

Constructive solution of a bilinear control problem

Lucie Baudouin^a, Julien Salomon^b

^a*LAAS - CNRS, 7 avenue du Colonel Roche, 31077 Toulouse Cedex 4, France*

^b*Laboratoire J.-L. Lions, Université P. & M. Curie, 175 rue du Chevaleret, 75013 Paris, France.*

Received ****; accepted after revision +++++

Presented by

Abstract

We present an optimization method of a quantum control problem giving rise to a sequence of controls increasing monotonically the values of a cost functional. We first claim some results about the regularity of *this* cost functional. Those enable to extend an inequality due to Lojasiewicz to the infinite dimensional case. Lastly, a sequence of inequalities proving the Cauchy character of the monotonic sequence is obtained, and we can also estimate the rate of convergence. The detailed proof will be given in [3]. *To cite this article: L. Baudouin, J. Salomon, C. R. Acad. Sci. Paris, Ser. ? ??? (200?).*

Résumé

Méthode constructive de résolution d'un problème de contrôle bilinéaire. Nous présentons une méthode d'optimisation d'un problème issu du contrôle quantique aboutissant à une suite de valeurs pour le contrôle faisant croître les valeurs d'une fonctionnelle de coût de façon monotone. Après avoir introduit la fonctionnelle de coût associée au problème, nous énonçons quelques propriétés sur sa régularité. Celles-ci permettent d'étendre une inégalité dû à Lojasiewicz au cadre de la dimension infinie. Une série de majorations démontrant la propriété de Cauchy pour la suite monotone est alors obtenue et nous pouvons également donner une estimation de son taux de convergence. Les détails des démonstrations seront donnés dans [3]. *Pour citer cet article : L. Baudouin, J. Salomon, C. R. Acad. Sci. Paris, Ser. ? ??? (200?).*

Version française abrégée

Soit $\alpha > 0$, $T > 0$, O un opérateur symétrique positif sur $L^2(\mathbb{R})$, ψ_0 dans $H^2(\mathbb{R}, \mathbb{C})$ et μ et V des fonctions de $W^{2,\infty}(\mathbb{R})$ avec $\mu(x) \xrightarrow{x \rightarrow \infty} 0$. Nous considérons le problème d'optimisation associé à la fonc-

Email addresses: baudouin@laas.fr (Lucie Baudouin), salomon@ann.jussieu.fr (Julien Salomon).

tionnelle de coût J définie sur $L^\infty(0, T)$ par : $J(\varepsilon) = \int_{\mathbb{R}} \overline{\psi(x, T)} O \psi(x, T) dx - \alpha \int_0^T \varepsilon^2(t) dt$ où $\psi \in L^\infty(0, T; H^2) \cap W^{1,\infty}(0, T; L^2)$ est la solution de l'équation de Schrödinger

$$\begin{cases} i\partial_t \psi(x, t) = [-\Delta + V(x) - \mu(x)\varepsilon(t)]\psi(x, t) \\ \psi(x, 0) = \psi_0(x). \end{cases}$$

L'existence d'un contrôle optimal a déjà été démontrée dans les références [2] et [4].

Cette fonctionnelle J est analytique et sa Hessienne peut s'écrire $\lambda(Id + \varphi)$ où Id est l'identité et φ un opérateur compact sur $L^\infty(0, T)$. Il est alors possible de reprendre un raisonnement exposé dans [5] pour établir une généralisation à la dimension infinie (7) d'une inégalité due à Łojasiewicz [6] valable pour les fonctions analytiques de \mathbb{R}^N . Nous considérons ainsi la suite $(\varepsilon^k)_{k \in \mathbb{N}}$ définie par (8-11), qui assure la croissance monotone des valeurs de la fonctionnelle de coût J . L'inégalité de Łojasiewicz généralisée permet alors d'obtenir :

Théorème 0.1 *La suite $(\varepsilon^k)_{k \in \mathbb{N}}$ définie par (8 – 9) est convergente dans $L^2(0, T)$.*

Par l'intermédiaire d'une seconde utilisation de l'inégalité (7), on peut enfin donner une estimation du taux de convergence de la suite (ε^k) .

Théorème 0.2 *Soit ε^∞ , la limite de $(\varepsilon^k)_{k \in \mathbb{N}}$ définie par (8 – 9), θ et κ les quantités apparaissant dans (7), avec $\tilde{C}_J = \{\varepsilon^\infty\}$.*

Si $\theta < \frac{1}{2}$, alors il existe $c > 0$ tel que : $\|\varepsilon^k - \varepsilon^\infty\|_{L^2(0, T)} \leq ck^{-\frac{\theta}{1-2\theta}}$.

Si $\theta = \frac{1}{2}$, alors il existe $c' > 0$ et τ tels que : $\|\varepsilon^k - \varepsilon^\infty\|_{L^2(0, T)} \leq c'e^{-\tau k}$.

1. Optimal control problem

We denote by H^2 and L^2 the spaces $H^2(\mathbb{R}, \mathbb{C})$ and $L^2(\mathbb{R}, \mathbb{C})$. We also use the notation $\langle . | . | . \rangle$ defined by: $\langle \psi | A | \chi \rangle = \int_{\mathbb{R}} \overline{\psi(x)} A \chi(x) dx$, where ψ and χ are in L^2 and A is an operator on L^2 .

Let μ and $V \in W^{2,\infty}(\mathbb{R})$, $\varepsilon \in L^\infty(0, T)$ and $\psi_0 \in H^2$. One can prove the existence of a unique solution $\psi \in L^\infty(0, T; H^2) \cap W^{1,\infty}(0, T; L^2)$ of the following Schrödinger equation [2]:

$$\begin{cases} i\partial_t \psi(x, t) = [-\Delta + V(x) - \mu(x)\varepsilon(t)]\psi(x, t) \\ \psi(x, 0) = \psi_0(x). \end{cases} \quad (1)$$

In what follows, we simply denote by $H = -\Delta + V$ the internal Hamiltonian of the system and we fix $\|\psi_0\|_{L^2} = 1$. Let O be a positive symmetric bounded operator on H^2 and α and T two positive real numbers. In this paper, we consider the optimal control problem corresponding to the cost functional J defined on $L^\infty(0, T)$ by:

$$J(\varepsilon) = \langle \psi(T) | O | \psi(T) \rangle - \alpha \int_0^T \varepsilon^2(t) dt. \quad (2)$$

The existence of a maximizer has been obtained in [2] and [4]. The gradient of J can be computed by introducing the Lagrange multiplier χ (also called *adjoint state*) corresponding to the constraint (1) and defined by:

$$\begin{cases} i\partial_t \chi(x, t) = [H - \mu(x)\varepsilon(t)]\chi(x, t) \\ \chi(x, T) = O\psi(x, T). \end{cases} \quad (3)$$

If we denote the usual inner product on $L^2(0, T)$ by (\cdot, \cdot) then we have (see [2]):

$$(\nabla J(\varepsilon), \varepsilon') = \int_0^T -2(\alpha\varepsilon(t) + Im\langle \chi(t)|\mu|\psi(t)\rangle)\varepsilon'(t)dt.$$

Thanks to the following lemma, one can prove that the set C_J of the critical points of J is compact in $L^\infty(0, T)$ (see a similar result in [1], Theorem 3.6).

Lemma 1.1 *Let be $(\varepsilon^n)_{n \in \mathbb{N}}$ a weakly convergent sequence in $L^2(0, T)$ and $(\psi^n)_{n \in \mathbb{N}}$ and $(\chi^n)_{n \in \mathbb{N}}$ the corresponding sequences of solutions of (1) and (3). Then $(\psi^n)_{n \in \mathbb{N}}$ and $(\chi^n)_{n \in \mathbb{N}}$ strongly converge in $C([0, T], H_{loc}^1)$.*

2. Properties of J

We present now some necessary results about the regularity of the cost functionnal J .

Theorem 2.1 *The functional $\phi : \varepsilon \in L^\infty(0, T) \mapsto \psi \in L^\infty(0, T; L^2)$ (where ψ is the solution of (1) corresponding to ε) is analytic.*

Sketch of the proof: Consider $\varepsilon, \varepsilon' \in L^\infty(0, T)$ with $\|\varepsilon'\|_{L^1(0, T)} \leq \min\left(\frac{1}{2\|\mu\|_{L^\infty(\mathbb{R})}}, 1\right)$ and the sequence $(\psi^l)_{l \in \mathbb{N}} \in (H^2)^\mathbb{N}$ defined recursively by $\psi^0 = \phi(\varepsilon)$ and for $l > 0$:

$$\begin{cases} i\partial_t \psi^l(x, t) = [H - \mu(x)\varepsilon(t)]\psi^l(x, t) - \mu(x)\varepsilon'(t)\psi^{l-1}(x, t) \\ \psi^l(x, 0) = 0. \end{cases} \quad (4)$$

The existence of the solutions of (4) is obtained by fixed-point method. It can also be proved recursively that:

$$\forall l \geq 1, \forall t \in [0, T], \|\psi^l(t)\|_{L^2} \leq \|\mu\|_{L^\infty(\mathbb{R})}^l \|\varepsilon'\|_{L^1(0, T)}^l. \quad (5)$$

Thus, for any $N > 0$:

$$\left\| \phi(\varepsilon + \varepsilon')(t) - \sum_{l=0}^N \psi^l(t) \right\|_{L^2} \leq \|\mu\|_{L^\infty(\mathbb{R})}^N \|\varepsilon'\|_{L^1(0, T)}^N \leq 2^{-N}$$

and the functional ϕ reads now: $\phi(\varepsilon + \varepsilon') = \sum_{l=0}^\infty \psi^l$. Since $\varepsilon' \mapsto \psi^l$ is l linear, the theorem follows.

Theorem 2.2 *The functional J is analytic on $L^\infty(0, T)$.*

Keeping the notations of the latter proof, one can define in the same way the sequence $(\chi^l)_{l \in \mathbb{N}} \in (H^2)^\mathbb{N}$ by $\chi^0 = \chi$, where χ is the solution of (3), and χ^l is the solution of

$$\begin{cases} i\partial_t \chi^l(x, t) = [H - \mu(x)\varepsilon(t)]\chi^l(x, t) - \mu(x)\varepsilon'(t)\chi^{l-1}(x, t) \\ \chi^l(x, T) = O\psi^l(x, T) \end{cases} \quad (6)$$

in order to prove that $\phi' : \varepsilon \in L^\infty(0, T) \mapsto \chi \in L^\infty(0, T; L^2)$ is analytic.

For some reasons that will appear in section 3, it can be useful to study the Hessian of J . As it was the case for the gradient, one can obtain an explicit formula.

Similar arguments enable to obtain the following result.

Lemma 2.3 *The functional $\gamma : \varepsilon \mapsto \text{Im}\langle \chi(t) | \mu | \psi(t) \rangle$ is differentiable on $L^\infty(0, T)$ and one has:*

$$\begin{aligned} D\gamma(\varepsilon) : L^\infty(0, T) &\rightarrow L^\infty(0, T) \\ \varepsilon' &\mapsto (t \mapsto \text{Im}\langle \chi^1(t) | \mu | \psi(t) \rangle + \text{Im}\langle \chi(t) | \mu | \psi^1(t) \rangle), \end{aligned}$$

where ψ and χ are the solutions of (1) and (3), and ψ^1 and χ^1 are the solutions of (4) and (6) for $l = 1$. Furthermore, the functional $D\gamma(\varepsilon)$ is compact on $L^\infty(0, T)$.

The Hessian operator of J is then given by : $H_J(\varepsilon) = \varepsilon' \mapsto -2(\alpha\varepsilon' + D\gamma(\varepsilon)(\varepsilon'))$.

3. Łojasiewicz inequality

The result we generalize here is the following one (cf [6,7]):

Theorem 3.1 *Let N be an integer and $\Gamma : \mathbb{R}^N \rightarrow \mathbb{R}$ be an analytic function in a neighborhood of a point $a \in \mathbb{R}^N$. Then there exists $\sigma' > 0$ and $\theta' \in]0, \frac{1}{2}]$ such that*

$$\forall x \in \mathbb{R}^N, \|x - a\| < \sigma', \quad \|\nabla \Gamma(x)\| \geq |\Gamma(x) - \Gamma(a)|^{1-\theta'}.$$

Following the work [5] of M. A. Jendoubi (which simplifies the theorem of Łojasiewicz-Simon [10]) the latter theorem can be generalized in infinite dimension. The key points of the proof are the compactness of $D\gamma(\varepsilon)$ and the analyticity of J . Moreover, thanks to compactness of the set C_J of the critical points of the cost functionnal J , one can prove the global version of the Łojasiewicz theorem:

Theorem 3.2 *Let denote by \tilde{C}_J a connex component of C_J in $L^\infty(0, T)$ and by l the value of the J on \tilde{C}_J . There exist $\sigma > 0$, $\kappa > 0$ and $\theta \in]0, \frac{1}{2}]$ such that:*

$$\forall \varepsilon \in \mathbb{R}^N, d(\varepsilon, \tilde{C}_J) < \sigma, \quad \|\nabla J(\varepsilon)\|_{L^1(0, T)} \geq \kappa |\tilde{J}(\varepsilon)|^{1-\theta}, \quad (7)$$

where d is the distance associated to the $L^\infty(0, T)$ norm and $\tilde{J}(\varepsilon) = l - J(\varepsilon)$.

4. Optimizing sequence

In [8] (see also [12] and [11]), Maday *et al.* have defined an optimizing sequence $(\varepsilon^k)_{k \in \mathbb{N}}$ of J as follows. Consider $(\delta, \eta) \in]0, 2[\times]0, 2[$, $\varepsilon^0 \in L^\infty(0, T)$ and $\tilde{\varepsilon}^0 \in L^\infty(0, T)$. The functions ε^k and $\tilde{\varepsilon}^k$ are computed by solving iteratively:

$$\begin{cases} i\partial_t \psi^k(x, t) = (H(x) - \varepsilon^k(t)\mu(x))\psi^k(x, t) \\ \psi^k(x, t=0) = \psi_0(x) \end{cases} \quad (8)$$

$$\varepsilon^k(t) = (1 - \delta)\tilde{\varepsilon}^{k-1}(t) - \frac{\delta}{\alpha} \operatorname{Im} \langle \chi^{k-1}(t) | \mu | \psi^k(t) \rangle \quad (9)$$

$$\begin{cases} i\partial_t \chi^k(x, t) = (H(x) - \tilde{\varepsilon}^k(t)\mu(x))\chi^k(x, t) \\ \chi^k(x, t=T) = O\psi^k(x, T) \end{cases} \quad (10)$$

$$\tilde{\varepsilon}^k(t) = (1 - \eta)\varepsilon^k(t) - \frac{\eta}{\alpha} \operatorname{Im} \langle \chi^k(t) | \mu | \psi^k(t) \rangle. \quad (11)$$

It can be proved by induction that each system of equations of this algorithm has a unique solution. A first interesting property of $(\varepsilon^k)_{k \in \mathbb{N}}$ and $(\tilde{\varepsilon}^k)_{k \in \mathbb{N}}$ is that these sequences are bounded.

Lemma 4.1 *Given an initial field $\varepsilon^0 \in L^\infty(0, T)$, there exists M depending on $\|\varepsilon^0\|_{L^\infty(0, T)}$, δ , η , α , O and μ such that $\|\varepsilon^k\|_{L^\infty(0, T)} \leq M$, $\|\tilde{\varepsilon}^k\|_{L^\infty(0, T)} \leq M$.*

A second property of $(\varepsilon^k)_{k \in \mathbb{N}}$ is given by the following lemma (see [8]) and a result analogous to Lemma 1.1 is given in the next one.

Lemma 4.2 *The sequence $(\varepsilon^k)_{k \in \mathbb{N}}$ defined by (8 – 9) ensures the monotonic convergence of the cost functional J in the sense that:*

$$\begin{aligned} J(\varepsilon^{k+1}) - J(\varepsilon^k) &= \langle \psi^{k+1}(T) - \psi^k(T) | O | \psi^{k+1}(T) - \psi^k(T) \rangle \\ &\quad + \left(\frac{2}{\eta} - 1 \right) \|\varepsilon^{k+1} - \tilde{\varepsilon}^k\|_{L^2(0, T)}^2 + \left(\frac{2}{\delta} - 1 \right) \|\tilde{\varepsilon}^k - \varepsilon^k\|_{L^2(0, T)}^2, \end{aligned} \quad (12)$$

and there exists l_{ε^0} such that $\lim_{k \rightarrow +\infty} J(\varepsilon^k) = l_{\varepsilon^0}$.

Lemma 4.3 *Let $(\varepsilon^{k_n})_{n \in \mathbb{N}}$ be a weakly convergent subsequence of $(\varepsilon^k)_{k \in \mathbb{N}}$ in $L^2(0, T)$. Then $(\varepsilon^{k_n})_{n \in \mathbb{N}}$ converges in $L^\infty(0, T)$ towards a critical point of the functional J .*

Let us denote by $C_{\varepsilon^0} \subset C_J$ the set of the limit points of $(\varepsilon^{k_n})_{n \in \mathbb{N}}$. A standard argument of compactness applied to C_{ε^0} enables to obtain the following result.

Lemma 4.4 *Let denote by d the distance corresponding to the $L^\infty(0, T)$ norm. One has:*

$$d(\varepsilon^k, C_{\varepsilon^0}) \rightarrow 0. \quad (13)$$

Note that, thanks to the monotonic property, $J = l_{\varepsilon^0}$ on C_{ε^0} . It can also be proved that C_{ε^0} is connected (see [9]). Lastly, the gradient of the cost functional can be estimated in each point ε^k as follows:

Lemma 4.5 *There exists $\lambda > 0$, depending on μ , O , α , δ , η and T , such that:*

$$\|\nabla J(\varepsilon^k)\|_{L^1(0, T)} \leq \lambda (\|\varepsilon^k - \tilde{\varepsilon}^{k-1}\|_{L^2(0, T)} + \|\tilde{\varepsilon}^{k-1} - \varepsilon^{k-1}\|_{L^2(0, T)}).$$

This result is obtained using estimate (5) with $l = 1$, $\varepsilon = \varepsilon^k$, $\varepsilon' = \varepsilon^{k+1} - \varepsilon^k$, $\psi^l = \psi^{k+1} - \psi^k$ and a corresponding estimate with χ .

5. Convergence of $(\varepsilon^k)_{k \in \mathbb{N}}$

It is now possible to prove the convergence of the sequence $(\varepsilon^k)_{k \in \mathbb{N}}$ by a Cauchy argument.

Theorem 5.1 *The sequence $(\varepsilon^k)_{k \in \mathbb{N}}$ defined by (8 – 9) is convergent in $L^2(0, T)$.*

Sketch of the proof: Suppose first that $\forall k \in \mathbb{N}$, $\tilde{J}(\varepsilon^k) \neq 0$. By (13), there exists k_0 such that (7) holds (with $\tilde{C}_J = C_{\varepsilon^0}$) for all ε^k with $k \geq k_0$. Consider an integer $k \geq k_0$. Thanks to the results mentioned above and the concavity of $s \mapsto s^\theta$:

$$\begin{aligned} (\tilde{J}(\varepsilon^k))^\theta - (\tilde{J}(\varepsilon^{k+1}))^\theta &\geq \frac{\theta}{(\tilde{J}(\varepsilon^{k+1}))^{1-\theta}} (J(\varepsilon^{k+1}) - J(\varepsilon^k)) \\ &\geq \frac{\kappa\theta}{\|\nabla J(\varepsilon^{k+1})\|_{L^1(0,T)}} \left(\left(\frac{2}{\delta} - 1 \right) \|\varepsilon^{k+1} - \tilde{\varepsilon}^k\|_{L^2(0,T)}^2 + \left(\frac{2}{\eta} - 1 \right) \|\tilde{\varepsilon}^k - \varepsilon^k\|_{L^2(0,T)}^2 \right) \\ &\geq \frac{\kappa\theta a_{(\delta,\eta)}}{\|\nabla J(\varepsilon^{k+1})\|_{L^1(0,T)}} (\|\varepsilon^{k+1} - \tilde{\varepsilon}^k\|_{L^2(0,T)} + \|\tilde{\varepsilon}^k - \varepsilon^k\|_{L^2(0,T)})^2 \\ &\geq \frac{\kappa\theta a_{(\delta,\eta)}}{\lambda} \|\varepsilon^{k+1} - \varepsilon^k\|_{L^2(0,T)}, \end{aligned}$$

where $a_{(\delta,\eta)} = \frac{1}{\max(\delta,\eta)} - \frac{1}{2}$. Since $\left((\tilde{J}(\varepsilon^k))^\theta \right)_{k \in \mathbb{N}}$ is a Cauchy sequence (as a monotonic sequence bounded by $\|O\|_* + \alpha TM^2$, where $\|O\|_*$ is the norm of the operator O on L^2), we obtain that $(\varepsilon^k)_{k \in \mathbb{N}}$ is also a Cauchy sequence.

If there exists k_1 such that $\tilde{J}(\varepsilon^{k_1}) = 0$, the monotonicity of the algorithm implies that

$$J(\varepsilon^{k_1}) = J(\varepsilon^{k_1+1}) = J(\varepsilon^{k_1+2}) = \dots$$

and by (12) the sequence $(\varepsilon^k)_{k \in \mathbb{N}}$ is constant for $k \geq k_1$.

A second use of the Lojasiewicz inequality enables to obtain estimates of the rate of convergence of the sequence $(\varepsilon^k)_{k \in \mathbb{N}}$. In particular we have the following result:

Theorem 5.2 *Let us denote by ε^∞ , the limit of $(\varepsilon^k)_{k \in \mathbb{N}}$ defined by (8 – 9) and θ , κ the real numbers appearing in (7), where $C_{\varepsilon^0} = \{\varepsilon^\infty\}$.*

If $\theta < \frac{1}{2}$, then there exists $c > 0$ such that: $\|\varepsilon^k - \varepsilon^\infty\|_{L^2(0,T)} \leq ck^{-\frac{\theta}{1-2\theta}}$.

If $\theta = \frac{1}{2}$, then there exist $c' > 0$ and τ such that: $\|\varepsilon^k - \varepsilon^\infty\|_{L^2(0,T)} \leq c'e^{-\tau k}$.

Acknowledgements

We acknowledge helpful discussions that we had on this topic with J. Bolte (Laboratoire de Combinatoire et Optimisation, Université Paris 6), G. Turinici (CEREMADE, Université Paris Dauphine) and O. Kavian (Laboratoire de Mathématiques Appliquées, Université de Versailles Saint-Quentin).

References

- [1] J.M. BALL, J.E. MARDSEN, M. SLEMROD, *Controllability for distributed bilinear systems*, SIAM J.Control and Optimization, **20**, No 4 (1982), 575–597 .

- [2] L. BAUDOUIN, O. KAVIAN and J.-P. PUEL, *Regularity for a Schrödinger equation with singular potentials and application to bilinear optimal control*, Journal of Differential Equations, 216 Issue 1(2005), 188-222.
- [3] L. BAUDOUIN, J. SALOMON, *Constructive solution of a bilinear quantum control problem*, in preparation (2005).
- [4] E. CANCES, C. LE BRIS, M. PILOT, *Optimal bilinear control for a Schrödinger equation*, C. R. Acad. Sci. Paris, Série 1, **330** (2000), 567-571.
- [5] M. A. JENDOUBI, *A simple unified approach to some convergence theorems of L. Simon.*, J. Funct. Anal., **153** (1998), 187–202.
- [6] S. LOJASIEWICZ, *Une propriété topologique des sous-ensembles analytiques réels*, Colloques internationaux du CNRS. Les équations aux dérivées partielles, **117** (1963).
- [7] S. LOJASIEWICZ, *Sur la géométrie semi- et sous-analytique*, Ann. Inst. Fourier, **43** (1993), 1575–1595.
- [8] Y. MADAY, G. TURINICI, *New formulations of monotonically convergent quantum control algorithms*, J. Chem. Phys, **118** No 18 (2003), 8191–8196.
- [9] J. SALOMON, *Limit points of the monotonic schemes in quantum control*, to appear in Proceedings of the 44th IEEE Conference on Decision and Control, Sevilla, 2005.
- [10] L. SIMON, *Asymptotics for a class of non-linear evolution equations, with applications to geometric problems*, Ann. of Math., **118** (1983), 525–571.
- [11] D. TANNOR, V. KAZAKOV, V. ORLOV, *Control of Photochemical Branching: Novel Procedures for Finding Optimal Pulses and Global Upper Bounds*, in J. Broeckhove and L. Lathouwers editors, *Time Dependent Quantum Molecular Dynamics*, Plenum, 1992, 347–360.
- [12] W. ZHU, H. RABITZ, *A rapid monotonically convergent algorithm for quantum optimal control over the expectation value of a definite operator*, J. Chem. Phys., **109** (1998), 385–391.