SIAM J. CONTROL OPTIM.
Vol. 46, No. 1, pp. 274–287

OPTIMAL BILINEAR CONTROL OF AN ABSTRACT SCHRÖDINGER EQUATION*

KAZUFUMI ITO† AND KARL KUNISCH‡

Abstract. Well-posedness of abstract quantum mechanical systems is considered and the existence of optimal control of such systems is proved. First order optimality systems are derived. Convergence of the monotone scheme for the solution of the optimality system is proved.

Key words. Schrödinger equation, C_0-groups, optimal control, optimality systems, monotone scheme

AMS subject classifications. 35Q40, 49K20, 65M12

DOI. 10.1137/05064254X

1. Introduction. We consider a quantum mechanical system with internal Hamiltonian H_0 prepared in the initial state $\Psi_0(x)$, where x denotes the relevant spatial coordinate. The state $\Psi(x,t)$ satisfies the time-dependent Schrödinger equation (we set $h = 1$). In the presence of an external interaction taken as an electric field, modeled by a coupling operator with amplitude $\epsilon(t) \in \mathbb{R}$ and a time-independent dipole moment operator $\hat{\mu}$, the new Hamiltonian $H_0 - \mu(t)$ gives rise to the control system

$$i\,\frac{\partial}{\partial t}\Psi(x,t) = (H_0 - \mu(t))\Psi(x,t), \quad \Psi(x,0) = \Psi_0(x), \tag{1.1}$$

where $\mu(t) = \epsilon(t)\hat{\mu}$. Here $\mu(t)$ represents a controlled Hamiltonian which can be a distributed control. The optimal control approach (see, e.g., [MT], [PDR], [TKO], [ZR]) allows us to assess the fitness of the final state $\Psi(T)$ to a prescribed goal. This is achieved through the introduction of a performance index J which is maximized. One possible choice for a cost functional is given by

$$J(\mu) = \frac{1}{2}\langle\Psi(T)|O|\Psi(T)\rangle - \frac{\alpha}{2}\int_0^T |\mu(t)|^2\,dt, \tag{1.2}$$

where $\alpha > 0$ and O is the observable operator that encodes the goal. The larger the value $\langle\Psi(T)|O|\Psi(T)\rangle$ is, the better the control objective is met. Here we used the notation $\langle\Psi(T)|O|\Psi(T)\rangle = \int_\Omega \overline{\Psi(T,x)}\,O\Psi(T,x)\,dx$. The conditions that we utilize for H_0, $\mu(\cdot)$ and O will be given in the following section. Maximization of $\langle\Psi(T)|O|\Psi(T)\rangle$ is at the price of a large laser influence $\int_0^T |\mu(t)|^2\,dt$. The optimally controlled evolution must therefore balance between the expense for the laser influence and the desire that the observable has an acceptably large value.

*Received by the editors October 12, 2005; accepted for publication (in revised form) September 6, 2006; published electronically April 13, 2007.
http://www.siam.org/journals/sicon/46-1/64254.html

†Department of Mathematics, North Carolina State University, Raleigh, NC 27695-8205 (kito@unity.ncsu.edu). This research was partially supported by the Army Research Office under DAAD19-02-1-0394.

‡Institute for Mathematics and Scientific Computing, Karl-Franzens-Universität Graz, A-8010 Graz, Austria (karl.kunisch@uni-graz.at). This research was supported in part by the Radon Institute, Linz, Austria.

An alternative cost is given by

$$J(\mu) = -\frac{1}{2}\left(|\Psi(T) - \bar{\Psi}(T)|^2 + \alpha\int_0^T |\mu(t)|^2\,dt\right),$$

where $\bar{\Psi}$ is a target state. Since $|\Psi|_{L^2} = 1$, it is equivalent to

$$J(\mu) = \mathrm{Re}\,(\Psi, \bar{\Psi}) - \frac{\alpha}{2}\int_0^T |\mu(t)|^2\,dt. \tag{1.3}$$

In section 2 we shall establish well-posedness results for (1.1) based on a semigroup framework in a form that will facilitate the optimal control treatment. Section 3 is devoted to the precise statement of the optimal control problem, including the class of admissible control operators μ which are considered, and a proof for the existence of optimal solutions. First order necessary optimality conditions are derived in section 4. In section 5 we describe the monotone scheme for the general class of optimal problems that is considered in this paper. Well-posedness and subsequential convergence of the scheme are proved.

To point at some of the relevant literature for the problem under investigation we mention the pioneering work of Rabitz and collaborators; see, e.g., [PDR], [ZR], and the references given there. For existence of optimal controls we refer to [BP]. Differently from our semigroup approach, the work in [BP] is based on partial differential equation techniques, and requires higher regularity in time. Many important aspects of the monotone scheme for the solution of the optimality system were investigated in, e.g., [MST], [MT], [S], [TKO]. However, except for [S], which treats the case of scalar-valued controls, convergence proofs of the optimal controls and states have received little attention so far. The technique of proof in [S] and in the present work are different. While the key ingredient for the convergence proof in [S] is a convergence result in [BMS] for the convolution of a Hilbert-space valued function with a sequence of weakly convergent scalar-valued functions, our results are based on compactness arguments. This allows for finite dimensional (in space) as well as infinite dimensional (distributed) control action.

2. Well-posedness. Setting $\Psi(t,x) = \Psi_1(t,x) + \Psi_2(t,x)$ and $\Psi = (\Psi_1, \Psi_2)$, system (1.1) can equivalently be written as

$$\begin{aligned} &\frac{\partial}{\partial t}\Psi_1(t,x) = (H_0 - \mu(t))\,\Psi_2(t,x), \\ &\frac{\partial}{\partial t}\Psi_2(t,x) = -(H_0 - \mu(t))\,\Psi_1(t,x) \quad \text{ for } (t,x) \in (0,T] \times \Omega. \end{aligned} \tag{2.1}$$

Here $T > 0$ and $\Omega = \mathbb{R}^n$ or Ω is a bounded subset of $\mathbb{R}^n$. The behavior of Ψ at the boundary of Ω is defined through the domain of the operator H_0. We refer to section 3 for specific examples. Throughout it is assumed that H_0 is a densely defined, self-adjoint positive semidefinite operator in a real Hilbert space H, consisting of functions defined over the domain Ω. Typically H is $L^2(\Omega)$. If H_0 satisfies the above assumptions it is necessarily closed. We define the closed linear operator A_0 in $X = H \times H$ by

$$A_0 = \begin{pmatrix} 0 & H_0 \\ -H_0 & 0 \end{pmatrix},$$

with $dom\,(A_0) = dom\,(H_0) \times dom\,(H_0)$. Note that A_0 is skew-adjoint, i.e.,

$$(A_0\Psi, \hat{\Psi}) = -(A_0\hat{\Psi}, \Psi) \text{ for all } \Psi, \hat{\Psi} \in dom\,(A_0).$$

Consequently by Stone's theorem [HP] A_0 generates a C_0-group $S(t)$ on X satisfying $|S(t)\Psi|_X = |\Psi|_X$ for all $\Psi \in X$ and $t \geq 0$. Let

$$V = dom\,(H_0^{\frac{1}{2}}) \quad \text{and} \quad \mathcal{V} = V \times V.$$

Then $H_0 \in \mathcal{L}(V, V^*)$ and thus $A_0 \in \mathcal{L}(\mathcal{V}, \mathcal{V}^*)$, where

$$V^* \quad \text{and} \quad \mathcal{V}^* = V^* \times V^*$$

denote the dual space of V and $\mathcal{V}$, respectively, with H and X as pivot spaces. V is equipped with

$$|\phi|_V^2 = \langle H_0\phi, \phi\rangle_{V^*\times V} + |\phi|_H^2$$

as norm. Then the restriction of $S(t)$ to $\mathcal{V}$ is again a C_0-group. The dual $S^*(-t)$ is the extension of $S(t)$ to $\mathcal{V}^*$ and forms a C_0-group on $\mathcal{V}^*$. Moreover, for the extension group on $\mathcal{V}^*$ the domain of the generator is given by $dom_{\mathcal{V}^*}(A_0) = \mathcal{V}^*$.

Suppose that $\mu(t) \in \mathcal{L}(H)$ is self-adjoint for almost every $t \in (0, T)$ and define

$$B(t) = \begin{pmatrix} 0 & \mu(t) \\ -\mu(t) & 0 \end{pmatrix}.$$

In the context of an external interaction with an electric field, as mentioned in the introduction, $\mu(t) = \epsilon(t)\hat{\mu}$, where ϵ denotes a scalar-valued amplitude and $\hat{\mu} = \hat{\mu}(x)$ is a multiplication operator representing the dipole moment [MT], [MST], [ZR].

By a fixed point argument it can be argued that for every $T > 0$, $\mu \in L^2(0, T; \mathcal{L}(H))$, and $\Psi_0 \in X$ there exists a unique mild solution $\Psi \in C(0, T; X)$ to (2.1) satisfying

$$\Psi(t) = S(t)\Psi_0 - \int_0^t S(t-s)\,B(s)\Psi(s)\,ds \quad \text{for} \quad t \in [0, T]. \tag{2.2}$$

Here $C(0, T; X)$ stands for $C([0, T]; X)$. Moreover, if $\hat{\Psi} \in C(0, T; X)$ denotes the mild solution to (2.1) corresponding to $(\hat{\Psi}_0, \hat{\mu}) \in X \times L^2(0, T; H)$, then by Gronwall's inequality

$$|\Psi - \hat{\Psi}|_{C(0,T;X)} \leq \tilde{M} \left(|\Psi_0 - \hat{\Psi}_0|_X + \int_0^T |\mu(t) - \hat{\mu}(t)|_{\mathcal{L}(H)}\,dt \right), \tag{2.3}$$

for a constant $\tilde{M}$ depending continuously on $|\mu|_{L^1(0,T;\mathcal{L}(H))}$ and $|\Psi_0|_X$.

THEOREM 2.1. *If $\Psi_0 \in \mathcal{V}$ and $\mu \in L^2(0, T; \mathcal{L}(V) \cap \mathcal{L}(H))$, then the mild solution $\Psi \in C(0, T; X)$ to (2.2) satisfies*

$$\Psi(t) \in H^1(0, T; \mathcal{V}^*) \cap C(0, T; \mathcal{V})$$

and

$$\frac{d}{dt}\Psi(t) = (A_0 - B(t))\Psi(t) \text{ a.e. in } (0, T).$$

Moreover $|\Psi(t)|_X = |\Psi_0|_X$ *for all* $t \in [0,T]$*;*

$$|\Psi(t)|_{\mathcal{V}} \le K_1 \exp\left(K_2 \int_0^t |\mu(s)|_{\mathcal{L}(V)}\, ds\right) |\Psi_0|_{\mathcal{V}}$$

for constants K_i *independent of* μ *and* Ψ_0*, and for some* M_1 *depending continuously on its arguments*

$$\left|\frac{d}{dt}\Psi(t)\right|_{L^2(0,T;\mathcal{V}^*)} \le M_1\left(|\mu|_{L^2(0,T;\mathcal{L}(\mathcal{V})\cap\mathcal{L}(H))}, |\Psi_0|_{\mathcal{V}}\right). \tag{2.4}$$

Proof. Consider

$$A_0\Psi(t) = S(t)A_0\Psi_0 - \int_0^t S(t-s)\, A_0 B(s)\Psi(s)\, ds \text{ in } \mathcal{V}^*. \tag{2.5}$$

Adding this equation to (2.2) we find the a priori estimate

$$|\Psi(t)|_{\mathcal{V}} \le K_1|\Psi_0|_{\mathcal{V}} + K_2\int_0^t |B(s)|_{\mathcal{L}(\mathcal{V})}|\Psi(s)|_{\mathcal{V}}\, ds$$

for embedding constants K_1, K_2. By Gronwall's inequality we have

$$|\Psi(t)|_{\mathcal{V}} \le K_1|\Psi_0|_{\mathcal{V}} \exp\left(K_2\int_0^t |\mu(s)|_{\mathcal{L}(V)}\, ds\right) \text{ for } t\in(0,T).$$

This estimate allows us to verify existence of a solution to (2.5) in $C(0,T;\mathcal{V})$, which coincides with the solution to (2.2). By construction we have that $\Psi \in C(0,T; dom_{\mathcal{V}^*}(A_0))$. It follows with standard arguments (see, e.g., [P, p. 107]) applied to (2.2) that Ψ is differentiable almost everywhere in $(0,T)$ and that

$$\frac{d}{dt}\Psi(t) = A_0\Psi(t) - B(t)\Psi(t) \text{ in } \mathcal{V}^* \text{ for a.e. in } (0,T).$$

Hence $\Psi \in H^1(0,T;X)\cap C(0,T;\mathcal{V})$. In fact we have

$$\left|\frac{d}{dt}\Psi\right|_{L^2(0,T;\mathcal{V}^*)} \le K(|\Psi|_{L^2(0,T;\mathcal{V})} + |\mu|_{L^2(0,T;\mathcal{L}(H))}|\Psi|_{C(0,T;H)}),$$

which implies (2.4). Since

$$\frac{1}{2}\frac{d}{dt}|\Psi(t)|_X^2 = \left\langle \frac{d}{dt}\Psi(t), \Psi(t)\right\rangle_{\mathcal{V}^*,\mathcal{V}} = \langle (A_0 - B(t))\,\Psi(t), \Psi(t)\rangle_{\mathcal{V}^*,\mathcal{V}} = 0$$

for a.e. $t\in(0,T)$, it follows that $|\Psi(t)|_X = |\Psi_0|_X$ for all $t\in[0,T]$. ∎

3. Existence of an optimal solution. In this section we provide sufficient conditions for the existence of a solution to

$$\begin{cases} \max\ J(\mu) \text{ over } \mu\in L^2(0,T;U) \\ \text{subject to (2.2),} \end{cases} \tag{3.1}$$

where $J(\mu) = \frac{1}{2}\langle\Psi(T)|O|\Psi(T)\rangle - \frac{\alpha}{2}\int_0^T |\mu(t)|^2\, dt$, with $O\in\mathcal{L}(X)\cap\mathcal{L}(\mathcal{V})$ a self-adjoint positive definite operator. Here $\langle\Psi(T)|O|\Psi(T)\rangle$ stands for $(\Psi(T), O\Psi(T))_X$, with $(\cdot,\cdot)_X$ denoting the inner product in X.

Here U is a closed Hilbert space continuously embedded in $\{\mu \in \mathcal{L}(H) \cap \mathcal{L}(V) : \mu \text{ is self-adjoint}\}$. We assume that there exists a closed subspace $H_1 \subset H$ such that for $X_1 = H_1 \times H_1$ we have

$$\mathcal{V} \cap X_1 \text{ is compactly embedded into } X \tag{3.2}$$

and

$$|\Psi|_{L^2(0,T;\mathcal{V}\cap X_1)} \le M\,(|\Psi_0|_{\mathcal{V}\cap X_1},\, |\mu|_{L^2(0,T;U)}), \tag{3.3}$$

where M depends continuously on its arguments, and Ψ denotes the solution to (2.2). Since

$$J(\mu) \to -\infty \text{ as } |\mu|_{L^2(0,T;U)} \to \infty,$$

there exists a maximizing sequence $\{\mu_n\}$ to (3.1), i.e.,

$$\lim_{n\to\infty} J(\mu_n) = \sup_{\mu \in L^2(0,T;U)} J(\mu) \quad \text{ and } \quad |\mu_n|_{L^2(0,T;U)} \le K,$$

for some K independent of n. Hence there exists a subsequence of $\{\mu_n\}$ denoted by the same symbol and $\bar{\mu} \in L^2(0,T;U)$ such that

$$\mu_n \to \bar{\mu} \text{ weakly in } L^2(0,T;U). \tag{3.4}$$

By (2.4) and (3.3) the sequence $\{\Psi_n\}$ is bounded in $L^2(0,T;X_1\cap\mathcal{V})$ and the sequence $\{\frac{d}{dt}\Psi_n\}$ is bounded in $L^2(0,T;\mathcal{V}^*)$, where $\Psi_n = \Psi(\mu_n)$ denotes the solution to (2.2) with μ replaced by μ_n. By Aubin's lemma, e.g., [CF], there exists $\bar{\Psi} \in H^1(0,T;\mathcal{V}^*)\cap L^2(0,T;\mathcal{V}\cap X_1)$ such that for a further subsequence

$$\Psi_n \to \bar{\Psi} \text{ strongly in } L^2(0,T;X) \tag{3.5}$$

and weakly in $L^2(0,T;\mathcal{V})$. For φ and ψ in X the mapping $B \to (B\varphi,\psi)_X, B \in U$, defines a bounded linear functional in U. Hence by the Riesz representation theorem there exists $F = F(\varphi,\psi) \in U$ such that

$$(B\varphi,\psi)_X = (F(\varphi,\psi),\mu)_U \text{ for all } \mu \in U, \text{ where } B = \begin{pmatrix} 0 & \mu \\ -\mu & 0 \end{pmatrix}. \tag{3.6}$$

Note that $F : X \times X \to U$ is a continuous, bilinear mapping satisfying

$$F(\varphi,\psi) = -F(\psi,\varphi).$$

Moreover, if $\psi_n \to \psi$ strongly in $L^2(0,T;X)$ and $\varphi_n \to \varphi$ strongly in $C(0,T;X)$ we have

$$F(\varphi_n,\psi_n) \to F(\varphi,\psi) \text{ in } L^2(0,T;U). \tag{3.7}$$

Taking the inner product in $L^2(0,T;X)$ of

$$\Psi_n(t) = S(t)\Psi_0 - \int_0^t S(t-s)\,B_n(s)\,\Psi_n(s)\,ds$$

with an arbitrary $\Phi \in L^2(0,T;X)$ implies that

$$\int_0^T (\Psi_n(t), \Phi(t))_X\, dt = \int_0^T (S(t)\Psi_0, \Phi(t))_X\, dt + \int_0^T \left(F\left(\int_\cdot^T S^*(t-\cdot)\Phi(t)\, dt, \Psi_n \right), B_n \right)_U ds.$$

From (3.4), (3.5), and (3.7) we deduce that

$$\begin{aligned}\int_0^T (\Psi(t), \Phi(t))_X\, dt &= \int_0^T (S(t)\Psi_0, \Phi(t))_X\, dt + \int_0^T \left(F\left(\int_\cdot^T S^*(t-\cdot)\Phi(t)\, dt, \Psi \right), B \right)_U ds \\ &= \int_0^T (S(t)\Psi_0, \Phi(t))_X\, dt - \int_0^T \left(\int_0^t S(t-s)\, B(s)\, \Psi(s)\, ds, \Phi(t) \right)_X dt.\end{aligned}$$

Since Φ was arbitrary we find

$$\bar\Psi(t) = S(t)\Psi_0 - \int_0^t S(t-s)\, \bar B(s)\, \bar\Psi(s)\, ds,$$

and thus $\bar\Psi$ is the unique solution to (2.2) with μ replaced by $\bar\mu$.

We next verify that

$$\Psi_n(T) \to \bar\Psi(T) \text{ strongly in } X. \tag{3.8}$$

For this purpose set $\Phi_n = \Psi_n - \bar\Psi$, and choose K such that

$$\max(|\Phi_n|_{L^2(0,T;\mathcal{V}^*)}, |\Phi_n|_{C(0,T;\mathcal{V}\cap X_1)}) \le K.$$

Due to (3.2) there exists [CF, p. 96], for every $\epsilon > 0$, a constant c_ϵ such that

$$|\Phi_n(T)|_X \le \epsilon |\Phi_n(T)|_{\mathcal{V}\cap X_1} + c_\epsilon |\Phi_n(T)|_{\mathcal{V}^*} \le \epsilon K + c_\epsilon |\Phi_n(T)|_{\mathcal{V}^*}. \tag{3.9}$$

By Hölder's inequality we have

$$\begin{aligned} |\ \Phi_n(T)|_{\mathcal{V}^*} &= \left| \frac{1}{\epsilon} \int_{T-\epsilon}^T \Phi_n(s)\, ds + \frac{1}{\epsilon} \int_{T-\epsilon}^T (s-T+\epsilon) \frac{d}{ds} \Phi_n'(s)\, ds \right|_{\mathcal{V}^*} \\ &\le \frac{1}{\epsilon} \left| \int_{T-\epsilon}^T \Phi_n(s)\, ds \right|_{\mathcal{V}^*} + \frac{1}{\epsilon} \left(\int_{T-\epsilon}^T (s-T+\epsilon)^2\, ds \right)^{\frac12} \left(\int_{T-\epsilon}^T \left| \frac{d}{ds} \Phi'(s) \right|_{\mathcal{V}^*} ds \right)^{\frac12} \\ &\le \frac{1}{\epsilon} \left| \int_{T-\epsilon}^T \Phi_n(s)\, ds \right|_{\mathcal{V}^*} + \frac{\sqrt{\epsilon}\, K}{\sqrt{3}}, \end{aligned}$$

and with (3.9)

$$|\Phi_n(T)|_X \leq \epsilon K + \frac{\sqrt{\epsilon}\, K}{\sqrt{3}} + \frac{1}{\epsilon}\left|\int_{T-\epsilon}^{T} \Phi_n(s)\, ds\right|_{\mathcal{V}^*}.$$

Since $\Phi_n \to 0$ weakly in $L^2(0,T;\mathcal{V})$ we have $\frac{1}{\epsilon}|\int_{T-\epsilon}^{T} \Phi_n(s)\, ds|_{\mathcal{V}^*} \to 0$ as $n \to \infty$ for every fixed $\epsilon > 0$. We conclude that (3.8) holds.

Weak lower-semicontinuity of norms and (3.8) imply that

$$J(\bar{\mu}) \geq \sup_{\mu} J(\mu)$$

and hence $\bar{\mu}$ is an optimal solution to (3.1). We thus proved the following result.

THEOREM 3.1. *If $\Psi_0 \in X_1 \cap \mathcal{V}$ and (3.2), (3.3) hold, then (3.1) admits a solution $\bar{\mu} \in L^2(0,T;U)$.*

Example 3.1. The control space in (3.1) is $\mathcal{U} = L^2(0,T;U)$. Here we consider the special case of a scalar-valued control coupling a time-dependent control amplitude ϵ with a fixed time-independent self-adjoint moment operator $\tilde{\mu} \in \mathcal{L}(V) \cap \mathcal{L}(H)$, i.e., we consider the closed subspace of $\mathcal{U}$ given by

$$\widehat{\mathcal{U}} = \{\epsilon\tilde{\mu} : \epsilon \in L^2(0,T;\mathbb{R})\},$$

which is isomorphic to $L^2(0,T;\mathbb{R})$. In this case U is the one dimensional space $\{\epsilon\tilde{\mu} : \epsilon \in \mathbb{R}\}$, which is endowed with the inner product of $\mathbb{R}$. The resulting control cost is $\frac{\alpha}{2}\int_0^T |\epsilon(t)|^2 dt$ and the bilinear mapping $F : X \times X \to U = \mathbb{R}$ is given by

$$F(\phi,\psi) = (\tilde{B}\phi,\psi)_X = (\tilde{\mu}(\phi_2),\psi_1)_H - (\tilde{\mu}(\phi_1),\psi_2)_H,$$

with $\tilde{B} = \left(\begin{smallmatrix} 0 & \tilde{\mu} \\ -\tilde{\mu} & 0 \end{smallmatrix}\right)$. The resulting optimality condition has the form

$$\alpha\bar{\epsilon} + (\tilde{B}\bar{\Psi}(t),\bar{\chi})_X = 0.$$

Example 3.2. Let $H = L^2(\Omega)/\mathbb{R}$ with $\Omega = (0,1)$ and $H_0 = -\Delta$ with periodic boundary conditions. Then $V = H^1_P(\Omega)$, the space of $H^1(\Omega)$ functions with periodic boundary conditions $\phi(0) = \phi(1)$. The control space is taken as multiplication operators by elements $\mu \in H^1_P(\Omega)$ and we identify U with $H^1(\Omega)_p$. Note that $\phi \to \mu\phi$ defines a self-adjoint element in $\mathcal{L}(H) \cap \mathcal{L}(V)$, since $H^1(\Omega)$ is a Banach algebra in dimension one. For $\phi \in X = H \times H$ and $\psi \in X = H \times H$ the element $F(\phi,\psi) \in V$ is the solution to

$$(F(\phi,\psi),\mu)_{H^1} = (\mu\phi^2,\psi^1)_H - (\mu\phi^1,\psi^2)_H \text{ for all } \mu \in V.$$

Thus the optimality condition can be expressed as

$$\alpha\mu(t) + (-\Delta + I)^{-1}(\Psi^2(t)\chi^1(t) - \Psi^1(t)\chi^2(t)) = 0,$$

where $\Psi, \chi \in C(0,T;\mathcal{V})$. Note that this implies additional spatial regularity of the optimal solution.

Example 3.3. Let H_0, H, V, and Ω be as in the previous example. Define

$$\tilde{U} = \{\tilde{\mu} \in L^2(\Omega) : \tilde{\mu}(x) = \tilde{\mu}(-x) \text{ for } x \in \Omega\}$$

endowed with the canonical inner product. Each $\tilde\mu$ can be uniquely identified with a self-adjoint operator $\mu \in \mathcal{L}(H)$ given by

$$\mu(\phi)(x) = \int_\Omega \tilde\mu(x-y)\phi(y)\,dy,$$

where $\tilde\mu$ is extended periodically from Ω to $\mathbb{R}$. All such operators also satisfy $\mu \in \mathcal{L}(V)$. The set of all these operators constitutes the control space U. The resulting penalty term in the cost functional J has the form

$$\frac{\alpha}{2}\int_0^T |\tilde\mu(t,\cdot)|^2_{L^2(\Omega)}\,dt.$$

Using symmetry of $\tilde\mu$ it can be shown that for ϕ, ψ in $X = H \times H$ the element $F \in L^2(\Omega)$ satisfying

$$(F(\phi,\psi),\tilde\mu)_{L^2(\Omega)} = (\mu\phi^2,\psi^1)_{L^2(\Omega)} - (\mu\phi^1,\psi^2)_{L^2(\Omega)} \text{ for all } \mu \in U$$

is given by

$$F(\phi,\psi)(x) = \frac{1}{2}\int_\Omega \big(\phi^2(y)\psi^1(x+y) + \phi^2(y)\psi^1(-x+y) \\ - \phi^1(y)\psi^2(x+y) - \phi^1(y)\psi^2(-x+y)\big)\,dy.$$

The resulting optimality condition is

$$\alpha\tilde\mu(t,x) + \frac{1}{2}\int_\Omega \big(\Psi^2(t,y)\chi^1(t,x+y) + \Psi^2(t,y)\chi^1(t,-x+y) \\ - \Psi^1(t,y)\chi^2(t,x+y) - \Psi^1(t,y)\chi^2(t,-x+y)\big)\,dy = 0.$$

Analogous results can be obtained with $\Omega = (0,1)$ replaced by bounded cubes in $\mathbb{R}^n$ with H_0 satisfying periodic boundary conditions, or with $\Omega = \mathbb{R}^n$.

Example 3.4. Let $H_0 = -\Delta$ in $H = L^2(\mathbb{R}^n)$. Then H_0 is densely defined with $dom(H_0) = H^2(\mathbb{R}^n)$ and self-adjoint (see, e.g., [K]), with spectrum consisting of continuous spectrum given by $[0,\infty)$. We set $\mathcal{H} = \{\varphi \in L^2(\mathbb{R}^n) : \int_{\mathbb{R}^n}(1+|x|^2)\varphi(x)^2 < \infty\}$. To verify (3.2) let $\{f_n\}_{n=1}^\infty$ be a bounded sequence in $H_1 = V \cap \mathcal{H} = dom(H_0^{\frac{1}{2}}) \cap \mathcal{H}$. For $r \in N$ set $\Omega_r = \{x \in \mathbb{R}^n : |x|_{\mathbb{R}^n} \le r\}$. Extract a subsequence of $\{f_n\}$ that converges weakly in H_1 to some $f \in H_1$. Using compactness of $\{\phi|_{\Omega_r} : \phi \in V\}$ in $L^2(\Omega_r)$ successively extract further subsequences whose restriction to Ω_r converges strongly in $L^2(\Omega_r)$ to f, for $r = 1, 2, \ldots$. Let $\{f_{n_k}\}$ denote the sequence which arises from diagonalization of the above procedure. The restriction to Ω_r of this sequence converges strongly in $L^2(\Omega_r)$ to the restriction of f to Ω_r for each $r \in N$. Strong convergence of $\{f_{n_k}\}$ to $\{f\}$ in $L^2(\mathbb{R}^n)$ follows from the following estimate:

$$\int_{\mathbb{R}^n} |f - f_{n_k}|^2\,dx = \int_{\Omega_r} |f - f_{n_k}|^2\,dx + \int_{\mathbb{R}^n\setminus\Omega_r} |f - f_{n_k}|^2\,|x|^2\,\frac{dx}{|x|^2} \\ \le \int_{\Omega_r} |f - f_{n_k}|^2\,dx + \frac{1}{r^2}\int_{\mathbb{R}^n\setminus\Omega_r} |f - f_{n_k}|^2|x|^2\,dx \le \int_{\Omega_r} |f - f_{n_k}|^2\,dx + \frac{4}{r^2}C,$$

where C is the common bound for $\{f_{n_k}\}$ and f in H_1. Hence $dom(H_0^{\frac{1}{2}}) \cap \mathcal{H}$ is compactly embedded in H and (3.2) follows.

Turning to (3.3), consider, for $X = L^2(\mathbb{R}^n) \times L^2(\mathbb{R}^n)$,

$$\begin{aligned}
&\langle \tfrac{d}{dt}\Psi(t), |x|^2\Psi(t)\rangle = \tfrac{1}{2}\tfrac{d}{dt}\langle \Psi(t), |x|^2\Psi(t)\rangle \\
&= \langle A_0\Psi(t), |x|^2\Psi(t)\rangle - (B(t)\Psi(t), |x|^2\Psi(t))_X \\
&= (-\Delta\Psi_2, |x|^2\Psi_1)_H + (\Delta\Psi_1, |x|^2\Psi_2)_H - ((\mu(t)\Psi_2, |x|^2\Psi_1)_H - (\mu(t)\Psi_1, |x|^2\Psi_2)_H) \\
&= 2(\nabla\Psi_2(t), x\Psi_1(t))_H - 2(\nabla\Psi_1(t), x\Psi_2(t))_H \\
&\le |\nabla\Psi_1(t)|_H^2 + |\nabla\Psi_2(t)|_H^2 + \big|\,|x|\Psi_1(t)\big|_H^2 + \big|\,|x|\Psi_2(t)\big|_H^2,
\end{aligned}$$

and hence

$$\frac{1}{2}\frac{d}{dt}\big|\,|x|\Psi(t)\big|_X^2 \le K|\Psi|_{\mathcal{V}}^2 + \big|\,|x|\Psi(t)\big|_X^2$$

for a constant K satisfying $|\nabla\phi| \le K|\phi|_{\mathcal{V}}$ for all $\phi \in \mathcal{V}$. Gronwall's inequality and Theorem 2.1 imply the existence of a constant $\tilde{M} = \tilde{M}(|\Psi_0|_{\mathcal{V}\cap X_1}, |B|_{L^2(0,T;\mathcal{L}(\mathcal{V})\cap\mathcal{L}(X))})$ such that

$$|\Psi|_{C(0,T;\mathcal{V}\cap X_1)} \le \tilde{M},$$

which, in particular, implies (3.3).

4. Necessary optimality condition.

We now derive a first order necessary optimality system for (3.1).

THEOREM 4.1. *Let* $(\bar{\mu}, \bar{\Psi}) = (\bar{\mu}, \Psi(\bar{\mu}))$ *be an optimal pair for* (3.1) *and assume that* $\Psi_0 \in \mathcal{V}$ *and* $O\,\bar{\Psi}(T) \in \mathcal{V}$. *Then*

$$\begin{aligned}
&\tfrac{d}{dt}\,\bar{\Psi}(t) = (A_0 - \bar{B}(t))\bar{\Psi}(t), && \bar{\Psi}(0) = \Psi_0 && \textit{(primal equation)},\\
&\tfrac{d}{dt}\,\bar{\chi}(t) = (A_0 - \bar{B}(t))\bar{\chi}(t), && \chi(T) = O\bar{\Psi}(T) && \textit{(adjoint equation)},\\
&\alpha\bar{\mu}(t) + F(\bar{\Psi}(t),\, \bar{\chi}(t)) = 0 && && \textit{(optimality)},
\end{aligned}$$

where the adjoint state satisfies $\bar{\chi} \in H^1(0,T;\mathcal{V}^*) \cap C(0,T;\mathcal{V})$ *and* $\bar{B} = \begin{pmatrix} 0 & \bar{\mu} \\ -\bar{\mu} & 0 \end{pmatrix}$.

Proof. For any $\mu \in L^2(0,T;U)$ we have

$$J(\mu) - J(\bar{\mu}) = -\alpha\,(\bar{\mu}, \mu - \bar{\mu})_{L^2(0,T;U)} - \frac{\alpha}{2}|\mu - \bar{\mu}|^2_{L^2(0,T;U)}$$

$$+(\Psi(T) - \bar{\Psi}(T), O\bar{\Psi}(T))_X + \frac{1}{2}(\Psi(T) - \bar{\Psi}(T), O(\Psi(T) - \bar{\Psi}(T))\,)_X.$$

Let $\bar{\chi}(t) \in H^1(0,T;\mathcal{V}^*) \cap C(0,T; dom\,\mathcal{V})$ be the solution to the adjoint equation

$$\frac{d}{dt}\bar{\chi}(t) = (A_0 - \bar{B}(t))\bar{\chi}(t), \quad \chi(T) = O\bar{\Psi}.$$

Then,

$$\begin{aligned}
&(\Psi(T) - \bar{\Psi}(T), O\bar{\Psi}(T)) = \int_0^T \left\langle \frac{d}{dt}(\Psi(t) - \bar{\Psi(t)}), \bar{\chi}(t)\right\rangle + \left\langle \Psi(t) - \bar{\Psi(t)}, \frac{d}{dt}\bar{\chi}(t)\right\rangle\, dt \\
&= \int_0^T [\langle (A_0 - B(t))\Psi(t) - (A_0 - \bar{B}(t))\bar{\Psi}(t), \bar{\chi}(t)\rangle + \langle \Psi(t) - \bar{\Psi}(t), (A_0 - \bar{B}(t))\bar{\chi}(t)\rangle]\, dt \\
&= -\int_0^T ((B(t) - \bar{B}(t))\Psi(t), \bar{\chi}(t))_X\, dt \\
&= -\int_0^T \big((B(t) - \bar{B}(t))(\Psi(t) - \bar{\Psi}(t)), \bar{\chi}(t)\big)_X\, dt - \int_0^T \big((B(t) - \bar{B}(t))\bar{\Psi}(t), \bar{\chi}(t)\big)_X\, dt,
\end{aligned}$$

where $\langle\cdot,\cdot\rangle$ denotes the duality pairing between $\mathcal{V}$ and $\mathcal{V}^*$. Hence

$$J(\mu)-J(\bar\mu)=-\int_0^T\left(\alpha\bar\mu(t)+F(\bar\Psi(t),\bar\chi(t)),\mu(t)-\bar\mu(t)\right)_U$$
$$-\int_0^T\left((B(t)-\bar B(t))(\Psi(t)-\bar\Psi(t)),\bar\chi(t)\right)_X dt$$
$$-\frac{\alpha}{2}\,|\mu-\bar\mu|^2_{L(0,T;U)}+\frac{1}{2}\,(\Psi(T)-\bar\Psi(T),O(\Psi(T)-\bar\Psi(T))\,)_X.$$

Taking the limit $\mu\to\bar\mu$ and using (2.3) we obtain the claim. □

5. An algorithm and its convergence. The following algorithm for solving the optimality system in case of scalar-valued controls was proposed in [ZR] and further developed in [TKO], [MT].

ALGORITHM.

(i) Choose $\delta\in[0,2]$, $\eta\in[0,2]$, $\tilde\mu^0\in L^2(0,T;U)$, $\chi^0\in C(0,T;X)$.

For $k=1,2,\ldots$ until convergence

(ii)

$$\tfrac{d}{dt}\Psi^k(t)=(A_0-B^k(t))\Psi^k(t),\quad \Psi^k(0)=\Psi_0,$$

$$\mu^k=(1-\delta)\tilde\mu^{k-1}-\tfrac{\delta}{\alpha}F(\Psi^k,\chi^{k-1}),$$

(iii)

$$\tfrac{d}{dt}\chi^k(t)=(A_0-\tilde B^k(t))\chi^k(t),\quad \chi^k(T)=O\Psi^k(T),$$

$$\tilde\mu^k=(1-\eta)\,\mu^k-\tfrac{\eta}{\alpha}F(\Psi^k,\chi^k).$$

First we prove the well-posedness of the algorithm.

PROPOSITION 5.1. *Let $\psi_0\in\mathcal{V}$, $\mu\in L^2(0,T;U)$, and $\chi\in C(0,T;X)$. Then there exists a unique solution $\Psi\in H^1(0,T;\mathcal{V}^*)\cap C(0,T;\mathcal{V})$ to*

$$\Psi(t)=S(t)\Psi_0-\int_0^t S(t-s)B(\Psi)(s)\Psi(s)\,ds, \tag{5.1}$$

where $B=B(\mu)$, with $\mu(\Psi)(t)=(1-\delta)\mu(t)-\frac{\delta}{\alpha}F(\Psi(t),\chi(t))$. Analogously, if $\Psi\in C(0,T;X)$, then there exists a unique solution $\chi\in H^1(0,T;\mathcal{V}^*)\cap C(0,T;\mathcal{V})$ to

$$\chi(t)=S^*(T-t)O\Psi(T)+\int_t^T S^*(s-t)\tilde\mu(\chi)(s)\,ds,$$

where $\tilde\mu(\chi)(t)=(1-\eta)\mu(t)-\frac{\eta}{\alpha}F(\Psi(t),\chi(t))$.

Proof. We verify the first claim by a continuation argument. The second one can be proved analogously. For any Ψ and $\hat\Psi$ in $C(0,T;X)$ we have

$$|B(\Psi)(t)-B(\hat\Psi)(t)|\le M|\Psi(t)-\hat\Psi(t)|_X,$$

where $M=\tilde M\frac{\delta}{\alpha}|\chi|_{C(0,T;X)}$ and $\tilde M$ is an embedding constant. Consider the iteration

$$\Psi_n=S(t)\Psi_0+\int_0^t S(t-s)B(\Psi_{n-1})(s)\Psi_n(s)\,ds,$$

which is initialized by the constant with value Ψ_0. It is well defined by Theorem 2.1, and $|\Psi_n(t)|_X = |\Psi_0|_X$ for all n and $t \geq 0$. For consecutive iterates we find

$$\begin{aligned}
&\tfrac{1}{2}\tfrac{d}{dt}|\Psi_{n+1}(t) - \Psi_n(t)|_X^2 \\
&= ((A_0 - B(\Psi_n))(t)(\Psi_{n+1}(t) - \Psi_n(t)) \\
&\quad -(B(\Psi_n)(t) - B(\Psi_{n-1})(t))\Psi_n(t), \Psi_{n+1}(t) - \Psi_n(t)) \\
&\quad \leq \tfrac{M^2}{2}|\Psi_{n+1}(t) - \Psi_n(t)|^2 + \tfrac{1}{2}|\Psi_n(t) - \Psi_{n-1}(t)|^2.
\end{aligned}$$

Hence for every $\tau \in (0, T]$ and $t \in (0, \tau]$

$$|\Psi_{n+1}(t) - \Psi_n(t)|_X^2 \leq \frac{1}{M^2}(e^{M^2\tau} - 1) \max_{t\in[0,\tau]} |\Psi_n(t) - \Psi_{n-1}(t)|_X.$$

Selecting $\tau > 0$ sufficiently small so that $\theta = \frac{1}{M^2}(e^{M^2\tau} - 1) < 1$ implies that

$$|\Psi_{n+1} - \Psi_n|_{C(0,\tau;X)} \leq \theta^n |\Psi_1 - \Psi_0|_{C(0,T;X)} \to 0$$

as $n \to \infty$. By standard arguments existence of a solution to (5.1) on $[0, \tau]$ follows. Since τ only depends on M, this solution can be extended to a solution $\Psi \in C(0, T; X)$. Uniqueness follows by Gronwall's inequality. Another application of Theorem 2.1 guarantees that $\Psi \in H^1(0, T; \mathcal{V}^*) \cap C(0, T; \mathcal{V})$. □

THEOREM 5.2. *Assume that* $(\delta, \eta) \neq (0, 0)$, *that* $\Psi_0 \in \mathcal{V} \cap X_1$, *and that* (3.2), (3.3) *hold. Then the sequence* $\{\mu^k, \tilde{\mu}^k, \Psi^k, \chi^k\}$ *contains a subsequence which converges strongly in* $L^2(0, T; U) \times L^2(0, T; U) \times C(0, T; X) \times C(0, T; X)$ *and every such subsequence converges to some* (μ, μ, Ψ, χ), *where* (μ, Ψ, χ) *is a solution of the optimality system.*

Proof. For $k \geq 2$ and $\delta, \eta \in [0, 2]$

$$\begin{aligned}
J(\mu^k) - J(\mu^{k-1}) &= \tfrac{1}{2}(\Psi^k(T) - \Psi^{k-1}(T), O(\Psi^k(T) - \Psi^{k-1}(T)))_X \\
&+\tfrac{\alpha}{2}\int_0^T (\tfrac{2}{\delta} - 1)|\mu^k - \tilde{\mu}^{k-1}|_U^2 + (\tfrac{2}{\eta} - 1)|\mu^{k-1} - \tilde{\mu}^{k-1}|_U^2\, dt \geq 0.
\end{aligned} \tag{5.2}$$

If $\delta = 0$ or $\eta = 0$, then $\mu^k = \tilde{\mu}^{k-1}$, respectively, $\mu^{k-1} = \tilde{\mu}^{k-1}$, and the corresponding terms in (5.2) are dropped. This inequality will be verified at the end of the proof, in an analogous way as in the scalar case which was treated in [ZR], [MT].

From (5.2) it follows that $J(\mu^k)$ is monotonically increasing. Since $J(\mu)$ is bounded from above this implies that $\lim_{k\to\infty} J(\mu^k)$ exists. Recall that $|\Psi^k(t)|_X = |\Psi_0|_X$ and $|\chi^k(t)|_X \leq \|O\||\Psi_0|_X$ for all k and $t \in [0, T]$. It thus follows that

$$J(\mu^0) \leq J(\mu^k) = \frac{1}{2}(\Psi^k(T), O\Psi^k(T))_X - \frac{\alpha}{2}|\mu^k|_{L^2(0,T;U)}^2,$$

and hence

$$\frac{\alpha}{2}|\mu^k|_{L^2(0,T;U)}^2 \leq \frac{1}{2}|\Psi_0|_X^2\|O\|_{\mathcal{L}(X)} - J(\mu^0).$$

Moreover,

$$|\tilde{\mu}^k|_{L^2(0,T;U)} \leq |1 - \eta|\, |\mu^k|_{L^2(0,T;U)} + \frac{\eta}{2}|\Psi_0|_X^2\|O\|_{\mathcal{L}(X)},$$

and hence

$$\{\mu^k\}_{k=1}^\infty \text{ and } \{\tilde{\mu}^k\}_{k=1}^\infty \text{ are bounded in } L^2(0, T; U). \tag{5.3}$$

From Theorem 2.1 and assumptions (3.2) and (3.3), therefore,

$$\{\Psi^k\}_{k=1}^\infty \text{ and } \{\chi^k\}_{k=1}^\infty \text{ are bounded in } H^1(0,T;\mathcal{V}^*)\cap L^2(0,T;\mathcal{V}\cap X_1).$$

By Aubin's lemma there exists a subsequence $\{k^n\}$ of $\{k\}$ and $\Psi \in C(0,T;X)$, $\chi \in C(0,T;X)$ such that

$$\Psi^{k_n} \to \Psi \text{ and } \chi^{k_n} \to \chi \text{ strongly in } L^2(0,T;X).$$

Using the boundedness of $\{\Psi^{k_n}\}$ and $\{\chi^{k_n}\}$ in $C(0,T;X)$ and the properties of F one argues that $F(\Psi^{k_n},\chi^{k_n}) \to F(\Psi,\chi)$ strongly in $L^2(0,T;U)$. From (iii) of the algorithm we have

$$\eta\mu^{k_n} = \mu^{k_n} - \tilde{\mu}^{k_n} - \frac{\eta}{\alpha}F(\Psi^{k_n},\chi^{k_n}).$$

Since $\mu^{k_n} - \tilde{\mu}^{k_n} \to 0$ in $L^2(0,T;U)$ by (5.2), it follows, for $\eta \neq 0$, that μ^{k_n} converges strongly in $L^2(0,T;U)$ to some μ, as $k_n \to \infty$. For each k_n we have the following by (ii) of the algorithm:

$$\Psi^{k_n}(t) = S(t)\Psi_0 - \int_0^t S(t-s)B^{k_n}(s)\Psi^{k_n}(s)\,ds. \tag{5.4}$$

Let $\Psi \in C(0,T;X)$ denote the solution to

$$\Psi(t) = S(t)\Psi_0 - \int_0^t S(t-s)B(s)\Psi(s)\,ds. \tag{5.5}$$

From Gronwall's inequality it follows that $\Psi^{k_n} \to \Psi$ in $C(0,T;X)$. By (5.2) the sequence $\{\tilde{\mu}^{k_n}\}$ converges strongly in $L^2(0,T;U)$ to μ. Step (iii) of the algorithm implies that

$$\chi^{k_n}(t) = S^*(T-t)O\Psi^{k_n}(T) + \int_t^T S^*(s-t)\tilde{B}^{k_n}(s)\chi^{k_n}(s)\,ds. \tag{5.6}$$

Let χ in $C(0,T;X)$ denote the solution to

$$\chi(t) = S^*(T-t)O\Psi(T) + \int_t^T S^*(s-t)B(s)\chi(s)\,ds. \tag{5.7}$$

Again by Gronwall's lemma we find that $\chi^{k_n} \to \chi$ in $C(0,T;X)$. Passing to the limit in the second equation of (iii) implies that

$$\alpha B + F(\Psi,\chi) = 0. \tag{5.8}$$

For $\eta = 0$ there exists a subsequence $\{k^n\}$ of $\{k\}$ and $\bar{\Psi} \in C(0,T;X)$, $\bar{\chi} \in C(0,T;X)$ such that

$$\Psi^{k_n} \to \bar{\Psi} \text{ and } \chi^{k_n} \to \bar{\chi} \text{ strongly in } L^2(0,T;X).$$

By (5.2) and since $\tilde{\mu}^k = \mu^k$ for $\eta = 0$ we have $\lim_{n\to\infty} \mu^{k_n-1} - \mu^{k_n} = 0$ in $L^2(0,T;U)$. From

$$\mu^{k_n} = (1-\delta)\mu^{k_n-1} - \frac{\delta}{\alpha}F(\Psi^{k_n},\chi^{k_n-1})$$

it therefore follows that μ^{k_n-1} converges strongly to some μ in $L^2(0,T;U)$. By (5.2) also $\lim_{n\to\infty}\mu^{k_n} = \mu$ in $L^2(0,T;U)$. As before, the solutions to (5.4) and (5.6) converge strongly in $C(0,T;X)$ to the solutions of (5.5) and (5.7), and (5.8) also holds for $\eta = 0$. From (5.5), (5.7), and (5.8) we conclude that (μ,Ψ,χ) is a solution to the optimality system.

We now provide the proof of (5.2) for the case $\eta \neq 0, \delta \neq 0$. The remaining cases follow easily. We have

$$J(\mu^{k+1}) - J(\mu^k) = \frac{1}{2}(\,\Psi^{k+1}(T) - \Psi^k(T), O\,(\Psi^{k+1}(T) - \Psi^k(T))\,)_X$$
$$+(\Psi^{k+1}(T) - \Psi^k(T), O\,\Psi^k(T))_X + \frac{\alpha}{2}\int_0^T |\mu^{k+1}|^2 - \frac{\alpha}{2}\int_0^T |\mu^k|^2.$$

Suppressing the dependence of Ψ^k and μ^k on t we find

$$\begin{aligned}
&(\Psi^{k+1}(T) - \Psi^k(T), O\,\Psi^k(T))_X = (\Psi^{k+1}(T) - \Psi^k(T), \chi^k(T))_X \\
&= \int_0^T \left(\frac{\partial}{\partial t}(\Psi^{k+1} - \Psi^k), \chi^k\right)_X + \left(\Psi^{k+1} - \Psi^k, \frac{\partial}{\partial t}\chi^k\right)_X \\
&= \int_0^T ((A_0 - B^{k+1})\Psi^{k+1} - (A_0 - B^k)\Psi^k, \chi^k)_X + (\Psi^{k+1} - \Psi^k, (A_0 - \tilde{B}^k)\chi^k)_X \\
&= \int_0^T ((\tilde{B}^k - B^{k+1})\Psi^{k+1}, \chi^k)_X + ((B^k - \tilde{B}^k)\Psi^k, \chi^k)_X \\
&= \int_0^T (F(\Psi^{k+1}, \chi^k), \tilde{\mu}^k - \mu^{k+1})_U + (F(\Psi^k, \chi^k), \mu^k - \tilde{\mu}^k)_U \\
&= \alpha\int_0^T \frac{1}{\delta}(\tilde{\mu}^k - \mu^{k+1}, (1-\delta)\tilde{\mu}^k - \mu^{k+1})_U + \frac{1}{\eta}(\tilde{\mu}^k - \mu^k, (1-\eta)\mu^k - \tilde{\mu}^k)_U \\
&= \alpha\int_0^T \frac{1}{\delta}|\tilde{\mu}^k - \mu^{k+1}|_U^2 + \frac{1}{\eta}|\tilde{\mu}^k - \mu^k|_U^2 - (\tilde{\mu}^k - \mu^{k+1}, \tilde{\mu}^k)_U - (\mu^k - \tilde{\mu}^k, \mu^k)_U.
\end{aligned}$$

Hence we find

$$\begin{aligned}
&J(\mu^{k+1}) - J(\mu^k) = \frac{1}{2}(\,\Psi^{k+1}(T) - \Psi^k(T), O\,(\Psi^{k+1}(T) - \Psi^k(T))\,)_X \\
&+(\,\Psi^{k+1}(T) - \Psi^k(T), O\,\Psi^k(T)\,)_X - \frac{\alpha}{2}\int_0^T |\mu^{k+1}|_U^2 + \frac{\alpha}{2}\int_0^T |\mu^k|^2 \\
&= \frac{1}{2}(\,\Psi^{k+1}(T) - \Psi^k(T), O\,(\Psi^{k+1}(T) - \Psi^k(T))\,)_X \\
&+\frac{\alpha}{2}\int_0^T \left(\left(\frac{2}{\delta} - 1\right)|\tilde{\mu}^k - \mu^{k+1}|_U^2 + \left(\frac{2}{\eta} - 1\right)|\mu^k - \tilde{\mu}^k|_U^2\right)dt \geq 0. \qquad \square
\end{aligned}$$

In [S] it is argued that the set of limit points is in fact compact. Moreover, if the penalty parameter α is sufficiently large, then the limit set consists of a singleton.

In the previous theorem subsequential convergence followed under the assumption of compactness of the orbits implied by (3.2), (3.3). Alternatively a compactness assumption for U as a subset of $\mathcal{L}(X)$ also implies convergence.

THEOREM 5.3. *Assume that $(\delta,\eta) \neq (0,0)$, that $\Psi_0 \in \mathcal{V}$, $\chi^0 \in H^1(0,T;X)$, $\tilde{\mu} \in H^1(0,T;U)$, and that U is a compact subset of $\mathcal{L}(X)$. Then the conclusion of Theorem 5.2 holds.*

Proof. As in the proof of Theorem 5.2 $\{\mu^k\}_{k=1}^\infty$ and $\{\tilde{\mu}^k\}_{k=1}^\infty$ are bounded in $L^2(0,T;U)$, and by Theorem 3.1

$$\{\Psi^k\}_{k=1}^\infty \text{ and } \{\chi^k\}_{k=1}^\infty \text{ are bounded in } H^1(0,T;\mathcal{V}^*) \cap C(0,T;\mathcal{V}).$$

This implies that $\{F(\Psi^k,\chi^{k-1})\}_{k=1}^\infty$ and $\{F(\Psi^k,\chi^k)\}_{k=1}^\infty$ are bounded in $H^1(0,T;U)$. If $\delta=\eta=1$, then $\{\mu^k\}$ and $\{\tilde{\mu}^k\}$ are bounded in $H^1(0,T;U)$. Otherwise

$$\tilde{\mu}^k = (1-\eta)(1-\delta)\tilde{\mu}^{k-1} + (1-\eta)\frac{\delta}{\alpha}F(\Psi^k,\chi^{k-1}) - \frac{\eta}{\alpha}F(\Psi^k,\chi^k),$$

with $|(1-\eta)(1-\delta)| < 1$. It follows that μ^k and $\tilde{\mu}^k$ are bounded in $H^1(0,T;U)$. Hence there exists a subsequence $\{k_n\}$ of $\{k\}$ and $\mu \in H^1(0,T;U), \tilde{\mu} \in H^1(0,T;U)$ such that

$$\mu^{k_n} \to \mu, \quad \text{and} \quad \tilde{\mu}^{k_n} \to \tilde{\mu} \text{ strongly in } L^2(0,T;\mathcal{L}(X)).$$

By (5.2) we have $|\mu_k - \tilde{\mu}_k|_{L^2(0,T;\mathcal{L}(X))} \to 0$ if $\eta \neq 0$, whereas $\mu_k = \tilde{\mu}_k$ if $\eta = 0$. In either case it follows that $\mu = \tilde{\mu}$. The proof can now be completed as the one for Theorem 5.2. ∎

Acknowledgments. We would like to thank Prof. A. Borzi for interesting discussions on various aspects of this paper and Dr. J. Salomon for providing us with a preprint of [S].

REFERENCES

[BMS] J. M. Ball, J. M. Marsden, and M. Slemrod, *Controllability for distributed bilinear systems*, SIAM J. Control Optim., 20 (1982), pp. 575–597.

[BP] L. Baudouin, O. Kavian, and J.-P. Puel, *Regularity for a Schrödinger equation with singular potentials and application to bilinear optimal control*, J. Differential Equations, 216 (2005), pp. 188–222.

[CF] P. Constantin and C. Foias, *Navier-Stokes Equations*, University of Chicago Press, Chicago, 1988.

[HP] E. Hille and R. S. Phillips, *Functional Analysis and Semi-Groups*, AMS, Providence, RI, 1957.

[K] T. Kato, *Perturbation Theory for Linear Operators*, Springer-Verlag, Berlin, 1980.

[MST] Y. Maday, J. Salomon, and G. Turinici, *Monotonic time-discretized schemes*, Numer. Math., 103 (2006), pp. 323–338.

[MT] Y. Maday and G. Turinici, *New formulations of monotonically convergent quantum control algorithms*, J. Chem. Phys., 118 (2003), pp. 8191–8196.

[P] A. Pazy, *Semi-Groups of Linear Operators and Applications to Partial Differential Equations*, Springer-Verlag, Heidelberg, 1983.

[PDR] A. P. Peirce, M. A. Dahleh, and H. Rabitz, *Optimal control of quantum-mechanical systems: Existence, numerical approximation, and applications*, Phys. Rev. A, 37 (1988), pp. 4950–4967.

[S] J. Salomon, *Limit points of the monotonic schemes in quantum control*, in Proceedings of the 44th Annual IEEE Conference on Decision and Control, Seville, Spain, 2005, CD-ROM. Available online at http://www.ceremade.dauphine.fr/~salomon/ar/proceeding.pdf.

[TKO] D. Tannor, V. Kazakov, and V. Orlov, *Control of photochemical branching: Novel procedures for finding optimal pulses and global upper bounds*, in Time Dependent Quantum Molecular Dynamics, J. Broeckhove and L. Lathouwers, eds., Plenum Press, New York, 1992, pp. 347–360.

[ZR] W. Zhu and H. Rabitz, *A rapid monotonically convergent iteration algorithm for quantum optimal control over the expectation value of a positive definite operator*, J. Chem. Phys., 109 (1998), pp. 385–391.