllability problems governed by the Liouville–von Neumann master equation is presented. The proposed control framework is based on a new optimisation formulation of exact-controllability quantum spin problems that allows the application of efficient computational techniques. This formulation results in an optimality system with four differential equations and an optimality condition. The differential equations are approximated with an appropriate modified Crank–Nicholson scheme and the resulting discretised optimality system is solved with a matrix-free Krylov–Newton scheme combined with a cascadic nonlinear conjugate gradient initialisation. Results of numerical experiments demonstrate the ability of the proposed framework to solve quantum spin exact-controllability control problems.

Keywords: quantum spin systems; Liouville–von Neumann master equation; exact-controllability problem; optimal control theory; optimality conditions; modified Crank–Nicholson scheme; Krylov–Newton scheme

1. Introduction

In many applications, the need of controlling a dynamical system to steer it from an initial state to a desired target state at a given final time arises. Such objective is performed by means of exact-control functions. This class of control problems arises, for example, in nuclear magnetic resonance (NMR) spectroscopy and quantum information processing; for a review, see e.g. Borzì (2012) and Dong and Petersen (2010b). In these applications, the dynamical system is modelled by the Liouville–von Neumann master (LvNM) equation that describes the time evolution of the density operator representing the quantum state.

Mathematically, this class of problems is known as exact-controllability. In particular, in quantum mechanics, we deal with dynamical systems with bilinear control structure, and exact-controllability problems can be also formulated as optimal control problems. A controllability problem aims to establish the reachability of a given target. On the other hand, an optimal control problem has the purpose of computing control functions such that an appropriate tracking error is minimised.

Many theoretical results are available concerning controllability of quantum systems. In particular, general controllability results for bilinear systems evolving on Lie groups are given in Jurdjevic and Sussmann (1972). For controllability results regarding quantum systems. see e.g. Albertini and D'Alessandro (2002), D'Alessandro (2003), Beauchard, Coron, and Rouchon (2010), Dirr and Helmke (2008), Dong and Petersen (2009,2010a,b), and Turinici and Rabitz (2001). The problems to estimate a final time that guarantees controllability and an optimal time are studied in, for example, Agrachev and Chambrion (2006), Dirr, Helmke, Hüper, and Kleisteuber (2006), Dong, Lam, and Petersen (2009), Khaneja, Glaser, and Brockett (2002), and Khaneja, Brockett, and Glaser (2001). We distinguish exact-controllability problems from optimal control problems where it is required to minimise a cost functional subject to the constraint given by a differential model. In the latter case, recent results (Borzì, Salomon, & Volkwein, 2008; Ditz & Borzì, 2008; Ho & Rabitz, 2010; Khaneja et al., 2005) show that optimisation techniques can be successfully applied, while in the exact-controllability case much less is known on how to solve efficiently these problems. It is the focus of this paper to develop an efficient strategy capable to solve exact-controllability quantum spin problems governed by the LvNM equation.

Pioneering works in the development of quantum optimal control algorithms can be found in Konnov and Krotov (1999), Tannor, Kazakov, and Orlov (1992), and Zhu and Rabitz (1998). Further progress in the development of efficient control schemes is documented in, for example, Eitan, Mundt, and Tannor (2011), Ho and Rabitz (2010), Khaneja

*Corresponding author. Email: julien.salomon@dauphine.fr

et al. (2005), Maday, Salomon, and Turinici (2007), Maximov, Salomon, Turinici, and Nielsen (2010), and Sklarz and Tannor (2002). Advanced optimisation methods for quantum control problems are discussed in Borzì et al. (2008) and de Fouquieres, Schirmer, Glaser, and Kuprov (2011).

The aim of our work is to develop an efficient and robust computational framework capable to solve exact-controllability problems governed by the LvNM equation that models closed quantum spin systems and investigates theoretical properties of such a control problem. For this purpose, we reformulate the exact-controllability problem in such a way that it is suitable for application of efficient optimisation techniques. We focus on NMR spectroscopy applications, where the need arises to determine the radiofrequencies of magnetic control fields to be applied in such a way to excite particular quantum spin states to reach the given target configurations.

Our work is organised in four sections. In Section 2, we discuss the formulation of an exact-controllability problem. Section 3 focuses on the reformulation of the exact-control problem in an optimal control problem. We discuss the relationship between the original control problem and its new reformulation. Further, we derive the optimality system and give a detailed discussion on the Hessian operator corresponding to the new formulation. In the new setting, we are able to prove regularity properties of the Hessian operator and some properties of the solutions to the original exact-control problem. This theoretical result is fundamental to guarantee an efficient behaviour of the optimisation algorithm. In Section 4, we address the problem of computing numerical solutions of our new formulation of quantum spin control problems. A modified Crank–Nicholson method and the first-discretise-then-optimise strategy are presented as an adequate discretisation framework of the optimality system that characterises the first-order optimality conditions. We present a Krylov–Newton method, including implementation details. Moreover, we discuss the nonlinear conjugate gradient (NCG) method combined with a cascadic approach (Borzì & Schulz, 2012) to obtain an accurate initialisation to the Newton method. Section 5 validates the proposed computational framework with three applications, demonstrating the ability of our method to solve quantum spin exact-controllability problems. A section of conclusions completes this work.

2. Exact-controllability of quantum spin systems

In many applications, including NMR spectroscopy, dynamical systems with a bilinear control structure appear as follows (Cavanagh, Fairbrother, Palmer III, Rance, & Skelton, 2007):

$$\dot{x} = \left[A + \sum_{n=1}^{N_C} B_n u_n \right] x, \tag{1}$$

where $A \in \mathbb{R}^{N\times N}$ is the drift matrix, $B_n \in \mathbb{R}^{N\times N}$ are the input matrices, N is the dimension of the differential system, N_C is the number of controls, x is the state, and u is the control vector function. In this paper, we focus on closed quantum spin systems, where (1) represents a real matrix representation of the LvNM equation (Cavanagh et al., 2007). Hence, the matrices A and B_n are skew-symmetric and the dynamics of (1) is norm preserving.

The exact-controllability problem associated to (1) is to find a control vector function u such that the following problem is solved:

$$\dot{x} = \left[A + \sum_{n=1}^{N_C} B_n u_n \right] x, \quad t \in (0, T], \quad x(0) = x_0, \quad x(T) = x_T. \tag{2}$$

Notice that, since (2) is a time-boundary-value problem, it is possible to solve it using the class shooting methods (Stoer & Bulirsch, 1993), although these methods have been less investigated in the case of bilinear control. However, problem (2) may admit many solutions, and it becomes necessary to complement the problem with a constraint on u.

In this paper, we present a computational framework to solve (2) with the additional requirement that the control functions have minimal energy. For this purpose, we consider the following steps:

(a) We embed (2) in an exact-controllability problem with minimum-norm problem, that is, (3).
(b) We write the first-order optimality system of (3) given by (5).
(c) We embed (5) in the optimisation problem (7).
(d) We derive the first-order optimality system of (7) in Proposition 2.
(e) We write problem (7) in the reduced form, that is, (13), having optimality system given by Proposition 4.
(f) We solve (13), with an NCG-cascadic initialised Krylov–Newton method.

A suitable way to constraint the controls is to consider (2) embedded in an optimisation problem. For this reason, we focus on the following equations:

$$\begin{aligned} \min_{x,u} \quad & J(x,u) := \frac{1}{2} \sum_{n=1}^{N_C} \|u_n\|_{L^2}^2 \\ \text{s.t.} \quad & \dot{x} = \left[A + \sum_{n=1}^{N_C} B_n u_n \right] x, \ t \in (0, T], \\ & x(0) = x_0, \ x(T) = x_T x \in H^1((0,T);\mathbb{R}^N) \text{ and} \\ & u \in L^2((0,T);\mathbb{R}^{N_C}). \end{aligned} \tag{3}$$

We notice that (3) admits a solution if the target x_T belongs to the set of all points reachable at time T from a given starting point x_0. We remark that problems (2) and (3) are not equivalent. A solution of (3) is a minimum L^2-norm solution and solves also (2). On the other hand, a solution of (2) is not necessarily a solution to (3).

Controllability theory is fundamental in addressing problems (2) and (3). Notice that (1) is the induced system of a bilinear control system evolving on the Lie group SO. Moreover, a real representation of the LvNM equation can also be considered, whose induced system evolves on the Lie group of unitary operators SU. Hence, there are several results providing necessary and sufficient conditions for controllability (see e.g. Dirr & Helmke, 2008; Dong & Petersen, 2010b). Now, we remark that, for quantum spin systems, there exist few results concerning the estimation of a time T capable to guarantee the existence of a control steering the trajectory to the given target in exactly T-units of time (Agrachev & Chambrion, 2006; Dirr & Helmke, 2008; Dirr et al., 2006; Dong et al., 2009; Khaneja et al., 2001, 2002). However, since the mentioned Lie groups are compact and semi-simple (Hall, 2003), we can make use of Theorem 7.2 in Jurdjevic and Sussmann (1972) which guarantees controllability at T-units of time choosing a sufficiently large $T > 0$. For this reason, we make the following assumption.

Assumption 1: *The target point x_T belongs to the reachable set, that is, the set of all points reachable from the given initial condition x_0. Moreover, the time T is assumed to be large enough to guarantee controllability in T-units of time.*

Further, we need the following assumption regarding the existence of Lagrange multipliers corresponding to problem (3).

Assumption 2: *There exist Lagrange multipliers $p_T \in \mathbb{R}^N$ and $p \in H^1((0, T); \mathbb{R}^N)$ corresponding to the constraint equation of the optimisation problem* (3). *Moreover, p satisfies the following adjoint equation:*

$$-\dot{p} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right]^* p, \quad t \in [0, T), \quad p(T) = p_T. \tag{4}$$

In Assumption 2, we assume that there exists a vector p_T such that the corresponding solution p is the Lagrange multiplier associated with the state x. Notice that p_T is unknown and p is uniquely determined by p_T and the control u. Further, notice that, once the existence of $p \in H^1((0, T); \mathbb{R}^N)$ is assumed, then (4) can be obtained by means of the standard Lagrange function approach.

A solution of (3) is characterised by the following first-order optimality system:

$$\dot{x} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right] x, \quad x(0) = x_0, \quad x(T) = x_T \tag{5a}$$

$$-\dot{p} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right]^* p, \quad p(T) = p_T \tag{5b}$$

$$u_n - \langle B_n x, p\rangle = 0, \quad n = 1, \ldots, N_C, \tag{5c}$$

where $\langle \cdot, \cdot \rangle$ represents the Euclidean scalar product.

Because of (5a), there is no clear approach of how to solve (5). For this reason, in the next section, we reformulate (5) in such a way that it can be solved by using appropriate optimisation techniques.

In this paper, we use the following notation. Given $m \in \mathbb{N}$, we denote with $\langle \cdot, \cdot \rangle$ the Euclidean inner product and with $\langle \cdot, \cdot \rangle_{L^2}$ the inner product defined by

$$\langle x, y \rangle_{L^2} := \int_0^T \langle x(t), y(t) \rangle dt, \quad \text{for every } x, y \in L^2((0, T); \mathbb{R}^m).$$

Moreover, $\| \cdot \|_2$ denotes the Euclidean norm and $\| \cdot \|_{L^2}$ denotes the norm induced by $\langle \cdot, \cdot \rangle_{L^2}$. Notice that m is equal to N for the state space and to N_C for the control space. Consider any pair $a, b \in L^2((0, T); \mathbb{R}^{N_C}) \times \mathbb{R}^N$ given by $a = (a_1, a_2)$ and $b = (b_1, b_2)$, we define the inner product $(\cdot, \cdot)_G$ and the corresponding induced norm $|||\cdot|||$ is as follows:

$$(a, b)_G := \sum_{n=1}^{N_C} \langle a_{1,n}, b_{1,n} \rangle_{L^2} + \langle a_2, b_2 \rangle, \quad \text{and, } |||a||| := \sqrt{(a, a)_G}.$$

3. Reformulation of the exact-controllability spin problem

In this section, in order to address the exact-controllability of (1), we define a new optimisation problem, which is equivalent to (5) under certain conditions, and amenable to numerical optimisation. First, we analyse the reformulated problem from a theoretical point of view and derive the corresponding optimality conditions. Then, we describe its reduced form, which is suitable for the numerical optimisation. Further, the corresponding Hessian operator and its action are discussed.

In order to solve (5), we consider the map $\mathcal{G} : H^1((0, T); \mathbb{R}^N) \times L^2((0, T); \mathbb{R}^{N_C}) \times H^1((0, T); \mathbb{R}^N) \to L^2((0, T); \mathbb{R}^{N_C}) \times \mathbb{R}^N$ defined as follows:

$$\mathcal{G}(x, u, p) := \begin{pmatrix} u_1 - \langle B_1 x, p \rangle \\ \vdots \\ u_{N_C} - \langle B_{N_C} x, p \rangle \\ x(T) - x_T \end{pmatrix}. \tag{6}$$

Since this map is obtained by using the gradient component (5c) and the terminal condition of (5a), a triple (x, u, p) is a solution of (5), and a stationary point for (3), if and only if, it is a root of $\mathcal{G}$ with x and p solutions to (5a) and (5b), respectively.

We remark that, it could be possible to compute a root for $\mathcal{G}$ using a Newton method, however, according to our experience, the corresponding Jacobian operator is not sufficiently regular to be used successfully in computational algorithms. For this reason, in order to compute a root (x, u, p) of $\mathcal{G}$, we define our main optimisation problem as follows:

$$\begin{aligned}
&\min_{x,u,p} \quad G(x, u, p) : \\
&= \frac{1}{2}|||\mathcal{G}(x, u, p)|||^2 = \frac{1}{2}\sum_{n=1}^{N_C} \|u_n - \langle B_n x, p\rangle\|^2_{L^2} \\
&+ \frac{1}{2}\|x(T) - x_T\|_2^2 \text{s.t.} \\
&\dot{x} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right] x,\ t \in (0, T], x(0) = x_0 \\
&-\dot{p} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right]^* p, \\
&t \in [0, T),\ p(T) = p_T \\
&x, p \in H^1((0, T); \mathbb{R}^N) \text{ and} \\
&u \in L^2((0, T); \mathbb{R}^{N_C}).
\end{aligned} \tag{7}$$

We remark that a solution $(\hat{x}, \hat{u}, \hat{p})$ of (7) with $G(\hat{x}, \hat{u}, \hat{p}) = 0$ is a root of $\mathcal{G}$, and hence a solution of the optimality system (5). Moreover, in the sequel of this paper, we prove and discuss some regularity properties of (7), which are important for the solution of (5), and useful for the characterisation of stationary points of (3).

We address the forward equation in x and the backward equation in p as constraint equations in the minimisation problem (7).

Existence and uniqueness of solutions $x, p \in H^1((0, T); \mathbb{R}^N)$ of the constraint equations of (7) for any $T > 0$ and any initial and terminal condition, corresponding to a given $u \in L^2((0, T); \mathbb{R}^{N_C})$, can be proved by standard techniques (see e.g. Sontag, 1998). Hence, the solutions x and p are uniquely determined by the controls and the initial and terminal conditions, respectively. We have that $x = x(u, x_0)$ and $p = p(u, p_T)$. Consequently, we remark that the unknowns of (5) are the control $u \in L^2((0, T); \mathbb{R}^{N_C})$ and the terminal condition for the adjoint equation $p_T \in \mathbb{R}^N$.

In the following proposition, we state the existence of a solution of (7). Moreover, we analyse the relationship between the problems (3) and (7). In particular, the condition $G = 0$ is required to guarantee that a solution to (7) is a stationary point for (3).

Proposition 1: *A triple $(x, u, p) \in H^1((0, T); \mathbb{R}^N) \times L^2((0, T); \mathbb{R}^{N_C}) \times H^1((0, T); \mathbb{R}^N)$, with $x = x(u, x_0)$ and $p = p(u, p_T)$, is a solution of* (7) *with $G(x, u, p) = 0$, if and only if, it is a stationary point of* (3).

The proof of Proposition 1 is omitted for brevity. We remark that a solution of (7) with $G = 0$ is only a stationary point for (3), hence it is not guaranteed that it is a minimum norm solution of (3).

3.1 *Optimality system and necessary conditions*

In this section, we discuss the optimality conditions used to characterise a solution to (7). To obtain the first-order optimality system, we follow the Lagrange multiplier approach. We denote with $y, q \in H^1((0, T); \mathbb{R}^N)$ the Lagrange multipliers corresponding to x and p, respectively. The existence of such functions can be ensured by means of standard techniques (Sontag, 1998).

The Lagrange function corresponding to (7) is given by

$$\begin{aligned}
L(x, u, p, y, q) = G(x, u, p) &+ \left\langle \dot{x} - \left[A + \sum_{n=1}^{N_C} B_n u_n\right] x, y \right\rangle_{L^2} \\
&+ \left\langle -\dot{p} - \left[A + \sum_{n=1}^{N_C} B_n u_n\right]^* p, q \right\rangle_{L^2},
\end{aligned} \tag{8}$$

By means of (8), the optimality conditions for (7) are given by the following proposition.

Proposition 2: *The optimality system corresponding to* (7) *is given by*

$$\dot{x} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right] x, \quad x(0) = x_0, \tag{9a}$$

$$-\dot{p} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right]^* p, \ p(T) = p_T, \tag{9b}$$

$$\begin{aligned}
-\dot{y} &= \left[A + \sum_{n=1}^{N_C} B_n u_n\right]^* y + \sum_{n=1}^{N_C} [(u_n - \langle B_n x, p\rangle) B_n^* p], \\
y(T) &= -(x(T) - x_T),
\end{aligned} \tag{9c}$$

$$\begin{aligned}
\dot{q} &= \left[A + \sum_{n=1}^{N_C} B_n u_n\right] q \\
&+ \sum_{n=1}^{N_C} [(u_n - \langle B_n x, p\rangle) B_n x], \quad q(0) = 0,
\end{aligned} \tag{9d}$$

$$\begin{aligned}
&u_n - \langle B_n x, p\rangle - \langle B_n x, y\rangle - \langle B_n^* p, q\rangle = 0, \\
&n = 1, \ldots, N_C,
\end{aligned} \tag{9e}$$

where (9*a*) *and* (9*b*) *are the constraint equations,* (9*c*) *and* (9*d*) *are the corresponding adjoint equations, and* (9*e*) *gives the components of the gradient.*

Proof: Since $L(x,u,p,y,q)$ is linear with respect to the adjoint variables y and q, we obtain the constraint equations (9a) and (9b) as follows:

$$\left\langle \nabla_y L(x,u,p,y,q), \delta y \right\rangle_{L^2} = \left\langle \dot{x} - \left[A + \sum_{n=1}^{N_C} B_n u_n \right] x, \delta y \right\rangle_{L^2},$$

and

$$\begin{aligned}&\left\langle \nabla_q L(x,u,p,y,q), \delta q \right\rangle_{L^2} \\ &= \left\langle -\dot{p} - \left[A + \sum_{n=1}^{N_C} B_n u_n \right]^* p, \delta q \right\rangle_{L^2}.\end{aligned}$$

For optimality, the two inner products $\left\langle \nabla_y L(x,u,p,y,q), \delta y \right\rangle_{L^2}$ and $\left\langle \nabla_q L(x,u,p,y,q), \delta q \right\rangle_{L^2}$ have to be equal to zero for all $\delta y \in L^2((0,T);\mathbb{R}^N)$ and $\delta q \in L^2((0,T);\mathbb{R}^N)$, respectively, thus (9a) and (9b) follow.

To obtain the adjoint equations (9c) and (9d), we consider the derivative with respect to x and p along the two directions δx and δp, respectively. We obtain (9c) as follows:

$$\begin{aligned}&\left\langle \nabla_x L(x,u,p,y,q), \delta x \right\rangle_{L^2} = \langle \delta x(T), x(T) - x_T \rangle \\ &\quad + \int_0^T \langle \dot{\delta x} - \left[A + \sum_{n=1}^{N_C} B_n u_n \right] \delta x, y \rangle dt \\ &\quad - \int_0^T \left\langle \sum_{n=1}^{N_C} (u_n - \langle B_n x, p \rangle) B_n \delta x, p \right\rangle dt \\ &= \langle \delta x(T), x(T) - x_T \rangle + \left[\langle \delta x, y \rangle \right]_0^T \\ &\quad + \int_0^T \langle -\dot{y} - \left[A + \sum_{n=1}^{N_C} B_n u_n \right]^* y \\ &\quad - \sum_{n=1}^{N_C} (u_n - \langle B_n x, p \rangle) B_n^* p, \delta x \rangle dt \\ &= \langle \delta x(T), x(T) - x_T \rangle + \left[\langle \delta x, y \rangle \right]_0^T \\ &\quad + \left\langle -\dot{y} - \left[A + \sum_{n=1}^{N_C} B_n u_n \right]^* y \right. \\ &\quad \left. - \sum_{n=1}^{N_C} (u_n - \langle B_n x, p \rangle) B_n^* p, \delta x \right\rangle_{L^2}.\end{aligned}$$

Since the product $\left\langle \nabla_x L(x,u,p,y,q), \delta x \right\rangle_{L^2}$ has to be equal to zero for all $\delta x \in L^2((0,T);\mathbb{R}^N)$, and we have that $\delta x(0) = 0$, we obtain the terminal condition $y(T) = -(x(T) - x_T)$ and the adjoint equation (9c).

To obtain the adjoint problem (9d), we proceed as follows:

$$\begin{aligned}&\left\langle \nabla_p L(x,u,p,y,q), \delta p \right\rangle_{L^2} \\ &= \int_0^T \langle -\dot{\delta p} - \left[A + \sum_{n=1}^{N_C} B_n u_n \right]^* \delta p, q \rangle dt \\ &\quad - \int_0^T \left\langle \sum_{n=1}^{N_C} (u_n - \langle B_n x, p \rangle) B_n x, \delta p \right\rangle dt \\ &= -\left[\langle \delta p, q \rangle \right]_0^T + \int_0^T \langle \dot{q} - \left[A + \sum_{n=1}^{N_C} B_n u_n \right] q \\ &\quad - \sum_{n=1}^{N_C} (u_n - \langle B_n x, p \rangle) B_n x, \delta p \rangle dt \\ &= -\left[\langle \delta p, q \rangle \right]_0^T + \left\langle \dot{q} - \left[A + \sum_{n=1}^{N_C} B_n u_n \right] q \right. \\ &\quad \left. - \sum_{n=1}^{N_C} (u_n - \langle B_n x, p \rangle) B_n x, \delta p \right\rangle_{L^2}.\end{aligned}$$

The product $\left\langle \nabla_p L(x,u,p,y,q), \delta p \right\rangle_{L^2}$ has to be equal to zero for all $\delta p \in L^2((0,T);\mathbb{R}^N)$ with $\delta p(T) = 0$. As a consequence, we have that $q(0) = 0$ and we obtain the adjoint equation (9d).

We derive the n-component of the gradient (9e) by means of the variation of the Lagrangian with respect to the control u_n as follows:

$$\begin{aligned}&\left\langle \nabla_{u_n} L(x,u,p,y,q), \delta u_n \right\rangle_{L^2} \\ &= \int_0^T (u_n - \langle B_n x, p \rangle) \delta u_n \\ &\quad - \langle B_n x, y \rangle \delta u_n - \left\langle B_n^* p, q \right\rangle \delta u_n dt \\ &= \left\langle u_n - \langle B_n x, p \rangle - \langle B_n x, y \rangle - \left\langle B_n^* p, q \right\rangle, \delta u_n \right\rangle_{L^2}.\end{aligned}$$

Since this product has to be equal to zero for all $\delta u_n \in L^2(0,T)$, we obtain the optimality condition (9e). □

In the following proposition, we discuss the existence and uniqueness of solutions to the adjoint problems (9c) and (9d).

Proposition 3: *Given y_T and q_0, consider the following problems:*

$$\begin{aligned}&-\dot{y} = \left[A + \sum_{n=1}^{N_C} B_n u_n \right]^* y + \sum_{n=1}^{N_C} [(u_n - \langle B_n x, p \rangle) B_n^* p], \\ &y(T) = y_T, \end{aligned} \tag{10}$$

and

$$\dot{q} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right] q + \sum_{n=1}^{N_C} [(u_n - \langle B_n x, p\rangle) B_n x],$$
$$q(0) = q_0, \tag{11}$$

with $y, q, x, p \in H^1((0,T);\mathbb{R}^N)$ *and* $u \in L^2((0,T);\mathbb{R}^{N_C})$. *Then,* (10) *and* (11) *admit unique solutions for any* $T > 0$ *and any* y_T *and* q_0*, respectively.*

Moreover, assume that $(x(u, x_0), u, p(u, p_T))$ *is a stationary point for* (3)*, then the problem* (9c)*, which corresponds to problem* (10) *with* $y_T = 0$*, and* (9d)*, which corresponds to* (11) *with* $q_0 = 0$*, admits the unique solutions* $y(t) = 0$ *and* $q(t) = 0$*, for all* $t \in [0, T]$*, for any* $T > 0$ *and any control* $u \in L^2((0,T);\mathbb{R}^{N_C})$.

Proof: The existence and uniqueness of solution of (10) and (11) can be proved by means of known results (see e.g. Sontag, 1998).

Next, consider problem (9d). Since $(x(u, x_0), u, p(u, p_T))$ is a stationary point for (3), we have that $u_n - \langle B_n x, p\rangle = 0$, for $n = 1, \ldots, N_C$; hence, the forcing terms in the differential equations in (9c) and (9d) are zero. Consequently, since A and B_n are skew-symmetric, the dynamics are norm preserving, we have that (10) with $y_T = 0$ and (11) with $q_0 = 0$ admit the unique solutions $y = 0$ and $q = 0$ for any $T > 0$ and any u.

Now, we discuss the reduced form of problem (7), which is suitable to be solved by means of appropriate numerical optimi'sation methods. As mentioned in the previous section, the solutions of the constraint equations (9a) and (9b) are uniquely determined by the initial and terminal conditions, that are $x(0) = x_0$ and $p(T) = p_T$, respectively, and by the control vector function u. We have

$$x = x(u) \ \text{ and } \ p = p(u, p_T), \tag{12}$$

where the dependence of x from x_0 is omitted because it is an input of the problem. Consequently, problem (7) can be equivalently expressed in the following reduced form:

$$\begin{aligned} &\min_{u, p_T} \quad G_r(u, p_T) := G(x(u), u, p(u, p_T)) \\ &\text{s.t.} \quad (x(u), p(u, p_T)) \in \mathcal{S}_{ad} := \big\{(x, p) \,\big|\, x \text{ solves } (9a) \\ &\ \text{and } p \text{ solves } (9b)\big\}\,. \end{aligned} \tag{13}$$

We characterise a solution of (13) with the first-order optimality conditions given in the following result, which follows directly from Theorem 2.

Proposition 4: *The optimality system corresponding to problem* (13) *is given by*

$$\nabla_{u_n} G_r(u, p_T) := u_n - \langle B_n x, p\rangle - \langle B_n x, y\rangle - \langle B_n^* p, q\rangle = 0, \ n = 1, \ldots, N_C, \tag{14a}$$

$$\nabla_{p_T} G_r(u, p_T) := -q(T) = 0, \tag{14b}$$

such that x, p, y, *and* q *solve the following problems:*

$$\dot{x} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right] x, \quad x(0) = x_0, \tag{14c}$$

$$-\dot{p} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right]^* p, \ \ p(T) = p_T, \tag{14d}$$

$$-\dot{y} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right]^* y + \sum_{n=1}^{N_C} [(u_n - \langle B_n x, p\rangle) B_n^* p],$$
$$y(T) = -(x(T) - x_T), \tag{14e}$$

$$\dot{q} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right] q + \sum_{n=1}^{N_C} [(u_n - \langle B_n x, p\rangle) B_n x],$$
$$q(0) = 0\,. \tag{14f}$$

Proof: Consider Theorem 2 and its proof. We remark that the gradient component of the reduced problem with respect to p_T is obtained from the fact that $\langle \nabla_{p_T} G_r(u, p_T), \delta q(T)\rangle = \langle -q(T), \delta q(T)\rangle = 0$ for all $\delta q(T)$. Notice that, unlike in (7), in (13) p_T is not fixed, hence $\delta q(T)$ is not fixed to 0.

Next, we investigate the reduced Hessian operator corresponding to (13). For this purpose, we first discuss the Hessian of problem (7), then we consider its reduced form corresponding to (13). In particular, we focus on its action on a given vector function. This aspect will be crucial in the development of the Krylov–Newton method discussed in the next section.

By computing the second directional derivative of the Lagrange function (8), we write that

$$\left\langle H(x, u, p) \begin{pmatrix} \delta x \\ \delta u \\ \delta p \\ \delta y \\ \delta q \end{pmatrix}, \begin{pmatrix} \delta x \\ \delta u \\ \delta p \\ \delta y \\ \delta q \end{pmatrix} \right\rangle_{L^2} = \left\langle \begin{pmatrix} H_x \\ H_u \\ H_p \\ H_y \\ H_q \end{pmatrix}, \begin{pmatrix} \delta x \\ \delta u \\ \delta p \\ \delta y \\ \delta q \end{pmatrix} \right\rangle_{L^2}, \tag{15}$$

where $(\delta x, \delta u, \delta p, \delta y, \delta q)^T \in H^1((0,T);\mathbb{R}^N) \times L^2((0,T);\mathbb{R}^{N_C}) \times H^1((0,T);\mathbb{R}^N) \times H^1((0,T);\mathbb{R}^N) \times H^1((0,T);\mathbb{R}^N)$ and H_x, H_u, H_p, H_y, and H_q denote the following equations:

$$H_x = -\dot{\delta y} - \left[A + \sum_{n=1}^{N_C} B_n u_n\right]^* \delta y - \left[\sum_{n=1}^{N_C} B_n \delta u_n\right]^* y - \sum_{n=1}^{N_C} (u_n - \langle B_n x, p\rangle) B_n^* \delta p - \sum_{n=1}^{N_C} (\delta u_n - \langle B_n \delta x, p\rangle - \langle B_n x, \delta p\rangle) B_n^* p, \quad \text{with} \quad \delta y(T) = -\delta x(T), \tag{16}$$

$$H_{u_n} = \delta u_n - \langle B_n \delta x, p\rangle - \langle B_n x, \delta p\rangle - \langle B_n \delta x, y\rangle - \langle B_n x, \delta y\rangle - \langle B_n^* \delta p, q\rangle - \langle B_n^* p, \delta q\rangle, \tag{17}$$

$$H_p = \dot{\delta q} - \left[A + \sum_{n=1}^{N_C} B_n u_n\right] \delta q - \left[\sum_{n=1}^{N_C} B_n \delta u_n\right] q - \sum_{n=1}^{N_C} (u_n - \langle B_n x, p\rangle) B_n \delta x - \sum_{n=1}^{N_C} (\delta u_n - \langle B_n \delta x, p\rangle - \langle B_n x, \delta p\rangle) B_n x, \quad \text{with} \quad \delta q(0) = 0, \tag{18}$$

$$H_y = \dot{\delta x} - \left[A + \sum_{n=1}^{N_C} B_n u_n\right] \delta x - \left[\sum_{n=1}^{N_C} B_n \delta u_n\right] x, \quad \text{with} \quad \delta x(0) = 0, \tag{19}$$

and

$$H_q = -\dot{\delta p} - \left[A + \sum_{n=1}^{N_C} B_n u_n\right]^* \delta p - \left[\sum_{n=1}^{N_C} B_n \delta u_n\right]^* p, \quad \text{with} \quad \delta p(T) = \delta p_T\ . \tag{20}$$

Notice that H_x, H_u, H_p, H_y, and H_q represent the residuals of the linearised optimality system.

Now, we consider the reduced problem (13) and we denote with $\nabla^2 G_r(x, u, p)$ the corresponding reduced Hessian operator. We recall that the unknowns are the control u and the terminal condition p_T. Consequently, the action of $\nabla^2 G_r(x, u, p)$ on a vector $(\delta u, \delta p_T)^T \in L^2((0, T); \mathbb{R}^{N_C}) \times \mathbb{R}^N$ is given as follows:

$$\nabla^2 G_r(u, p_T) \begin{pmatrix} \delta u_1 \\ \vdots \\ \delta u_{N_C} \\ \delta p_T \end{pmatrix} = \begin{pmatrix} H_{u_1}(x, u, p) \\ \vdots \\ H_{u_{N_C}}(x, u, p) \\ H_{p_T}(x, u, p) \end{pmatrix} \tag{21}$$

where δx, δp, δy, and δq are solutions obtained by cancelling (19), (20), (16), and (18), respectively, and $H_{p_T}(x, u, p) = -\delta q(T)$. Hence, the action of the reduced Hessian operator can be obtained by solving the linearised equations (16) and (18)–(20) and the assembling (21).

With the following theorem, we prove the regularity of the reduced Hessian operator.

Theorem 1: *Let (u, p_T) be a solution of (13) with $G_r(u, p_T) = 0$, then the reduced Hessian operator $\nabla^2 G_r(u, p_T)$ is positive semi-definite.*

Proof: We denote with $x = x(u)$ and $p = p(u, p_T)$ the unique solutions of the constraint equations (14c) and (14d), respectively, and with $y = y(x, u, p)$ and $q = q(x, u, p)$, the unique solutions of the adjoint equations (14e) and (14f), respectively. We prove the claim in two steps.

Step 1: Since (u, p_T) is a solution of (13) with $G_r(u, p_T) = 0$, then we have that $u_n - \langle B_n x, p\rangle = 0$ for $n = 1, \ldots, N_C$. Moreover, by Proposition 3, we know that $y = 0$ and $q = 0$. Consequently, the linearised adjoint equations $H_x = 0$ and $H_p = 0$ become as follows:

$$-\dot{\delta y} = \left[A + \sum_{n=1}^{N_C} u_n B_n\right]^* \delta y + \sum_{n=1}^{N_C} \big(\delta u_n - \langle B_n \delta x, p\rangle - \langle B_n x, \delta p\rangle\big) B_n^* p, \tag{22}$$

with $\delta y(T) = -\delta x(T)$, and

$$\dot{\delta q} = \left[A + \sum_{n=1}^{N_C} u_n B_n\right] \delta q + \sum_{n=1}^{N_C} \big(\delta u_n - \langle B_n \delta x, p\rangle - \langle B_n x, \delta p\rangle\big) B_n x, \tag{23}$$

with $\delta q(0) = 0$. Now, define $\mathcal{O}(u) : H^1((0, T); \mathbb{R}^N) \to L^2((0, T); \mathbb{R}^N)$:

$$\mathcal{O}(u) := \frac{d}{dt} - \left[A + \sum_{n=1}^{N_C} B_n u_n\right], \tag{24}$$

whose adjoint is given by

$$\mathcal{O}(u)^* = -\frac{d}{dt} - \left[A + \sum_{n=1}^{N_C} B_n u_n\right]^*. \tag{25}$$

Recall that solving the equations $H_y = 0$ and $H_p = 0$, we have

$$\begin{aligned} \mathcal{O}(u)(\delta x + \delta q) &= \dot{\delta x} + \dot{\delta q} - \left[A + \sum_{n=1}^{N_C} B_n u_n\right](\delta x + \delta q) \\ &= \sum_{n=1}^{N_C} \delta u_n B_n x + \sum_{n=1}^{N_C} \big(\delta u_n - \langle \delta x, B_n^* p\rangle - \langle x, B_n^* \delta p\rangle\big) B_n x \\ &= \sum_{n=1}^{N_C} \big(2\delta u_n - \langle \delta x, B_n^* p\rangle - \langle x, B_n^* \delta p\rangle\big) B_n x, \end{aligned} \tag{26}$$

and analogously, solving $H_x = 0$ and $H_q = 0$, we have

$$\mathcal{O}(u)^*(\delta p + \delta y) = -\dot{\delta p} - \dot{\delta y} - \left[A + \sum_{n=1}^{N_C} B_n u_n\right]^* (\delta p + \delta y) = \sum_{n=1}^{N_C} (2\delta u_n - \langle \delta x, B_n^* p\rangle - \langle x, B_n^* \delta p\rangle) B_n^* p\ . \quad (27)$$

Step 2: Using (21) and (17) and the fact that $y = 0$ and $q = 0$, we have

$$\left\langle \nabla^2 G_r(u, p_T)\begin{pmatrix}\delta u\\ \delta p_T\end{pmatrix}, \begin{pmatrix}\delta u\\ \delta p_T\end{pmatrix}\right\rangle_{L^2} = = \left\langle \begin{pmatrix} \delta u_1 - \langle B_1 \delta x, p\rangle - \langle B_1 x, \delta p\rangle - \langle B_1 x, \delta y\rangle - \langle B_1^* p, \delta q\rangle \\ \vdots \\ \delta u_{N_C} - \langle B_{N_C} \delta x, p\rangle - \langle B_{N_C} x, \delta p\rangle - \langle B_{N_C} x, \delta y\rangle - \left\langle B_{N_C}^* p, \delta q\right\rangle \\ -\delta q(T)\end{pmatrix}, \times \begin{pmatrix}\delta u_1 \\ \vdots \\ \delta u_{N_C} \\ \delta p_T\end{pmatrix}\right\rangle_{L^2}$$
$$= \left\langle \begin{pmatrix} \delta u_1 - \langle B_1 x, \delta p + \delta y\rangle - \langle B_1^* p, \delta x + \delta q\rangle \\ \vdots \\ \delta u_{N_C} - \langle B_{N_C} x, \delta p + \delta y\rangle - \left\langle B_{N_C}^* p, \delta x + \delta q\right\rangle \\ -\delta q(T)\end{pmatrix}, \begin{pmatrix}\delta u_1 \\ \vdots \\ \delta u_{N_C} \\ \delta p_T\end{pmatrix}\right\rangle_{L^2}$$
$$= -\langle \delta q(T), \delta p_T\rangle + \sum_{n=1}^{N_C}\int_0^T \delta u_n^2 dt - \sum_{n=1}^{N_C}\int_0^T (\langle B_n x, \delta p + \delta y\rangle + \langle B_n^* p, \delta x + \delta q\rangle)\delta u_n dt = -\langle \delta q(T), \delta p_T\rangle + \sum_{n=1}^{N_C}\int_0^T \delta u_n^2 dt$$
$$- \int_0^T \left(\left\langle \sum_{n=1}^{N_C} \delta u_n B_n x, \delta p + \delta y\right\rangle + \left\langle \sum_{n=1}^{N_C} \delta u_n B_n^* p, \delta x + \delta q\right\rangle\right) dt$$
$$= -\langle \delta q(T), \delta p_T\rangle + \sum_{n=1}^{N_C}\int_0^T \delta u_n^2 dt - \int_0^T (\langle \mathcal{O}(u)(\delta x), \delta p + \delta y\rangle + \langle \mathcal{O}(u)^*(\delta p), \delta x + \delta q\rangle) dt. \quad (28)$$

The latter equation follows from solving $H_y = 0$, $H_q = 0$ and (24) and (25). Now, integrating by parts, we obtain

$$\left\langle \nabla^2 G_r(u, p_T)\begin{pmatrix}\delta u\\ \delta p_T\end{pmatrix}, \begin{pmatrix}\delta u\\ \delta p_T\end{pmatrix}\right\rangle_{L^2}$$
$$= -\langle \delta q(T), \delta p_T\rangle + \sum_{n=1}^{N_C}\int_0^T \delta u_n^2 dt - \left[\langle \delta x, \delta p + \delta y\rangle\right]_0^T - \int_0^T \langle \delta x, \mathcal{O}(u)^*(\delta p + \delta y)\rangle dt + \left[\langle \delta p, \delta x + \delta q\rangle\right]_0^T - \int_0^T \langle \delta p, \mathcal{O}(u)(\delta x + \delta q)\rangle dt$$
$$= -\langle \delta q(T), \delta p_T\rangle + \sum_{n=1}^{N_C}\int_0^T \delta u_n^2 dt - \langle \delta x(T), \delta p_T + \delta y(T)\rangle - \int_0^T \langle \delta x, \mathcal{O}(u)^*(\delta p + \delta y)\rangle dt + \langle \delta p_T, \delta x(T) + \delta q(T)\rangle - \int_0^T \langle \delta p, \mathcal{O}(u)(\delta x + \delta q)\rangle dt$$
$$= -\langle \delta x(T), \delta y(T)\rangle + \sum_{n=1}^{N_C}\int_0^T \delta u_n^2 dt - \int_0^T \langle \delta x, \mathcal{O}(u)^*(\delta p + \delta y)\rangle dt - \int_0^T \langle \delta p, \mathcal{O}(u)(\delta x + \delta q)\rangle dt$$
$$= \|\delta x(T)\|_2^2 + \sum_{n=1}^{N_C}\int_0^T \delta u_n^2 dt - \int_0^T \left\langle \delta x, \sum_{n=1}^{N_C} (2\delta u_n - \langle \delta x, B_n^* p\rangle - \langle x, B_n^* \delta p\rangle) B_n^* p\right\rangle dt - \int_0^T \left\langle \delta p, \sum_{n=1}^{N_C} (2\delta u_n - \langle \delta x, B_n^* p\rangle - \langle x, B_n^* \delta p\rangle) B_n x\right\rangle dt, \quad (29)$$

where we use (26) and (27) and the fact that $\delta y(T) = -\delta x(T)$. We have the following equations:

$$\left\langle \nabla^2 G_r(u, p_T)\begin{pmatrix}\delta u\\ \delta p_T\end{pmatrix}, \begin{pmatrix}\delta u\\ \delta p_T\end{pmatrix}\right\rangle_{L^2}$$
$$= \|\delta x(T)\|_2^2 + \sum_{n=1}^{N_C}\int_0^T [\delta u_n^2 - 2\delta u_n \langle \delta x, B_n^* p\rangle + (\langle \delta x, B_n^* p\rangle + \langle x, B_n^* \delta p\rangle)\langle \delta x, B_n^* p\rangle - 2\delta u_n \langle \delta p, B_n x\rangle + (\langle \delta x, B_n^* p\rangle + \langle x, B_n^* \delta p\rangle)\langle \delta p, B_n x\rangle] dt$$
$$= \|\delta x(T)\|_2^2 + \sum_{n=1}^{N_C}\int_0^T (\delta u_n - \langle \delta x, B_n^* p\rangle - \langle x, B_n^* \delta p\rangle)^2 dt, \quad (30)$$

which implies that

$$\left\langle \nabla^2 G_r(u, p_T)\begin{pmatrix}\delta u\\ \delta p_T\end{pmatrix}, \begin{pmatrix}\delta u\\ \delta p_T\end{pmatrix}\right\rangle_{L^2}$$
$$= \|\delta x(T)\|_2^2 + \sum_{n=1}^{N_C} \|\delta u_n - \langle \delta x, B_n^* p\rangle - \langle x, B_n^* \delta p\rangle\|_{L^2}^2 \ . \quad (31)$$

Consequently, we have

$$\left\langle \nabla^2 G_r(u, p_T)\begin{pmatrix}\delta u\\ \delta p_T\end{pmatrix}, \begin{pmatrix}\delta u\\ \delta p_T\end{pmatrix}\right\rangle_{L^2} \geq 0, \quad \forall(\delta u, \delta p_T) \ . \quad (32)$$

□

3.2 *Complementary results on coercivity and second-order sufficient conditions*

A property that plays an important role in the solution of optimisation problems is the coercivity of the reduced Hessian operator. From the coercivity property, two benefits arise: first, coercivity is a second-order sufficient optimality condition; second, coercivity implies regularity of the Hessian operator, which guarantees an optimal behaviour, namely a superlinear or quadratic convergence, of second-order optimisation algorithms in the neighbourhood of a minimum point.

In this section, the coercivity of the reduced Hessian operator (21) is discussed. According to Theorem 1, the Hessian in (21) is positive-semi-definite for all the pairs $(\delta u, \delta p_T)$. To improve this result, we characterise in Corollary 1 the set of all points in which (21) is indefinite and we discuss the relationship between (21) and the end-point map $\delta u \mapsto \delta x(T; \delta u)$. Next, we provide sufficient conditions for the coercivity of the reduced Hessian operator (21) (see Theorem 2 and Corollary 2).

Moreover, the coercivity of the reduced Hessian operator (21) allows us to characterise solutions to the minimum norm exact-control problem (3) as isolated points. This property is shown in Corollary 4.

In the sequel, we denote with $\|\cdot\|$ the Hilbert–Schmidt norm.

Corollary 1: *Consider the assumptions of Theorem 1. Then, we have that*

$$\left\langle \nabla^2 G_r(u, p_T)\begin{pmatrix}\delta u\\ \delta p_T\end{pmatrix}, \begin{pmatrix}\delta u\\ \delta p_T\end{pmatrix}\right\rangle_{L^2} = 0, \quad (33)$$

for all $(\delta u, \delta p_T)$ *belonging to a convex neighbourhood of* $(0, 0)$. *Moreover, if the map* $\delta u \mapsto \delta x(T; \delta u)$ *is injective in a neighbourhood* $\mathcal{N}$ *of* $\delta u = 0$, *then* $\nabla^2 G_r(u, p_T)$ *is positive definite in* $\mathcal{N}$.

Proof: To prove the first claim, we consider the following optimisation problem:

$$\min_{\delta u, \delta p_T} \quad F(\delta u, \delta p_T)$$
$$:= \|\delta x(T)\|_2^2 + \sum_{n=1}^{N_C} \|\delta u_n - \langle \delta x, B_n^* p\rangle - \langle x, B_n^* \delta p\rangle\|_{L^2}^2$$
$$\text{s.t.} \quad \dot{\delta x} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right]\delta x + \left[\sum_{n=1}^{N_C} B_n \delta u_n\right] x,$$
$$\delta(0) = 0, \quad -\dot{\delta p} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right]^* \delta p + \left[\sum_{n=1}^{N_C} B_n \delta u_n\right]^* p,$$
$$\delta p(T) = \delta p_T, \quad (\delta u, \delta p_T) \in S \subset L^2((0, T); \mathbb{R}^N) \times \mathbb{R}^{N_C}, \quad (34)$$

where $(x(u), u, p(u, p_T))$ is a solution of (13) with $G_r(u, p_T) = 0$ and S is a closed, convex, and bounded subset of $L^2((0, T); \mathbb{R}^N) \times \mathbb{R}^{N_C}$. The existence of a solution of (34) follows from the fact that $F(\delta u, \delta p_T) \geq 0$ and $F(0, 0) = 0$. Hence $(\delta u, \delta p_T) = (0, 0)$ is a global minimum of (34).

Now, notice that the maps $(\delta x, \delta u_n, \delta p) \mapsto \delta u_n - \langle \delta x, B_n^* p\rangle - \langle x, B_n^* \delta p\rangle$ and $\delta u \mapsto \delta x(T; \delta u)$ preserve convex combinations. Hence, the convexity of the norms implies that F is convex. Since, C is a convex set and F a convex function, then the set of global minima of F is convex. Consequently, we obtain that $F(\delta u, \delta p_T) = 0$ for all $(\delta u, \delta p_T)$ belonging to a convex neighbourhood of $(0, 0)$ included in S.

To prove the second argument, we consider the following. If $\delta u \mapsto \delta x(T; \delta u)$ is injective in a neighbourhood $\mathcal{N}$ of $\delta u = 0$, then in $\mathcal{N}$, we have that $\delta u = 0$, if and only if $\|\delta x(T; \delta u)\|_2 = 0$. Consequently, the positive definiteness of (21) follows. □

Lemma 1: *Let* $(\tilde{u}, \tilde{p}_T)$ *be a solution of* (13) *with* $G_r(\tilde{u}, \tilde{p}_T) = 0$. *If* $\tilde{p}_T = 0$, *then* $\tilde{u} = 0$, *that is,* $(\tilde{u}, \tilde{p}_T)$ *is a trivial solution of* (13).

Proof: Assuming that $\tilde{p}_T = 0$ and recalling that (9b) is norm preserving, we get that $\tilde{p}(t; \tilde{p}_T) = 0$ a.e. on $(0, T)$. Since $(\tilde{u}, \tilde{p}_T)$ be a solution of (13) with $G_r(\tilde{u}, \tilde{p}_T) = 0$, we have that $\tilde{u}_n = \langle B_n x, \tilde{p}\rangle$ for $n = 1, \ldots, N_C$. Consequently, we obtain that $\tilde{u} = 0$. □

Lemma 2: *Let* (u, p_T) *be a solution of* (13) *with* $G_r(u, p_T) = 0$. *Let* δx *and* δp *be the unique solutions of* $H_y = 0$ *and* $H_q = 0$, *respectively. Then the following estimates hold:*

$$\|\delta x\|_{L^2} \leq 2TM\|x(0)\|_2\|\delta u\|_{L^2}, \quad (35)$$

and

$$\|\delta p\|_{L^2} \leq 2TM\|p_T\|_2\|\delta u\|_{L^2} + \sqrt{T}\|\delta p_T\|_2, \quad (36)$$

where $M := \sqrt{N_C}\sum_{n=1}^{N_C}\|B_n\|$.

Proof: We start proving (35). Consider the linearised equation $H_y = 0$, that is,

$$\dot{\delta x} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right]\delta x + \left[\sum_{n=1}^{N_C} B_n \delta u_n\right]x,\quad \text{with } \delta x(0) = 0\ . \tag{37}$$

by multiplying (37) to the left with δx, we obtain

$$\langle \delta x, \dot{\delta x}\rangle = \left\langle \delta x, \left[A + \sum_{n=1}^{N_C} B_n u_n\right]\delta x\right\rangle + \left\langle \delta x, \left[\sum_{n=1}^{N_C} B_n \delta u_n\right]x\right\rangle. \tag{38}$$

Now, considering that $\langle \delta x(t), \dot{\delta x}(t)\rangle = \frac{1}{2}\frac{d}{dt}\|\delta x(t)\|_2^2$ and recalling the skew-symmetry of A and B_n, we get

$$\frac{1}{2}\frac{d}{dt}\|\delta x(t)\|_2^2 = \left\langle \delta x, \left[\sum_{n=1}^{N_C} B_n \delta u_n\right]x\right\rangle . \tag{39}$$

Integrating over $(0, t)$, and using that $\delta x(0) = 0$, (1) is norm preserving and the Cauchy–Schwarz inequality, we obtain

$$\begin{aligned}\|\delta x(t)\|_2^2 &= 2\int_0^t \left\langle \delta x, \left[\sum_{n=1}^{N_C} B_n \delta u_n\right]x\right\rangle dt\\ &= 2\sum_{n=1}^{N_C}\int_0^t \delta u_n\langle \delta x, B_n x\rangle dt\\ &\le 2\sum_{n=1}^{N_C}\int_0^t |\delta u_n||\langle \delta x, B_n x\rangle| dt\\ &\le 2\sum_{n=1}^{N_C}\int_0^T |\delta u_n||\langle \delta x, B_n x\rangle| dt\\ &\le 2\sum_{n=1}^{N_C}\int_0^T |\delta u_n|\|\delta x\|_2\|B_n x\|_2 dt\\ &\le 2\sum_{n=1}^{N_C}\int_0^T |\delta u_n|\|\delta x\|_2\|B_n\|\|x(0)\|_2 dt\\ &\le 2\|x(0)\|_2\sum_{n=1}^{N_C}\|B_n\|\int_0^T |\delta u_n|\|\delta x\|_2 dt\\ &\le 2\|x(0)\|_2 M\|\delta u\|_{L^2}\|\delta x\|_{L^2},\end{aligned} \tag{40}$$

where $M := \sqrt{N_C}\sum_{n=1}^{N_C}\|B_n\|$. Now, integrating over $(0, T)$, we obtain (35) as follows:

$$\begin{aligned}\int_0^T \|\delta x(t)\|_2^2 dt \ &\le\ 2\int_0^T \|x(0)\|_2 M\|\delta u\|_{L^2}\|\delta x\|_{L^2} dt\\ &\Rightarrow \|\delta x\|_{L^2}^2 \le 2T\|x(0)\|_2 M\|\delta u\|_{L^2}\|\delta x\|_{L^2}\\ &\Rightarrow \|\delta x\|_{L^2} \le 2T\|x(0)\|_2 M\|\delta u\|_{L^2}\ .\end{aligned} \tag{41}$$

Next, we prove (36). Consider the linearised equation $H_y = 0$, that is,

$$-\dot{\delta p} = \left[A + \sum_{n=1}^{N_C} B_n u_n\right]^*\delta p + \left[\sum_{n=1}^{N_C} B_n \delta u_n\right]^* p,\quad \text{with } \delta p(T) = \delta p_T\ . \tag{42}$$

By multiplying this equation from the left with δp, and using the same arguments as above for δx, we have

$$\begin{aligned}\|\delta p(t)\|_2^2 &= \|\delta p(T)\|_2^2 - 2\int_t^T \left\langle \delta p, \left[\sum_{n=1}^{N_C} B_n \delta u_n\right]p\right\rangle dt\\ &\le \|\delta p_T\|_2^2 + 2\sum_{n=1}^{N_C}\int_0^T |\delta u_n||\langle \delta p, B_n p\rangle| dt\\ &\le \|\delta p_T\|_2^2 + 2\sum_{n=1}^{N_C}\int_0^T |\delta u_n|\|\delta p\|_2\|B_n\|\|p_T\|_2 dt\\ &\le \|\delta p_T\|_2^2 + 2\|p_T\|_2\sum_{n=1}^{N_C}\|B_n\|\int_0^T |\delta u_n|\|\delta p\|_2 dt\\ &\le \|\delta p_T\|_2^2 + 2\|p_T\|_2 M\|\delta u\|_{L^2}\|\delta p\|_{L^2}\ .\end{aligned} \tag{43}$$

Now, integrating over $(0, T)$, we obtain

$$\begin{aligned}&\int_0^T \|\delta p(t)\|_2^2 dt\\ &\le T\|\delta p_T\|_2^2 + 2\int_0^T \|p_T\|_2 M\|\delta u\|_{L^2}\|\delta p\|_{L^2} dt\\ &\Rightarrow \|\delta p\|_{L^2}^2 \le T\|\delta p_T\|_2^2 + 2T\|p_T\|_2 M\|\delta u\|_{L^2}\|\delta p\|_{L^2}\\ &\Rightarrow \|\delta p\|_{L^2}^2 - 2T\|p_T\|_2 M\|\delta u\|_{L^2}\|\delta p\|_{L^2} - T\|\delta p_T\|_2^2\\ &\le 0.\end{aligned} \tag{44}$$

For a non-trivial solution (u, p_T) of (13), the discriminant of the previous quadratic inequality is

$$\Delta = 4T^2M^2\|p_T\|_2^2\|\delta u\|_{L^2}^2 + 4T\|\delta p_T\|_2^2 > 0\ \ \forall(\delta u, \delta p_T) \ne (0, 0), \tag{45}$$

where we use Lemma 1 to guarantee that $\|p_T\|_2 \neq 0$. Consequently, inequality (44) is satisfied for

$$\|\delta p\|_{L^2} \leq TM\|p_T\|_2\|\delta u\|_{L^2} + \sqrt{T^2M^2\|p_T\|_2^2\|\delta u\|_{L^2}^2 + T\|\delta p_T\|_2^2}. \tag{46}$$

The previous inequality (46) allows us to write that

$$\begin{aligned}\|\delta p\|_{L^2} &\leq TM\|p_T\|_2\|\delta u\|_{L^2} + \sqrt{T^2M^2\|p_T\|_2^2\|\delta u\|_{L^2}^2 + T\|\delta p_T\|_2^2 + 2(TM\|p_T\|_2\|\delta u\|_{L^2})\sqrt{T}\|\delta p_T\|_2} \\ &\leq 2TM\|p_T\|_2\|\delta u\|_{L^2} + \sqrt{T}\|\delta p_T\|_2,\end{aligned} \tag{47}$$

which concludes the proof. □

Theorem 2: *Let (u, p_T) be a solution of* (13) *with $G_r(u, p_T) = 0$. Let $M_n := \|B_n\|$, $M = \sqrt{N_C}\sum_{n=1}^{N_C}\|B_n\|$, and*

$$\tilde{K}_n := M_n\|x(0)\|_2\sqrt{T}, \tag{48}$$

and

$$K_n := 1 - 4MTM_n\|p_T\|_2\|x(0)\|_2, \tag{49}$$

and assume that

$$C_1 := 1 + \tilde{K}_n(16TM^2\|p_T\|_2^2\tilde{K}_n - 8\sqrt{T}M\|p_T\|_2 - 1 + 4\sqrt{T}M\|p_T\|_2\tilde{K}_n) > 0, \tag{50}$$

and

$$C_2 := \tilde{K}_n + 4\sqrt{T}M\tilde{K}_n\|p_T\|_2 - 1 > 0, \tag{51}$$

for $n = 1, \ldots, N_C$. Then, the reduced Hessian operator $\nabla^2 G_r(u, p_T)$ is coercive as follows:

$$\left\langle \nabla^2 G_r(u, p_T)\begin{pmatrix}\delta u\\ \delta p_T\end{pmatrix}, \begin{pmatrix}\delta u\\ \delta p_T\end{pmatrix}\right\rangle_{L^2} \geq \alpha\left(\|\delta u\|_{L^2}^2 + \|\delta p_T\|_2^2\right), \quad \forall(\delta u, \delta p_T) \neq 0, \tag{52}$$

where $\alpha > 0$ is given by

$$\alpha := \min_n\left\{(K_n^2 - K_n\tilde{K}_n),\ (\tilde{K}_n^2 - K_n\tilde{K}_n)\right\}. \tag{53}$$

Moreover, $\nabla^2 G_r(u, p_T)$ is invertible in a neighbourhood of (u, p_T).

Proof: Consider the norm $\|\delta u_n - \langle\delta x, B_n^* p\rangle - \langle x, B_n^*\delta p\rangle\|_{L^2}$ which appears in (31). We have that

$$\begin{aligned}&\|\delta u_n - \langle\delta x, B_n^* p\rangle - \langle x, B_n^*\delta p\rangle\|_{L^2} \\ &\geq \|\delta u_n\|_{L^2} - \|\langle\delta x, B_n^* p\rangle\|_{L^2} - \|\langle B_n x, \delta p\rangle\|_{L^2}.\end{aligned} \tag{54}$$

Now, recalling that (14c) and (14d) are norm preserving and using the estimates (35) and (36), we obtain

$$\|\langle\delta x, B_n^* p\rangle\|_{L^2} \leq M_n\|p_T\|_2 2TM\|x(0)\|_2\|\delta u\|_{L^2}, \tag{55}$$

and

$$\|\langle B_n x, \delta p\rangle\|_{L^2} \leq M_n\|p_T\|_2 2TM\|x(0)\|_2\|\delta u\|_{L^2} + M_n\sqrt{T}\|x(0)\|_2\|\delta p_T\|_2. \tag{56}$$

Replacing (55) and (56) in (54), we have

$$\|\delta u_n - \langle\delta x, B_n^* p\rangle - \langle x, B_n^*\delta p\rangle\|_{L^2} \geq K_n\|\delta u\|_{L^2} - \tilde{K}_n\|\delta p_T\|_2. \tag{57}$$

Taking the square and using the Cauchy inequality, we obtain

$$\begin{aligned}&\|\delta u_n - \langle\delta x, B_n^* p\rangle - \langle x, B_n^*\delta p\rangle\|_{L^2}^2 \\ &\geq K_n^2\|\delta u\|_{L^2}^2 + \tilde{K}_n^2\|\delta p_T\|_2^2 - 2K_n\tilde{K}_n\|\delta u\|_{L^2}\|\delta p_T\|_2 \\ &\geq K_n^2\|\delta u\|_{L^2}^2 + \tilde{K}_n^2\|\delta p_T\|_2^2 - K_n\tilde{K}_n\left(\|\delta u\|_{L^2}^2 + \|\delta p_T\|_2^2\right).\end{aligned} \tag{58}$$

Now, we take the sum over n and we look for a positive α such that the following holds:

$$\begin{aligned}&\sum_{n=1}^{N_C}\|\delta u_n - \langle\delta x, B_n^* p\rangle - \langle x, B_n^*\delta p\rangle\|_{L^2}^2 \\ &\geq \sum_{n=1}^{N_C}\left[K_n^2\|\delta u\|_{L^2}^2 + \tilde{K}_n^2\|\delta p_T\|_2^2 - K_n\tilde{K}_n\left(\|\delta u\|_{L^2}^2 + \|\delta p_T\|_2^2\right)\right] \\ &= \left[\sum_{n=1}^{N_C}\left(K_n^2 - K_n\tilde{K}_n\right)\right]\|\delta u\|_{L^2}^2 + \left[\sum_{n=1}^{N_C}\left(\tilde{K}_n^2 - K_n\tilde{K}_n\right)\right]\|\delta p_T\|_2^2 \\ &\geq \alpha\left(\|\delta u\|_{L^2}^2 + \|\delta p_T\|_2^2\right).\end{aligned} \tag{59}$$

We consider α defined in (53) and we notice that K_n, defined in (49), can be written as follows:

$$K_n = 1 - 4TMM_n\|x(0)\|_2\|p_T\|_2 = 1 - 4\sqrt{T}M\tilde{K}_n\|p_T\|_2. \tag{60}$$

To guarantee the positivity of α, we have to require that $(K_n^2 - K_n\tilde{K}_n) > 0$ and $(\tilde{K}_n^2 - K_n\tilde{K}_n) > 0$. From these requirements, we derive the conditions (50) and (51) as follows:

$$\begin{aligned} K_n^2 - K_n\tilde{K}_n &= \left(1 - 4\sqrt{T}M\tilde{K}_n\|p_T\|_2\right)^2 \\ &\quad -\left(1 - 4\sqrt{T}M\tilde{K}_n\|p_T\|_2\right)\tilde{K}_n \\ &= 1 + 16TM^2\|p_T\|_2^2\tilde{K}_n^2 - 8\sqrt{T}M\|p_T\|_2\tilde{K}_n \\ &\quad - \tilde{K}_n + 4\sqrt{T}M\|p_T\|_2\tilde{K}_n^2 > 0 \\ &\Leftrightarrow 1 + \tilde{K}_n\big(16TM^2\|p_T\|_2^2\tilde{K}_n \\ &\quad - 8\sqrt{T}M\|p_T\|_2 - 1 \\ &\quad + 4\sqrt{T}M\|p_T\|_2\tilde{K}_n\big) > 0, \end{aligned} \tag{61}$$

and

$$\begin{aligned} \tilde{K}_n^2 - K_n\tilde{K}_n > 0 &\Leftrightarrow \tilde{K}_n\left(\tilde{K}_n - K_n\right) > 0 \\ &\Leftrightarrow \left(\tilde{K}_n - K_n\right) > 0 \\ &\Leftrightarrow \tilde{K}_n + 4\sqrt{T}M\tilde{K}_n\|p_T\|_2 - 1 > 0\,. \end{aligned} \tag{62}$$

Finally, (31) and (59) imply that

$$\begin{aligned} &\left\langle \nabla^2 G_r(u, p_T)\begin{pmatrix}\delta u \\ \delta p_T\end{pmatrix}, \begin{pmatrix}\delta u \\ \delta p_T\end{pmatrix}\right\rangle_{L^2} \\ &\geq \|\delta x(T)\|_2^2 + \sum_{n=1}^{N_C}\|\delta u_n - \langle \delta x, B_n^* p\rangle - \langle x, B_n^*\delta p\rangle\|_{L^2}^2 \\ &\geq \|\delta x(T)\|_2^2 + \alpha\left(\|\delta u\|_{L^2}^2 + \|\delta p_T\|_2^2\right) \\ &\geq \alpha\left(\|\delta u\|_{L^2}^2 + \|\delta p_T\|_2^2\right),\ \forall(\delta u, \delta p_T) \neq 0, \end{aligned} \tag{63}$$

which implies that $\nabla^2 G_r$ is invertible in (u, p_T). Since $(u, p_T) \mapsto \nabla^2 G_r(u, p_T)$ is continuous, inverse function theorem enables to conclude that $\nabla^2 G_r$ is invertible in a neighbourhood of (u, p_T). □

In the next corollary, we give a sufficient condition for the two assumptions (50) and (51) in Theorem 1 to hold.

Corollary 2: *Let (u, p_T) be a solution of* (13) *with $G_r(u, p_T) = 0$. Let M_n, M, K_n, and $\tilde{K}_n$ be defined as in Theorem 1. Assume that*

$$C_{12} := 4\sqrt{T}M\tilde{K}_n\|p_T\|_2 - 1 > 0 \tag{64}$$

for $n = 1, \ldots, N_C$. Then, the conditions (50) *and* (51) *are satisfied; hence the reduced Hessian operator $\nabla^2 G_r(u, p_T)$ is coercive with α given by* (53).

Proof: Condition (51) follows immediately from (64) and the positivity of $\tilde{K}_n$.

Next, we show that (64) implies also (50). For this purpose, we write (50) as follows:

$$\begin{aligned} 16TM^2\tilde{K}_n^2\|p_T\|_2^2 &+ \left(4\sqrt{T}M\tilde{K}_n^2 - 6\sqrt{T}M\tilde{K}_n\right)\|p_T\|_2 \\ &+ (1 - \tilde{K}_n) > 0\,. \end{aligned} \tag{65}$$

The discriminant of the previous quadratic inequality is

$$\begin{aligned} \Delta &= \left(4\sqrt{T}M\tilde{K}_n^2 - 8\sqrt{T}M\tilde{K}_n\right)^2 - 64TM^2\tilde{K}_n^2(1 - \tilde{K}_n) \\ &= 16TM^2\tilde{K}_n^4 > 0\,. \end{aligned} \tag{66}$$

Consequently, (65) is fulfilled if the following holds:

$$\|p_T\|_2 > \frac{1}{2\sqrt{T}M\tilde{K}_n}, \tag{67}$$

which is equivalent to (64). □

We remark that condition (64) is in agreement with Assumption 1: replacing $\tilde{K}_n$ in C_{12}, we obtain that

$$C_{12} = 4TMM_n\|x(0)\|_2\|p_T\|_2 - 1,$$

from which it is clear that a 'sufficiently large' T contributes to the fulfilment of (64).

The next corollary, which follows directly from Theorem 2, provides a relaxation on the conditions (50) and (51). The proof is similar to the one of Theorem 2, hence we omit it for brevity.

Corollary 3: *Let the assumptions of Theorem 1 hold, and assume the following equation:*

$$\begin{aligned} C_3 &:= \sum_{n=1}^{N_C}\left(K_n^2 - K_n\tilde{K}_n\right) > 0 \quad \textit{and} \\ C_4 &:= \sum_{n=1}^{N_C}\left(\tilde{K}_n^2 - K_n\tilde{K}_n\right) > 0\,. \end{aligned} \tag{68}$$

Then, the reduced Hessian operator $\nabla^2 G_r(u, p_T)$ is coercive with

$$\alpha := \min\left\{\sum_{n=1}^{N_C}\left(K_n^2 - K_n\tilde{K}_n\right),\ \sum_{n=1}^{N_C}\left(\tilde{K}_n^2 - K_n\tilde{K}_n\right)\right\}.$$

We remark that, if Theorem 2, Corollary 2, and Corollary 3 hold, then (u, p_T), such that $G_r(u, p_T) = 0$, is an isolated global minimum in a ball of finite radius centred in (u, p_T). This fact is expressed by the following corollary, its proof can be obtained by known result, hence we omit it for brevity.

Corollary 4: *Let (u, p_T) be a solution of* (13) *with $G_r(u, p_T) = 0$. Let the assumptions of Theorem 2 hold. Then, there exists a positive constant $\rho > 0$ such that*

$$G_r(\hat{u}, \hat{p}_T) \geq G_r(u, p_T) + \rho\left(\|\hat{u} - u\|_{L^2}^2 + \|\hat{p}_T - p_T\|_2^2\right), \tag{69}$$

for all $(\hat{u}, \hat{p}_T)$ belonging to a ball centred in (u, p_T).

Corollary 4 has the important purpose of characterising minimum points of (3). In fact, its meaning is as follows. By

Proposition 1, we know that global minima of (13) are stationary points of the minimum-norm problem (3). Hence, under the assumptions of Corollary 4, global minima of (13) are isolated points, which implies that stationary points of (3) are isolated points, which means that minima of (3) are isolated points.

4. Discretisation of the optimality system

In this section, we discuss the discretisation of the optimality system (14). Specifically, we illustrate the discretisation of the constraint equations (9a) and (9b), and follow the first-discretise-then-optimise strategy (see e.g. Borzì & Schulz, 2012). In the sequel, we use the following notation:

$$\nabla G_r(u, p_T) := (\nabla_u G_r(u, p_T), \nabla_{p_T} G_r(u, p_T)) .$$

To discretise the constraint, we implement a modified Crank–Nicholson (MCN) scheme. As discussed in Hochbruck and Lubich (2003), von Winckel, Borzì, and Volkwein (2009), and von Winckel and Borzì (2010), this method is appropriate for discretising quantum evolution operators with time-dependent control functions. In particular, the MCN scheme is norm preserving and second-order accurate.

Consider a time interval $[0, T]$ with a uniform mesh of size $h = \frac{T}{N_t - 1}$ and N_t points, such that $0 = t^1 < \cdots < t^{N_t} = T$. The MCN discretisation of the bilinear equation (1) is given by

$$\frac{x^j - x^{j-1}}{h} = \frac{1}{4}\left(2A + \sum_{n=1}^{N_C} B_n \left(u_n^j + u_n^{j-1}\right)\right)(x^j + x^{j-1}), \tag{70}$$

where $j = 2, \ldots, N_t$ and a given starting point $x^1 = x(0)$.

To obtain the discrete optimality system and the corresponding linearised equations, we consider the so-called first-discretise-then-optimise strategy (see e.g. Borzì & Schulz, 2012; von Winckel et al., 2009). We consider the following discrete $(L^2(0, T))^m$-scalar product:

$$\langle a, b\rangle_{L_h^2} := h \sum_{j=2}^{N_t} \langle a^j, b^j\rangle, \tag{71}$$

where a and b are the discretisations of any two functions belonging to the $L^2((0, T); \mathbb{R}^m)$ space, and m is equal to N for the state and N_C for the control.

The discretisation of problem (13) is as follows:

$$\begin{aligned}
&\min_{x,u,p} \quad G(x, u, p)\\
&:= \frac{1}{2}\|x^{N_t} - x_T\|_2^2 + \frac{1}{2} h \sum_{n=1}^{N_C} \sum_{j=2}^{N_t} (u_n^j - \langle Bx^j, p^j\rangle)^2 \text{s.t.} \quad \frac{x^j - x^{j-1}}{h}\\
&= \frac{1}{4}\left(2A + \sum_{n=1}^{N_C} B_n \left(u_n^j + u_n^{j-1}\right)\right)(x^j + x^{j-1}) \text{ for}\\
&j = 2, \ldots, N_t \ \text{ and with } \ x^1 = x(0) - \frac{p^{j+1} - p^j}{h}\\
&= \frac{1}{4}\left(2A + \sum_{n=1}^{N_C} B_n (u_n^{j+1} + u_n^j)\right)^* (p^{j+1} + p^j) \text{ for}\\
&j = N_t - 1, \ldots, 1 \ \text{ and with } \ p^{N_t} = p_T \ .
\end{aligned} \tag{72}$$

Now, we define the constraint functions $c_x(x, u)$ and $c_p(p, u)$ as follows:

$$c_x^j(x, u) := (x^j - x^{j-1})/h - \frac{1}{4}\left(2A + \sum_{n=1}^{N_C} B_n (u_n^j + u_n^{j-1})\right)(x^j + x^{j-1}), \tag{73}$$

for $j = 2, \ldots, N_t$, and

$$c_p^j(p, u) := -(p^j - p^{j-1})/h - \frac{1}{4}\left(2A + \sum_{n=1}^{N_C} B_n (u_n^j + u_n^{j-1})\right)^* (p^j + p^{j-1}), \tag{74}$$

for $j = N_t - 1, \ldots, 1$. The corresponding discrete Lagrangian is given by

$$\begin{aligned}
&L_h(x, u, p)\\
&:= \frac{1}{2}\|x^{N_t} - x_T\|_2^2 + \frac{1}{2} h \sum_{n=1}^{N_C} \sum_{j=2}^{N_t} (u_n^j - \langle Bx^j, p^j\rangle)^2\\
&\quad + h \sum_{j=2}^{N_t} \langle y^j, c_x^j(x, u)\rangle + h \sum_{j=2}^{N_t} \langle q^{j-1}, c_p^j(p, u)\rangle.
\end{aligned} \tag{75}$$

With this Lagrange function, we derive the following discrete optimality system.

The discrete adjoint systems, corresponding to the continuous equations (14e) and (14f), respectively, are given by

$$\begin{aligned}
\frac{y^j - y^{j+1}}{h} &= \frac{1}{4}\left(2A + \sum_{n=1}^{N_C} B_n (u_n^j + u_n^{j+1})\right)^* y^{j+1}\\
&\quad + \frac{1}{4}\left(2A + \sum_{n=1}^{N_C} B_n (u_n^j + u_n^{j-1})\right)^* y^j\\
&\quad + \sum_{n=1}^{N_C} (u_n^j - \langle B_n x^j, p^j\rangle) B_n^* p^j
\end{aligned} \tag{76}$$

for $j = N_t - 1, \dots, 2$ and with

$$\frac{x^{N_t} - x_T}{h} - \sum_{n=1}^{N_C} \left(u_n^{N_t} - \langle B_n x^{N_t}, p^{N_t}\rangle\right) B_n^* p^{N_t} + \left(\frac{1}{h} I - \frac{1}{4}\left(2A + \sum_{n=1}^{N_C} B_n (u_n^{N_t-1} + u_n^{N_t})\right)^*\right) y^{N_t} = 0, \quad (77)$$

and

$$\frac{q^j - q^{j-1}}{h} = \frac{1}{4}\left(2A + \sum_{n=1}^{N_C} B_n \left(u_n^j + u_n^{j-1}\right)\right)^* q^{j-1} + \frac{1}{4}\left(2A + \sum_{n=1}^{N_C} B_n \left(u_n^j + u_n^{j+1}\right)\right)^* q^j + \sum_{n=1}^{N_C} \left(u_n^j - \langle B_n x^j, p^j\rangle\right) B_n x^j \quad (78)$$

for $j = 2, \dots, N_t - 1$ and with $q^1 = 0$.

The discrete gradient, corresponding to the continuous equations (14a) and (14b), is given by

$$\nabla_u G_r(u, p_T)_n^j = u_n^j - \langle B_n x^j, p^j\rangle - \frac{1}{4}\langle B_n\left(x^{j+1} + x^j\right), y^{j+1}\rangle - \frac{1}{4}\langle B_n\left(x^j + x^{j-1}\right), y^j\rangle - \frac{1}{4}\left\langle B_n^*\left(p^{j+1} + p^j\right), q^j\right\rangle - \frac{1}{4}\left\langle B_n^*\left(p^j + p^{j-1}\right), q^{j-1}\right\rangle, \quad (79)$$

for $j = 2, \dots, N_t - 1$ and $n = 1, a \dots, N_C$,

$$\nabla_u G_r(u, p_T)_n^{N_t} = u_n^{N_t} - \langle B_n x^{N_t}, p^{N_t}\rangle - \frac{1}{4}\langle B_n\left(x^{N_t} + x^{N_t-1}\right), y^{N_t}\rangle - \frac{1}{4}\langle B_n^*\left(p^{N_t} + p^{N_t-1}\right), q^{N_t-1}\rangle, \quad (80)$$

for $n = 1, \dots, N_C$ and

$$\nabla_{p_T} G_r(u, p_T) = -\sum_{n=1}^{N_C} h \left(u_n^{N_t} - \langle B_n x^{N_t}, p^{N_t}\rangle\right) B_n x^{N_t} - q^{N_t-1} - \left(2A + \sum_{n=1}^{N_C} B_n \left(u_n^{N_t} + u_n^{N_t-1}\right)\right)^* q^{N_t-1}. \quad (81)$$

The discrete linearised constraint equations, corresponding to $H_y = 0$ and $H_q = 0$, respectively, are given by

$$\frac{\delta x^j - \delta x^{j-1}}{h} = \frac{1}{4}\left(2A + \sum_{n=1}^{N_C} B_n (u_n^j + u_n^{j-1})\right)(\delta x^j + \delta x^{j-1}) + \frac{1}{4}\left(\sum_{n=1}^{N_C} B_n (\delta u_n^j + \delta u_n^{j-1})\right)(x^j + x^{j-1}) \quad (82)$$

for $j = 2, \dots, N_t$ and with $\delta x^1 = 0$, and

$$-\frac{\delta p^{j+1} - \delta p^j}{h} = \frac{1}{4}\left(2A + \sum_{n=1}^{N_C} B_n (u_n^{j+1} + u_n^j)\right)^* (\delta p^{j+1} + \delta p^j) + \frac{1}{4}\left(\sum_{n=1}^{N_C} B_n (\delta u_n^{j+1} + \delta u_n^j)\right)^* (p^{j+1} + p^j) \quad (83)$$

for $j = N_t - 1, \dots, 1$ and with $\delta p^{N_t} = \delta p_T$.

The discrete linearised adjoint equations, corresponding to $H_x = 0$ and $H_p = 0$, are given by

$$\frac{\delta y^j - \delta y^{j+1}}{h} = \frac{1}{4}\left(2A + \sum_{n=1}^{N_C} B_n (u_n^j + u_n^{j+1})\right)^* \delta y^{j+1} + \frac{1}{4}\left(2A + \sum_{n=1}^{N_C} B_n (u_n^j + u_n^{j-1})\right)^* \delta y^j + \frac{1}{4}\left(\sum_{n=1}^{N_C} B_n (\delta u_n^j + \delta u_n^{j+1})\right)^* y^{j+1} + \frac{1}{4}\left(\sum_{n=1}^{N_C} B_n (\delta u_n^j + \delta u_n^{j-1})\right)^* y^j + \sum_{n=1}^{N_C} (\delta u_n^j - \langle B_n \delta x^j, p^j\rangle - \langle B_n x^j, \delta p^j\rangle) B_n^* p^j + \sum_{n=1}^{N_C} (u_n^j - \langle B_n x^j, p^j\rangle) B_n^* \delta p^j \quad (84)$$

for $j = N_t - 1, \dots, 2$ and with

$$\frac{\delta x^{N_t}}{h} - \sum_{n=1}^{N_C} (u_n^{N_t} - \langle B_n x^{N_t}, p^{N_t}\rangle) B_n^* \delta p^{N_t} - \frac{1}{4}\left(\sum_{n=1}^{N_C} B_n (\delta u_n^{N_t-1} + \delta u_n^{N_t})\right)^* y^{N_t}$$

$$- \sum_{n=1}^{N_C} (\delta u_n^{N_t} - \langle B_n \delta x^{N_t}, p^{N_t} \rangle - \langle B_n x^{N_t}, \delta p^{N_t} \rangle) B_n^* p^{N_t} + \left(\frac{1}{h} I - \frac{1}{4} \left(2A + \sum_{n=1}^{N_C} B_n \left(u_n^{N_t - 1} + u_n^{N_t} \right) \right)^* \right) \delta y^{N_t} = 0, \tag{85}$$

and

$$\begin{aligned} \frac{\delta q^j - \delta q^{j-1}}{h} &= \frac{1}{4} \left(2A + \sum_{n=1}^{N_C} B_n \left(u_n^j + u_n^{j-1} \right) \right)^* \delta q^{j-1} \\ &+ \frac{1}{4} \left(\sum_{n=1}^{N_C} B_n \left(\delta u_n^j + \delta u_n^{j-1} \right) \right)^* q^{j-1} \\ &+ \frac{1}{4} \left(2A + \sum_{n=1}^{N_C} B_n \left(u_n^j + u_n^{j+1} \right) \right)^* \delta q^j \\ &+ \frac{1}{4} \left(\sum_{n=1}^{N_C} B_n \left(\delta u_n^j + \delta u_n^{j+1} \right) \right)^* q^j \\ &+ \sum_{n=1}^{N_C} (\delta u_n^j - \langle B_n \delta x^j, p^j \rangle - \langle B_n x^j, \delta p^j \rangle) B_n q^j \\ &+ \sum_{n=1}^{N_C} (u_n^j - \langle B_n x^j, p^j \rangle) B_n \delta q^j \end{aligned} \tag{86}$$

for $j = 2, \ldots, N_t - 1$ and with $\delta q^1 = 0$.

The action of the discrete reduced Hessian operator, corresponding to (17) and (21), on the vector $(\delta u, \delta p_T)$ is given by

$$\begin{aligned} H_{u_n}^j &= \delta u_n^j - \langle B_n \delta x^j, p^j \rangle - \langle B_n x^j, \delta p^j \rangle \\ &- \frac{1}{4} \langle B_n \left(\delta x^{j+1} + \delta x^j \right), y^{j+1} \rangle \\ &- \frac{1}{4} \langle B_n \left(x^{j+1} + x^j \right), \delta y^{j+1} \rangle \\ &- \frac{1}{4} \langle B_n \left(\delta x^j + \delta x^{j-1} \right), y^j \rangle \\ &- \frac{1}{4} \langle B_n \left(x^j + x^{j-1} \right), \delta y^j \rangle \\ &- \frac{1}{4} \langle B_n^* \left(\delta p^{j+1} + \delta p^j \right), q^j \rangle \\ &- \frac{1}{4} \langle B_n^* \left(p^{j+1} + p^j \right), \delta q^j \rangle \\ &- \frac{1}{4} \langle B_n^* \left(\delta p^j + \delta p^{j-1} \right), q^{j-1} \rangle \\ &- \frac{1}{4} \langle B_n^* \left(p^j + p^{j-1} \right), \delta q^{j-1} \rangle, \end{aligned} \tag{87}$$

for $j = 2, \ldots, N_t - 1$ and $n = 1, \ldots, N_C$,

$$\begin{aligned} H_{u_{N_C}}^{N_t} &= \delta u_n^{N_t} - \langle B_n \delta x^{N_t}, p^{N_t} \rangle - \langle B_n x^{N_t}, \delta p^{N_t} \rangle \\ &- \frac{1}{4} \langle B_n \left(\delta x^{N_t} + \delta x^{N_t - 1} \right), y^{N_t} \rangle \\ &- \frac{1}{4} \langle B_n \left(x^{N_t} + x^{N_t - 1} \right), \delta y^{N_t} \rangle \\ &- \frac{1}{4} \langle B_n^* \left(\delta p^{N_t} + \delta p^{N_t - 1} \right), q^{N_t - 1} \rangle \\ &- \frac{1}{4} \langle B_n^* \left(p^{N_t} + p^{N_t - 1} \right), \delta q^{N_t - 1} \rangle, \end{aligned} \tag{88}$$

for $n = 1, \ldots, N_C$,

$$\begin{aligned} H_{p_T} &= - \sum_{n=1}^{N_C} h \big(\delta u_n^{N_t} - \langle B_n \delta x^{N_t}, p^{N_t} \rangle - \langle B_n x^{N_t}, \delta p^{N_t} \rangle \big) B_n x^{N_t} - \delta q^{N_t - 1} \\ &- \left(\sum_{n=1}^{N_C} B_n \left(\delta u_n^{N_t} + \delta u_n^{N_t - 1} \right) \right)^* q^{N_t - 1} \\ &- \left(2A + \sum_{n=1}^{N_C} B_n \left(u_n^{N_t} + u_n^{N_t - 1} \right) \right)^* \delta q^{N_t - 1} . \end{aligned} \tag{89}$$

5. Optimisation schemes

In this section, discuss a numerical scheme which is specific for the formulation (4). For this purpose, we make use of a cascadic NCG scheme (Borzì & Schulz, 2012; Hager & Zhang, 2005) as an initialisation procedure for a Krylov–Newton method. For completeness, we give all details regarding these procedures.

See Borzì et al. (2008), Khaneja et al. (2005), Tersigni, Gaspard, and Rice (1990) for previous works on the use of NCG schemes to solve quantum control problems. We refer to Borzì et al. (2008), Dai and Yuan (1999), Hager and Zhang (2005), and references therein, for details about the convergence of this method. In our case, the iterative NCG procedure to solve (13) is given by the following algorithm.

In Algorithm 1, given (u, p_T), the gradient ∇G_r is obtained using the following algorithm.

Algorithm 1 (NCG scheme)

Require: u^0, p_T^0, $k = 0$, $k_{\max}$, tol;
Call Algorithm 2 to compute $\nabla G_r(u^0, p_T^0)$;
Set $d^0 = -\nabla G_r(u^0, p_T^0)$;
while $k < k_{\max}$ and $|||\nabla G_r(u^k, p_T^k)||| > \text{tol}$ **do**
- Call Algorithm 3 to compute α along the direction d^k;
- Set $(u^{k+1}, p_T^{k+1}) = (u^k, p_T^k) + \alpha\, d^k$;
- Call Algorithm 2 to compute $\nabla G_r(u^{k+1}, p_T^{k+1})$;
- Compute $y^k = \nabla G_r(u^{k+1}, p_T^{k+1}) - \nabla G_r(u^k, p_T^k)$;
- Compute $\sigma^{k+1} = y^k - 2d^k \frac{(y^k, y^k)_G}{(d^k, y^k)_G}$;
- Compute $\beta^{k+1} = \frac{(\nabla G_r(u^{k+1}, p_T^{k+1}), \sigma^{k+1})_G}{(d^k, y^k)_G}$;
- Set $d^{k+1} = -\nabla G_r(u^{k+1}, p_T^{k+1}) + \beta^{k+1} d^k$;
- Set $k = k + 1$;

end while

Algorithm 2 (Evaluation of the gradient)

Require: u,p_T;
- Integrate the constraint (14c) forward;
- Integrate the constraint (14d) backward;
- Integrate the adjoint (14e) backward;
- Integrate the adjoint (14f) forward;
- Assemble $\nabla_u G_r(u, p_T)$ using (14a);
- Assemble $\nabla_{p_T} G_r(u, p_T)$ using (14b);

Algorithm 3 (Backtracking line-search scheme with Armijio's condition)

Input $G_r(u, p_T)$, $\nabla G_r(u, p_T)$, d, u, $it = 0$, $it_{\max}$, $\gamma \in (0, 1)$, $c_1 \in (0, 1)$;
Set $\alpha = 1$;
while $it < it_{\max}$ and $G_r((u, p_T) + \alpha d) > G_r(u, p_T) + c_1\alpha(d, \nabla G_r(u, p_T))_G$ **do**
- Evaluate $G_r((u, p_T) + \alpha d)$;
- If (90) is satisfied, then break;
- Set $\alpha = \gamma\alpha$;
- Set $it = it + 1$;

end while

We implement a line-search strategy based on the Armijio's condition (see e.g. Nocedal & Wright, 2006; Grippo & Sciandrone, 2011; von Winckel & Borzì, 2010), that is, we use a step-length α that satisfies

$$G_r((u, p_T) + \alpha d) \leq G_r(u, p_T) + c_1\alpha(d, \nabla G_r(u, p_T))_G \ . \tag{90}$$

More precisely, we implement a backtracking strategy, as shown in the next algorithm.

According to our experience, Algorithm 1 shows a slow convergence in solving problem (13). In order to accelerate it, we embed it in the cascadic scheme. For a detailed discussion about this method, see e.g. Borzì et al. (2008) and Borzì and Schulz (2012). The NCG-cascadic procedure is given in the following algorithm.

We use the NCG-cascadic scheme to perform an adequate initialisation of a fast Newton method, which is discussed next.

We implement a matrix-free Krylov–Newton method applied to (13). Convergence results can be found in Hinze, Pinnau, Ulbrich, and Ulbrich (2011) and Malanowski (2004), whereas, there exist much less results regarding the application of the Newton method for solving bilinear quantum control problem (we refer to von Winckel et al., 2009; von Winckel & Borzì, 2010). The crucial feature of a matrix-free Newton-type method is that the Hessian operator is not stored in the computer: Krylov-based solvers are used for the solution of the Newton linear system in such a way that only the action of the Hessian operator is computed without the storage of any matrix.

In order to define a matrix-free procedure, we consider the reduced problem (13) with $x = x(u)$ and $p = p(u, p_T)$. Consequently, the Newton procedure consists, at a given

Algorithm 4 (Cascadic scheme)

Require: u^0, p_T^0, $k = 1$, $k_{\max}$;
Require: Coarse space discretisation grid;
Call Algorithm 1 to solve the problem and obtain u^1 and p_T^1;
while $k < k_{\max}$ **do**
- Refine the discretisation grid;
- Obtain a guess solution u^{k+1}, by interpolating u^k on the new grid;
- Call Algorithm 1 to solve the problem and obtain u^{k+1} and p_T^{k+1};
- Set $k = k + 1$;

end while

step k, of solving

$$\nabla^2 G_r\left(u^k, p_T^k\right) d^k = -\nabla G_r\left(u^k, p_T^k\right)\left(u^{k+1}, p_T^{k+1}\right) = \left(u^k, p_T^k\right) + d^k \ . \tag{91}$$

A globalised implementation of this procedure is given by the following algorithm.

The following algorithm is used to solve the Newton linear system.

The action of the reduced Hessian can be evaluated by the following algorithm.

Algorithm 5 (Krylov–Newton scheme)

Require: u^0, p_T^0, $k = 0$, $k_{\max}$, tol;
while $k < k_{\max}$ and $|||\nabla G_r(u^k, p_T^k)||| >$ tol **do**
- Call Algorithm 2 to compute $\nabla G_r(u^{k+1}, p_T^{k+1})$;
- Call Algorithm 6 to solve $\nabla^2 G_r(u^k, p_T^k)d^k = -\nabla G_r(u^k, p_T^k)$;
- Call Algorithm 3 to compute α along the direction d^k;
- Set $(u^{k+1}, p_T^{k+1}) = (u^k, p_T^k) + \alpha\, d^k$;
- Set $k = k + 1$;

end while

Algorithm 6 (Solve the Newton linear system)

Input u, p_T, $\nabla G_r(u, p_T)$;
- Guess an initial value of d;
- Compute d by solving $\nabla^2 G_r(u, p_T)d = -\nabla G_r(u, p_T)$: use a Krylov-based linear system solver, for example, GMRES or CG, calling Algorithm 7 to apply the reduced Hessian;
- If d is an ascending direction, then set $d = -d$;

Algorithm 7 (Action of the reduced Hessian)

Require: $d = (\delta u, \delta p_T)$;
- Integrate the linearised constraint (19) forward;
- Integrate the linearised constraint (20) backward;
- Integrate the linearised adjoint (16) backward;
- Integrate the linearised adjoint (17) forward;
- Assemble $\nabla^2 G_r(u, p_T)d$ using (18);

6. Numerical experiments

We present the numerical results of experiments used to investigate the efficiency and robustness of our computational framework. For this purpose, we consider systems of coupled Ising spin-$\frac{1}{2}$. For more details regarding this class of spin systems, see e.g. Cavanagh et al. (2007) and Stefanatos, Glaser, and Khaneja (2005). We solve (13) using Algorithm 4 to initialise the optimisation procedure, and apply both the NCG Algorithm 1 and the Krylov–Newton Algorithm 5, to compare the performance of these two schemes.

We consider three cases. Case 1 represents the analysis of a one spin-$\frac{1}{2}$ system. The bilinear system describing this model is as follows:

$$\dot{x} = \left[A + u_1 B_1 + u_2 B_2\right] x,$$

where u_1 and u_2 are the control functions, and the matrices A, B_1, and B_2 are given by

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad B_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \text{ and}$$

$$B_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}.$$

We consider the following starting and target vectors:

$$x(0) = \begin{pmatrix} 0 & 0 & 0 & 1 \end{pmatrix}^T, \; x_T = \begin{pmatrix} 0 & 1 & 0 & 0 \end{pmatrix}^T,$$

and we fix $T = 10$.

In Figure 1, the controls resulting from (13) are depicted.

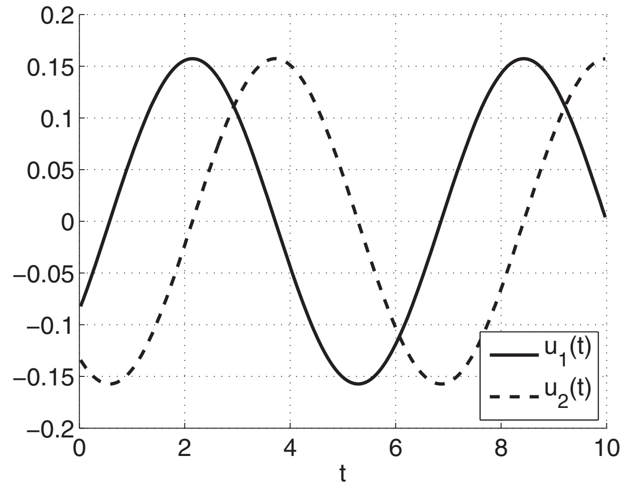

Figure 1. Case 1: exact-control functions resulting from (13).

In Case 2, we control a system of two coupled spin-$\frac{1}{2}$. For details, we refer to Khaneja et al. (2001) and Stefanatos et al. (2005). The corresponding bilinear system is $\dot{x} = \left[A + \sum_{n=1}^{4} u_n B_n\right] x$, where u_n are the control functions, and A and B_n are skew-symmetric matrices in $\mathbb{R}^{16\times 16}$. We consider the following starting and target vectors:

$$x(0) = \begin{pmatrix} 0\,0\,0\,1\,0\,0\,0\,0\,0\,0\,0\,0\,1\,0\,0\,0 \end{pmatrix}^T$$
$$x_T = \begin{pmatrix} 0\,1\,0\,0\,1\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0 \end{pmatrix}^T,$$

and we fix $T = 10$.

In Figure 2, the controls resulting from (13) are depicted.

Case 3 corresponds to the control of a system of three coupled spin-$\frac{1}{2}$. For details, see Khaneja et al. (2002) and Stefanatos et al. (2005). The corresponding bilinear system

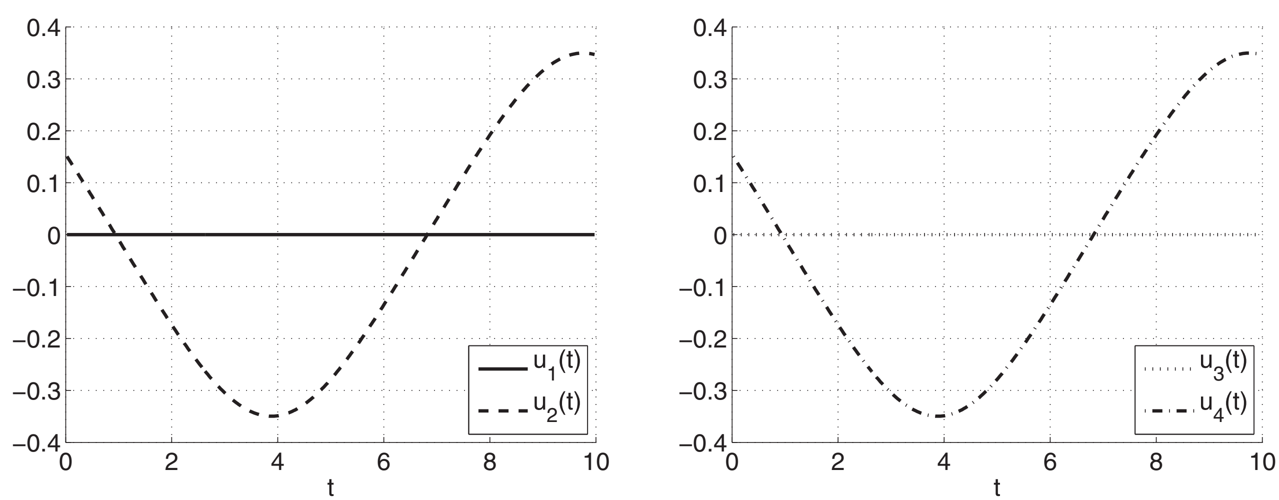

Figure 2. Case 2: exact-control functions resulting from (13).

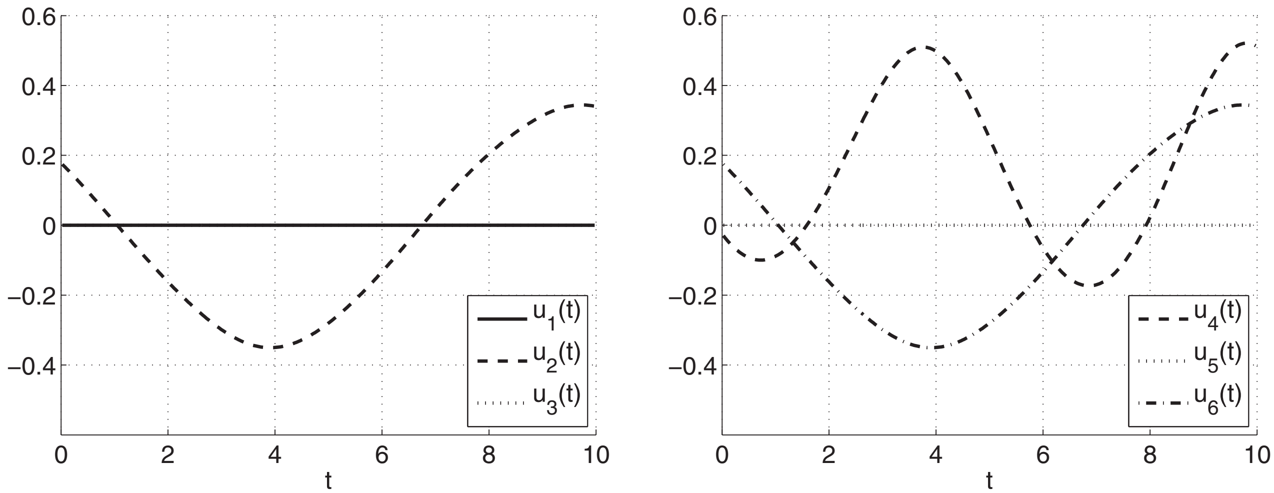

Figure 3. Case 3: exact-control functions resulting from (13).

Table 1. Characteristics and computational effort for the initialisation procedure performed using the cascadic approach are shown. These results obtained show that the NCG-cascadic approach is capable to provide an efficient initialissation: this fact results from the obtained values of G and CPU time.

Test	N_t − start	Cascadic iter	NCG tol	G	CPU time
Case 1	51	3	1.00e−003	1.28e−007	3.82
Case 2	51	3	1.00e−003	7.19e−008	9.79
Case 3	51	3	1.00e−003	1.38e−005	67.36

is $\dot{x} = \left[A + \sum_{n=1}^{6} u_n B_n\right]x$, where u_n are the control functions, and A and B_n are skew-symmetric matrices in $\mathbb{R}^{64\times 64}$. We consider the starting and target vectors $x(0)$, $x_T \in \mathbb{R}^{64}$, having all components zero, except for $x_4(0) = x_{13}(0) = x_{49}(0) = 1$ and $x_{2,T} = x_{5,T} = x_{17,T} = 1$. We compute the control functions corresponding to $T = 10$.

In Figure 3, the controls resulting from (13) are depicted.

Next, we investigate the numerical performance of our computational framework and demonstrate the validity of the assumptions of our theoretical results. For this purpose, we show more details regarding the optimisation of the three test cases.

In Table 1, details of the cascadic approach and its computational effort needed to perform the initialisation are shown. In particular, 'N_t − start' is the number of discretisation points corresponding to the starting coarse grid; 'Cascadic iter' represents the number of mesh refinements; 'NCG tol' is the tolerance required to NCG; 'G' is the obtained value of the cost functional of (13); 'CPU time' represents the time needed for the overall initialisation process. All the optimisation were performed on an Intel Core i7-2620M (2.7 GHz) with 8 GB of RAM computer using MATLAB R2012b. Notice that we consider as starting condition for all cases $u = 0$ and $p_T = 0$.

In Table 2, we compare the computational performance of the NCG-cascadic as stand-alone solver and the NCG-cascadic initialised Krylov–Newton schemes to solve (13) corresponding to the considered cases. The tolerance required to NCG and Krylov–Newton is fixed to 10^{-8}. The maximum number of iterations allowed to NCG and Krylov–Newton are 1000 and 40, respectively.

In Table 3, we consider an a-posteriori analysis concerning the sufficient second-order optimality conditions given in Theorem 2 and Corollary 2. In particular, we computed

Table 2. Computational efforts of the NCG and Krylov–Newton schemes for the solution of (13) are shown. These results obtained show that, after the cascadic initialisation, the Krylov–Newton method is more efficient and accurate than NCG in solving the optimisation problem. Further, the norms of the solutions of the adjoint equations are shown: these validate numerically Proposition 3.

Test	NCG iter	G	CPU time	Newton iter	G	CPU time	$\|y\|_{L^2}^2$	$\|q\|_{L^2}^2$
Case 1	33	1.37e−017	8.43	2	9.30e−026	3.82	3.01e−026	1.86e−024
Case 2	30	1.31e−017	13.71	2	1.15e−023	9.33	3.17e−023	3.75e−022
Case 3	588	3.34e−009	1911.50	5	3.34e−009	570.29	4.16e−009	1.14e−019

Table 3. In this table, conditions of Theorem 2 and Corollary 2 regarding the positivity of C_1, C_2, C_3, and C_4. In particular, the norms of the terminal conditions p_T, the time T, the coefficient M, and the coefficients C_1, C_2, C_3, and C_4 are shown. According to Theorem 2 and Corollary 2, the positivity of C_1, C_2, C_3, and C_4 guarantees that the computed stationary points of (13) in the three different cases are isolated global minima.

Test	$\|p_T\|_2$	T	M	C_1	C_2	C_3	C_4
Case 1	0.18	10	2.82	4.36e+002	1.15e+002	8.72e+002	1.42e+002
Case 2	0.53	10	8.00	5.88e+004	4.56e+002	2.35e+005	4.38e+003
Case 3	3.43	10	14.70	1.22e+007	1.02e+003	7.32e+007	1.15e+005

Table 4. Results of the optimisation performed on Case 1. The obtained values of G and the computed fidelity C show that for all values of T we are able to compute exact-control functions.

T	N_t-start	Cascadic	Newton iter	G	C
1	51	3	2	3.16e−020	1.0000
2	51	3	2	2.43e−024	1.0000
5	51	3	2	2.50e−026	1.0000
8	51	3	2	1.21e−023	1.0000
10	51	3	2	9.30e−026	1.0000
20	51	3	2	8.84e−026	1.0000

C_1 and C_2 given by (50) and (51), respectively, and C_3 and C_4 given by (68). Notice that, all these coefficients are positive; hence, according to Theorem 2 and Corollary 2, the computed stationary points for the three cases are (global) minima of (13).

Next, we want to study the dependence of the problem on the time T. For this purpose, we show results of numerical optimisation performed for different values of time T. In particular, we are interested in studying the behaviour of the optimisation when T is smaller than the considered value used in the previous tests. In particular, we consider values of T between 1 and 20. We make this choice because Khaneja et al. (2001) and Dirr et al. (2006) estimate the optimal time needed for specific transitions of two coupled spins equal to $T = 3/2$. Moreover, Khaneja et al. (2002) estimate the optimal time for specific transitions of three coupled spins to be equal to $T = 3\sqrt{2}/2$.

Table 5. Results of the optimisation performed on Case 2. We observe that the convergence requires more computational effort when T is smaller. The obtained values of G and the computed fidelity C show that for $T = 1$ the control solution is not an exact-control function. In the other cases, the computed controls are exact-control functions and global solutions of (13).

T	N_t-start	Cascadic	Newton iter	G	C
1	51	3	40	4.66e−003	0.9976
2	51	3	33	4.67e−015	1.0000
5	51	3	17	1.38e−017	1.0000
8	51	3	3	4.20e−019	1.0000
10	51	3	2	1.15e−023	1.0000
20	51	3	2	2.94e−024	1.0000

Table 6. Results of the optimisation performed on Case 3. We observe that the convergence requires more computational effort when T is smaller. In particular, for $T = 1$, $T = 2$, $T = 5$, and $T = 8$, the optimisation is stopped because the maximum number of allowed iterations is reached. The obtained values of G and the computed fidelity C show that the computed controls are exact-control functions or capable to steer the trajectory in a very small neighbourhood of the target.

T	N_t-start	Cascadic	Newton iter	G	C
1	51	3	40	1.60e−002	0.9946
2	51	3	40	1.50e−003	0.9995
5	51	3	40	7.71e−003	0.9973
8	51	3	40	4.82e−009	1.0000
10	51	3	5	3.34e−009	1.0000
20	101	3	3	2.14e−008	1.0000

We remark that the maximum number of iterations allowed to NCG, used in the cascadic approach, and Krylov–Newton are 100 and 40, respectively.

The results obtained show that smaller the T is, harder the problem is to solve. From the results obtained that shown in the next tables, it is evident that the problem is harder to solve when T decreases. To analyse the results in a way which is of interest for NMR experiments, we compute the so-called fidelity, defined as

$$C := \frac{\langle x(T), x_T \rangle}{\|x(T)\|_2 \|x_T\|_2} . \tag{92}$$

Table 4 shows that for a system of one spin we are able to steer the trajectory to the target exactly, for any considered value of time T.

Table 5 shows that that in Case 2 with $T = 1$, the optimisation is stopped because the maximum number of iterations is reached, and the computed control functions are not a global solution of (13); this is evident from the fact that the value of the cost functional evaluated in the solution obtained is $G \gg 0$. On the other hand, the fidelity obtained shows that we reached a small neighbourhood of the target. Further, the number of iteration performed by the Newton method shows that the convergence requires more computational effort when T is smaller.

Table 6 shows that in Case 3 with $T = 1$, 2, 5, and 8, we observe that the optimisation algorithm is stopped because the maximum number of iterations is reached. The computed controls allow to obtain high values of the fidelity, which means that the trajectory is steered in a very small neighbourhood of the target.

7. Conclusions

Although there are many results that prove the existence of controls for exact controllability, much less is known on the construction of these controls. In fact, apart of special cases, where the controls can be constructed analytically, in most cases, a numerical approach is necessary. For this purpose, we propose an efficient and robust computational framework that is supported by theoretical evidence. Moreover, our methodology appears to be of general applicability. In particular, it could be applied to solve exact-controllability problems governed by infinite-dimensional quantum models and other time-dependent partial differential equation models.

In this paper, the proposed methodology was applied to solve exact-controllability problems governed by the LvNM equation that was presented. Moreover, theoretical results were presented for the analysis of first-order and second-order optimality conditions and for characterising the set of exact-controllability functions with minimum norm as a set of isolated points.

For the numerical implementation, the differential models were approximated with a modified Crank–Nicholson scheme and the resulting discretised optimality system was solved with a matrix-free Krylov–Newton scheme combined with an NCG-cascadic initialisation. Results of numerical experiments demonstrated the ability of the proposed framework to solve quantum spin exact-controllability problems.

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