Optimal control of Nuclear Magnetic Resonance periodic systems

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***Abstract*— In this paper, we consider an optimal control problem for quantum systems with a periodic time evolution. In this non-classical problem both the initial and final state are unknown (and equal). We first prove the existence of periodic solution of this problem for a fixed period and study the associated optimal periodic control problem.**

I. INTRODUCTION

We consider in this paper a question arising from NMR and MRI [1], [2], [3], [4], namely the maximization of the signal-to-noise ratio per unit time (SNR) of spin as 1/2 particles. In the experiments, the SNR is practically enhanced in spin systems by using a multitude of identical cycles. In this periodic regime, the SNR increases as the square root of the number of scans. Each period of control is composed of a detection time and of a control period where the spin is subjected to a radio-frequency magnetic pulse, the latter being used to guarantee the periodic character of the overall process. A pioneering work in this field has been done by R. Ernst and his co-workers [4] in the sixties by establishing an optimal control law made of a δ-pulse characterized by a specific rotation angle, called the *Ernst angle solution*. This pulse sequence is nowadays currently used in magnetic resonance spectroscopy and imaging. Related control procedures, known as SSFP (Steady State Free Precession) have been also intensively investigated in the literature for medical applications (See, among others, Ref. [5], [6], [7], [8], [9], [10], [11], [12]).

From a mathematical point of view, some works have tackled the exact local controllability of the linear Schrdinger equation, see for example [13], [14] in the case of non-periodic processes. In the context of the periodic systems, there are also several works applied on different domains [15], [16], [17], [18], [19].

In a recent paper [20], an optimal control algorithm for periodic spin dynamics has been proposed to deal with the maximization of SNR in the framework of the control of an ensemble of inhomogeneous ensemble of spins. This complex optimization problem involves the design of a control field, while finding the initial state of the dynamics associated with periodic trajectories. This work was rather related to numerical aspects and above all to applications to medical imaging.

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The goal of the present paper is to provide a mathematical framework and analyse the problem of the maximization of SNR in the case of periodic spin systems. Though we consider an only spin, all what follows also holds for an inhomogeneous ensemble of spins. More precisely, we prove in Section II the existence and uniqueness of a solution of a periodic version of the Bloch equation for a fixed control. In Section III, we prove the existence of an optimal control for the maximization of SNR and present the associated optimality system. We conclude with some numerical experiments in section IV.

Throughout this paper, we use the following notations: $\mathbb{R}^3$ denotes the canonical 3-dimensional linear space on $\mathbb{R}$, $\langle \cdot, \cdot \rangle$ the usual Euclidean scalar product on $\mathbb{R}^3$ and $\| \cdot \|_2$ the corresponding norm, $L^2_{T_c}(0, T; \mathbb{R}^2)$ indicates the subspace of the Lebesgue space $L^2(0, T; \mathbb{R}^2)$ of functions cancelling on $[T_c, T]$, $L^\infty(0, T; \mathbb{R}^3)$ denotes the usual Lebesgue's functional space, and $\mathcal{C}(0, T; \mathbb{R}^3)$ the space of continuous functions of $[0, T]$ taking values in $\mathbb{R}^3$.

II. THE PERIODIC BLOCH EQUATION

The optimization of the SNR per time unit that we consider corresponds to a simple scenario, described in Fig. 1 (see Ref. [21], [22] for details). In this picture , the point M reached at the end of the control process is the measurement point for the spin of offset ω. The corresponding spin has then a free evolution from this point to the steady state S where the pulse sequence starts. The times T_d and T_c denote the detection time (fixed by the experimental setup) and the control time, respectively.

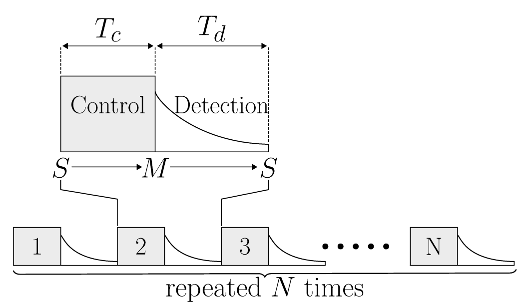

Fig. 1. Schematic representation of the cyclic process used in the maximization of the SNR.

We consider a spin 1/2 particle [3]. In a rotating frame, the motion for the spin follows the Bloch equation:

$$\begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix} = \begin{pmatrix} -2\pi x/T_2 \\ -2\pi y/T_2 \\ 2\pi(1-z)/T_1 \end{pmatrix} + \begin{pmatrix} -\omega y + u_y(t) z \\ \omega x - u_x(t) z \\ u_x(t) y - u_y(t) x \end{pmatrix},$$

where the Bloch vector $X := (x, y, z)^\intercal$ corresponds to the state of the spin, T_1 and T_2 are the two relaxation parameters, ω the offset term and $u_x(t)$, $u_y(t)$ the two control fields. Defining $u = (u_x, u_y)$ and normalizing the time by the detection time T_d (see below for the definition) and setting $\gamma = 2\pi T_d/T_1$ and $\Gamma = 2\pi T_d/T_2$, we arrive at:

$$\dot{X} = A(u)\,X + D \tag{1}$$

where $D := (0, 0, \gamma)^\intercal$ and $A(u)$ is a 3×3- matrix:

$$A(u) := \begin{pmatrix} -\Gamma & -\omega & u_y(t) \\ \omega & -\Gamma & -u_x(t) \\ -u_y(t) & u_x(t) & -\gamma \end{pmatrix},$$

with $u(t) = (u_x(t), u_y(t))$.

In our periodic problem, the initial state $X_0 = X(0)$ is an unknown of the problem, that must satisfy

$$X(T) = X_0. \tag{2}$$

A. The Cauchy problem associated with the non-periodic Bloch equation

We first consider the Cauchy problem associated with Eq. (1). Given $u \in L^2_{T_c}(0, T; \mathbb{R}^2)$ and an initial state $X_0 \in \mathbb{R}^3$, this one reads:

Find $X \in \mathcal{C}(0, T; \mathbb{R}^3)$ *such that*

$$\begin{cases} \dot{X}(t) &= A(u(t))\,X(t) + D,\ t \in [0, T] \\ X(0) &= X_0 \end{cases} \tag{3}$$

The next theorem gives existence and uniqueness of a solution of this problem.

Theorem 1: There exists a unique weak solution of (3), i.e. a function $X \in \mathcal{C}(0, T; \mathbb{R}^3)$ satisfying

$$X(t) = X_0 + \int_0^t A(u(s))\,X(s) + D\,ds, \tag{4}$$

for all $t \in [0, T]$.

Proof: Define the matrices

$$B := \begin{pmatrix} -\Gamma & -\omega & 0 \\ \omega & -\Gamma & 0 \\ 0 & 0 & -\gamma \end{pmatrix}, \tag{5}$$

and

$$C(u(t)) := \begin{pmatrix} 0 & 0 & u_y(t) \\ 0 & 0 & -u_x(t) \\ -u_y(t) & u_x(t) & 0 \end{pmatrix}. \tag{6}$$

Note $C(u(t))$ that depends linearly on $u(t)$, so that there exists $\kappa > 0$ such that for all $Z_0 \in \mathbb{R}^3$

$$\|C(u(t))Z_0\|_2 \le \kappa \|u(t)\|_2 \|Z_0\|_2. \tag{7}$$

Consider the mapping:

$$\Phi : \begin{cases} \mathcal{C}(0, T; \mathbb{R}^3) \to \mathcal{C}(0, T; \mathbb{R}^3) \\ X \mapsto \Phi(X), \end{cases}$$

where $\Phi(X)$ is defined for $t \in [0, T]$ by the Duhamel's formula:

$$\Phi(X)(t) = \exp(tB)X_0 + \int_0^t \exp((t-s)B)\,(C(u(s))\,X(s) + D)\,ds. \tag{8}$$

The operator Φ is well-defined: indeed since $X \in \mathcal{C}(0, T; \mathbb{R}^3)$ and $u \in L^2_{T_c}(0, T; \mathbb{R}^2)$, $s \mapsto A(u(s))\,X(s) + D$ is Lebesgue integrable, and $t \mapsto \Phi(X)(t) \in \mathcal{C}(0, T; \mathbb{R}^3)$ according to the fundamental theorem of calculus ($\Phi(X)$ is actually absolutely continuous). Consider now the contraction property of Φ. Let X_1 and $X_2 \in \mathcal{C}(0, T; \mathbb{R}^3)$. As we know that $\exp((t-s)B)$ is a bounded function, we note by μ its upper bound such that

$$\|\exp((t-s)B)\| \le \mu. \tag{9}$$

Using (8), (7) and (9), we obtain

$$\|\Phi(X_2) - \Phi(X_1)\|_{L^\infty(0,T;\mathbb{R}^3)} \le \sqrt{T}\mu\kappa \|u\|_{L^2(0,T;\mathbb{R}^2)} \|X_2 - X_1\|_{L^\infty(0,T;\mathbb{R}^3)}.$$

If $\|u\|_{L^2(0,T;\mathbb{R}^2)}$ is small enough, the latter inequality implies that Φ is a contraction. We deduce from the Banach fixed point theorem that Φ has a unique fixed point, hence (3) admits a unique solution $X \in \mathcal{C}(0, T; \mathbb{R}^3)$.

If $\|u\|_{L^2(0,T;\mathbb{R}^2)}$ is not small, we consider the partition $[0, T] = \cup_{l=0}^{N-1} [T_l, T_{l+1}]$, with $T_0 = 0$ and $T_N = T$, such that $\|u\|_{L^2(T_l, T_{l+1};\mathbb{R}^2)}$ is small enough. The existence is obtained by applying the previous result on each interval $[T_l, T_{l+1}]$ for all $l \in \{0, \cdots, N-1\}$.

Finally, remark that if X is a fixed point of Φ, then the right-hand sides of (4) and (8) are almost everywhere differentiable and that there derivatives are almost everywhere equal. A weak solution (3) consequently consists in a fixed point of Φ. The result follows. ■

B. The periodic problem

We now consider a variant of the previous Cauchy problem, where the initial condition must also satisfy the periodicity condition (2). Given $u \in L^2_{T_c}(0, T; \mathbb{R}^2)$, this problem reads:

Find $(X_0, X) \in \mathbb{R}^3 \times \mathcal{C}(0, T; \mathbb{R}^3)$ *such that*

$$\begin{cases} \dot{X}(t) &= A(u(t))\,X(t) + D,\ t \in [0, T] \\ X(0) &= X_0 = X(T). \end{cases}$$

To prove the existence and uniqueness of a (weak) solution of this problem, we need the following result.

Lemma 1: let $Z_0 \in \mathbb{R}^3$ and $Z(t) \in \mathcal{C}(0, T; \mathbb{R}^3)$ be the weak solution of (3) in the case $X_0 = Z_0$ and $D = 0$. For $t \in [0, T]$:

$$\|Z(t)\|_2 \le e^{-\min(\Gamma,\gamma)t} \|Z_0\|_2. \tag{10}$$

Proof: The result will be obtained by a Gronwall-type estimate. Let $t \in [0, T]$. As a weak solution of (3), the function Z is almost everywhere differentiable and a direct calculation gives

$$\frac{d\|Z(t)\|_2^2}{dt} = 2\langle Z(t), A(u(t))\, Z(t)\rangle \leq -2\min(\Gamma,\gamma)\|Z(t)\|_2^2, \quad (11)$$

where we have used the fact that the symmetric part of $A(u(t))$ is diagonal, with negative coefficients. Defining $h(t) := \frac{d\|Z(t)\|_2^2}{dt} + 2\min(\Gamma,\gamma)\|Z(t)\|_2^2$ and multiplying both sides by $e^{2\min(\Gamma,\gamma)t}$, we obtain:

$$\frac{d(e^{2\min(\Gamma,\gamma)t}\|Z(t)\|_2^2)}{dt} = e^{2\min(\Gamma,\gamma)t}\, h(t),$$

which gives by integration over $[0,t]$

$$\|Z(t)\|_2^2 = e^{-2\min(\Gamma,\gamma)t}\|Z_0\|_2^2 + \int_0^t e^{2\min(\Gamma,\gamma)(s-t)}\, h(s)ds.$$

Because of (11), $h(t) \leq 0$ and the result follows. ■

We can now state an existence and uniqueness result in the periodic case.

Theorem 2: There exists a unique couple $(X_0, X) \in \mathbb{R}^3 \times \mathcal{C}(0,T;\mathbb{R}^3)$ satisfying

$$\begin{cases} X(t) &= X_0 + \int_0^t A(u(s))\, X(s) \,+\, D\, ds, \\ X(T) &= X_0, \end{cases} \quad (12)$$

for all $t \in [0,\, T]$.

Proof: Introduce the mapping $\Psi : \mathbb{R}^3 \to \mathbb{R}^3$ defined by

$$\Psi(X_0) := X(T),$$

where X is the weak solution of (3) obtained in Theorem 1.

Given $X_0^1 \in \mathbb{R}^3$ and $X_0^2 \in \mathbb{R}^3$, define $Z_0 = X_0^2 - X_0^1$ and $Z(t) = X^2(t) - X^1(t)$, where X^2 and X^1 are the weak solutions obtained by Theorem 1 with $X_0 = X_0^2$ and $X_0 = X_0^1$, respectively. Substracting the corresponding weak representations (4), we see that Z satisfies the assumptions of Lemma 1 so that (10) holds. As a consequence,

$$\|X^2(T) - X^1(T)\|_2 \leq e^{-\min(\Gamma,\gamma)T}\|X_0^2 - X_0^1\|_2,$$

which implies that Ψ is a contraction. Applying Banach fixed-point theorem, it follows that there exists a unique $X_0 \in \mathbb{R}^3$ such that $\Psi(X_0) = X_0$. The corresponding weak solution X of (3) satisfies (12). ■

Remark 1: Theorem 2 remains true if $D \in L^1(0,T;\mathbb{R}^3)$.

We can actually bound X, as stated in the next lemma.

Lemma 2: Let $(X_0, X) \in \mathbb{R}^3 \times \mathcal{C}(0,T;\mathbb{R}^3)$ be the unique solution of (12) and $t \in [0,T]$. We have

$$\|X(t)\|_2 \leq \frac{1}{\min(\Gamma,\gamma)}\|D\|_2. \quad (13)$$

Proof: The first step of the proof is similar to the one of Lemma 1. As a weak solution of (3), the function X is almost everywhere differentiable and we have for $t \in [0,T]$,

$$\begin{aligned}\frac{d\|X(t)\|_2^2}{dt} =& 2\langle X(t), A(u(t))X(t) + D\rangle \\ \leq& -2\min(\Gamma,\gamma)\|X(t)\|_2^2 + 2\|X(t)\|_2\|D\|_2 \\ \leq& -2\min(\Gamma,\gamma)\|X(t)\|_2^2 + \varepsilon\|X(t)\|^2 + \frac{1}{\varepsilon}\|D\|_2^2,\end{aligned}$$

where ε is on the interval $]0,\, 2\min(\Gamma,\gamma)[$. Multiplying both sides by $e^{(2\min(\Gamma,\gamma)-\varepsilon)t}$, we obtain:

$$\frac{d(e^{(2\min(\Gamma,\gamma)-\varepsilon)t}\|X(t)\|_2^2)}{dt} \leq e^{(2\min(\Gamma,\gamma)-\varepsilon)t}\,\frac{1}{\varepsilon}\|D\|_2^2, \quad (14)$$

which gives by integration over $[0,T]$

$$\begin{aligned}\|X(T)\|_2^2 \leq& e^{(-2\min(\Gamma,\gamma)+\varepsilon)T}\|X_0\|_2^2 \\ &+ \int_0^T e^{(2\min(\Gamma,\gamma)-\varepsilon)(s-T)}\,\frac{1}{\varepsilon}\|D\|_2^2 ds.\end{aligned}$$

Since $X(T) = X_0$, we deduce

$$\|X_0\|_2^2 \leq \frac{1}{(2\min(\Gamma,\gamma)-\varepsilon)\,\varepsilon}\|D\|_2^2$$

We then set $\varepsilon = \min(\Gamma,\gamma)$ to get

$$\|X_0\|_2 \leq \frac{1}{\min(\Gamma,\gamma)}\|D\|_2. \quad (15)$$

Using again (14), we obtain by integration over $[0,t]$:

$$\begin{aligned}\|X(t)\|_2^2 \leq& e^{-\min(\Gamma,\gamma)t}\|X_0\|_2^2 \\ &+ \frac{1}{\min(\Gamma,\gamma)^2}\left(1 - e^{-\min(\Gamma,\gamma)t}\right)\|D\|_2^2.\end{aligned}$$

Eq. (13) then follows by estimating $\|X_0\|_2$ using (15). ■

In the rest of this paper, we note by $H^1_{per}(0,T;\mathbb{R}^3)$ a subspace of $\mathcal{C}(0,T;\mathbb{R}^3)$ defined as follows:

$$H^1_{per}(0,T;\mathbb{R}^3) := \{X \in H^1(0,T;\mathbb{R}^3) \backslash X(0) = X(T)\}.$$

Corollary 1: For every $u \in L^2_{T_c}(0,T;\mathbb{R}^2)$ and $X \in \mathcal{C}(0,T;\mathbb{R}^3)$ solution of (12), X is in $H^1_{per}(0,T;\mathbb{R}^3)$.

Proof: Because of (8) and the fact that $\phi(X) = X$, the solution X is well-defined. Moreover, it is almost everywhere differentiable and we have:

$$\dot{X}(t) = B\exp(tB)X_0 + (C(u(t))\, X(t) \,+\, D)\,.$$

Since $X \in \mathcal{C}(0,T;\mathbb{R}^3)$ and $u \in L^2_{T_c}(0,T;\mathbb{R}^2)$, X and $\dot{X}$ are in $L^2(0,T;\mathbb{R}^3)$. ■

III. OPTIMIZATION PROBLEM

In this section, we are interested here in presenting an optimal control problem [23], [24], [25], [26] that amounts to maximizing a functional. In this way, we define:

$$F(u) := \langle X(T_c)|O|X(T_c)\rangle - \alpha\|u\|^2_{L^2_{T_c}(0,T;\mathbb{R}^2)}, \quad (16)$$

where $X \in H^1_{per}(0,T;\mathbb{R}^3)$ is the solution of (12), $\alpha > 0$, $0 < T_c < T$ and O is a self-adjoint matrix of spectral radius λ_O. The optimal control problem we consider is:

Find $u^\star$ solving the maximization problem:

$$\max_{u\in L^2_{T_c}(0,T;\mathbb{R}^2)} F(u), \quad (17)$$

In what follows, we prove the existence of a solution of this problem and obtain optimality conditions.

A. Maximizing sequence

Consider a maximizing sequence $(u^k)_{k\in\mathbb{N}}$ associated with (17) and $(X_0^k, X^k)_{k\in\mathbb{N}}$ the corresponding sequence of solutions of (12). Because of (13), we have

$$\langle X^k(T_c)|O|X^k(T_c)\rangle \leq \frac{\lambda_O}{\min(\Gamma,\gamma)^2}\|D\|_2^2,$$

so that if $\|u^k\|_{L^2(0,T;\mathbb{R}^2)} \to +\infty$, then $F(u^k) \to -\infty$. This contradicts the definition of $(u^k)_{k\in\mathbb{N}}$. As a consequence, we can extract a subsequence, that we still denote by $(u^k)_{k\in\mathbb{N}}$, that weakly converges in $L^2(0,T;\mathbb{R}^2)$ to some control u^∞. Considering again (13), we see that $(X_0^k)_{k\in\mathbb{N}}$ is necessarily bounded, so that -up to a supplementary extraction- we can also assume that $(X_0^k)_{k\in\mathbb{N}}$ converges to some state X_0^∞.

B. Existence of an optimum

We now prove that the sequence $(X^k)_{k\in\mathbb{N}}$ of weak solutions of (12) defined in the previous section actually strongly converges in $\mathcal{C}(0,T;\mathbb{R}^3)$.

Theorem 3: We keep the previous notations. The sequence $(X^k)_{k\in\mathbb{N}}$ converges strongly in $\mathcal{C}(0,T;\mathbb{R}^3)$ to X^∞, where X^∞ is the solution of (12) with $u = u^\infty$.

Proof: Consider the mapping:

$$\begin{aligned}\mathbb{R}^3 \times L^2_{T_c}(0,T;\mathbb{R}^2) &\to \mathcal{C}(0,T;\mathbb{R}^3)\\ \varphi : (X_0,u) &\mapsto X,\end{aligned}$$

where X is defined as the solution of (4) associated with X_0. We have

$$\begin{aligned}X^\infty - X^k =& \varphi(X_0^\infty,u^\infty) - \varphi(X_0^k,u^k)\\ =& \varphi(X_0^\infty,u^\infty) - \varphi(X_0^\infty,u^k)\\ &+ \varphi(X_0^\infty,u^k) - \varphi(X_0^k,u^k).\end{aligned}$$

Let $\eta > 0$. We first consider the term $Z^k := \varphi(X_0^\infty,u^k) - \varphi(X_0^k,u^k)$. Substracting the weak representations (4) corresponding to $\varphi(X_0^\infty,u^k)$ and $\varphi(X_0^k,u^k)$, we see that Z^k satisfies the assumptions of Lemma 1 so that (10) holds. As a consequence,

$$\|\varphi(X_0^\infty,u^k) - \varphi(X_0^k,u^k)\|_2 \leq e^{-\min(\Gamma,\gamma)T}\|X_0^\infty - X_0^k\|_2,$$

meaning that there exists k_1, such that for all $k \geq k_1$ $\|\varphi(X_0^\infty,u^k) - \varphi(X_0^k,u^k)\|_2 \leq \frac{\eta}{2}$.

Let us now consider the term $W^k := \varphi(X_0^\infty,u^\infty) - \varphi(X_0^\infty,u^k)$. Following the reasoning in the proof of Theorem 1, we obtain the Duhamel formula for $t \in [0,T]$:

$$\begin{aligned}W^k(t) =& \int_0^t \exp\left((t-s)B\right)\left(C(u^k(s) - u^\infty(s))\right)X^\infty(s)ds\\ &+ \int_0^t \exp\left((t-s)B\right)C(u^k(s))W^k(s)ds, \qquad (18)\end{aligned}$$

where B and $C(\cdot)$ have been defined in (5) and (6). Define $\widetilde{X}^k \in \mathcal{C}(0,T;\mathbb{R}^3)$ by $\widetilde{X}^k(t) := \int_0^t \exp\left(-sB\right)\left(C(u^k(s) - u^\infty(s))\right)X^\infty(s)ds$.

We aim at showing that $(\widetilde{X}^k)_{k\in\mathbb{N}}$ converges strongly in $\mathcal{C}(0,T;\mathbb{R}^3)$ using the compact embedding of $H^1(0,T;\mathbb{R})$ in $\mathcal{C}(0,T;\mathbb{R})$. According to the fundamental theorem of calculus $\widetilde{X}^k \in \mathcal{C}(0,T;\mathbb{R}^3)$, so that $\widetilde{X}^k \in L^2(0,T;\mathbb{R}^3)$. Moreover, this function is differentiable almost everywhere and we have:

$$\dot{\widetilde{X}}^k(t) = \exp\left(-tB\right)\left(C(u^k(t) - u^\infty(t))\right)X^\infty(t). \qquad (19)$$

As X^∞ and $t \mapsto \exp\left(-tB\right)$ are two bounded continuous functions on $[0,T]$ and $u^k - u^\infty \in L^2_{T_c}(0,T;\mathbb{R}^2)$, $\dot{\widetilde{X}}^k$ belongs to $L^2(0,T;\mathbb{R}^3)$. Thus, $\widetilde{X}^k \in H^1(0,T;\mathbb{R}^3)$.

Let us now show that $\widetilde{X}^k$ converges weakly to 0 in $H^1(0,T;\mathbb{R})$. Given $U \in H^1(0,T;\mathbb{R}^3)$, we have:

$$\begin{aligned}\langle U,\widetilde{X}^k\rangle_{H^1(0,T;\mathbb{R}^3)} =& \int_0^T \langle U(t),\widetilde{X}^k(t)\rangle_{\mathbb{R}^3}dt \qquad (20)\\ &+ \int_0^T \langle \dot{U}(t),\dot{\widetilde{X}}^k(t)\rangle_{\mathbb{R}^3}dt.\end{aligned}$$

The first member in the right-hand side could be written as follows:

$$\int_0^T \langle U(t),\widetilde{X}^k(t)\rangle_{\mathbb{R}^3}dt = \int_0^T \langle \varphi(s),\dot{\widetilde{X}}^k(s)\rangle_{\mathbb{R}^3}ds$$

where $\varphi(s) := \int_s^T U(t)dt$ so that $\varphi \in L^\infty(0,T;\mathbb{R}^3) \subset L^2(0,T;\mathbb{R}^3)$. It follows then from (19) that both terms of the right-hand side of (20) consist in sums of integrals of products of functions in $L^2(0,T;\mathbb{R})$ with components of $u^k - u^\infty$. Since $u^k - u^\infty$ converges weakly to 0, the two terms converge to 0. As a consequence, $(\widetilde{X}^k)_{k\in\mathbb{N}}$ weakly converges to 0 in $H^1(0,T;\mathbb{R}^3)$. From Sobolev embedding $H^1(0,T;\mathbb{R}) \to \mathcal{C}(0,T;\mathbb{R})$ applied to the components of $\widetilde{X}^k$, we have

$$d_k := \sup_{t\in[0,T]}\left\|\exp\left(-tB\right)\widetilde{X}^k(t)\right\|_2 \to 0 \qquad (21)$$

On the other hand, we can estimate the second integral of $W^k(t)$ in (18) by

$$\begin{aligned}&\left\|\int_0^t \exp\left((t-s)B\right)C(u^k(s))W^k(s)ds\right\|_2\\ &\leq \mu\int_0^t \left\|C(u^k(s))W^k(s)\right\|_2 ds\\ &\leq \sqrt{T}\kappa\mu\|u^k\|_{L^2_{T_c}(0,T;\mathbb{R}^2)}\int_0^t \left\|W^k(s)\right\|_2 ds,\end{aligned}$$

where κ and μ has been introduced in (7) and (9), respectively. Summarizing these results, we get:

$$\|W^k(t)\|_2 \leq d_k + \sqrt{T}\kappa\|u^k\|_{L^2_{T_c}(0,T;\mathbb{R}^2)}\int_0^t \|W^k(s)\|_2 ds.$$

Since $W^k(0) = 0$, Gronwall's inequality then gives $\forall t \in [0,T]$

$$\|W^k(t)\|_2 \leq d_k \exp(T^{\frac{3}{2}}\kappa\|u^k\|_{L^2_{T_c}(0,T;\mathbb{R}^2)}).$$

It follows from (21) that there exists k_2, such that for all $k \geq k_2$, $\|\varphi(X_0^\infty,u^\infty) - \varphi(X_0^\infty,u^k)\|_2 \leq \frac{\eta}{2}$. This leads to obtain

$$\|X^\infty(t) - X^k(t)\|_2 \leq \eta.$$

Hence the result. ■

We can now prove the existence of solution of (17).

Theorem 4: There exists a solution $u \in L^2_{T_c}(0,T;\mathbb{R}^2)$ of Problem (17).

Proof: Let still denote by $(u^k)_{k\in\mathbb{N}}$ and $(X^k)_{k\in\mathbb{N}}$ the sequences introduced in Section III-A. Because of Theorem 3, $\lim_{k\to\infty} X^k(T_c) = X^\infty(T_c)$. We have

$$\begin{aligned} F(u^\infty) =& \langle X^\infty(T_c)|O|X^\infty(T_c)\rangle - \alpha\|u^\infty\|^2_{L^2_{T_c}(0,T;\mathbb{R}^2)}, \\ \geq& \lim_{k\to\infty} \langle X^k(T_c)|O|X^k(T_c)\rangle \\ &- \alpha \limsup_{k\to\infty} \|u^k\|^2_{L^2_{T_c}(0,T;\mathbb{R}^2)} \\ =& \limsup_{k\to\infty} F(u^k), \end{aligned}$$

where we have used the lower-semicontinuity of the L^2-norm. Since $(u^k)_{k\in\mathbb{N}}$ is a maximizing sequence, we have proved that u^∞ is a solution of (17). The result follows. ■

C. Optimality system

We finally characterize an optimum by means of an optimality system. The corresponding Euler-Lagrange equations are given in the next theorem.

Theorem 5: Let u be a solution of Problem (17), and $X \in H^1_{per}(0,T;\mathbb{R}^3)$ the corresponding solution of (12). Then, there exists $Y \in L^2(0,T;\mathbb{R}^3)$ and continuous everywhere except T_c such that:

$$\begin{cases} \dot{X}(t) = & A(u(t))\,X(t) \,+\, D \\ \dot{Y}(t) = & -A^\intercal(u(t))\,Y(t) \\ Y(T_c^+) = & Y(T_c^-) - 2OX(T_c) \\ Y(t)^\intercal \partial_{u(t)} A(u(t))X(t) = & 2\alpha u(t). \end{cases} \quad (22)$$

Proof: We start by introducing $K : H^1_{per}(0,T;\mathbb{R}^3) \times L^2_{T_c}(0,T;\mathbb{R}^2) \to L^2(0,T;\mathbb{R}^3)$ is defined by:

$$(X,u) \mapsto A(u(.))X(.) + D - \dot{X}(.),$$

so that $K(X,u) = 0$ is equivalent to (12). Let us show that F and K are Fréchet-differentiable and the linearization $\nabla K(v)$ is surjective [27] for every $v = (X,u) \in H^1_{per}(0,T;\mathbb{R}^3)\times L^2_{T_c}(0,T;\mathbb{R}^2)$. First, let recall that $H^1(0,T;\mathbb{R}^3)$ is continuously embedded into $\mathcal{C}(0,T;\mathbb{R}^3)$ so that there exists an embedding constant $c_1 > 0$ satisfying:

$$\|\phi\|_{L^\infty(0,T;\mathbb{R}^3)} \leq c_1 \|\phi\|_{H^1_{per}(0,T;\mathbb{R}^3)}.$$

Let $v = (X,u)$ and $h_v = (h_X,h_u)$ belong to $H^1_{per}(0,T;\mathbb{R}^3) \times L^2_{T_c}(0,T;\mathbb{R}^2)$. We start by the function F. Note that

$$\begin{aligned} F(v{+}h_v){-}F(v){-}2\langle X(T_c)|O|h_X(T_c)\rangle{-}2\alpha\langle u,h_u\rangle_{L^2(0,T;\mathbb{R}^2)} \\ = \langle h_X(T_c)|O|h_X(T_c)\rangle - \alpha\|h_u\|^2_{L^2_{T_c}(0,T;\mathbb{R}^2)}, \end{aligned}$$

which leads to

$$\begin{aligned} |F(v{+}h_v){-}F(v){-}2\langle X(T_c)|O|h_X(T_c)\rangle{-}2\alpha\langle u,h_u\rangle_{L^2(0,T;\mathbb{R}^2)}| \\ \leq \lambda_O \|h_X(T_c)\|_2^2 + \alpha\|h_u\|^2_{L^2_{T_c}(0,T;\mathbb{R}^2)} \\ \leq \lambda_O c_1 \|h_X\|^2_{H^1_{per}(0,T;\mathbb{R}^3)} + \alpha\|h_u\|^2_{L^2_{T_c}(0,T;\mathbb{R}^2)} \\ \leq c_2\left(\|h_X\|^2_{H^1_{per}(0,T;\mathbb{R}^3)} + \|h_u\|^2_{L^2_{T_c}(0,T;\mathbb{R}^2)}\right) \\ = c_2\|h_v\|^2_{H^1_{per}(0,T;\mathbb{R}^3)\times L^2_{T_c}(0,T;\mathbb{R}^2)} \to 0, \end{aligned}$$

where $c_2 = \lambda_O c_1 + \alpha$. Thus, F is Fréchet-differentiable and its Fréchet-derivative $\nabla F(v)$ is:

$$\nabla F(v)(h_v) = 2\langle X(T_c)|O|h_X(T_c)\rangle - 2\alpha\langle u, h_u\rangle_{L^2(0,T;\mathbb{R}^2)}$$

Similarly, we prove that the Fréchet-derivative of the function K satisfies

$$\nabla K(v)(h_v) = A(u(.))h_X(.) + A(h_u(.))X(.) - \dot{h}_X(.).$$

We now prove the surjectivity of the function $\nabla K(v)$ for every $v = (X,u) \in H^1_{per}(0,T;\mathbb{R}^3)\times L^2_{T_c}(0,T;\mathbb{R}^2)$. Let $g \in L^2(0,T;\mathbb{R}^3)$ be arbitrary. Then, $\nabla K(X,u)(h_X,h_u) = g$ is equivalent to:

$$\dot{h}_X = A(u(.))h_X + A(h_u(.))X - g.$$

Using Remark 1 and Corollary 1, we see that there exists $h_X \in H^1_{per}(0,T;\mathbb{R}^3)$ satisfying the latter equation with $h_u = 0$. As a consequence, $\nabla K(v)$ is surjective.

We have assumed that u is a solution of (17) and $X \in H^1_{per}(0,T;\mathbb{R}^3)$ satisfies (12). Finally, thanks to the surjectivity (see [27], Section 1.3) of $\nabla K(X,u)$ there exists an adjoint vector $Y \in L^2(0,T;\mathbb{R}^3)$ such that for δX in $H^1_{per}(0,T;\mathbb{R}^3)$, we get the usual Karush-Kuhn-Tucker condition:

$$\nabla F(u)(\delta X, 0) = \int_0^T \langle Y(t), \nabla K(X,u)(\delta X, 0)\rangle$$

meaning that

$$\begin{aligned} \int_0^T \langle Y(t),\, \delta\dot{X}(t)\rangle\, dt =& 2\langle X(T_c)|O|\delta X(T_c)\rangle \\ &+ \int_0^T \langle A(u(t))^\intercal Y(t),\, \delta X(t)\rangle\, dt. \end{aligned}$$

Consider now a function ϕ such that $\dot{\phi}(t) = -A(u(t))^\intercal Y(t)$ and $\phi(T_c^-) - \phi(T_c^+) = 2OX(T_c)$. By integrating $\langle\phi(t),\, \delta\dot{X}(t)\rangle$ on the interval $[T_c^+,\, T_c^-]$ (in the periodic sense), we obtain

$$\begin{aligned} \int_{T_c^+}^{T_c^-} \langle \phi(t),\, \delta\dot{X}(t)\rangle\, dt = \langle \phi(T_c^-) - \phi(T_c^+)), \delta X(T_c)\rangle \\ - \int_{T_c^+}^{T_c^-} \langle \dot{\phi}(t),\, \delta X(t)\rangle\, dt. \end{aligned}$$

by identification, we conclude that $Y = \phi$. Hence the equation on Y. ■

IV. NUMERICAL RESULTS

We finally investigate here some results about the L^2-norm of optimal field for different values of penalty parameter α and time T_c, respectively. For the numerical solving of the evolution equation in X we use a Crank-Nicholson time-discretization scheme, with 50 steps in $[0, T_c]$. To compute the optimal controls u, we apply the gradient method described in [20]. The values of the parameters we consider are also taken from the latter. The implementation is carried out with Octave [28].

First test : We consider a range of values α in the interval $[10^{-2}, 4]$ and we solve iteratively the optimization problem for increasing values of α; the previous optimal field is used as a guess field to initialize the next optimization. Figure 2 (left) shows that the L^2-norm of the optimal control field decrease with α. We observe a polynomial convergence of the norm of the control with respect to α, more precisely, we find that $\|u\|_{L^2(0,T;\mathbb{R}^2)} = \frac{a}{\alpha}$ asymptotically for some $a > 0$.

Second test : We consider the same procedure as in the previous test, and solve the optimization problem for various values of T_c. More precisely, we consider values of T_c in the interval $[10^{-4}, 10^{-2}]$. Figure 2 (right) shows that the norm of control field increases with T_c. We observe a relation of the form:

$$\log(\|u\|_{L^2(0,T;\mathbb{R}^2)}) = a\log(T_c) + b,$$

where the coefficients a and b can be determined with the blue line. In this test, we observe that $a \approx 0.5$.

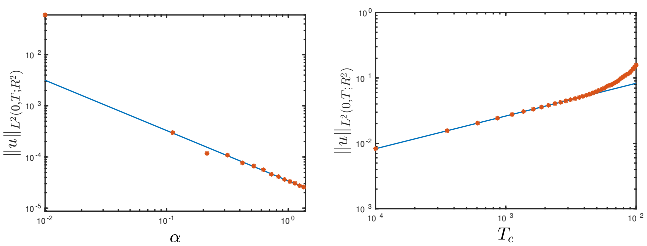

Fig. 2. Evolution of the $\|u\|_{L^2(0,T;\mathbb{R}^2)}$ (Red), for $\omega = 0$, $\Gamma = 1.8$ and $\gamma = 1$, with respect to α (Left, $T_c = 10^{-2}$ and $T = 1 + T_c$). and to T_c (Right, $\alpha = 10^{-5}$ and $T = 1 + T_c$).

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