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OPTIMAL CONTROL OF PDES IN A COMPLEX SPACE SETTING; APPLICATION TO THE SCHRÖDINGER EQUATION *

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May 4, 2016

Abstract. In this paper we discuss optimality conditions for abstract optimization problems over complex spaces. We then apply these results to optimal control problems with a semigroup structure. As an application we detail the case when the state equation is the Schrödinger one, with pointwise constraints on the "bilinear" control. We derive first and second order optimality conditions and address in particular the case that the control enters the state equation and cost function linearly.

Key words. Optimal control, partial differential equations, optimization in complex Banach spaces, second-order optimality conditions, Goh-transform, semigroup theory, Schrödinger equation, bilinear control systems.

AMS subject classifications. 49J20, 49K20, 35J10, 93C20.

1. Introduction. In this paper we derive no gap second order optimality conditions for optimal control problems in a complex Banach space setting with pointwise constraints on the control. This general framework includes, in particular, optimal control problems for the bilinear Schrödinger equation.

Let us consider $T>0$, $\Omega\subset\mathbb{R}^n$ an open bounded set, $n\in\mathbb{N}$, $Q:=(0,T)\times\Omega$, and $\Sigma=(0,T)\times\partial\Omega$. The Schrödinger equation is given by

$$i\dot{\Psi}(t,x)+\Delta\Psi(t,x)-u(t)B(x)\Psi(t,x)=0,\quad \Psi(x,0)=\Psi_0(x), \tag{1.1}$$

where $t\in(0,T)$, $x\in\Omega$, and with $u:[0,T]\to\mathbb{R}$ the time-dependent electric field, $\Psi:[0,T]\times\Omega\to\mathbb{C}$ the wave function, and $B:\Omega\to\mathbb{R}$ the coefficient of the magnetic field. The system describes the probability of position of a quantum particle subject to the electric field u; that will be considered as the control throughout this paper. The wave function Ψ belongs to the unitary sphere in $L^2(\Omega;\mathbb{C})$.

For $\alpha_1\in\mathbb{R}$ and $\alpha_2\geq 0$, the optimal control problem is given as

$$\begin{cases}\min J(u,\Psi):=\frac{1}{2}\displaystyle\int_\Omega|\Psi(T)-\Psi_{dT}|^2dx+\frac{1}{2}\int_Q|\Psi-\Psi_d|^2dxdt\\ \qquad\qquad\qquad+\displaystyle\int_0^T(\alpha_1u(t)+\tfrac{1}{2}\alpha_2u(t)^2)dt,\ \text{subject to (1.1) and } u\in\mathcal{U}_{\rm ad},\end{cases} \tag{1.2}$$

with $\mathcal{U}_{\rm ad}:=\{u\in L^\infty(0,T):u_m\leq u(t)\leq u_M \text{ a.e. in } (0,T)\}$, $u_m,u_M\in\mathbb{R}$, $u_m<u_m$ and $|z|:=\sqrt{z\bar{z}}$ for $z\in\mathbb{C}$, and desired running and final states $\Psi_d\colon(0,T)\times\Omega\to\mathbb{C}$ and $\Psi_{dT}\colon\Omega\to\mathbb{C}$, resp. The control of the Schrödinger equation is an important question in quantum physics. For the optimal control of semigroups, the reader is

*The second and third author were supported by the project "Optimal control of partial differential equations using parameterizing manifolds, model reduction, and dynamic programming" funded by the Foundation Hadamard/Gaspard Monge Program for Optimization and Operations Research (PGMO).

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referred to Li et al. [37, 38], Fattorini et al. [29, 28] and Goldberg and Tröltzsch [33]. In the context of optimal control of partial differential equations for systems in which the control enters linearly in both the state equation and cost function (we speak of control-linear problems), in a companion paper [3], we have extended the results of Bonnans [17] (about necessary and sufficient second order optimality conditions for a bilinear heat equation) to problems governed by general bilinear systems in a real Banach space setting, and presented applications to the heat and wave equation.

The contribution of this paper is the extension to a complex Banach space setting of the optimality conditions of a general class of optimization problems and of the framework developed in [3]. More precisely, we consider optimal control problems governed by a strongly continuous semigroup operator defined in a complex Banach space and derive necessary and sufficient optimality conditions. In particular (i) the study of strong solutions when $\alpha_2 > 0$, and (ii) the control-affine case, i.e. when $\alpha_2 = 0$, are addressed. The results are applied to the Schrödinger equation.

While the literature on optimal control of the heat equation is quite rich (see, e.g., the monograph by Tröltzsch [43]), much less is available for the optimal control of the Schrödinger equation. We list some references on optimal control of Schrödinger equation and related topics. In Ito and Kunisch [35] necessary optimality conditions are derived and an algorithm is presented to solve the unconstrained problem, in Baudouin et al. [7] regularity results for the Schrödinger equation with a singular potential are presented, further regularity results can be found in Baudouin et al. [8] and Boscain et al. [21] and in particular in Ball et al. [5]. For a minimum time problem and controllability problems for the Schrödinger equation see Beauchard et al. [12, 13, 11]. For second order analysis for control problems of control-affine ordinary differential systems see [2, 32]. About the case of optimal control of nonlinear Schrödinger equations of Gross-Pitaevskii type arising in the description of Bose-Einstein condensates, see Hintermüller et al. [34]; for sparse controls in quantum systems see Friesecke et al. [31].

The paper is organized as follows. In Section 2 necessary optimality conditions for general minimization problems in complex Banach spaces are formulated. In Section 3 the abstract control problem is introduced in a semigroup setting and some basic calculus rules are established. In Section 4 first order optimality conditions, in Section 5 sufficient second order optimality conditions are presented; sufficient second order optimality conditions for singular problems are presented in Section 6, again in a general semigroup setting. Section 7 presents the application, resp. the control of the Schrödinger equation and Section 8 a numerical tests supporting the possibility of existence of a singular arc.

2. Optimality conditions in complex spaces.

2.1. Real and complex spaces. We consider complex Banach spaces which can be identified with the product of two identical real Banach spaces. That is, with a real Banach space X we associate the complex Banach space $\overline{X}$ with element represented as $x_1 + ix_2$, with x_1, x_2 in X and $i = \sqrt{-1}$, and the usual computing rules for complex variable, in particular, for $\gamma = \gamma_1 + i\gamma_2 \in \mathbb{C}$ with γ_1, γ_2 real, we define $\gamma x = \gamma_1 x_1 - \gamma_2 x_2 + i(\gamma_2 x_1 + \gamma_1 x_2)$. Define the real and imaginary parts of a $x \in \overline{X}$ by $\Re x$ and $\Im x$, resp.

Let X be a real Banach space and $\overline{X}$ the corresponding complex one. We denote by $\langle \cdot, \cdot \rangle_X$ (resp. $\langle \cdot, \cdot \rangle_{\overline{X}}$) the duality product (resp. antiduality product, which is linear w.r.t. the first argument, and antilinear w.r.t. the second). The dual (resp. antidual) of X (resp. $\overline{X}$), i.e. the set of linear (resp. antilinear) forms, is denoted by X^* (resp. $\overline{X}^*$).

2.2. Optimality conditions. We next adress the questions of optimality conditions analogous to the obtained in the case of real Banach spaces [19]. Consider the problem

$$\operatorname*{Min}_{u,x} f(u,x); \quad g(u,x) \in K_g; \quad h(u,x) \in K_h. \tag{2.1}$$

Here U and W are real Banach space, $\overline{X}$ and $\overline{Y}$ are complex Banach spaces, and K_g, K_h are nonempty, closed convex subsets of $\overline{Y}$ and W resp. The mappings f, g, h from $U \times \overline{X}$ to respectively, $\mathbb{R}$, $\overline{Y}$, and W are of class C^1. As said before, the complex space $\overline{X}$ can be identified to a pair $X \times X$ of real Banach spaces, with dual $X^* \times X^*$. Let $x^* := (x_1^*, x_2^*) \in X \times X$, $\hat{x} := (x_1^*, x_2^*) \in X^* \times X^*$. Setting $x := x_1 + ix_2$ and $x^* := x_1^* + ix_2^*$ observe that (by linearity/antilinearity of $\langle \cdot, \cdot \rangle_{\overline{X}}$) that

$$\langle x^*, x \rangle_{\overline{X}} = \langle x_1^*, x_1 \rangle_X + \langle x_2^*, x_2 \rangle_X + i \left(\langle x_2^*, x_1 \rangle_X - \langle x_1^*, x_2 \rangle_X \right), \tag{2.2}$$

and therefore the 'real' duality product in $X \times X$ given by $\langle x^*, x \rangle_{X \times X} = \langle x_1^*, x_1 \rangle_X + \langle x_2^*, x_2 \rangle_X$ satisfies

$$\langle x^*, \hat{x} \rangle_{X \times X} = \Re \langle x^*, x \rangle_{\overline{X}}. \tag{2.3}$$

Let $\overline{X}$, $\overline{Y}$ be two complex spaces associated with the real Banach spaces X and Y. The conjugate transpose of $A \in \mathcal{L}(\overline{X}, \overline{Y})$ is the operator $A^* \in \mathcal{L}(\overline{Y}^*, \overline{X}^*)$ defined by

$$\langle y^*, Ax \rangle_{\overline{Y}} = \langle A^* y^*, x \rangle_{\overline{X}}, \text{ for all } (x, y^*) \text{ in } \overline{X} \times \overline{Y}^*. \tag{2.4}$$

If $A \in L(U, \overline{Y})$, identifying the real Banach space U with the space of real parts of the corresponding complex Banach space $\bar{U}$, we may define $A^* \in \mathcal{L}(\overline{Y}^*, \bar{U}^*)$ by

$$\langle A^* y^*, u \rangle_{\bar{U}} = \langle y^*, Au \rangle_{\overline{Y}}. \tag{2.5}$$

Combining this relation with (2.3), we deduce that

$$\Re \langle y^*, Au \rangle_{\overline{Y}} = \Re \langle A^* y^*, u \rangle_{\bar{U}} = \langle \Re A^* y^*, u \rangle_U. \tag{2.6}$$

We deduce the following expression of normal cones, for $y \in \overline{Y}$:

$$N_{K_g}(y) = \{ y^* \in \overline{Y}^*; \ \Re \langle y^*, z - y \rangle_{\overline{Y}} \le 0, \text{ for all } z \in K_g \}. \tag{2.7}$$

For $\lambda \in \overline{Y}$ and $\mu \in W$ the Lagrangian of the problem is defined as

$$L(u, x, \lambda, \mu) := f(u, x) + \Re \langle \lambda, g(u, x) \rangle_{\overline{Y}} + \langle \mu, h(u, x) \rangle_W. \tag{2.8}$$

LEMMA 2.1. *The partial derivatives of the Lagrangian are as follows:*

$$\left\{ \begin{aligned} \frac{\partial L}{\partial u} &= \frac{\partial f}{\partial u} + \Re \left(\frac{\partial g}{\partial u}^* \lambda \right) + \frac{\partial h}{\partial u}^\top \mu, \\ \frac{\partial L}{\partial x_r} &= \frac{\partial f}{\partial x_r} + \Re \left(\frac{\partial g}{\partial x}^* \lambda \right) + \frac{\partial h}{\partial x_r}^\top \mu, \\ \frac{\partial L}{\partial x_i} &= \frac{\partial f}{\partial x_i} + \Im \left(\frac{\partial g}{\partial x}^* \lambda \right) + \frac{\partial h}{\partial x_i}^\top \mu. \end{aligned} \right. \tag{2.9}$$

In particular, we have that

$$\frac{\partial L}{\partial x_r} + i\frac{\partial L}{\partial x_i} = \frac{\partial f}{\partial x_r} + i\frac{\partial f}{\partial x_i} + \frac{\partial g}{\partial x}^* \lambda + \left(\frac{\partial h}{\partial x_r} + i\frac{\partial h}{\partial x_i}\right)^\top \mu. \tag{2.10}$$

Proof. We have that, skipping arguments:

$$\begin{aligned} \frac{\partial L}{\partial u} v &= \frac{\partial f}{\partial u} v + \Re(\lambda, \frac{\partial g}{\partial u} v)_{\overline{Y}} + (\mu, \frac{\partial h}{\partial u} v)_W \\ &= \frac{\partial f}{\partial u} v + \Re(\frac{\partial g}{\partial u}^* \lambda, v)_U + (\frac{\partial h}{\partial u}^\top \mu, v)_U \\ &= \left(\frac{\partial f}{\partial u} + \Re(\frac{\partial g}{\partial u}^* \lambda) + \frac{\partial h}{\partial u}^\top \mu, v\right)_U \end{aligned} \tag{2.11}$$

for all $v \in U$. We have used that setting $\frac{\partial g}{\partial u} = a + ib$ and $\lambda = \lambda_r + i\lambda_i$, then

$$\begin{aligned} \left(\Re\left(\frac{\partial g}{\partial u}^* \lambda\right), v\right)_U &= (\Re(a^\top - ib^\top)(\lambda_r + i\lambda_i), v)_U \\ &= (a^\top \lambda_r + b^\top \lambda_i), v)_U \\ &= \Re\left(\tfrac{\partial g}{\partial u}^* \lambda, v\right)_U. \end{aligned} \tag{2.12}$$

Now, for $z_r \in X$:

$$\begin{aligned} \frac{\partial L}{\partial x_r} z_r &= \frac{\partial f}{\partial x_r} z_r + \Re(\lambda, \frac{\partial g}{\partial x} z_r)_{\overline{Y}} + (\mu, \frac{\partial h}{\partial x_r} z_r)_W \\ &= \frac{\partial f}{\partial x_r} z_r + \Re(\frac{\partial g}{\partial x}^* \lambda, z_r)_{\overline{X}} + (\frac{\partial h}{\partial x_r}^\top \mu, z_r)_{\overline{X}} \\ &= \left(\frac{\partial f}{\partial x_r} + \Re(\frac{\partial g}{\partial x}^* \lambda) + \frac{\partial h}{\partial x_r}^\top \mu, z_r\right)_{\overline{X}} \end{aligned} \tag{2.13}$$

and for all $z_i \in X$:

$$\begin{aligned} \frac{\partial L}{\partial x_i} z_i &= \frac{\partial f}{\partial x_i} z_i + \Re(\lambda, \frac{\partial g}{\partial x_i} i z_i)_{\overline{Y}} + (\mu, \frac{\partial h}{\partial x_i} z_i)_W \\ &= \frac{\partial f}{\partial x_i} z_i - \Re(i\frac{\partial g}{\partial x_i}^* \lambda, z_i)_{\overline{X}} + (\frac{\partial h}{\partial x_i}^\top \mu, z_i)_{\overline{X}} \\ &= \frac{\partial f}{\partial x_i} z_i + \Im(\frac{\partial g}{\partial x}^* \lambda, z_i)_{\overline{X}} + (\frac{\partial h}{\partial x_i}^\top \mu, z_i)_{\overline{X}} \\ &= \left(\frac{\partial f}{\partial x_i} + \Im(\frac{\partial g}{\partial x}^* \lambda) + \frac{\partial h}{\partial x_i}^\top \mu, z_i\right)_{\overline{X}}. \end{aligned} \tag{2.14}$$

The result follows. □

REMARK 2.2. *Not surprisingly, we obtain the same optimality system as if we had represented the constraint $g(u, x) = 0$ as an element of the product of real spaces. The advantage of the complex setting is to allow more compact formulas.*

3. The abstract control problem in a semigroup setting. Given a complex Banach space $\overline{\mathcal{H}}$, we consider optimal control problems for equations of type

$$\dot{\Psi} + \mathcal{A}\Psi = f + u(\mathcal{B}_1 + \mathcal{B}_2\Psi); \quad t \in (0, T); \quad \Psi(0) = \Psi_0, \tag{3.1}$$

where

$$\Psi_0 \in \overline{\mathcal{H}};\;\; f \in L^1(0,T;\overline{\mathcal{H}});\;\; \mathcal{B}_1 \in \overline{\mathcal{H}};\;\; u \in L^1(0,T);\;\; \mathcal{B}_2 \in \mathcal{L}(\overline{\mathcal{H}}), \tag{3.2}$$

and $\mathcal{A}$ is the generator of a strongly continuous semigroup on $\overline{\mathcal{H}}$, in the sense that, denoting by $e^{-t\mathcal{A}}$ the semigroup generated by $\mathcal{A}$, we have that

$$\mathrm{dom}(\mathcal{A}) := \left\{ y \in \overline{\mathcal{H}};\;\; \lim_{t\downarrow 0} \frac{y - e^{-t\mathcal{A}}y}{t} \text{ exists} \right\} \tag{3.3}$$

is dense and for $y \in \mathrm{dom}(\mathcal{A})$, $\mathcal{A}y$ is equal to the above limit. Then $\mathcal{A}$ is closed. Note that we choose to define $\mathcal{A}$ and not its opposite as the generator of the semigroup. We have then

$$\|e^{-t\mathcal{A}}\|_{\mathcal{L}(\overline{\mathcal{H}})} \leq c_{\mathcal{A}} e^{\lambda_{\mathcal{A}} t}, \quad t > 0, \tag{3.4}$$

for some positive $c_{\mathcal{A}}$ and $\lambda_{\mathcal{A}}$. For the semigroup theory in a complex space setting we refer to Dunford and Schwartz [27, Ch. VIII]. The solution of (3.1) in the *semigroup sense* is the function $\Psi \in C(0,T;\overline{\mathcal{H}})$ such that, for all $t \in [0,T]$:

$$\Psi(t) = e^{-t\mathcal{A}}\Psi_0 + \int_0^t e^{-(t-s)\mathcal{A}}\big(f(s) + u(s)(\mathcal{B}_1 + \mathcal{B}_2\Psi(s))\big)\mathrm{d}s. \tag{3.5}$$

This fixed-point equation (3.5) is well-posed in the sense that it has a unique solution in $C(0,T;\overline{\mathcal{H}})$, see [3]. We recall that the conjugate transpose of $\mathcal{A}$ has domain

$$\mathrm{dom}(\mathcal{A}^*) := \{\varphi \in \overline{\mathcal{H}}^*;\;\; \text{for some } c > 0\text{:}\;\; |\langle \varphi, \mathcal{A}y\rangle| \leq c\|y\|, \;\; \text{for all } y \in \mathrm{dom}(\mathcal{A})\}, \tag{3.6}$$

with antiduality product $\langle \cdot,\cdot\rangle := \langle \cdot,\cdot\rangle_{\overline{\mathcal{H}}}$. Thus, $y \mapsto \langle \varphi, \mathcal{A}y\rangle$ has a unique extension to a linear continuous form over $\overline{\mathcal{H}}$, which by the definition is $\mathcal{A}^*\varphi$. This allows to define weak solutions, extending to the complex setting the definition in [6]:

DEFINITION 3.1. *We say that* $\Psi \in C(0,T;\overline{\mathcal{H}})$ *is a* weak solution *of* (3.1) *if* $\Psi(0) = \Psi_0$ *and, for any* $\phi \in \mathrm{dom}(\mathcal{A}^*)$*, the function* $t \mapsto \langle \phi, \Psi(t)\rangle$ *is absolutely continuous over* $[0,T]$ *and satisfies*

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \phi, \Psi(t)\rangle + \langle \mathcal{A}^*\phi, \Psi(t)\rangle = \langle \phi, f + u(t)(\mathcal{B}_1 + \mathcal{B}_2\Psi(t))\rangle, \;\; \textit{for a.a. } t \in [0,T]. \tag{3.7}$$

We recall the following result, obvious extension to the complex setting of the corresponding result in [6]:

THEOREM 3.2. *Let* $\mathcal{A}$ *be the generator of a strongly continuous semigroup. Then there is a unique weak solution of* (3.7) *that coincides with the semigroup solution.*

So in the sequel we can use any of the two equivalent formulations (3.5) or (3.7). The control and state spaces are, respectively,

$$\mathcal{U} := L^1(0,T); \quad \mathcal{Y} := C(0,T;\overline{\mathcal{H}}). \tag{3.8}$$

For $s \in [1,\infty]$ we set $\mathcal{U}_s := L^s(0,T)$. Let $\hat{u} \in \mathcal{U}$ be given and $\hat{\Psi}$ solution of (3.1). The *linearized state equation* at $(\hat{\Psi}, \hat{u})$, to be understood in the semigroup sense, is

$$\dot{z}(t) + \mathcal{A}z(t) = \hat{u}(t)\mathcal{B}_2 z(t) + v(t)(\mathcal{B}_1 + \mathcal{B}_2\hat{\Psi}(t)); \quad z(0) = 0, \tag{3.9}$$

where $v \in \mathcal{U}$. It is easily checked that given $v \in \mathcal{U}$, the equation (3.9) has a unique solution denoted by $z[v]$, and that the mapping $u \mapsto \Psi[u]$ from $\mathcal{U}$ to $\mathcal{Y}$ is of class C^∞, with $D\Psi[u]v = z[v]$.

The results above may allow to prove higher regularity.

DEFINITION 3.3 (Restriction property). *Let E be a Banach space, with norm denoted by $\|\cdot\|_E$ with continuous inclusion in $\overline{\mathcal{H}}$. Assume that the restriction of $e^{-t\mathcal{A}}$ to E has image in E, and that it is a continuous semigroup over this space. We let $\mathcal{A}'$ denote its associated generator, and $e^{-t\mathcal{A}'}$ the associated semigroup. By* (3.3) *we have that*

$$\operatorname{dom}(\mathcal{A}') := \left\{ y \in E;\ \lim_{t\downarrow 0} \frac{e^{-t\mathcal{A}}y - y}{t} \text{ exists} \right\} \tag{3.10}$$

so that $\operatorname{dom}(\mathcal{A}') \subset \operatorname{dom}(\mathcal{A})$*, and $\mathcal{A}'$ is the restriction of $\mathcal{A}$ to* $\operatorname{dom}(\mathcal{A}')$*. We have that*

$$\|e^{-t\mathcal{A}'}\|_{\mathcal{L}(E)} \leq c_{\mathcal{A}'} e^{\lambda_{\mathcal{A}'} t} \tag{3.11}$$

for some constants $c_{\mathcal{A}'}$ and $\lambda_{\mathcal{A}'}$. Assume that $\mathcal{B}_1 \in E$, and denote by $\mathcal{B}_2'$ the restriction of $\mathcal{B}_2$ to E, which is supposed to have image in E and to be continuous in the topology of E, that is,

$$\mathcal{B}_1 \in E; \quad \mathcal{B}_2' \in \mathcal{L}(E). \tag{3.12}$$

In this case we say that E has the restriction property.

3.1. Dual semigroup. Since $\overline{\mathcal{H}}$ is a reflexive Banach space it is known, e.g. [40, Ch. 1, Cor. 10.6], that $\mathcal{A}^*$ generates another strongly continuous semigroup called the *dual (backward) semigroup* on $\overline{\mathcal{H}}^*$, denoted by $e^{-t\mathcal{A}^*}$, which satisfies

$$(e^{-t\mathcal{A}})^* = e^{-t\mathcal{A}^*}. \tag{3.13}$$

The reference [40] above assumes a real setting, but the arguments have an immediate extension to the complex one. Let (z,p) be solution of the forward-backward system

$$\left\{ \begin{array}{lll} \text{(i)} & \dot{z} + \mathcal{A}z & = az + b, \\ \text{(ii)} & -\dot{p} + \mathcal{A}^* p & = a^* p + g, \end{array} \right. \tag{3.14}$$

where

$$\left\{ \begin{array}{l} b \in L^1(0,T;\overline{\mathcal{H}}), \\ g \in L^1(0,T;\overline{\mathcal{H}}^*), \\ a \in L^\infty(0,T;\mathcal{L}(\overline{\mathcal{H}})), \end{array} \right. \tag{3.15}$$

and for a.a. $t \in (0,T)$, $a^*(t)$ is the conjugate transpose operator of $a(t)$, element of $L^\infty(0,T;\mathcal{L}(\overline{\mathcal{H}}^*))$.

The solutions of (3.14) in the semigroup sense are $z \in C(0,T;\overline{\mathcal{H}})$, $p \in C(0,T;\overline{\mathcal{H}}^*)$, and for a.a. $t \in (0,T)$:

$$\left\{ \begin{array}{ll} \text{(i)} & z(t) = e^{-t\mathcal{A}} z(0) + \displaystyle\int_0^t e^{-(t-s)\mathcal{A}}(a(s)z(s) + b(s))\mathrm{d}s, \\ \text{(ii)} & p(t) = e^{-(T-t)\mathcal{A}^*} p(T) + \displaystyle\int_t^T e^{-(s-t)\mathcal{A}^*}(a^*(s)p(s) + g(s))\mathrm{d}s. \end{array} \right. \tag{3.16}$$

The following integration by parts (IBP) lemma follows:

LEMMA 3.4. *Let* $(z,p) \in C(0,T;\overline{\mathcal{H}}) \times C(0,T;\overline{\mathcal{H}}^*)$ *satisfy* (3.14)-(3.15). *Then,*

$$\langle p(T), z(T)\rangle + \int_0^T \langle g(t), z(t)\rangle \mathrm{d}t = \langle p(0), z(0)\rangle + \int_0^T \langle p(t), b(t)\rangle \mathrm{d}t. \tag{3.17}$$

Proof. This is an obvious extension of [3, Lemma 2.9] to the complex setting. ∎

4. First order optimality conditions.

4.1. The optimal control problem. Let q and q_T be continuous quadratic forms over $\overline{\mathcal{H}}$, with associated symmetric and continuous operators Q and Q_T in $\mathcal{L}(\overline{\mathcal{H}}, \overline{\mathcal{H}}^*)$, such that $q(y) = \Re\langle Qy, y\rangle$ and $q_T(y) = \Re\langle Q_T y, y\rangle$, where the operators Q and Q_T are self-adjoint, i.e.,

$$\langle Qx, y\rangle = \overline{\langle Qy, x\rangle} \quad \text{for all } x,\ y \text{ in } \overline{\mathcal{H}}. \tag{4.1}$$

Observe that the derivative of q at y in direction x is

$$Dq(y)x = 2\Re\langle Qy, x\rangle. \tag{4.2}$$

Similar relations for q_T hold.

REMARK 4.1. *The bilinear form associated with the quadratic form q is*

$$\tfrac{1}{2}(q(x+y) - q(x) - q(y)) = \Re\langle Qx, y\rangle. \tag{4.3}$$

Then

$$\Im\langle Qx, y\rangle = \Re(-i\langle Qx, y\rangle) = \Re\langle Qx, iy\rangle = \tfrac{1}{2}(q(x+iy) - q(x) - q(iy)). \tag{4.4}$$

Given

$$\Psi_d \in L^\infty(0,T;\overline{\mathcal{H}}); \quad \Psi_{dT} \in \overline{\mathcal{H}}, \tag{4.5}$$

we introduce the cost function, where $\alpha_1 \in \mathbb{R}$ and $\alpha_2 \geq 0$, assuming that $u \in L^2(0,T)$ if $\alpha_2 \neq 0$:

$$J(u,\Psi) := \int_0^T (\alpha_1 u(t) + \tfrac{1}{2}\alpha_2 u(t)^2)\mathrm{d}t + \tfrac{1}{2}\int_0^T q(\Psi(t) - \Psi_d(t))\mathrm{d}t + \tfrac{1}{2} q_T(\Psi(T) - \Psi_{dT}) \tag{4.6}$$

The costate equation is

$$-\dot{p} + \mathcal{A}^* p = Q(\Psi - \Psi_d) + u\mathcal{B}_2^* p; \quad p(T) = Q_T(\Psi(T) - \Psi_{dT}). \tag{4.7}$$

We take the solution in the (backward) semigroup sense:

$$p(t) = e^{(t-T)\mathcal{A}^*} Q_T(\Psi(T) - \Psi_d(T)) + \int_t^T e^{(t-s)\mathcal{A}^*}\big(Q(\Psi(s) - \Psi_d(s)) + u(s)\mathcal{B}_2^* p(s)\big)\mathrm{d}s. \tag{4.8}$$

The reduced cost is

$$F(u) := J(u, \Psi[u]). \tag{4.9}$$

The set of feasible controls is

$$\mathcal{U}_{ad} := \{u \in \mathcal{U};\ u_m \leq u(t) \leq u_M \text{ a.e. on } [0,T]\}, \tag{4.10}$$

with $u_m < u_M$ given real constants. The optimal control problem is

$$\operatorname*{Min}_u F(u); \quad u \in \mathcal{U}_{ad}. \tag{P}$$

Given $(f, y_0) \in L^1(0,T;\overline{\mathcal{H}}) \times \overline{\mathcal{H}}$, let $y[y_0, f]$ denote the solution in the semigroup sense of

$$\dot{y}(t) + \mathcal{A}y(t) = f(t), \quad t \in (0,T), \qquad y(0) = y_0. \tag{4.11}$$

The *compactness hypothesis* is

$$\left\{ \begin{array}{l} \text{For given } y_0 \in \mathcal{H}, \text{ the mapping } f \mapsto \mathcal{B}_2 y[y_0, f] \\ \text{is compact from } L^2(0,T;\overline{\mathcal{H}}) \text{ to } L^2(0,T;\overline{\mathcal{H}}). \end{array} \right. \tag{4.12}$$

THEOREM 4.2. *Let* (4.12) *hold. Then problem* (P) *has a nonempty set of solutions.*

Proof. Similar to [3, Th. 2.15]. □

We set

$$\Lambda(t) := \alpha_1 + \alpha_2 \hat{u}(t) + \Re\langle p(t), \mathcal{B}_1 + \mathcal{B}_2 \hat{\Psi}(t)\rangle. \tag{4.13}$$

THEOREM 4.3. *The mapping $u \mapsto F(u)$ is of class C^∞ from $\mathcal{U}$ to $\mathbb{R}$ and we have that*

$$DF(u)v = \int_0^T \Lambda(t)v(t)\mathrm{d}t, \qquad \textit{for all } v \in \mathcal{U}. \tag{4.14}$$

Proof. That $F(u)$ and J are of class C^∞ follows from classical arguments based on the implicit function theorem, as in [3]. This also implies that, setting $\Psi := \Psi[u]$ and $z := z[u]$:

$$\begin{aligned} DF(u)v = \ & \int_0^T (\alpha_1 + \alpha_2 u(t))v(t))\mathrm{d}t + \int_0^T \Re\langle Q(\Psi(t) - \Psi_d(t)), z(t)\rangle \mathrm{d}t \\ & + \Re\langle Q_T(\Psi(T) - \Psi_{dT}), z(T)\rangle. \end{aligned} \tag{4.15}$$

We deduce then (4.14) from lemma 3.4. □ Let for $u \in \mathcal{U}_{ad}$ and $I_m(u)$ and $I_M(u)$ be the associated contact sets defined, up to a zero-measure set, as

$$\left\{ \begin{array}{l} I_m(u) := \{t \in (0,T) : u(t) = u_m\}, \\ I_M(u) := \{t \in (0,T) : u(t) = u_M\}. \end{array} \right. \tag{4.16}$$

The first order optimality necessary condition is given as follows.

PROPOSITION 4.4. *Let $\hat{u}$ be a local solution of problem* (P)*. Then, up to a set of measure zero there holds*

$$\{t;\ \Lambda(t) > 0\} \subset I_m(\hat{u}), \quad \{t;\ \Lambda(t) < 0\} \subset I_M(\hat{u}). \tag{4.17}$$

Proof. Same proof as in [3, Proposition 2.17]. □

5. Second order optimality conditions.

5.1. Technical results. Set $\delta\Psi := \Psi - \hat{\Psi}$. Since $u\Psi - \hat{u}\hat{\Psi} = u\delta\Psi + v\hat{\Psi}$, we have, in the semigroup sense:

$$\frac{\mathrm{d}}{\mathrm{d}t}\delta\Psi(t) + \mathcal{A}\delta\Psi(t) = \hat{u}(s)\mathcal{B}_2\delta\Psi(s) + v(t)(\mathcal{B}_1 + \mathcal{B}_2\hat{\Psi}(t) + \mathcal{B}_2\delta\Psi(s)). \tag{5.1}$$

Thus, $\eta := \delta\Psi - z$ is solution of

$$\dot{\eta}(t) + \mathcal{A}\eta(t) = \hat{u}\mathcal{B}_2\eta(t) + v(s)\mathcal{B}_2\delta\Psi(s). \tag{5.2}$$

We get the following estimates.

LEMMA 5.1. *The linearized state z solution of* (3.9)*, the solution $\delta\Psi$ of* (5.1)*, and $\eta = \delta\Psi - z$ solution of* (5.2) *satisfy, whenever v remains in a bounded set of $L^1(0,T)$:*

$$\|z\|_{L^\infty(0,T;\overline{\mathcal{H}})} = O(\|v\|_1), \tag{5.3}$$
$$\|\delta\Psi\|_{L^\infty(0,T;\overline{\mathcal{H}})} = O(\|v\|_1), \tag{5.4}$$
$$\|\eta\|_{L^\infty(0,T;\overline{\mathcal{H}})} = O(\|\delta\Psi\, v\|_{L^1(0,T;\overline{\mathcal{H}})}) = O(\|v\|_1^2). \tag{5.5}$$

Proof. Similar to the proof of lemma 2.18 in [3]. □

For $(\hat{\Psi}, \hat{u})$ solution of (3.1), $\hat{p}$ the corresponding solution of (4.8), $v \in L^1(0,T)$, and $z \in C(0,T;\overline{\mathcal{H}})$, let us set

$$\mathcal{Q}(z,v) := \int_0^T \Big(q(z(t)) + \alpha_2 v(t)^2 + 2v(t)\Re\langle\hat{p}(t), \mathcal{B}_2 z(t)\rangle\Big)\mathrm{d}t + q_T(z(T)). \tag{5.6}$$

PROPOSITION 5.2. *Let u belong to $\mathcal{U}$. Set $v := u - \hat{u}$, $\hat{\Psi} := \Psi[\hat{u}]$, $\Psi := \Psi[u]$. Then*

$$F(u) = F(\hat{u}) + DF(\hat{u})v + \tfrac{1}{2}\mathcal{Q}(\delta\Psi, v). \tag{5.7}$$

Proof. We can expand the cost function as follows:

$$\begin{aligned} F(u) =& F(\hat{u}) + \tfrac{1}{2}\int_0^T \alpha_2 v(t)^2 + q(\delta\Psi(t)))\mathrm{d}t + \tfrac{1}{2}q_T(\delta\Psi(T)) \\ &+ \int_0^T (\alpha_1 + \alpha_2\hat{u}(t))v(t)\mathrm{d}t \\ &+ \Re\left(\int_0^T \langle Q(\hat{\Psi}(t) - \Psi_d(t)), \delta\Psi\rangle\mathrm{d}t + \langle Q_T(\hat{\Psi}(T) - \Psi_d(T)), \delta\Psi(T)\rangle\right). \end{aligned} \tag{5.8}$$

Applying lemma 3.4 to the pair $(\delta\Psi, \hat{p})$, where z is solution of the linearized equation (3.9), and using the expression of Λ in (4.13), we obtain the result. □

COROLLARY 5.3. *We have that*

$$F(u) = F(\hat{u}) + DF(\hat{u})v + \tfrac{1}{2}\mathcal{Q}(z,v) + O(\|v\|_1^3), \tag{5.9}$$

where $z := z[v]$.

Proof. We have that

$$\begin{aligned}\mathcal{Q}(\delta\Psi, v) - \mathcal{Q}(z, v) \quad &= \quad \Re\left(\int_0^T \langle Q(\delta\Psi(t) + z(t)), \eta(t)\rangle + 2v(t)\langle p(t), B_2\eta(t)\rangle \mathrm{d}t\right) \\ &\quad + \Re\left(\langle Q_T(\delta\Psi(T) + z(T)), \eta(T)\rangle\right).\end{aligned} \tag{5.10}$$

By (5.3)-(5.5) this is of order of $\|v\|_1^3$. The conclusion follows. □

5.2. Second order necessary optimality conditions. Given a feasible control u, the critical cone is defined as

$$C(u) := \left\{ \begin{array}{l} v \in L^1(0,T) \mid \Lambda(t)v(t) = 0 \text{ a.e. on } [0,T], \\ v(t) \geq 0 \text{ a.e. on } I_m(u),\ v(t) \leq 0 \text{ a.e. on } I_M(u) \end{array} \right\}. \tag{5.11}$$

THEOREM 5.4. *Let $\hat{u} \in \mathcal{U}$ be a local solution of* (P) *and $\hat{p}$ be the corresponding costate. Then there holds,*

$$\mathcal{Q}(z[v], v) \geq 0 \quad \textit{for all } v \in C(\hat{u}). \tag{5.12}$$

Proof. The proof is similar to the one of theorem 3.3 in [3]. □

5.3. Second order sufficient optimality conditions. In this subsection we assume that $\alpha_2 > 0$, and obtain second order sufficient optimality conditions. Consider the following condition: there exists $\alpha_0 > 0$ such that

$$\mathcal{Q}(z, v) \geq \alpha_0 \int_0^T v(t)^2 \mathrm{d}t, \quad \text{for all } v \in C(\hat{u}). \tag{5.13}$$

THEOREM 5.5. *Let $\hat{u} \in \mathcal{U}$ satisfy the first order optimality conditions of* (P)*, $\hat{p}$ being the corresponding costate, as well as* (5.13) *Then $\hat{u}$ is a local solution of problem (P), that satisfies the quadratic growth condition.*

Proof. It suffices to adapt the arguments in say [15, Thm. 4.3] or Casas and Tröltzsch [24]. □

Using the technique of Bonnans and Osmolovskiĭ [16] we can actually deduce from theorem 5.4 that $\hat{u}$ is a strong solution in the following sense (natural extension of the notion of strong solution in the sense of the calculus of variations).

DEFINITION 5.6. *We say that a control $\hat{u} \in \mathcal{U}_{ad}$ is a strong solution if there exists $\varepsilon > 0$ such that, if $u \in \mathcal{U}_{ad}$ and $\|y[u] - y[\hat{u}]\|_{C(0,T;\overline{\mathcal{H}})} < \varepsilon$, then $F(\hat{u}) \leq F(u)$.*

In the context of optimal control of PDEs, sufficient conditions for strong optimality were recently obtained for elliptic state equations in Bayen et al. [9], and for parabolic equations by Bayen and Silva [10], and by Casas and Tröltzsch [24].

We consider the part of the Hamiltonian depending on the control:

$$H(t, u) := \alpha_1 u + \tfrac{1}{2}\alpha_2 u^2 + u\Re\langle \hat{p}(t), \mathcal{B}(t)\rangle, \tag{5.14}$$

where $\mathcal{B}(t) := \mathcal{B}(t)_1 + \mathcal{B}(t)_2\hat{\Psi}(t)$. The Hamiltonian inequality reads

$$H(t, \hat{u}(t)) \leq H(t, u), \quad \text{for all } u \in [u_m, u_M], \text{ for a.a. } t \in [0, T]. \tag{5.15}$$

Since $\alpha_2 > 0$, $H(t, \cdot)$ is a strongly convex function, and therefore the Hamiltonian inequality follows from the first order optimality conditions and in addition we have the quadratic growth property

$$H(t,\hat{u}(t)) + \tfrac{1}{2}\alpha_2(u-\hat{u}(t))^2 \le H(t,u), \quad \text{for all } u \in [u_m,u_M], \text{ for a.a. } t\in[0,T]. \tag{5.16}$$

LEMMA 5.7. *Let $\hat{u}$ be feasible and satisfy the first order optimality conditions, with $\alpha_2 > 0$. Let u_k be also feasible such that the associated states $\hat{\Psi}_k := \Psi[u_k]$ converge to $\hat{\Psi}$ in $C(0,T;\overline{\mathcal{H}})$, and $\limsup_k F(u_k) \le F(\hat{u})$. Then $u_k \to \hat{u}$ in $L^2(0,T)$.*

Proof. Since u_k is bounded in $L^\infty(0,T)$, from the expression of the cost function of the optimal control problem in view of theorem 4.3 and corollary 5.3, it follows that

$$0 \ge \limsup_k (F(u_k) - F(\hat{u})) = \limsup_k \int_0^T (H(t,u_k(t)) - H(t,\hat{u}(t)))\mathrm{d}t. \tag{5.17}$$

Then the conclusion follows from the quadratic growth property (5.16). □

For u_k as in Lemma 5.7 we have

$$B_k := \{t\in(0,T);\ |u_k(t)-\hat{u}(t)| > \sqrt{\|u_k-\hat{u}\|_1}\}; \quad A_k := (0,T)\setminus B_k. \tag{5.18}$$

Note that

$$|B_k| \le \int_0^T \frac{|u_k(t)-\hat{u}(t)|}{\sqrt{\|u_k-\hat{u}\|_1}}\mathrm{d}t = \sqrt{\|u_k-\hat{u}\|_1}. \tag{5.19}$$

Set for a.a. t:

$$v_k^A(t) := (u_k(t)-\hat{u}(t))\mathbf{1}_{A_k}(t); \quad v_k^B(t) := (u_k(t)-\hat{u}(t))\mathbf{1}_{B_k}(t). \tag{5.20}$$

We now extend to the semigroup setting the *decomposition principle* from [16], which has been extended to the elliptic setting by [9], and to the parabolic setting by [10].

THEOREM 5.8 (Decomposition principle). *For u_k as in Lemma 5.7 we have that $|B_k| \to 0$, and*

$$F(u_k) = F(\hat{u}+v_k^A) + F(\hat{u}+v_k^B) - F(\hat{u}) + o(\|u_k-\bar{u}\|_2^2). \tag{5.21}$$

and also

$$F(\hat{u}+v_k^B) - F(\hat{u}) = \int_{B^k} (H(t,u_k(t)) - H(t,\hat{u}(t)))\mathrm{d}t + o(\|u_k-\bar{u}\|_2^2). \tag{5.22}$$

Proof. Remember the linearized state equation (3.9) whose solution is denoted by $z[v]$. Set

$$v_k := u_k - \hat{u};\ \ z_k := z[v_k];\ \ z_k^A := z[v_k^A];\ \ z_k^B := z[v_k^B]. \tag{5.23}$$

Since $A_k \cap B_k$ has null measure, we have that $z_k = z_k^A + z_k^B$. Also,

$$\|v_k^B\|_1 \le |B_k|^{1/2}\|v_k^B\|_2 = o(\|v_k^B\|_2), \tag{5.24}$$

since $|B_k| \to 0$ by lemma 5.7. Then, in view of lemma 5.1:

$$\|z_k^B\|_{C(0,T;\overline{\mathcal{H}})} = O(\|v_k^B\|_1) = o(\|v_k^B\|_2). \tag{5.25}$$

Combining with corollary 5.3 and using the fact that $v_k^A(t)v_k^B(t) = 0$ a.e., we deduce that

$$\begin{array}{rcl} F(u_k) - F(\hat{u}) & = & DF(\hat{u})v_k + \frac{1}{2}\mathcal{Q}(v_k, z_k) + o(\|v_k\|_2^2) \\ & = & DF(\hat{u})v_k + \frac{1}{2}\mathcal{Q}(v_k, z_k^A) + o(\|v_k\|_2^2) \\ & = & DF(\hat{u})v_k^A + \frac{1}{2}\mathcal{Q}(v_k^A, z_k^A) + DF(\hat{u})v_k^B + \frac{1}{2}\alpha\|v_k^B\|_2^2 \\ & & +2\displaystyle\int_0^T v_k^B(t)\Re\langle\hat{p}(t), \mathcal{B}_2 z_k^A(t)\rangle \mathrm{d}t + o(\|v_k\|_2^2) \\ & = & DF(\hat{u})v_k^A + \frac{1}{2}\mathcal{Q}(v_k^A, z_k^A) + DF(\hat{u})v_k^B + \frac{1}{2}\alpha\|v_k^B\|_2^2 + o(\|v_k\|_2^2), \end{array} \tag{5.26}$$

where we have used the fact that, by (5.24):

$$\left| \int_0^T v_k^B(t)\Re\langle\hat{p}(t), \mathcal{B}_2 z_k^A(t)\rangle \mathrm{d}t \right| = O(\|v_k^B\|_1 \|z_k^A\|_{C(0,T;\overline{\mathcal{H}})}) = o(\|v_k\|_2^2). \tag{5.27}$$

Now

$$F(\hat{u} + v_k^A) - F(\hat{u}) = DF(\hat{u})v_k^A + \tfrac{1}{2}\mathcal{Q}(v_k^A, z_k^A) + o(\|v_k^A\|_2^2), \tag{5.28}$$

and by (5.25)

$$F(\hat{u} + v_k^B) - F(\hat{u}) = DF(\hat{u})v_k^B + \tfrac{1}{2}\alpha_2\|v_k^B\|_2^2 + o(\|v_k^B\|_2^2). \tag{5.29}$$

Combining the above relations we get the desired result. □

DEFINITION 5.9. *We say that $\hat{u}$ satisfies the* quadratic growth condition for strong solutions *if there exists $\varepsilon > 0$ and $\varepsilon' > 0$ such that for any feasible control u:*

$$F(\hat{u}) + \varepsilon\|u - \hat{u}\|_2^2 \le F(u), \quad \textit{whenever } \|\Psi[u] - \Psi[\bar{u}]\|_{C(0,T;\overline{\mathcal{H}})} < \varepsilon'. \tag{5.30}$$

THEOREM 5.10. *Let $\hat{u}$ satisfy the first order necessary optimality condition* (4.17)*, and the second order sufficient condition* (5.13)*. Then $\hat{u}$ is a strong minimum that satisfies the above quadratic growth condition.*

Proof. If the conclusion is false, then there exists a sequence u_k of feasible controls such that $\Psi_k \to \hat{\Psi}$ in $C(0,T;\overline{\mathcal{H}})$, where $\Psi_k := \Psi[u_k]$, and $F(u_k) \le F(\hat{u}) + o(\|u_k - \hat{u}\|_2^2)$. By lemma 5.7, $u_k \to \hat{u}$ in $L^2(0,T)$. By the decomposition theorem 5.8 and since $DF(\hat{u})v_k^B \ge 0$, it follows that

$$\alpha_2\|v_k^B\|_2^2 + F(\hat{u} + v_k^A) - F(\hat{u}) \le o(\|v_k\|_2^2). \tag{5.31}$$

We next distinguish two cases.
(a) Assume that $\|v_k^A\|_2/\|v_k\|_2 \to 0$. We know that

$$F(\hat{u} + v_k^A) - F(\hat{u}) = DF(\hat{u})v_k^A + \tfrac{1}{2}\mathcal{Q}(v_k^A, z_k^A) + o(\|v_k^A\|_2^2). \tag{5.32}$$

Since (by the first order optimality conditions) $DF(\hat{u})v_k^A \ge 0$ and $\mathcal{Q}(v_k^A, z_k^A) = O(\|v_k^A\|_2^2) = o(\|v_k\|_2^2)$ by hypothesis, it follows with (5.31) that $\|v_k^B\|_2^2 = o(\|v_k\|_2^2) = o(\|v_k^B\|_2^2)$ which gives a contradiction.
(b) Otherwise, $\liminf_k \|v_k^A\|_2/\|v_k\|_2 > 0$ (extracting if necessary a subsequence). It follows from (5.31) that

$$F(\hat{u} + v_k^A) - F(\hat{u}) \le o(\|v_k^A\|_2). \tag{5.33}$$

Since $\|v_k^A\|_\infty \to 0$, we obtain a contradiction with theorem 5.4. □

REMARK 5.11. *A shorter proof for theorem 5.8 is obtained by combining lemma 5.7 and the Taylor expansion in corollary 5.3, which implies*

$$F(u) = F(\hat{u}) + DF(\hat{u})v + \tfrac{1}{2}\mathcal{Q}(z,v) + O(\|v\|_2^3), \tag{5.34}$$

from which we can state a sufficient condition for optimality in $L^2(0,T)$. On the other hand the present proof opens the way for dealing with non quadratic (w.r.t. the control) Hamiltonian functions, as in [9].

6. Second order optimality conditions for singular problems. In this section we assume that $\alpha_2 = 0$, so that the control enters linearly in both the state equation and cost function. For such optimal control problems there is an extensive theory in the finite dimensional setting, see Kelley [36], Goh [32], Dmitruk [25, 26], Poggiolini and Stefani [41], Aronna et al. [1], and Frankowska and Tonon [30]; the case of additional scalar state constraints was considered in Aronna et al. [2].

In the context of optimal control of PDEs, there exist very few papers on sufficient optimality conditions for affine-linear control problems, see Bergounioux and Tiba [14], Tröltzsch [42], Bonnans and Tiba [20], Casas [22] (and the related literature involving L^1 norms, see e.g. Casas et al. [23]). As mentioned in the introduction, here we will follow the ideas in [3, 17] by using in an essential way the Goh transform [32].

Let $E_1 \subset \mathcal{H}$ with continuous inclusion, having the restriction property (definition 3.3). We can denote the restriction of $\mathcal{B}_2$ to E_1 by $\mathcal{B}_2$ with no risk of confusion. In the rest of the paper we make the following hypothesis:

$$\begin{cases} \text{(i)} & \mathcal{B}_1 \in \operatorname{dom}(\mathcal{A}), \\ \text{(ii)} & \mathcal{B}_2 \operatorname{dom}(\mathcal{A}) \subset \operatorname{dom}(\mathcal{A}), \quad \mathcal{B}_2^* \operatorname{dom}(\mathcal{A}^*) \subset \operatorname{dom}(\mathcal{A}^*), \end{cases} \tag{6.1}$$

with $\mathcal{B}_i^k := (\mathcal{B}_i)^k$. So, we may define the operators below, with domains $\operatorname{dom}(\mathcal{A})$ and $\operatorname{dom}(\mathcal{A}^*)$, respectively:

$$\begin{cases} [\mathcal{A}, \mathcal{B}_2^k] := \mathcal{A}\mathcal{B}_2^k - \mathcal{B}_2^k\mathcal{A}, \\ [(\mathcal{B}_2^k)^*, \mathcal{A}^*] := (\mathcal{B}_2^k)^*\mathcal{A}^* - \mathcal{A}^*(\mathcal{B}_2^k)^*. \end{cases} \tag{6.2}$$

$$\begin{cases} \text{(i)} & \text{For } k = 1,2,\ \left[\mathcal{A}, \mathcal{B}_2^k\right] \text{ has a continuous extension to } E_1, \\ & \text{denoted by } M_k, \\ \text{(ii)} & f \in L^\infty(0,T;\overline{\mathcal{H}}); \quad M_k^*\hat{p} \in L^\infty(0,T;\overline{\mathcal{H}}^*),\ k=1,2, \\ \text{(iii)} & \hat{\Psi} \in L^2(0,T;E_1); \ \ [M_1, \mathcal{B}_2]\hat{\Psi} \in L^\infty(0,T;\overline{\mathcal{H}}). \end{cases} \tag{6.3}$$

REMARK 6.1. *Point* (6.1) *(ii) implies*

$$\mathcal{B}_2^k \operatorname{dom}(\mathcal{A}) \subset \operatorname{dom}(\mathcal{A}), \quad (\mathcal{B}_2^k)^* \operatorname{dom}(\mathcal{A}^*) \subset \operatorname{dom}(\mathcal{A}^*), \qquad \textit{for } k = 1,2. \tag{6.4}$$

So, $[\mathcal{A}, \mathcal{B}_2]$ is well-defined as operator with domain $\operatorname{dom}(\mathcal{A})$, and point (iii) makes sense.

We also assume that

$$\begin{cases} \text{(i)} & \mathcal{B}_2^2 f \in C(0,T;\overline{\mathcal{H}}); \ \ \Psi_d \in C(0,T;\overline{\mathcal{H}}), \\ \text{(ii)} & M_k^*\hat{p} \in C(0,T;\overline{\mathcal{H}}^*), \ \ k=1,2. \end{cases} \tag{6.5}$$

Let $\xi \in C(0,T;\overline{\mathcal{H}})$ be (semigroup) solution of the following equation

$$\dot{\xi} + \mathcal{A}\xi = \hat{u}\mathcal{B}_2\xi + wb_z^1; \quad \xi(0) = 0, \tag{6.6}$$

where

$$b_z^1 := -\mathcal{B}_2 f - M_1\hat{\Psi} - \mathcal{A}\mathcal{B}_1. \tag{6.7}$$

Note that $b_z^1 \in C(0,T;\overline{\mathcal{H}})$, so that equation (6.6) has a unique solution. Consider the space

$$W := \big(L^2(0,T;E_1) \cap C([0,T];\mathcal{H})\big) \times L^2(0,T) \times \mathbb{R}. \tag{6.8}$$

We define the continuous quadratic forms over W, defined by

$$\widehat{\mathcal{Q}}(\xi,w,h) = \widehat{\mathcal{Q}}_T(\xi,h) + \widehat{\mathcal{Q}}_a(\xi,w) + \widehat{\mathcal{Q}}_b(w), \tag{6.9}$$

where $\widehat{\mathcal{Q}}_b(w) := \int_0^T w^2(t)R(t)\mathrm{d}t$ and

$$\widehat{\mathcal{Q}}_T(\xi,h) := q_T(\xi(T) + h\mathcal{B}(T)) + h^2\Re\langle\hat{p}(T), \mathcal{B}_2\mathcal{B}_1 + \mathcal{B}_2^2\hat{\Psi}(T)\rangle + h\Re\langle\hat{p}(T), \mathcal{B}_2\xi(T)\rangle, \tag{6.10}$$

$$\widehat{\mathcal{Q}}_a(\xi,w) := \Re\int_0^T \Big(q(\xi) + 2w\langle Q\xi,\mathcal{B}\rangle + 2w\langle Q(\hat{\Psi} - \Psi_d), \mathcal{B}_2\xi\rangle - 2w\langle M_1^*\hat{p},\xi\rangle\Big)\mathrm{d}t, \tag{6.11}$$

with $R \in L^\infty(0,T)$ given by

$$\begin{cases} R(t) := q(\mathcal{B}) + \Re\langle Q(\hat{\Psi} - \Psi_d), \mathcal{B}_2\mathcal{B}\rangle + \Re\langle\hat{p}(t), r(t)\rangle, \\ r(t) := \mathcal{B}_2^2 f(t) - \mathcal{A}\mathcal{B}_2\mathcal{B}_1 + 2\mathcal{B}_2\mathcal{A}\mathcal{B}_1 - \big[M_1,\mathcal{B}_2\big]\hat{\Psi}. \end{cases} \tag{6.12}$$

We write $PC_2(\hat{u})$ for the closure in the $L^2 \times \mathbb{R}$–topology of the set

$$PC(\hat{u}) := \{(w,h) \in W^{1,\infty}(0,T) \times \mathbb{R}, \dot{w} \in C(\hat{u});\ w(0) = 0,\ w(T) = h\}. \tag{6.13}$$

The final value of w becomes an independent variable when we consider this closure.

Definition 6.2 (Singular arc). *The control $\hat{u}(\cdot)$ is said to have a* singular arc *in a nonempty interval $(t_1,t_2) \subset [0,T]$ if, for all $\theta > 0$, there exists $\varepsilon > 0$ such that*

$$\hat{u}(t) \in [u_m + \varepsilon, u_M - \varepsilon], \quad \text{for a.a. } t \in (t_1+\theta, t_2-\theta). \tag{6.14}$$

We may also say that (t_1,t_2) is a singular arc itself. We call (t_1,t_2) a lower boundary arc *if $\hat{u}(t) = u_m$ for a.a. $t \in (t_1,t_2)$, and an* upper boundary arc *if $\hat{u}(t) = u_M$ for a.a. $t \in (t_1,t_2)$. We sometimes simply call them boundary arcs. We say that a boundary arc (c,d) is* initial *if $c = 0$, and* final *if $d = T$.*

Lemma 6.3. *For $v \in L^1(0,T)$ and $w \in AC(0,T)$, $w(t) = \int_0^t v(s)\mathrm{d}s$, there holds*

$$\mathcal{Q}(z[v],v) = \widehat{\mathcal{Q}}(\xi[w],w,w(T)). \tag{6.15}$$

For any $(w,h) \in L^2(0,T) \times \mathbb{R}$*:*

$$\widehat{\mathcal{Q}}(\xi[w], w, h) \geq 0 \quad \textit{for all } (w,h) \in PC_2(\hat{u}). \tag{6.16}$$

In addition, provided the mapping

$$w \mapsto \xi[w], \quad L^2(0,T) \to L^2(0,T;\overline{\mathcal{H}}) \tag{6.17}$$

is compact we have that $R(t) \geq 0$ *a.e. on singular arcs.*

Proof. Similar to [3, Lemma 3.9 and corollary 3.11]. □

In the following we assume that the following hypotheses hold:

1. *finite structure:*

$$\left\{ \begin{array}{l} \text{there are finitely many boundary and singular maximal arcs} \\ \text{and the closure of their union is } [0,T], \end{array} \right. \tag{6.18}$$

2. *strict complementarity* for the control constraint (note that Λ is a continuous function of time)

$$\left\{ \begin{array}{l} \Lambda \text{ has nonzero values over the interior of each boundary arc, and} \\ \text{at time } 0 \text{ (resp. } T\text{) if an initial (resp. final) boundary arc exists,} \end{array} \right. \tag{6.19}$$

Proposition 6.4. *Let* (6.18)–(6.19) *hold. Then*

$$PC_2(\hat{u}) = \left\{ \begin{array}{l} (w,h) \in L^2(0,T) \times \mathbb{R};\ w \textit{ is constant over boundary arcs,} \\ w = 0 \textit{ over an initial boundary arc} \\ \textit{and } w = h \textit{ over a terminal boundary arc} \end{array} \right\}. \tag{6.20}$$

Proof. Similar to the one of [1, Lemma 8.1]. □

Letting $\mathcal{T}_{BB}$ denote the *set of bang-bang junctions,* we assume in addition that

$$R(t) > 0, \quad t \in \mathcal{T}_{BB}. \tag{6.21}$$

Consider the following positivity condition: there exists $\alpha > 0$ such that

$$\Omega(\xi[w], w, h) \geq \alpha(\|w\|_2^2 + h^2), \quad \text{for all } (w,h) \in PC_2(\hat{u}). \tag{6.22}$$

We say that $\hat{u}$ satisfies a *weak quadratic growth condition* if there exists $\beta > 0$ such that for any $u \in \mathcal{U}_{ad}$, setting $v := u - \hat{u}$ and $w(t) := \int_0^T v(s)\mathrm{d}s$, we have

$$F(u) \geq F(\hat{u}) + \beta(\|w\|_2^2 + w(T)^2), \quad \text{if } \|v\|_1 \text{ is small enough.} \tag{6.23}$$

The word 'weak' makes reference to the fact that the growth is obtained for the L^2 norm of w, and not the one of v.

Theorem 6.5. *Let* (6.18)-(6.19) *and* (6.21) *hold. Then* (6.22) *holds iff the quadratic growth condition* (6.23) *is satisfied.*

Proof. Similar to the one in [3, Thm 4.5]. □

7. Application to Schrödinger equation.

7.1. Statement of the problem. The equation is formulated first in an informal way. Let $\Omega \subset \mathbb{R}^n$, $n \in \mathbb{N}$, open and bounded, and $T > 0$. The state equation, with $\Psi = \Psi(t, x)$, is

$$\begin{cases} \dot{\Psi}(t,x) - i \displaystyle\sum_{j,k=1}^{n} \frac{\partial}{\partial x_k}\left[a_{jk}(x)\frac{\partial \Psi(t,x)}{\partial x_j}\right] = -iub_2\Psi(t,x) + f & \text{in } (0,T)\times\Omega, \\ \Psi(0,x) = \Psi_0 & \text{in } \Omega, \\ \Psi(t,x) = 0 & \text{on } (0,T)\times\partial\Omega \end{cases} \tag{7.1}$$

with

$$\Psi_0 \in \bar{V}, \;\; b_2^k \in W_0^{2,\infty}(\Omega),\; k = 1, 2, \quad f \in L^2(0,T;\bar{V}) \cap C(0,T;\bar{H}) \tag{7.2}$$

and the complex-valued spaces $\bar{H} := L^2(\Omega;\mathbb{C})$ and $\bar{V} := H_0^1(\Omega;\mathbb{C})$. Note that although f is normally equal to zero, it is useful to introduce it since the sensitivity of the solution w.r.t. the r.h.s., that plays a role in the numerical analysis. Here the a_{jk} are C^1 functions over $\bar{\Omega}$ that satisfy, for each $x \in \bar{\Omega}$, the symmetry hypothesis $a_{jk} = a_{kj}$ for all j, k as well as the following coercivity hypothesis, that for some $\nu > 0$:

$$\sum_{j,k=1}^{n} a_{jk}(x)\xi_j\xi_k \geq \nu|\xi|^2, \quad \text{for all } \xi \in \mathbb{C}^n,\ x \in \Omega. \tag{7.3}$$

We apply the abstract setting with $\overline{\mathcal{H}} = \bar{H}$. Consider the unbouded operator in $\bar{H}$ defined by

$$(\mathcal{A}_0\Psi)(t,x) := -\sum_{j,k=1}^{n} \frac{\partial}{\partial x_k}\left[a_{jk}(x)\frac{\partial \Psi(t,x)}{\partial x_j}\right], \quad (t,x) \in (0,T)\times\Omega, \tag{7.4}$$

with domain $\operatorname{dom}(\mathcal{A}_0) := \bar{H}^2(\Omega) \cap \bar{V}$, where $\bar{H}^2(\Omega)$ denotes the complex valued Sobolev space $H^2(\Omega, \mathbb{C})$. One easily checks that this operator is self-adjoint, i.e., equal to the conjugate transpose. The PDE (7.1) enters in the semigroup framework, with generator

$$(\mathcal{A}_{\bar{H}}\Psi) := i\mathcal{A}_0\Psi, \quad \text{for all } \Psi \in \bar{H}. \tag{7.5}$$

LEMMA 7.1. *The operator $\mathcal{A}_{\overline{\mathcal{H}}}$, with domain $\operatorname{dom}(\mathcal{A}_{\overline{\mathcal{H}}}) := \bar{H}^2(\Omega) \cap \bar{V}$, is the generator of a unitary semigroup and* (7.1) *has a semigroup solution* $\Psi \in C(0,T;\bar{H})$.

Proof. That $\mathcal{A}_{\overline{\mathcal{H}}}$ is the generator of a contracting semigroup follows from the Hille Yosida characterization with $M = 1$, $n = 1$ and $\omega = 0$. The operator $\mathcal{A}_{\overline{\mathcal{H}}}$ being the opposite of its conjugate transpose it follows that the semigroup is norm preserving. □ We define then the following sesquilinear form over $\bar{V}$:

$$a(y,z) := \sum_{j,k=1}^{n} \int_\Omega a_{jk}(x)\frac{\partial y}{\partial x_j}\frac{\partial \bar{z}}{\partial x_k}\mathrm{d}x, \quad \text{for all } y,\ z \text{ in } \bar{V}, \tag{7.6}$$

which is self-adjoint in the sense that

$$\overline{a(y,z)} = a(z,y). \tag{7.7}$$

Furthermore, for y, z in $\operatorname{dom}(\mathcal{A}_0)$ we have that

$$\langle \mathcal{A}_0 y, z\rangle_{\bar{H}} = a(y,z) = \overline{a(z,y)} = \langle y, \mathcal{A}_0 z\rangle_{\bar{H}}. \tag{7.8}$$

so that is $\mathcal{A}_0$ also self-adjoint.

7.2. Link to variational setting and regularity for Schrödinger equation. We introduce the function space

$$\mathcal{X} := L^\infty(0,T;\bar{V}) \cap H^1(0,T;\bar{V}'), \tag{7.9}$$

endowed with the natural norm

$$\|\Psi\|_{\mathcal{X}} := \|\Psi\|_{L^\infty(0,T;\bar{V})} + \|\Psi\|_{H^1(0,T;\bar{V}')}. \tag{7.10}$$

There holds the following weak convergence result.

LEMMA 7.2. *Let Ψ_k be a bounded sequence in $\mathcal{X}$. Then there exists $\Psi \in \mathcal{X}$ such that a subsequence of Ψ_k converges to Ψ strongly in $L^2(0,T;\bar{H})$, and weakly in $L^2(0,T;\bar{V})$, and $H^1(0,T;\bar{V}')$. Finally, if u_k weakly$*$ converges to u in $L^\infty(0,T)$, then*

$$u_k b_2 \Psi_k \to u b_2 \Psi \quad \textit{weakly in } L^2(0,T;\bar{H}) \tag{7.11}$$

Proof. By the Aubin-Lions lemma [4], $\mathcal{X}$ is compactly embedded into $L^2(0,T;\bar{H})$. Thus, extracting a subsequence if necessary, we may assume that Ψ_k converges in $L^2(0,T;\bar{H})$ to some Ψ. Since Ψ_k is bounded in the Hilbert spaces $L^2(0,T;\bar{V})$ and $H^1(0,T;\bar{V}')$, re-extracting a subsequence if necessary, we may assume that it also weakly converges in these spaces.

Let C_R denote the closed ball of $L^\infty(0,T,\bar{V})$ of radius R. This is a closed subset of $L^2(0,T,\bar{V})$ that, for large enough R, contains the sequence Ψ_k. Since any closed convex set is weakly closed, $\Psi \in C_R$. Thus $\Psi \in \mathcal{X}$. That (7.11) holds follows from the joint convergence of u_k in $L^\infty(0,T)$ (endowed with the weak$*$ topology), and of Ψ_k in $L^2(0,T;\bar{H})$. □

The variational solution of (7.1) is given as $\Psi \in \mathcal{X}$ satisfying, for a.a. $t \in (0,T)$:

$$\langle \dot{\Psi}(t), z\rangle_{\bar{V}} + ia(\Psi(t), z) + iu(t)\langle b_2\Psi, z\rangle_{\bar{H}} = \langle f(t), z\rangle_{\bar{V}} \text{ for all } z \in \bar{V}, \tag{7.12}$$

and $\Psi(0) = \Psi_0 \in \bar{V}$.

For $(f, b_2, u, \Psi_0) \in L^2(0,T;\bar{V}) \times W^{1,\infty}(\Omega) \times L^\infty(\Omega) \times \bar{V}$ we set

$$\begin{aligned}\kappa[f,b_2,u,\Psi_0] = \;& \|f\|^2_{L^1(0,T;\bar{V})} + \|\Psi_0\|^2_{\bar{V}} + \\ & \|u\|^2_{L^\infty(0,T)} \|\nabla b_2\|^2_{L^\infty(\Omega)} (\|f\|^2_{L^2(0,T;\bar{H})} + \|\Psi_0\|^2_{\bar{V}}).\end{aligned} \tag{7.13}$$

There holds the following existence and regularity result for the unique solution of (7.12) (cf. [39]).

THEOREM 7.3. *Let $(f, b_2, u, \Psi_0) \in L^2(0,T;\bar{V}) \times W^{1,\infty}(\Omega) \times L^\infty(\Omega) \times \bar{V}$. Then there exists $c_0 > 0$ independent of (f, b_2, u, Ψ_0) such that (7.12) has a unique solution Ψ in $\mathcal{X}$, that satisfies the estimates*

$$\|\Psi\|_{C(0,T;\bar{H})} \le c_0\big(\|f\|_{L^1(0,T;\bar{H})} + \|\Psi_0\|_{\bar{H}}\big), \tag{7.14}$$

$$\|\Psi\|_{C(0,T;\bar{V})} + \|\dot{\Psi}(t)\|_{L^2(0,T;\bar{V}')} \le c_0\kappa[f,b_2,u,\Psi_0]. \tag{7.15}$$

Proof. Since Ω is bounded, there exists a Hilbert basis of $H^1_0(\Omega)$ (w_j, λ_j), $j \in \mathbb{N}$ of (real) eigenvalues and nonnegative eigenvectors of the operator $\mathcal{A}_0$ (with, by the definition, homogeneous Dirichlet conditions), i.e

$$-\sum_{j,k=1}^n \frac{\partial}{\partial x_k}\left[a_{jk}(x)\frac{\partial w_j(x)}{\partial x_j}\right] = \lambda_j w_j(x), \quad j = 1, \cdots, w_j \in H^1_0(\Omega), \quad \lambda_j \in \mathbb{R}_+. \tag{7.16}$$

Consider the associated Faedo-Galerkin discretization method; that is, let $\{\bar{V}_k\}$ be the finite dimensional subspaces of $\bar{V}$ generated by the (complex combinations of the) w_j, for $j \leq k$. The corresponding approximate solution $\Psi_k(t) = \sum_{j=1}^k \psi_k^j(t) w_j$ of (7.1), with $\psi_k^j(t) \in \mathbb{C}$, is defined as the solution of

$$\langle \dot{\Psi}_k(t), w_j \rangle_{\bar{H}} + ia(\Psi_k(t), w_j) + iu(t)\langle b_2 \Psi_k(t), w_j \rangle_{\bar{H}} = \langle f(t), w_j \rangle_{\bar{H}}, \tag{7.17}$$

for $j = 1, \dots, k$ and $t \in [0, T]$, with initial condition

$$\psi_k^j(0) = (\Psi_0, w_j), \quad \text{for } j = 1, \dots, k. \tag{7.18}$$

For each $k \in \mathbb{N}$, the above equations are a system of linear ordinary differential equations that has a unique solution $\psi_k = (\psi_k^1, \dots, \psi_k^k) \in C(0, T; \mathbb{C}^k)$. It follows that for any $\Phi(t) = \sum_{j=1}^k \phi^j(t) w_j$ (where $\phi^j(t) \in L^1(0, T)$ for $j = 1, \dots, k$) we have that

$$\langle \dot{\Psi}_k(t), \Phi(t) \rangle_{\bar{H}} + ia(\Psi_k(t), \Phi(t)) + iu(t)\langle b_2 \Psi_k(t), \Phi(t) \rangle_{\bar{H}} = \langle f(t), \Phi(t) \rangle_{\bar{H}}, \tag{7.19}$$

We derive *a priori* estimates by using different test functions Φ.

1. Testing with $\Phi(t) = \Psi_k(t)$ gives

$$\langle \dot{\Psi}_k(t), \Psi_k(t) \rangle_{\bar{H}} + ia(\Psi_k(t), \Psi_k(t)) + iu(t)\langle b_2 \Psi_k(t), \Psi_k(t) \rangle_{\bar{H}} = \langle f(t), \Psi_k(t) \rangle_{\bar{H}}. \tag{7.20}$$

Taking the real part in both sides in (7.20) we obtain

$$\tfrac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} \|\Psi_k(t)\|_{\bar{H}}^2 \leq C_1 \|f(t)\|_{\bar{H}} \|\Psi_k(t)\|_{\bar{H}} \leq C_2 (\|f(t)\|_{\bar{H}}^2 + \|\Psi_k(t)\|_{\bar{H}}^2). \tag{7.21}$$

By Gronwall's inequality we get the following estimate

$$\|\Psi_k\|_{L^\infty(0,T;\bar{H})}^2 \leq C_3 (\|f\|_{L^1(0,T;\bar{H})}^2 + \|\Psi_k(0)\|_{\bar{H}}^2). \tag{7.22}$$

2. Testing with $\Phi(t) = \sum_{j=1}^k \lambda_j \psi_k^j(t) w_j = \mathcal{A}_0 \Psi_k(t)$ gives

$$\langle \dot{\Psi}_k(t), \mathcal{A}_0 \Psi_k(t) \rangle_{\bar{H}} + ia(\Psi_k(t), \mathcal{A}_0 \Psi_k(t)) + iu(t)(b_2 \Psi_k(t) - f(t), \mathcal{A}_0 \Psi_k(t))_{\bar{H}} = 0. \tag{7.23}$$

Applying (7.8) (in both directions) we get

$$i\langle \mathcal{A}_0 \Psi_k(t), \mathcal{A}_0 \Psi_k(t) \rangle_{\bar{H}} + a(\dot{\Psi}_k(t), \Psi_k(t)) + iu(t) b_2 \Psi_k(t) - f(t)) = 0. \tag{7.24}$$

Since $a(\cdot, \cdot)$ is self-adjoint we have that

$$\begin{array}{rcl} \frac{\mathrm{d}}{\mathrm{d}t} a(\Psi_k(t), \Psi_k(t)) & = & a(\Psi_k(t), \dot{\Psi}_k(t)) + a(\dot{\Psi}_k(t), \Psi_k(t)) \\ & = & 2\Re \Big(a(\Psi_k(t), \dot{\Psi}_k(t)) \Big). \end{array} \tag{7.25}$$

So, taking real parts in (7.24) we get using Young's inequality and the coercivity of $a(\cdot, \cdot)$ over $\bar{V}$:

$$\begin{array}{rl} \frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} a(\Psi_k(t), \Psi_k(t)) & = -\Re \left(a(\Psi_k(t), iu(t) b_2 \Psi_k(t) - f(t)) \right) \\ & \leq c \|\Psi_k(t)\|_{\bar{V}} (\|\Psi_k(t)\|_{\bar{V}} + \|f(t)\|_{\bar{V}}) \\ & \leq c' (a(\Psi_k(t), \Psi_k(t)) + \|f(t)\|_{\bar{V}}). \end{array} \tag{7.26}$$

So, by Gronwall's estimate and using (7.22):

$$\|\Psi_k\|_{L^\infty(0,T;\bar{V})} \leq c_0 \kappa[f, b_2, u, \Psi_0]. \tag{7.27}$$

3. Any $\Phi \in \bar{V}$ can be written as $\Phi = \Phi^1 + \Phi^2$ with $\Phi^1 \in \bar{V}_j$ and Φ^2 orthogonal to $\bar{V}_j$ in both spaces $\bar{H}$ and $\bar{V}$. Recall the notation for the dual and antidual pairing introduced in Section 4.1. Then

$$\langle \dot{\Psi}_k(t), \Phi \rangle_{\bar{V}} = \langle \dot{\Psi}_k(t), \Phi \rangle_{\bar{H}} = \langle \dot{\Psi}_k(t), \Phi^1 \rangle_{\bar{H}} = \langle \dot{\Psi}_k(t), \Phi^1 \rangle_{\bar{V}}. \tag{7.28}$$

It follows from (7.19) that there exists $c'' > 0$ such that, when $\|\Phi\|_{\bar{V}} \leq 1$,

$$\langle \dot{\Psi}_k(t), \Phi \rangle_{\bar{V}} \leq c'' \left(\|\Psi_k(t)\|_{\bar{V}} + \|u\|_{L^\infty(0,T)} \|b_2\|_{L^\infty(\Omega)} \|\Psi_k(t)\|_{\bar{H}} + \|f(t)\|_{\bar{H}} \right). \tag{7.29}$$

Combining with the above estimates we obtain

$$\left\| \dot{\Psi}_k \right\|_{L^2(0,T;\bar{V}')} \leq c_0 \kappa[f, b_2, u, \Psi_0]. \tag{7.30}$$

By lemma 7.2 a subsequence of (Ψ_k) strongly converges in $L^2(0,T;\bar{H})$ and weakly in $L^2(0,T;\bar{V}) \cap H^1(0,T;\bar{V}')$, while $ub_2\Psi_k \to ub_2\Psi$ weakly in $L^2(0,T;\bar{H})$. Passing to the limit in (7.19) we obtain that Ψ is solution of the Schrödinger equation. That Ψ is unique, belongs to $\mathcal{X}$ and satisfies (7.14),(7.15) and (7.30) follows from the same techniques as those used in the study of the Faedo-Galerkin approximation. □

Lemma 7.4. *For $(f, b_2, u, \Psi_0) \in L^2(0,T;\bar{V}) \times W^{1,\infty}(\Omega) \times L^\infty(\Omega) \times \bar{V}$ the semigroup solution coincides with the variational solution.*

Proof.

That the variational and semigroup solution coincide can be shown by a similar argument as in [3, Lemma 5.4]. □

The corresponding data of the abstract theory are $\mathcal{B}_1 \in \bar{H}$ equal to zero, and $\mathcal{B}_2 \in \mathcal{L}(\bar{H})$ defined by $(\mathcal{B}_2 y)(x) := -ib_2(x)y(x)$ for y in $\bar{H}$ and $x \in \Omega$. The cost function is, given $\alpha_1 \in \mathbb{R}$:

$$\begin{aligned} J(u,y) := \quad & \alpha_1 \int_0^T u(t)\mathrm{d}t + \tfrac{1}{2} \int_{(0,T)\times\Omega} (y(t,x) - y_d(t,x))^2 \mathrm{d}x\mathrm{d}t \\ & + \tfrac{1}{2} \int_\Omega (y(T,x) - y_{dT}(x))^2 \mathrm{d}x. \end{aligned} \tag{7.31}$$

We assume that

$$y_d \in C(0,T;\bar{V}); \quad y_{dT} \in \bar{V}. \tag{7.32}$$

For $u \in L^1(0,T)$, write the reduced cost as $F(u) := J(u, y[u])$. The optimal control problem is, $\mathcal{U}_{ad}$ being defined in (4.10):

$$\operatorname{Min} F(u); \quad u \in \mathcal{U}_{ad}. \tag{7.33}$$

7.3. Compactness for the Schrödinger equation. To prove existence of an optimal control of (P) we have to verify the compactness hypothesis (4.12).

Proposition 7.5. *Problem* (P) *for equation* (7.1) *and cost function* (7.31) *has a nonempty set of solutions.*

Proof. This follows from theorem 4.2, whose compactness hypothesis holds thanks to lemma 7.2. □

7.4. Commutators. Given $y \in \mathrm{dom}(\mathcal{A}_{\overline{\mathcal{H}}})$, we have by (7.5) that

$$M_1 y \quad = \quad - \sum_{j,k=1}^{n} \left(\frac{\partial b_2}{\partial x_k} \left[a_{jk} \frac{\partial y}{\partial x_j} \right] + \frac{\partial}{\partial x_k} \left[a_{jk} y \frac{\partial b_2}{\partial x_j} \right] \right). \tag{7.34}$$

As expected, this commutator is a first order differential operator that has a continuous extension to the space $\bar{V}$. In a similar way we can check that $[M_1, \mathcal{B}_2]$ is the "zero order" operator given by

$$[M_1, \mathcal{B}_2] y = 2i \sum_{j,k=1}^{n} a_{j,k} \frac{\partial b_2}{\partial x_j} \frac{\partial b_2}{\partial x_k} y. \tag{7.35}$$

REMARK 7.6. *In the case of the Laplace operator, i.e. when $a_{jk} = \delta_{jk}$, we find that for $y \in \bar{V}$*

$$M_1 y = -2 \nabla b_2 \cdot \nabla y - y \Delta b_2; \quad [M_1, \mathcal{B}_2] y = 2iy |\nabla b_2|^2, \tag{7.36}$$

and then for $p \in \bar{V}$ we have

$$M_1^* p = 2 \nabla b_2 \cdot \nabla \bar{p} + \bar{p} \Delta b_2. \tag{7.37}$$

Similarly we have

$$\left\{ \begin{array}{ll} M_2 y & = 2i \nabla b_2^2 \cdot \nabla y + iy \Delta b_2^2; \\ {[M_2, \mathcal{B}_2]}\, y & = -2iy |\nabla b_2^2|^2, \\ M_2^* p & = -i(2 \nabla b_2^2 \cdot \nabla \bar{p} + \bar{p} \Delta b_2^2). \end{array} \right. \tag{7.38}$$

7.5. Analysis of optimality conditions. For the sake of simplicity we only discuss the case of the Laplace operator. The costate equation is then

$$-\dot{p} + i \Delta p = \Psi - \Psi_d + iub_2 p \ \text{ in } (0,T) \times \Omega; \quad p(T) = \Psi(T) - \Psi_{dT}. \tag{7.39}$$

Remembering the expression of b_z^1 in (6.7), we obtain that the equation for $\xi := \xi_z$ introduced in (6.6) reduces to

$$\dot{\xi} - i \Delta \xi = -i \hat{u} b_2 \xi + w(ib_2 f + 2 \nabla b_2 \cdot \nabla \Psi + \Psi \Delta b_2) \ \text{ in } (0,T) \times \Omega; \quad \xi(0) = 0. \tag{7.40}$$

The quadratic forms $\mathcal{Q}$ and $\widehat{\mathcal{Q}}$ defined in (5.6) and (6.9) are as follows. First

$$\mathcal{Q}(z,v) = \int_0^T \left(\|z(t)\|_{\bar{H}}^2 + 2v(t) \Re \langle \hat{p}(t), b_2 z(t) \rangle_{\bar{H}} \right) \mathrm{d}t + \|z(T)\|_{\bar{H}}^2, \tag{7.41}$$

and second,

$$\widehat{\mathcal{Q}}(\xi, w, h) = \widehat{\mathcal{Q}}_T(\xi, h) + \widehat{\mathcal{Q}}_a(\xi, w) + \widehat{\mathcal{Q}}_b(w); \quad \widehat{\mathcal{Q}}_b(w) := \int_0^T w^2(t) R(t) \mathrm{d}t. \tag{7.42}$$

Here $R \in C(0,T)$, and

$$\widehat{\mathcal{Q}}_T(\xi, h) := \left\| \xi(T) - ihb_2 \hat{\Psi}(T) \right\|_{\bar{H}}^2 - h^2 \Re \langle \hat{p}(T), b_2^2 \hat{\Psi}(T) \rangle_{\bar{H}} + h \Re \langle i \hat{p}(T), b_2 \xi(T) \rangle_{\bar{H}}, \tag{7.43}$$

$$\widehat{\mathcal{Q}}_a(\xi, w) := \int_0^T \left(\|\xi\|_{\bar{H}}^2 + 2w \Re (i \langle \xi, b_2 \hat{\Psi} \rangle_{\bar{H}} + i \langle \hat{\Psi} - \Psi_d, b_2 \xi \rangle_{\bar{H}} - \langle M_1^* \hat{p}, \xi \rangle_{\bar{H}}) \right) \mathrm{d}t, \tag{7.44}$$

$$R(t) := \left\| b_2 \hat{\Psi} \right\|_{\bar{H}}^2 - \Re \langle \hat{\Psi} - \Psi_d, b_2^2 \hat{\Psi} \rangle_{\bar{H}} + \Re \langle \hat{p}(t), -b_2^2 f(t) - 2i |\nabla b_2|^2 \hat{\Psi} \rangle_{\bar{H}}. \tag{7.45}$$

THEOREM 7.7. (i) *The second order necessary condition* (6.16) *holds, i.e.,*

$$\widehat{\mathcal{Q}}(\xi[w], w, h) \geq 0 \quad \textit{for all } (w, h) \in PC_2(\hat{u}). \tag{7.46}$$

(ii) $R(t) \geq 0$ *over singular arcs.*
(iii) *Let* (6.18)-(6.21) *hold. Then the second order optimality condition* (6.22) *holds iff the quadratic growth condition* (6.23) *is satisfied.*

Proof. (i) Conditions (6.1)(i) and (ii) are satisfied with (7.2). Since we have

$$\overline{[-i\Delta, (-ib_2)^k]}\hat{\Psi} = -(-i)^{k-1}(\Delta b_2^k \hat{\Psi} + 2\nabla b_2^k \nabla \hat{\Psi}), \quad k = 1, 2, \tag{7.47}$$

i.e. the commutator is a first order differential operator and has an extension to the space $\bar{V}$, we obtain (6.3)(i) with $E_1 = \bar{V}$. (6.3)(ii) and (iii) follow from the regularity assumptions in (7.2) and (7.32).

(ii) The compactness hypothesis (6.17) for

$$w \mapsto \xi[w], \quad L^2(0, T) \to L^2(0, T; \bar{H}) \tag{7.48}$$

follows from (7.2), since hence, $\xi[w] \in L^2(0, T; \bar{V}) \cap H^1(0, T; \bar{V}')$ which is compactly embedded in $L^2(0, T; \bar{H})$ by Aubin's lemma [4].

(iii) Condition (6.5) follows also from the assumptions in (7.2) and (7.32). ◻

REMARK 7.8. *It is not difficult to extend such results for more general differential operators of the type, where the a_{jk} are as before, $b \in L^\infty(\Omega)^n$ and $c \in L^\infty(\Omega)$:*

$$(\mathcal{A}_{\overline{\mathcal{H}}}\Psi)(t, x) = -i \sum_{j,k=1}^{n} \frac{\partial}{\partial x_k}\left[a_{jk}(x)\frac{\partial}{\partial x_j}\Psi(t, x)\right] + \sum_{j=1}^{n} \frac{\partial(b_j(x)\Psi(t, x))}{\partial x_j} + c\Psi(t, x). \tag{7.49}$$

8. Numerical example. The question of existence of a singular arc is not addressed here, it remains an open problem. Nevertheless, we analyze this issue numerically for the one-dimensional Schrödinger equation. We present a numerical example where a singular arc occurs and is stable with respect to the discretization. Let the spatial domain be given as $\Omega \subset \mathbb{R}$ and set $T = 10$. We discretize the problem by standard finite differences. In space we choose 40 steps and in time 200. For the computational realization we use the optimal control toolbox Bocop [18] which uses the nonlinear programming solver IPOPT, see [44]. In Figure 8.1 we see that singular arcs appear.

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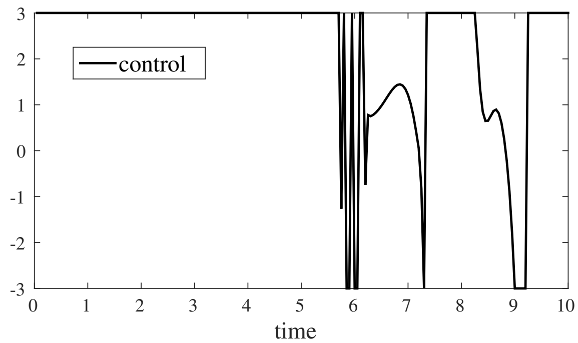

Fig. 8.1. *Singular arc*

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