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OPTIMAL CONTROL OF A SEMILINEAR PARABOLIC EQUATION WITH SINGULAR ARCS

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Abstract. This paper develops a theory of singular arc, and the corresponding second order necessary and sufficient conditions, for the optimal control of a semilinear parabolic equation with scalar control applied on the r.h.s. We obtain in particular an extension of Kelley's condition, and the characterization of a quadratic growth property for a weak norm.

Keywords parabolic equation, optimal control, singular arc, second order optimality conditions, characterization of quadratic growth.

1. Introduction

We consider in this paper an optimal control problem of a parabolic equation with a bound constrained scalar control, in which the state equation and integrand of cost function are affine functions of the control. Such *control affine problems* have been extensively studied in the ODE setting. Concerning second order optimality conditions which are the subject of the paper, in the totally singular case (the control is out of bounds at any time), the key results are the extended Legendre condition due to Kelley [20], and the Goh transform [18] allowing to obtain second order necessary conditions involving the primitive of the control rather than the control itself. Dmitruk [14] derived sufficient conditions for weak optimality, and in [15, 16] obtained necessary or sufficient optimality conditions in the case of a non unique multiplier. In the singular-bang setting, Poggiolini and Stefani [25] obtained second-order sufficient conditions for the strong local optimality in minimum time problem, and Aronna et al. [1, 2] obtained second-order necessary conditions and some sufficient conditions without uniqueness of the multiplier, and the local well-posedness of a shooting algorithm.

There are very few papers on the optimal control of PDEs for control affine systems. When the control is distributed, if the control is out of bounds on some open set, it is sometimes possible to give an explicit expression of the control: this is the theory of generalized bang-bang control, see Bergounioux and Tiba [3], Tröltzsch [27], Bonnans and Tiba [8].

In the elliptic case, Casas [10] considered the case of a distributed control and obtained second order sufficient conditions. While this technique is quite specific since time does not appear, these sufficients conditions are in the spirit of those obtained in Goh's theory, since they involve an Hilbert norm that is weaker than the L^2 norm of the control. Casas, Herzog and Wachsmuth [11] consider the case of an L^1 cost function, which may be viewed as an control affine problem if we take as new control the positive and negative parts of the original control. Casas, Clason

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and Kunisch [12] study related problems in the setting of a parabolic equation. See also the recent paper discussing several models [24], and the PhD dissertation [26].

Therefore there exists presently no analogous of the Goh theory in the setting of control of parabolic equations; our goal is to set some first steps in this direction. The paper is organized as follows. We present the problem, and derive the second order necessary conditions in Goh's form in section 2. Then we derive the second order sufficient conditions, that characterize quadratic growth in a weak norm, in section 3. Some numerical experiments, that give an experimental argument in favor of the existence of singular arcs for optimal control problems of parabolic equations, are presented in section 4. We conclude in section 5 by discussing some open problems and possible extensions.

2. Setting and classical results

2.1. **Setting.** Let Ω be a smooth open subset of $\mathbb{R}^n$, with $n \leq 3$. Set $Q := \Omega \times (0,T)$. We recall that, for $\mu \in [1,\infty]$ and $p \in \mathbb{N}$, $p \geq 1$, $W^{p,\mu}(\Omega)$ denotes the Sobolev space of functions in $L^\mu(\Omega)$ with derivatives up to order p (taken in the distribution sense) in $L^\mu(\Omega)$. We denote the closure of $\mathcal{D}(\Omega)$ (set of C^∞ functions over Ω with compact support) in $W^{p,\mu}(\Omega)$ by $W_0^{p,\mu}(\Omega)$, and set $H^p(\Omega) := W^{p,2}(\Omega)$ and $H_0^p(\Omega) := W_0^{p,2}(\Omega)$. Similarly, $W^{2,1,\mu}(Q)$ denotes the Sobolev space of function in $L^\mu(Q)$ whose second derivative in space and first derivative in time belong to $L^\mu(Q)$, and $H^{2,1}(Q) := W^{2,1,2}(Q)$. Set also $\Sigma := \partial\Omega \times (0,T)$, and

$$W_\Sigma^{2,1,\mu}(Q) := \{y \in W^{2,1,\mu}(Q); \quad y = 0 \text{ on } \Sigma\}. \tag{1}$$

The critical value

$$\mu_c := \tfrac{1}{2}(n+2) \tag{2}$$

is such that, see [21, Rem. 2.5, p. 21]:

$$W^{2,1,\mu}(Q) \subset L^\infty(Q), \text{ for all } \mu > \mu_c. \tag{3}$$

Fix $\gamma \geq 0$ and $T > 0$. We assume that

$$\text{(i) } y_0 \in W_0^{1,\infty}(\Omega); \quad \text{(ii) } B \in W_0^{2,\infty}(\Omega). \tag{4}$$

We consider the following semilinear parabolic controlled equation, close to those discussed in [21]:

$$\begin{cases} \dot{y}(x,t) - \Delta y(x,t) + \gamma y^3(x,t) = u(t)B(x) \quad \text{in } Q := \Omega \times [0,T], \\ y = 0 \text{ on } \Sigma; \quad y(\cdot,0) = y_0. \end{cases} \tag{5}$$

This is a prototype of a semilinear equation; taking the explicit nonlinearity y^3 allows to simplify the analysis of the nonlinearity and to concentrate on the essential features. Indeed, in the case when $\gamma = 0$, although the problem is convex, our characterization of quadratic growth is still of interest.

Consider the cost function

$$J(u,y) = \tfrac{1}{2}\int_Q (y(x,t) - y_d(x,t))^2 \mathrm{d}x\mathrm{d}t + \alpha \int_0^T u(t)\mathrm{d}t.$$

Here $\alpha \in \mathbb{R}$, the *desired state* y_d belongs to $L^{\bar\mu}(Q)$, for some $\bar\mu$ such that

$$\bar\mu > \mu_c. \tag{6}$$

We have control bounds

$$a \leq u(t) \leq b, \quad \text{for all } t \in (0,T), \tag{7}$$

for some real numbers $a < b$. The optimal control problem is therefore (we will be more precise on the functional framework later):

$$\underset{u,y}{\mathrm{Min}}\, J(u,y) \text{ s.t. } \quad (5) \text{ and } (7). \tag{P}$$

The well-posedness of the state equation can be deduced from the following result, in which we consider a more general r.h.s.:

$$\left\{ \begin{array}{l} \dot{y}(x,t) - \Delta y(x,t) + \gamma y^3(x,t) = f(x,t) \quad \text{in } Q := \Omega \times [0,T] \\ y = 0 \text{ on } \Sigma; \quad y(\cdot,0) = y_0. \end{array} \right. \tag{8}$$

Proposition 2.1. *Let $f \in L^\infty(Q)$ and $y_0 \in W_0^{1,\infty}$. Then* (8) *has a unique solution $y[[f]]$ in $W^{2,1,q}(Q)$ for all $q \in (2,\infty)$, and the mapping $f \mapsto y[[f]]$ is of class C^∞ from $L^\infty(Q)$ into $W^{2,1,q}(Q)$.*

Proof. We just give a sketch of the argument; see also e.g. [5, 21]. One classically obtains an priori estimate in $L^\infty(0,T,L^2(\Omega) \cap L^2(0,T,H_0^1(\Omega))$ by multiplying (8) by $y(x,t)$ and integrating over Q. More generally, for $q \in (2,\infty)$, with conjugate number q' such that $1/q + 1/q' = 1$, combining Hölder inequality and Young's inequality $ab \le a^{q'}/q' + b^q/q$, for any nonnegative a and b, we get

$$\int_\Omega |f||y|^{q-1} \le \|f\|_q \| |y|^{q-1} \|_{q'} = \|f\|_q \| \|y\|_q^{q/q'} \le \frac{1}{q}\|f(t)\|_q^q + \frac{1}{q'}\|y\|_q^q. \tag{9}$$

Multiplying (8) by $|y(x,t)|^{q-2} y(x,t)$, and integrating over Q, it follows that

$$\frac{1}{q}\frac{\mathrm{d}}{\mathrm{d}t}\|y\|_q^q + \gamma \int_\Omega |y|^{q+2} \le \frac{1}{q}\|f(t)\|_q^q + \frac{1}{q'}\|y\|_q^q. \tag{10}$$

Since $\|f(t)\|_q^q \in L^1(0,T)$, with Gronwall's lemma, this gives an a priori estimate of y in $L^\infty(0,T,L^q(\Omega))$. Taking $q = 3\bar{\mu}$, it follows that $y^3 \in L^{\bar{\mu}}(Q)$ and so $\dot{y} - \Delta y \in L^{\bar{\mu}}(Q)$ too. By the standard estimates for linear equations, we deduce that $y[[f]]$ belongs to $W^{2,1,\bar{\mu}}(Q)$, and so by (3), $y[[f]] \in L^\infty(Q)$. The existence is obtained by standard Galerkin type arguments.

The conclusion follows, in the spirit of [4], by applying the Implicit Function Theorem to the mapping $F : W_\Sigma^{2,1,q}(Q) \times L^\infty(Q) \to L^q(Q) \times W_0^{1,q}(\Omega)$,

$$F(y,f) := (\dot{y} - \Delta y + \gamma y^3 - f, y(\cdot,0) - y_0), \tag{11}$$

with $q > \mu_c$ so that $W_\Sigma^{2,1,q}(Q) \subset L^\infty(Q)$. This mapping is obviously of class C^∞. That its partial derivative w.r.t. y is an isomorphism is equivalent to check that, for any $(f,g) \in L^q(Q) \times W_0^{1,q}(\Omega)$, the linearized state equation below has a unique solution $z \in W_\Sigma^{2,1,q}(Q)$:

$$\left\{ \begin{array}{l} \dot{z} - \Delta z + 3\gamma y^2 z = f \quad \text{in } Q, \\ z = 0 \text{ on } \Sigma; \quad z(\cdot,0) = g. \end{array} \right. \tag{12}$$

Since $y \in L^\infty(Q)$ this is easily checked. □

A composition of C^∞ mappings being of class C^∞, we obtain that

Corollary 2.2. *With each $u \in L^\infty(0,T)$ is associated a unique state $y[u] \in W^{2,1,q}(Q)$, for all $q \in [2,\infty)$, and the mapping $u \mapsto y[u]$ is of class C^∞.*

Theorem 2.3. *The problem (P) has a nonempty set of solutions. If $\gamma = 0$, then the solution is unique.*

Proof. The existence is obtained by standard arguments based on minimizing sequences, passing to the limit on the nonlinearity of the state equation, see e.g. [5, 21]. If $\gamma = 0$ since the cost function is strictly convexity w.r.t. the state, the optimal state is unique, and then so is the optimal control. □

In the sequel we denote by $(\bar{u}, \bar{y})$ a solution of (P).

2.2. **First order optimality system.** The costate equation is

$$
\left\{\begin{array}{l} -\dot{\bar{p}} - \Delta \bar{p} + 3\gamma \bar{y}^2 \bar{p} = y - y_d \quad \text{in } Q \\ \bar{p} = 0 \text{ on } \Sigma; \quad \bar{p}(\cdot, T) = 0. \end{array}\right. \tag{13}
$$

Since $\bar{y} \in L^\infty(Q)$, and $y_d \in L^{\bar{\mu}}(Q)$, this equation has a unique solution $\bar{p} \in W^{2,1,\bar{\mu}}(Q) \subset L^\infty(Q)$. We denote by $F(u) := J(u, y[u])$ the cost viewed as function of the control only. This is a function of class C^∞ over $L^\infty(0,T)$. In the context of control affine problems, it is customary to call *switching function* the following amount in $L^\infty(0,T)$:

$$
\Psi(t) := \alpha + \int_\Omega B(x)\bar{p}(x,t)\mathrm{d}x. \tag{14}
$$

The linearized state equation is

$$
\left\{\begin{array}{l} \dot{z} - \Delta z + 3\gamma \bar{y}^2 z = v(t)B(x) \quad \text{in } Q, \\ z = 0 \text{ on } \Sigma; \quad z(\cdot, 0) = 0. \end{array}\right. \tag{15}
$$

For $v \in L^2(Q)$, it has a unique solution $z[v] \in H^{2,1}(Q)$. The following result is classical.

Lemma 2.4. *The switching function coincides with the derivative of F, in the sense that*

$$
DF(\bar{u})v = \int_0^T \Psi(t)v(t)\mathrm{d}t, \quad \textit{for all } v \in L^\infty(0,T). \tag{16}
$$

Proof. Let $z = z[v]$ denote the solution of the linearized state equation (15). By the chain rule, we have that using the integration by parts formula

$$
\begin{aligned}
DF(u)v &= \int_Q (y - y_d) z \mathrm{d}x\mathrm{d}t + \alpha \int_0^T v(t)\mathrm{d}t \\
&= \int_Q (-\dot{\bar{p}} - \Delta \bar{p} + 3\gamma \bar{y}^2 \bar{p})) z(x,t) \mathrm{d}x\mathrm{d}t + \alpha \int_0^T v(t)\mathrm{d}t \\
&= \int_Q \bar{p}(\dot{z} - \Delta z + 3\gamma \bar{y}^2 z) \mathrm{d}x\mathrm{d}t + \alpha \int_0^T v(t)\mathrm{d}t \\
&= \int_Q \bar{p}(x,t)B(x)v(t) \mathrm{d}x\mathrm{d}t + \alpha \int_0^T v(t)\mathrm{d}t.
\end{aligned} \tag{17}
$$

The conclusion follows. □

Denote the *contact set* (for the control constraints) by $I(\bar{u}) = I_a(\bar{u}) \cup I_b(\bar{u})$, where

$$
I_a(\bar{u}) := \{t \in (0,T);\; u(t) = a\}; \quad I_b(\bar{u}) := \{t \in (0,T);\; u(t) = b\}. \tag{18}
$$

These sets are defined up to a null measure set. The (classical) *first order optimality conditions* are as follows:

Proposition 2.5. *We have that up to a null measure set:*

$$
\{t; \Psi(t) > 0\} \subset I_a(\bar{u}); \quad \{t; \Psi(t) < 0\} \subset I_b(\bar{u}). \tag{19}
$$

Set

$$
\mathcal{U}_{a,b} := \{u \in L^\infty(0,T); \quad a \le u(t) \le b, \ \text{a.e.}\}.
$$

Proof. The differentiable function F attains its minimum over the convex set $\mathcal{U}_{a,b}$ at $\bar{u}$, and hence

$$
0 \le \lim_{\sigma \downarrow 0} \frac{F(\bar{u} + \sigma(v - \bar{u})) - F(\bar{u})}{\sigma} = DF(\bar{u})(v - \bar{u}). \tag{20}
$$

Since $DF(\bar{u})(v - \bar{u}) = \int_0^T \Psi(t)(v(t) - \bar{u}(t)\mathrm{d}t$, the conclusion follows easily. □

We next need to analyze the first and second derivative of the switching function. The switching function has a derivative in $L^2(0,T)$, and since $B \in W_0^{2,\infty}(\Omega)$, we have that

(21)
$$\left\{\begin{array}{ll} \dot\Psi(t) & := -\displaystyle\int_\Omega B(x)\Delta\bar p(x,t)\mathrm{d}x + \int_\Omega B(x)(3\gamma\bar y^2(x,t)\bar p(x,t) - \bar y(x,t) + y_d(x,t))\mathrm{d}x \\ & = -\displaystyle\int_\Omega \bar p(x,t)\Delta B(x)\mathrm{d}x + \int_\Omega B(x)(3\gamma\bar y^2(x,t)\bar p(x,t) - \bar y(x,t) + y_d(x,t))\mathrm{d}x. \end{array}\right.$$

As expected from the theory of control affine problems in the case of ODEs, the derivative of the switching function does not depend on the control. Set

$$\left\{\begin{array}{lll} \kappa(x,t) & := 1 - 6\gamma\bar p(x,t)\bar y(x,t), & (x,t)\in Q; \\ R(t) & := \displaystyle\int_\Omega \kappa(x,t)B(x)^2\mathrm{d}x. & \end{array}\right. \tag{22}$$

Obviously, $\kappa(x,t)$ and $R(t)$ are essentially bounded. By (21), if y_d is smooth enough, Ψ has a second derivative in $L^2(0,T)$. The latter is necessarily an affine function of the control, and it is easily checked that the following holds:

$$R(t) := -\frac{\partial\ddot\Psi(t)}{\partial u}. \tag{23}$$

In view of Kelley's result in [20], and of its extension to the case of control constraints in [1], we may expect that $R(t) \geq 0$ if the control constraints are not active near time t. We will indeed prove this, see remark 2.12.

2.3. **Standard second order expansion of the cost.** In the sequel we denote

$$\varphi(y) := \gamma y^3. \tag{24}$$

With problem (P) is associated the *Lagrangian function*

$$J(u,y) + \int_Q p(x,t)(\Delta y - \varphi(y) + uB - \dot y)\mathrm{d}x\mathrm{d}t + \int_\omega \hat p(x)(y(x,0) - y_0(x))\mathrm{d}x. \tag{25}$$

Let us consider the quadratic form corresponding to the Hessian of the Lagrangian, where κ was defined in (22):

$$\tilde Q(z) := \int_Q \kappa(x,t)z(x,t)^2\mathrm{d}t. \tag{26}$$

This is a continuous quadratic form over $L^2(Q)$. We denote by $F(P)$ the set of feasible control for problem (P), i.e., those that satisfy the control bounds.

Lemma 2.6. *If $\bar u + v \in F(P)$, then the following expansions holds:*

$$F(\bar u + v) = F(\bar u) + \int_0^T \Psi(t)v(t)\mathrm{d}t + \tfrac{1}{2}\tilde Q(\delta y) + O\left(\|\delta y\|_3^3\right). \tag{27}$$

Proof. Let $y = \bar y + \delta y$ be the state associated with the control $\bar u + v$. Indeed, we have that

$$J(\bar u + v, \bar y + \delta y) = J(\bar u, \bar y) + \int_O^T \left(\alpha v + (\bar y - y_d)\delta y + (\delta y)^2\right), \tag{28}$$

and since $\bar u + v \in F(P)$, the state y remains in a compact set, so that

$$\varphi(\bar y + \delta y) = \varphi(\bar y) + \varphi'(\bar y)\delta y + \tfrac{1}{2}\varphi''(\bar y)(\delta y)^2 + O(|\delta y|^3). \tag{29}$$

Multiplying the costate by the difference of state equations with the pairs (u, y) and $(\bar{u}, \bar{y})$, we get

(30)
$$\left\{\begin{array}{rcl} 0 & = & \int_Q \bar{p}\left(\Delta\delta y - \varphi(y) + \varphi(\bar{y}) + vB - \dot{\delta y}\right) \\ & = & \int_Q (\dot{\bar{p}} + \Delta\bar{p} - \varphi'(\bar{y})\bar{p})\,\delta y + \int_Q \left(\bar{p}vB - \frac{1}{2}\bar{p}\varphi''(\bar{y})(\delta y)^2\right) + O(\|\bar{p}\delta y\|_\infty^3) \\ & = & -\int_Q (\bar{y} - y_d)\delta y + \int_Q \left(\bar{p}vB - \frac{1}{2}\bar{p}\varphi''(\bar{y})(\delta y)^2\right) + O(\|\bar{p}\delta y\|_\infty^3) \end{array}\right.$$

Adding with (28), and using $\bar{p} \in L^\infty(Q)$ and (22), we prove our claim (27).

□

Corollary 2.7. *We have that*

$$F(\bar{u} + v) = F(\bar{u}) + \int_0^T \Psi(t)v(t)\mathrm{d}t + \tfrac{1}{2}\tilde{Q}(z) + O(\|v\|_\infty^3). \tag{31}$$

Proof. Let $q > \mu_c$. We have seen in the proof of proposition 2.1 that we can apply the Implicit Function Theorem to the state equation, so that $u \mapsto y[u]$, and consequently $F(u)$. is a function of class C^∞ over L^∞. It follows that

$$\|y[\bar{u} + v] - y[ub] - z[v]\|_2 = O(\|v\|_\infty^2) \tag{32}$$

where $z[v]$ denotes the solution of the linearized equation (12), so that, using the definition (26) of $\tilde{Q}$:

$$\left|\tilde{Q}(\delta y) - \tilde{Q}(z)\right| \leq \|\kappa\|_\infty \|\delta y + z\|_2 \|\delta y - z\|_2 = O(\|v\|_\infty^3). \tag{33}$$

Since also $\|\delta y\|_\infty = O(\|v\|_\infty)$, the conclusion follows. □

2.4. **Classical second order necessary conditions.** We recall that the linearized state equation and its solution denoted by $z[v]$ were defined in (15). The *critical cone* $C(\bar{u})$ is defined as

$$C(\bar{u}) = \{v \in L^\infty(0, T);\ \Psi(t)v(t) = 0, \text{ a.e.};\ v \geq 0 \text{ on } I_a(\bar{u});\ v \leq 0 \text{ on } I_b(\bar{u})\}, \tag{34}$$

where the above equality and inequalities should be understood a.e. The following quadratic form (where $\kappa \in L^\infty(Q)$ has been defined in (22)) is obviously well-defined and continuous over $L^2(\Omega)$:

$$Q(v) := \int_Q \kappa(x,t) z(x,t)^2 \mathrm{d}t. \tag{35}$$

Theorem 2.8. *We have that*

$$Q(v) \geq 0 \quad \textit{for all } v \in C(\bar{u}). \tag{36}$$

Proof. While this follows from general results on polyhedricity [19, 23] and [7, Section 6.3], we give a short direct proof. Let $v \neq 0$ be a critical direction. For $\varepsilon > 0$, set

$$v_\varepsilon(t) := \left\{\begin{array}{l} v(t) \text{ if } \bar{u}(t) \in (a + \varepsilon, b - \varepsilon), \\ 0 \text{ otherwise.} \end{array}\right. \tag{37}$$

Then $\bar{u} + \sigma v_\varepsilon \in \mathcal{U}_{a,b}$, whenever $0 < \sigma \leq \varepsilon / \|v\|_\infty$, and v_ε is critical so that $DF(\bar{u})v_\varepsilon = \int_0^T \Psi(t)v_\varepsilon(t)\mathrm{d}t = 0$. Setting $z_\varepsilon = z[v_\varepsilon]$, we deduce from corollary 2.7 that

$$0 \leq 2 \liminf_{\sigma \downarrow 0} \frac{F(\bar{u} + \sigma v_\varepsilon) - F(\bar{u})}{\sigma^2} = \tilde{Q}(z_\varepsilon). \tag{38}$$

When $\varepsilon \downarrow 0$, $z_\varepsilon \to z[v]$ in $L^2(Q)$, and since $\tilde{Q}$ is a continuous quadratic form over $L^2(Q)$, the conclusion follows.

□

2.5. **Goh transform.** We next extend the Goh transform theory [18] to the present setting as follows. Define the new "control" and "linearized state" resp. by

$$w(t) := \int_0^t v(t)\mathrm{d}t; \quad \xi(x,t) := z(x,t) - w(t)B(x). \tag{39}$$

We have that $\dot{\xi} = \dot{z} - uB = \Delta z - \varphi'(\bar{y})z$, and so ξ is solution of

$$\begin{cases} \dot{\xi}(x,t) - \Delta\xi(x,t) + \varphi'(\bar{y}(x,t))\xi(x,t) = w(t)\Delta B(x) - w(t)\varphi'(\bar{y}(x,t))B(x) \quad \text{in } \Omega, \\ \xi = 0 \text{ on } \Sigma; \quad \xi(\cdot,0) = 0. \end{cases} \tag{40}$$

Since $\varphi'(\bar{y}) \in L^\infty(Q)$, (40) has a unique solution $\xi[w] \in W^{2,1,s}(Q)$ whenever w belongs to $L^s(0,T)$, with $s \in [2,\infty)$. We define the set of *primitives of critical directions* with value 0 at time 0 as

$$PC(\bar{u}) := \{w \in W^{1,\infty}(0,T); \quad \dot{w} \in C(\bar{u}); \quad w(0) = 0\}. \tag{41}$$

Denote by $PC_2(\bar{u})$ the closure of $PC(\bar{u})$ in $L^2(0,T)$, and set

$$\hat{Q}(w) = \int_Q \kappa(x,t)(\xi[w](x,t) + w(t)B(x))^2\mathrm{d}t. \tag{42}$$

This quadratic form has a continuous extension over $L^2(0,T)$.

Lemma 2.9. *We have that $\hat{Q}(w) \geq 0$, for all $w \in PC_2(\bar{u})$.*

Proof. Let $w \in PC(\bar{u})$ with derivative $v \in C(\bar{u})$. By theorem 2.8, $Q(v) \geq 0$, and since $Q(v) = \tilde{Q}(z) = \tilde{Q}(\xi + wB) = \hat{Q}(w)$, we have that $\hat{Q}(w) \geq 0$, so that $\hat{Q}$ is nonnegative over $PC(\bar{u})$. Since $\hat{Q}$ is continuous over $L^2(0,T)$, the conclusion follows. □

Definition 2.10. Let t_1, t_2 belong to $[0,T]$ with $t_1 < t_2$. We say that (t_1,t_2) is a *singular arc* if, for all $\theta > 0$ small enough, there exists $\varepsilon > 0$ such that $\bar{u}(t) \in [a+\varepsilon, b-\varepsilon]$ for a.a. $t \in (t_1+\theta, t_2-\theta)$, a *lower bound arc* if $\bar{u}(t) = a$ for a.a. $t \in (t_1,t_2)$, and an *upper bound arc* if $\bar{u}(t) = b$ for a.a. $t \in (t_1,t_2)$. Lower and upper bound arcs are called boundary arcs.

Corollary 2.11. *Let (t_1,t_2) be a singular arc. Then*

$$R(t) \geq 0, \quad t \in (t_1,t_2). \tag{43}$$

Proof. Consider the problem of minimizing the quadratic form $\hat{Q}$ over the set

$$PC_2'(\bar{u}) = \{w \in L^2(0,T); \quad w(t) = 0, \ \ t \in (0,T) \setminus (t_1,t_2)\}. \tag{44}$$

Since $PC_2'(\bar{u}) \subset PC_2(\bar{u})$, by lemma 2.9, $\bar{w} = 0$ is solution of this problem. By the Legendre condition for this problem (itself a consequence of Pontryagin's principle [9]), we deduce that the conclusion holds. □

Remark 2.12. As in the finite dimensional setting we have recovered the Kelley condition [20]: when the control constraint is not active, (23) is nonnegative.

2.6. **Geometrical hypotheses.** We will next characterize $PC_2(\bar{u})$ under the following assumptions. This will be useful for the characterization of quadratic growth obtained in the next section. By *maximal arcs* we mean an arc that is not stricly included in another arc. Consider the hypotheses of *finite structure*:

$$\begin{cases} \text{There are finitely many boundary and singular maximal arcs} \\ \text{and the closure of their union is } [0,T], \end{cases} \tag{45}$$

and of *strict complementarity*:

$$\Psi \text{ has a.e. nonzero values over each boundary arc.} \tag{46}$$

Since these hypotheses hold in the sequel, by "arc" we will now mean "maximal arcs", and we then redefine "punctually" the contact sets $I_a(\bar{u})$ and $I_b(\bar{u})$ as

$$I_a(\bar{u}) = \{t \in [0,T];\ \Psi(t) > 0\}; \quad I_b(\bar{u}) = \{t \in [0,T];\ \Psi(t) < 0\}. \tag{47}$$

We say that the boundary arc (c,d) is *initial* if $c = 0$, and *final* if $d = T$.

Lemma 2.13. *If* (45)-(46) *holds, then*

$$PC_2(\bar{u}) = \left\{ \begin{array}{l} w \in L^2(0,T);\ w \textit{ is constant over boundary arcs} \\ \textit{and } w = 0 \textit{ over an initial boundary arc} \end{array} \right\}. \tag{48}$$

Proof. By the strict complementarity hypothesis (46), every $v \in C(\bar{u})$ has zero values over boundary arcs, and so every $w \in PC(\bar{u})$ is constant over boundary arcs, with zero value on an initial arc. Since the set of fonctions that are constant over a given arc is closed in $L^2(0,T)$, we deduce that $PC_2(\bar{u})$ is included in the r.h.s. of (48).

Conversely, we have to show that any w in the r.h.s. of (48) belongs to $PC_2(\bar{u})$. Let (c,d) be a singular arc with $0 \leq c < d < T$. The set of C^1 fonctions over (c,d) with value $w(c^-)$ (0 if $c = 0$) at point c and $w(d^+)$ at point d (when $d < T$) is a dense subset of $L^2(c,d)$. In view of (45), w is therefore the limit in $L^2(0,T)$ of a sequence w^k having the same (constant) values than w over boundary arcs, and of class C^1 with value 0 at 0, so that their derivative v^k is a critical direction. Therefore $w^k \in PC(\bar{u})$, and so the limit function w belongs to $PC_2(\bar{u})$ as was to be proved. ☐

3. Second order sufficient conditions

We first state the main result of this section. Consider the following condition:

$$\text{There exists } \rho > 0 \text{ such that } \hat{Q}(w) \geq \rho \|w\|_2^2, \text{ for all } w \in PC_2(\bar{u}). \tag{49}$$

Consider the *strong complementarity condition* (indeed stronger than (46)):

$$\left\{ \begin{array}{l} \Psi \text{ has nonzero values over the interior of each boundary arc} \\ \text{and at time 0 (resp. } T\text{) if an initial (resp. final) boundary arc exists,} \end{array} \right. \tag{50}$$

and the additional condition at bang-bang junctions:

$$R(\tau) \text{ has positive values for each bang-bang junction time } \tau. \tag{51}$$

We next state our sufficient optimality condition in the form of a characterization of quadratic growth.

Theorem 3.1. *Let* (50)-(51) *hold. Then* (49) *holds iff we have the following (weak) quadratic growth condition: there exists $\rho' > 0$ such that, if $u \in F(P)$, then setting $v := u - \bar{u}$ and $w(t) = \int_0^t v(s)\mathrm{d}s$, we have that*

$$J(\bar{u} + v) \geq J(\bar{u}) + \rho' \|w\|_2^2, \quad \textit{if } \|v\|_2 \textit{ is small enough.} \tag{52}$$

We first need to prove the following expansion of the cost function.

Proposition 3.2. *Let $\bar{u} + v$ be feasible, and set $w(t) = \int_0^t v(s)\mathrm{d}s$. Then we have that:*

$$J(\bar{u} + v) = J(\bar{u}) + \int_Q \Psi(t)v(t)\mathrm{d}(t) + \tfrac{1}{2}\hat{Q}(w) + O(\|y - \bar{y}\|_\infty \|w\|_2^2). \tag{53}$$

Remark 3.3. This is to be compared to the classical expansion stated in lemma 2.6.

Proof. We start from the expansion (27). Reminding that z is the solution of the linearized equation (12), we claim that

$$\left|\tilde{Q}(\delta y) - \tilde{Q}(z)\right| \leq O\left(\|\delta y\|_\infty \|w\|_2^2\right). \tag{54}$$

From (33) it follows that

$$\left|\tilde{Q}(\delta y) - \tilde{Q}(z)\right| = \|\kappa\|_\infty \left(\|\delta y\|_2 + \|z\|_2\right) \|\delta y - z\|_2. \tag{55}$$

We next obtain estimates for $\|\delta y\|_2 + \|z\|_2$ and $\|\delta y - z\|_2$. For this we apply a variant of the Goh transform to the state equation. Set $\hat{w}(t) := \int_0^t (\bar{u}(s) + v(s))\mathrm{d}s$. Then $\eta := y - \hat{w}B$ satisfies $\dot{\eta} = \dot{y} - (\bar{u} + v)B = \Delta y - \varphi(y)$, and so

$$\left\{ \begin{array}{l} \dot{\eta} - \Delta\eta + \varphi(\eta + \hat{w}B) = \hat{w}\Delta B \ \text{ in } Q, \\ \eta = 0 \text{ on } \Sigma; \quad \eta(\cdot, 0) = y_0. \end{array} \right. \tag{56}$$

Set $\bar{w}(t) := \int_0^t \bar{u}(s)\mathrm{d}s$, $\bar{\eta} = \bar{y} - \bar{w}B$, and $\delta\eta = \eta - \bar{\eta}$. We get, since $w = \hat{w} - \bar{w}$:

$$\left\{ \begin{array}{l} \dot{\delta\eta} - \Delta\delta\eta + \varphi(\eta + \hat{w}B) - \varphi(\bar{\eta} + \bar{w}B) = w\Delta B \ \text{ in } Q, \\ \delta\eta = 0 \text{ on } \Sigma; \quad \delta\eta(\cdot, 0) = y_0. \end{array} \right. \tag{57}$$

Since $\bar{u} + v \in F(P)$ a.e., the arguments of φ (equal to y and $\bar{y}$) are uniformly bounded, and so there exists $\theta[v]$ in a uniformly bounded subset of $L^\infty(Q)$ such that

$$\varphi(\eta + \hat{w}B) - \varphi(\bar{\eta} + \bar{w}B) = \theta[v](\delta\eta + wB). \tag{58}$$

Substituting this expression in (57), we get that $\|\delta\eta\|_{H^{2,1}(Q)} = O(\|w\|_2)$, and so

$$\|\delta y\|_2 = \|\delta\eta + wB\|_2 \leq \|\delta\eta\|_2 + \|B\|_\infty \|w\|_2 = O(\|w\|_2). \tag{59}$$

By similar arguments we get that

$$\|z\|_2 = \|\xi + wB\|_2 \leq \|\xi\|_2 + \|B\|_\infty \|w\|_2 = O(\|w\|_2). \tag{60}$$

Next, by (40) and (57), we have that $\chi := \delta\eta - \xi$ is solution of

$$\dot{\chi} - \Delta\chi + \varphi'(\bar{y})\chi = \varphi(\bar{y}) - \varphi(y) + \bar{\varphi}'(\bar{y})\delta y = c(x,t)(\delta y)^2, \tag{61}$$

for some bounded function c. If $\delta y = 0$, the conclusion obviously holds. Otherwise, $\hat{\chi} = \chi/\|\delta y\|_\infty$ is solution of

$$\dot{\hat{\chi}} - \Delta\hat{\chi} + \varphi'(\bar{y})\hat{\chi} = c(x,t)(\delta y)^2/\|\delta y\|_\infty. \tag{62}$$

The L^2 norm of the r.h.s. is by (59) of order $\|\delta y\|_2 = O(\|w\|_2)$, and so

$$\|\delta y - z\|_{H^{2,1}} = \|\delta\eta - \xi\|_{H^{2,1}} = \|\chi\|_{H^{2,1}} = \|\delta y\|_\infty \|\hat{\chi}\|_{H^{2,1}} = O(\|\delta y\|_\infty \|w\|_2). \tag{63}$$

Combining with (55) and (59)-(60), we deduce that the claim (54) holds.
c) We also have with (59) that

$$\|\delta y\|_3^3 \leq \|\delta y\|_\infty \|\delta y\|_2^2 = O\left(\|\delta y\|_\infty \|w\|_2^2\right). \tag{64}$$

We conclude by combining this inequality with (27) and (54). □

Proof of theorem 3.1. a) Assume that (49) holds, and let the sequence (v_k, w_k) contradict the weak quadratic growth condition (52), i.e., $\bar{u} + v_k \in F(P)$, $v_k \neq 0$, $\|v_k\|_2 \to 0$, w_k is the primitive of v_k with zero initial value, and

$$J(\bar{u} + v_k) \leq J(\bar{u}) + o\left(\|w_k\|_2^2\right). \tag{65}$$

Set $\hat{w}_k := w_k/\|w_k\|_2$. Extracting if necessary a subsequence, we may assume that $v_k \to 0$ a.e., and that the unit sequence $\hat{w}_k$ has a weak limit say $\hat{w}$ in $L^2(0,T)$. By the dominated convergence theorem, $v_k \to 0$ in $L^s(0,T)$ for all $s \in [1, \infty)$, and so

the associated state y_k uniformly converges to $\bar{y}$.
b) We claim that $\hat{w} \in PC_2(\bar{u})$. By proposition 3.2, we have that

$$J(\bar{u} + v_k) - J(\bar{u}) = \int_0^T \Psi(t) v_k(t) \mathrm{d}t + O(\|w_k\|_2^2). \tag{66}$$

By the first order optimality conditions, the above integral is nonnegative. Combining (65) and (66), we get that

$$\frac{1}{\|w_k\|_2} \int_0^T \Psi(t) v_k(t) \mathrm{d}t \to 0. \tag{67}$$

Let $(c, d) \subset (0, T)$ be a boundary arc, and let $\varphi \in \mathcal{D}_+(c, d)$, i.e., φ is of nonnegative, and of class C^∞ with compact support in (c, d). The integrand in (67) being nonnegative, we deduce that

$$\int_c^d \varphi(t)\Psi(t) \mathrm{d}\hat{w}_k(t) = \frac{1}{\|w_k\|_2} \int_c^d \varphi(t)\Psi(t) v_k(t) \mathrm{d}t \to 0. \tag{68}$$

Since $\varphi\Psi \in H^1(0, T)$, we may integrate by parts and we deduce that

$$0 = \lim_k \int_c^d \frac{\mathrm{d}}{\mathrm{d}t} \left(\varphi(t)\Psi(t)\right) \hat{w}_k(t) \mathrm{d}t = \int_c^d \frac{\mathrm{d}}{\mathrm{d}t} \left(\varphi(t)\Psi(t)\right) \hat{w}(t) \mathrm{d}t. \tag{69}$$

Assume for instance that $\bar{u} = a$ on (c, d). For some $\varepsilon > 0$ the support of φ is contained in $(c + \varepsilon, d - \varepsilon)$. On (c, d) we have that $v_k \geq 0$ and so w_k and $\hat{w}$ are nondecreasing. In particular, $\hat{w}$ has bounded variation on $(c + \varepsilon, d - \varepsilon)$. By the integration by parts formula with one of the function having only bounded variation, see [17, Vol. I, ch. 3, Theorem 22, p. 154], we get with (69) that

$$\int_{c+\varepsilon}^{d-\varepsilon} \varphi(t)\Psi(t) \mathrm{d}\hat{w}(t) = 0. \tag{70}$$

Over $[c + \varepsilon, d - \varepsilon]$, since $\Psi(t) > 0$ by the strict complementarity assumption (46), $\mathrm{d}\hat{w}(t) \geq 0$, and φ is an arbitrary element of $\mathcal{D}_+(c, d)$ with support in $(c + \varepsilon, d - \varepsilon)$, we deduce that $\hat{w}$ is constant over $(c+\varepsilon, d-\varepsilon)$. Since $\varepsilon > 0$ may be taken arbitrarily small, we see that $\hat{w}$ is constant over boundary arcs.

If $(0, d)$ is an initial boundary arc, then $\hat{w}$ is equal to some $\theta \in \mathbb{R}$ over $(0, d)$. Let $\varphi \in C^\infty([0, T])_+$ have support in $[0, d - \varepsilon)$ with $\varphi(0) = 1$. Since $\hat{w}_k(0) = 0$, by similar integrations by parts we deduce that $0 = \int_0^d \frac{\mathrm{d}}{\mathrm{d}t} \left(\varphi(t)\Psi(t)\right) \hat{w}(t) \mathrm{d}t = -\theta\Psi(0)$. Since $\Psi(0) \neq 0$ by (50), we deduce that $\theta = 0$, i.e., $\hat{w}$ vanishes on $(0, d)$. We deduce then our claim from lemma 2.13.
c) Let $I_S := [0, T] \setminus (I_a \cup I_b)$ denote the closure of the union of singular arcs, and $\mathcal{T}_{BB}$ denote the set of bang-bang junction points. For $\varepsilon > 0$, set

$$I_{SBB}^\varepsilon := \{t \in [0, T]; \quad \mathrm{dist}(t, I_S \cup \mathcal{T}_{BB}) \leq \varepsilon\}; \quad I_0^\varepsilon := [0, T] \setminus I_{SBB}^\varepsilon. \tag{71}$$

In view of the strong complementarity condition (50), and the condition (51) at bang-bang junctions, there exists $\beta > 0$ such that

$$|\psi(t)| > \beta \text{ is uniformy positive over } I_0^\varepsilon. \tag{72}$$

Now, let (c, d) be a connected component of I_0^ε. Take $\varepsilon > 0$ small enough, and set

$$\begin{cases} \varepsilon_1 & = 0 \quad \text{if } c = 0, \, \varepsilon_1 = \varepsilon \text{ otherwise}, \\ \varepsilon_2 & = 0 \quad \text{if } d = T, \, \varepsilon_2 = \varepsilon \text{ otherwise}. \end{cases} \tag{73}$$

By (67) and (72), we have that
(74)

$$0 = \lim_k \int_0^T \Psi(t) \mathrm{d}\hat{w}_k(t) \geq \lim_k \int_{c+\varepsilon_1}^{d-\varepsilon_2} \Psi(t) \mathrm{d}\hat{w}_k(t) \geq \beta \lim_k (\hat{w}_k(d - \varepsilon_2) - \hat{w}_k(c + \varepsilon_1))$$

and since $\hat{w}_k$ is monotonous over $[c+\varepsilon_1, d-\varepsilon_2]$, it follows that it uniformly converges over I_0^ε (we already know that the limit is constant over each maximal boundary arc).
d) Using (65), proposition 3.2, $\int_0^T \Psi(t)v_k(t)\mathrm{d}t \geq 0$, and $\|y_k - \bar{y}\|_\infty \to 0$, we deduce that

$$\limsup_k \hat{Q}(\hat{w}_k) \leq o(1). \tag{75}$$

Set, for $w \in PC_2(\bar{u})$, $\hat{Q}_\rho(w) := \hat{Q}(w) - \rho \int_0^T w(t)^2 \mathrm{d}t$. Applying corollary 2.11 to this quadratic form, we deduce that $R(t) \geq \rho$ over I_{SBB}. Since $R(t)$ is a continuous function, we deduce that there exists $\varepsilon > 0$ such that

$$R(t) \geq \tfrac{1}{2}\rho \ \text{ over } I_{SBB}^\varepsilon. \tag{76}$$

Now write, in view of (42),

$$\hat{Q}(\hat{w}_k) = \hat{Q}_1(\hat{w}_k) + \hat{Q}_2(\hat{w}_k) + \hat{Q}_3(\hat{w}_k), \tag{77}$$

with

$$\left\{ \begin{array}{lll} \hat{Q}_1(\hat{w}_k) & := & \displaystyle\int_Q \kappa(x,t)(\xi[w](x,t)^2 + 2\xi[w](x,t)w(t)B(x))\mathrm{d}x\mathrm{d}t, \\ \hat{Q}_2(\hat{w}_k) & := & \displaystyle\int_{I_{SBB}^\varepsilon} R(t)w(t)^2\mathrm{d}t, \quad \hat{Q}_3(\hat{w}_k) := \int_{I_0^\varepsilon} R(t)w(t)^2\mathrm{d}t. \end{array} \right. \tag{78}$$

Since the mapping $w \to \xi[w]$ is compact $L^2(0,T) \to L^2(Q)$ we have that $\hat{Q}_1$ is weakly continuous. By (76), $\hat{Q}_2$ restricted to $L^2(I_{SBB}^\varepsilon)$ is a Legendre form, in the sense that, it is weakly l.s.c. and satisfies

$$w_k \rightharpoonup w \text{ and } \hat{Q}(w_k) \to \hat{Q}(w) \text{ implies } w \to w \text{ in } L^2(I_{SBB}^\varepsilon). \tag{79}$$

So we have that (using the uniform convergence of $\hat{w}_k$ over I_0^ε):

$$\hat{Q}_1(\hat{w}) = \lim_k \hat{Q}_1(\hat{w}_k); \ \ \hat{Q}_2(\hat{w}) \leq \lim_k \hat{Q}_3(\hat{w}_k); \ \ \hat{Q}_3(\hat{w}) = \lim_k \hat{Q}_3(\hat{w}_k) = 0. \tag{80}$$

With (75) this implies that $\hat{Q}(\hat{w}) \leq 0$. Since $\hat{w} \in PC_2(\bar{u})$, by (49), $\hat{w} = 0$. By (80), $\hat{Q}_2(\hat{w}_k) \to \hat{Q}_2(\hat{w})$. We deduce with (79) that $\hat{w}_k \to \hat{w}$ in $L^2(0,T)$, in contradiction with the fact that $\hat{w}_k$ is a unit sequence and $\hat{w} = 0$.
e) Conversely, assume now that the weak quadratic growth condition (52) holds. For $v \in L^\infty(0,T)$, set $w[v](s) := \int_0^T v(s)\mathrm{d}s$. Applying the second order necessary condition (lemma 2.9) to the problem of minimizing $J(u,y) - \rho'\|w[u]\|_2^2$, that (49) holds. □

4. Numerical experiments

An open question is the existence of singular arcs. We could consider the convex case when $\gamma = 0$ and try to solve explicitly the optimality system; this however seems very difficult. We refer to Dhamo and Tröltzsch [13] for an example of an almost analytic resulution of an optimality sytem, in the context of parabolic equations.

On the other hand we can try numerical experiments and see if a singular arc seems to occur and is stable with respect to the discretization. We discretize the problem by standard finite differences, and solve the resulting optimal control problem with finitely many states using the optimal control toolbox BOCOP [6], which itself uses the nonlinear programming solver IPOPT [28].

The problem consists in controlling the one dimensional heat equation by the Neumann condition at one end. More precisely, the horizon is $T = 20$, $\Omega = (0,1)$, the control is the Neumann condition at $x = 0$, and the Neumann condition at

$x = 1$ is zero. We present the results obtained with 50 space steps, 200 time steps, the implicit Euler scheme, and taking $y_0 = 1$, $y_d = 0$, $\alpha = 0$. We display next the optimal control, and the states function of time. The control constraint is $u(t) \in [-1, 1]$, and we see that it is not active for $t \geq 5$. The same behavior is observed if we perturb the data and stepsize. So we may conjecture that this problem really has a singular arc.

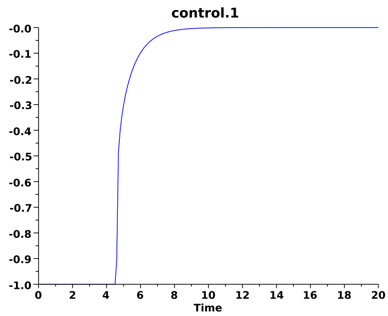

FIGURE 1. Optimal control: $u \in [-1, 1]$.

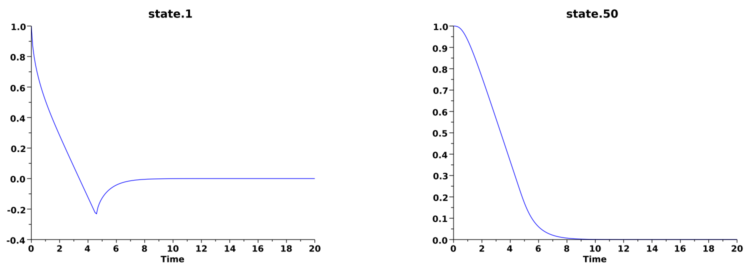

FIGURE 2. State at boundary $x = 0$.

5. CONCLUSION

We have established second order necessary and sufficient conditions for the local optimality of an optimal control problem of a parabolic equation, the Hamiltonian being affine w.r.t. the control, in the case when the optimal control has a singular arc. The main result is a characterization of a weak form of quadratic growth, that extends to the setting of control of parabolic equations the recent results and techniques in [1] (see in particular the proof of our key theorem 3.1).

It is not easy to prove if such singular arcs occur. However, we give strong numerical aguments supporting such an existence, actually in the case of a boundary control.

The present study deals with a simple case. It seems possible and of interest to extend our results in several directions: (i) the case of finitely many control variables, (ii) the case when the coefficients of the control, in the cost function and state equation, also depend on the state, (ii) the case when finitely many constraints on the terminal state are present.

Note also that, in real engineering devices, the action on the state equation is not the control itself, but rather the result of some integrations of the real control.

To be specific, we mignt consider the case when $\dot{u} = v$ where v is now the control, and u becomes a state variable, which is of course subject to bounds. This raises the question of extending the present framework to the case of state constraints. Let us observe that little is known, even in the ODE setting (see the analysis of optimality conditions in [22]).

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