

CONVERGENCE OF THE TIME-DISCRETIZED MONOTONIC SCHEMES *

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Abstract. Many numerical simulations in (bilinear) quantum control use the monotonically convergent Krotov algorithms (introduced by Tannor in [17]), Zhu & Rabitz ([20]) or their unified form described in [13]. In [12], a time discretization which preserves the propriety of monotonicity has been presented. This paper introduces a proof of the convergence of these schemes and some results regarding their rate of convergence.

Résumé. De nombreuses méthodes de simulation en contrôle quantique (biliénaire) utilisent les algorithmes monotones de Krotov, tels que ceux présentés par Tannor ([17]) et Zhu & Rabitz ([20]) ou ceux de la forme donnée dans [13]. Dans [12], une discrétisation conservant la propriété de monotonie a été présentée. Nous donnons dans cet article une preuve de la convergence de ces schémas ainsi que quelques résultats sur leur vitesse de convergence.

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INTRODUCTION

Quantum control has recently been subjected to significant developments through encouraging experimental results ([8,15]). At computational level ([4]), the introduction of monotonic Krotov algorithms (introduced by Tannor in [17]), Zhu & Rabitz ([20]) or the unified form proposed by Maday & Turinici in [13] has enabled us to design efficient methods being implemented to obtain laser fields that control the molecular dynamics ([6]). From a mathematical point of view, it can be proved that these procedures monotonically increase the values of a given criterium. Yet, few results are available about the convergence of the control sequences obtained by these schemes. In [14], a first necessary condition for convergence has been obtained in case of large penalization of the L^2 -norm of the control. A functional analysis of the schemes has been displayed in [7] in the abstract framework of semi-group theory. To complete these works, a first analysis of a time-discretized version of the monotonic algorithms is presented here.

Let us briefly introduce the model and the corresponding optimal control framework used in this paper. Consider a quantum system described by its wavefunction $\psi = \psi(x, t)$. The relevant spatial coordinates, denoted by x ,

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belong to a general space $\Omega \subset \mathbb{R}^{3p}$, where p is the number of particles considered (the symbol x will often be omitted in the following developments in order to make it simple). Absorbing boundary conditions [19] can be used to treat numerically the case of unbounded domains. In case $\Omega \neq \mathbb{R}^{3p}$ is bounded, we assume homogeneous Dirichlet boundary conditions. The dynamics of this system is characterized by its *internal Hamiltonian*:

$$H = H_0 + V.$$

In this equation H_0 is the kinetic part:

$$H_0 = -\frac{1}{2} \sum_{n=1}^p \frac{1}{m_n} \Delta_{r_n},$$

where m_n is the mass of the particle n and Δ_{r_n} the Laplace operator with respect to its coordinates. The operator $V = V(x)$ is the potential part. In case the domain is bounded with Dirichlet boundary conditions and V is smooth, the spectrum of H is discrete, see e.g. [2]. In corresponding numerical simulations, spectral decompositions can be used to discretize the wavefunction.

A way to control such a system is to light it with a laser pulse modelled by a scalar electric field $\varepsilon(t)$. The contribution of this laser field is taken into account by introducing a perturbative term in the Hamiltonian which then reads $H - \mu\varepsilon$. Like V , the *dipolar momentum* μ is a function of x . In many models, the value $\mu(x) = +\infty$ is only reached for $|x| = +\infty$. Neglecting the interactions with far-off particles, we suppose that the operator μ is bounded on $L^2(\Omega)$. The evolution of ψ is then governed by the Schrödinger equation (we are making use of atomic units, i.e. $\hbar = 1$):

$$\begin{aligned} i \frac{\partial}{\partial t} \psi &= H\psi - \mu\varepsilon\psi \\ \psi(t=0) &= \psi_{init}, \end{aligned} \quad (1)$$

where ψ_{init} is the initial condition for ψ , subjected to the constraint: $\|\psi_{init}\|_{L^2(\Omega)} = 1$. In numerical simulations, the ground state, i.e. a unitary eigenvector of H associated to the lowest eigenvalue, is generally taken as the initial state. The Hamiltonian being real, the evolution through (1) preserves the L^2 -norm of ψ so that

$$\|\psi(t)\|_{L^2(\Omega)} = 1. \quad (2)$$

Remark 0.1. *The analysis presented here after will be carried out in a general setting and prevails for all space discretizations preserving Propriety (2).*

In order to design relevant fields of control, the optimal control framework usually introduces a cost functional to assess their quality. A general example of such functional is given by:

$$J(\varepsilon) = \langle \psi(T) | O | \psi(T) \rangle - \alpha \int_0^T \varepsilon^2(t) dt, \quad (3)$$

where α and T are two positive real numbers and O is a positive symmetric operator, also called *observable*, that encodes the target: the larger the value $\langle \psi(T) | O | \psi(T) \rangle$ is, the better the control objectives are met (here and in what follows, we note $\langle f | A | g \rangle = \int_{\Omega} f(x) A g(x) dx$, where f and g are complex valued functions and A a given operator). In this paper, we assume that O is bounded on $L^2(\Omega)$. This assumption is true in many physical models. However, the analysis presented here after is relevant if O is only bounded on sub-domains containing the system. The Euler-Lagrange equations corresponding to J can be written by means of the introduction of

a Lagrange multiplier χ , called *adjoint state* in what follows. The system obtained by this way is [20]:

$$\begin{cases} i \frac{\partial}{\partial t} \psi = (H - \mu \varepsilon) \psi \\ \psi(t=0) = \psi_{init} \end{cases} \quad (4)$$

$$\begin{cases} i \frac{\partial}{\partial t} \chi = (H - \mu \varepsilon) \chi \\ \chi(t=T) = O \psi(T) \\ \alpha \varepsilon(t) = -Im < \chi(t) | \mu | \psi(t) > . \end{cases} \quad (5)$$

An efficient tool to solve these equations is provided by the monotonic schemes. A general formulation of these algorithms is given by the following system (see [13]), which is defined recursively:

$$\begin{cases} i \frac{\partial}{\partial t} \psi^k = (H - \mu \varepsilon^k) \psi^k \\ \psi^k(t=0) = \psi_{init} \\ \varepsilon^k(t) = (1 - \delta) \tilde{\varepsilon}^{k-1}(t) - \frac{\delta}{\alpha} Im < \chi^{k-1}(t) | \mu | \psi^k(t) > \\ i \frac{\partial}{\partial t} \chi^k = (H - \mu \tilde{\varepsilon}^k) \chi^k \\ \chi^k(t=T) = O \psi^k(T) \\ \tilde{\varepsilon}^k(t) = (1 - \eta) \varepsilon^k(t) - \frac{\eta}{\alpha} Im < \chi^k(t) | \mu | \psi^k(t) > , \end{cases} \quad (6)$$

where $\delta, \eta \in [0, 2]$, with $(\delta, \eta) \neq (0, 0)$. A significant propriety of these schemes is that the cost functional values monotonically increase during the iterations since:

$$\begin{aligned} J(\varepsilon^{k+1}) - J(\varepsilon^k) &= < \psi^{k+1}(T) - \psi^k(T) | O | \psi^{k+1}(T) - \psi^k(T) > \\ &+ \left(\frac{2}{\delta} - 1\right) \int_0^T \alpha (\varepsilon^{k+1}(t) - \tilde{\varepsilon}^k(t))^2 dt + \left(\frac{2}{\eta} - 1\right) \int_0^T \alpha (\tilde{\varepsilon}^k(t) - \varepsilon^k(t))^2 dt > 0. \end{aligned}$$

Implicit and explicit relevant time discretizations of these schemes have been designed and tested in [11, 12]. Their main propriety is to maintain the monotonic character at the discrete level. This paper aims at proving the convergence of these algorithms.

The paper is structured as follows: the time discretizations of the Schrödinger equation (1) and the cost functional defined in (3) will be presented in Section 1. In Section 2, we will study the variations in the discrete cost functional with respect to ε . In Section 3, we will recall the main features of the implicit time discretized monotonic schemes. Section 4 is dedicated to proving the convergence of these schemes. Finally, we will give some estimates of the rate of convergence in Section 5. Sufficient condition of convergence of the explicit scheme is provided in the appendix.

1. DISCRETE OPTIMAL CONTROL SETTING

For any given integer N , let us introduce the discretization parameter ΔT defined by $N \Delta T = T$ and $\varepsilon_j, \tilde{\varepsilon}_j, \psi_j, \chi_j$ that stand respectively for approximations of $\varepsilon(j \Delta T), \tilde{\varepsilon}(j \Delta T), \psi(j \Delta T), \chi(j \Delta T)$. We denote in the following $\varepsilon = (\varepsilon_j)_{0 \leq j \leq N-1}$, $\tilde{\varepsilon} = (\tilde{\varepsilon}_j)_{0 \leq j \leq N-1}$, $\psi = (\psi)_{0 \leq j \leq N}$ and $\chi = (\chi_j)_{0 \leq j \leq N}$.

To solve (1) numerically with enough accuracy, a propagation method based on the Strang's second-order split-operator technique ([16]) is generally used (see e.g. [1, 18, 20]). This method also simplifies algebraic manipulations as it will appear later in this study (see Equation (22)).

In this part, for any prescribed sequences $\varepsilon, \tilde{\varepsilon}$, the approximations of the state ψ and the adjoint state χ are thus defined by the semi-discretized propagation equations:

$$\begin{cases} \psi_{j+1}^\varepsilon &= e^{\frac{H_0 \Delta T}{2i}} e^{\frac{V - \mu \varepsilon_j}{i} \Delta T} e^{\frac{H_0 \Delta T}{2i}} \psi_j^\varepsilon \\ \psi_0^\varepsilon &= \psi_{init}, \end{cases} \quad (7)$$

$$\begin{cases} \chi_j^{\tilde{\varepsilon}} &= e^{-\frac{H_0 \Delta T}{2i}} e^{\frac{-V + \mu \tilde{\varepsilon}_j}{i} \Delta T} e^{-\frac{H_0 \Delta T}{2i}} \chi_{j+1}^{\tilde{\varepsilon}} \\ \chi_N^{\tilde{\varepsilon}} &= O \psi_N^\varepsilon. \end{cases} \quad (8)$$

Note that actually $\chi^{\tilde{\varepsilon}}$ also depends on ε . We omit this dependence for purpose of simplicity. We refer to [12] for more details about full discretization. This discretization of (4) and (5) preserves the L^2 -norm of the propagated vectors, which means:

$$\forall j = 0 \dots N-1, \quad \|\psi_j^\varepsilon\|_{L^2(\Omega)} = \|\psi_{init}\|_{L^2(\Omega)} = 1, \quad (9)$$

$$\|\chi_j^{\tilde{\varepsilon}}\|_{L^2(\Omega)} = \|\chi_N^{\tilde{\varepsilon}}\|_{L^2(\Omega)} \leq \|O\|_*, \quad (10)$$

where $\|O\|_*$ denotes the norm of the operator O over $L^2(\Omega)$. We consider the following time discretization of the cost functional defined in (3):

$$J_{\Delta T}(\varepsilon) = \langle \psi_N^\varepsilon | O | \psi_N^\varepsilon \rangle - \alpha \Delta T \sum_{j=0}^{N-1} |\varepsilon_j|^2.$$

Let us also introduce norms on \mathbb{R}^N corresponding to the time discretization:

$$\|\varepsilon\|_1 = \Delta T \sum_{j=0}^{N-1} |\varepsilon_j|, \quad \|\varepsilon\|_2 = \left(\Delta T \sum_{j=0}^{N-1} |\varepsilon_j|^2 \right)^{\frac{1}{2}}.$$

Note that the inner product associated with the norm $\|\cdot\|_2$ is defined by :

$$\varepsilon \cdot \varepsilon' = \Delta T \sum_{j=0}^{N-1} \varepsilon_j \varepsilon'_j.$$

2. VARIATIONS IN $J_{\Delta T}$

In this section, we investigate some variational proprieties of $J_{\Delta T}$.

2.1. Gradient of $J_{\Delta T}$

Given a field ε , the dependence of ψ_N^ε with respect to the field can be explicitly stated with the formula:

$$\psi_N^\varepsilon = \prod_{j=0}^{N-1} \left(e^{\frac{H_0 \Delta T}{2i}} e^{-i(V - \mu \varepsilon_j) \Delta T} e^{\frac{H_0 \Delta T}{2i}} \right) \psi_{init}.$$

The computation of the gradient of $J_{\Delta T}$ is simplified by the introduction of the adjoint state χ^ε . Indeed, note first that the partial derivative of $\langle \psi_N^\varepsilon | O | \psi_N^\varepsilon \rangle$ with respect to ε_{j_0} reads:

$$\frac{\partial \psi_N^\varepsilon}{\partial \varepsilon_{j_0}} = \Delta T \prod_{j=j_0+1}^{N-1} \left(e^{\frac{H_0 \Delta T}{2i}} e^{\frac{V - \mu \varepsilon_j}{i} \Delta T} e^{\frac{H_0 \Delta T}{2i}} \right) \times \left(e^{\frac{H_0 \Delta T}{2i}} e^{\frac{V - \mu \varepsilon_{j_0}}{i} \Delta T} i \mu e^{\frac{H_0 \Delta T}{2i}} \right) \times \prod_{j=0}^{j_0-1} \left(e^{\frac{H_0 \Delta T}{2i}} e^{\frac{V - \mu \varepsilon_j}{i} \Delta T} e^{\frac{H_0 \Delta T}{2i}} \right) \psi_{init}.$$

Consequently, the following equations apply:

$$\frac{\partial \langle \psi_N^\varepsilon | O | \psi_N^\varepsilon \rangle}{\partial \varepsilon_{j_0}} = 2Re \langle \frac{\partial \psi_N^\varepsilon}{\partial \varepsilon_{j_0}} | O | \psi_N^\varepsilon \rangle = -2\Delta T Im \langle \tilde{\chi}_{j_0}^\varepsilon | \mu | \check{\psi}_{j_0}^\varepsilon \rangle,$$

where:

$$\tilde{\chi}_j^\varepsilon = e^{\frac{H_0 \Delta T}{2i}} \chi_j^\varepsilon, \check{\psi}_j^\varepsilon = e^{\frac{H_0 \Delta T}{2i}} \psi_j^\varepsilon.$$

The gradient of $J_{\Delta T}$ is then given by:

$$\nabla J_{\Delta T}(\varepsilon) \cdot \delta \varepsilon = -2\Delta T \sum_{j=0}^{N-1} (Im \langle \tilde{\chi}_j^\varepsilon | \mu | \check{\psi}_j^\varepsilon \rangle + \alpha \varepsilon_j) \delta \varepsilon_j. \quad (11)$$

The previous computation allows us to define set C of the critical points of $J_{\Delta T}$:

$$C = \left\{ \varepsilon / \forall j = 0 \dots N-1, Im \langle \tilde{\chi}_j^\varepsilon | \mu | \check{\psi}_j^\varepsilon \rangle + \alpha \varepsilon_j = 0 \right\}. \quad (12)$$

2.2. About the Hessian of $J_{\Delta T}$

For some reasons that will be developed in Section 4.1, it can be useful to find conditions to make sure that the Hessian matrix $H_{J_{\Delta T}}(\varepsilon)$ of $J_{\Delta T}$ is invertible.

Denoting by $(\nabla J_{\Delta T}(\varepsilon))_\ell$ the ℓ -th component of $\nabla J_{\Delta T}(\varepsilon)$, the following equations prevails:

$$\frac{\partial}{\partial \varepsilon_m} (\nabla J_{\Delta T}(\varepsilon))_\ell = -2 \left(Im \langle \frac{\partial}{\partial \varepsilon_m} \tilde{\chi}_\ell^\varepsilon | \mu | \check{\psi}_\ell^\varepsilon \rangle + Im \langle \tilde{\chi}_\ell^\varepsilon | \mu | \frac{\partial}{\partial \varepsilon_m} \check{\psi}_\ell^\varepsilon \rangle + \alpha \delta_{\ell,m} \right),$$

where $\delta_{\ell,m}$ is the Kronecker's symbol. Repeating the analysis carried out in the previous section, we find out that $H_{J_{\Delta T}}(\varepsilon)$ reads:

$$H_{J_{\Delta T}}(\varepsilon) = -2(S(\varepsilon) + \alpha Id),$$

where Id is the identity matrix and $S(\varepsilon) = (s_{\ell,m})_{\substack{\ell=0 \dots N-1 \\ m=0 \dots N-1}}$ has the following propriety (see (9) and (10)):

$$|s_{\ell,m}| \leq 2\Delta T \|\mu\|_*^2 \|O\|_*, \quad (13)$$

where $\|\mu\|_*$ is the norm of the operator μ on $L^2(\Omega)$. This estimate enables us to claim the following result.

Lemma 2.1. *Let be $\varepsilon \in \mathbb{R}^N$. Suppose that $\alpha > 2\|\mu\|_*^2 \|O\|_* T$. Then $H_{J_{\Delta T}}(\varepsilon)$ is invertible.*

Proof. : Let us denote by $h_{\ell,m}$ the coefficients of $H_{J_{\Delta T}}(\varepsilon)$. According to (13), we obtain, for any $\ell = 0 \dots N-1$:

$$\begin{aligned} |h_{\ell,\ell}| &\geq 2(\alpha - 2\Delta T \|\mu\|_*^2 \|O\|_*) \\ &> 4\|\mu\|_*^2 \|O\|_* (T - \Delta T) \\ &\geq \sum_{m=0, m \neq \ell}^{N-1} |h_{m,\ell}|. \end{aligned}$$

Thus, $H_{J_{\Delta T}}(\varepsilon)$ is a dominant diagonal matrix and the result comes as a consequence. \square

2.3. Variations in ψ^ε and χ^ε

The variations in the state ψ^ε and adjoint state χ^ε with respect to ε can also be estimated by means of direct computations. Given two discrete fields ε' and ε , the difference $\psi_{j+1}^{\varepsilon'} - \psi_{j+1}^\varepsilon$ reads:

$$\begin{aligned} \psi_{j+1}^{\varepsilon'} - \psi_{j+1}^\varepsilon &= e^{\frac{H_0 \Delta T}{2i}} \left(e^{\frac{V - \mu \varepsilon'_j}{i} \Delta T} - e^{\frac{V - \mu \varepsilon_j}{i} \Delta T} \right) e^{\frac{H_0 \Delta T}{2i}} \psi_j^\varepsilon \\ &\quad + e^{\frac{H_0 \Delta T}{2i}} e^{\frac{V - \mu \varepsilon'_j}{i} \Delta T} e^{\frac{H_0 \Delta T}{2i}} (\psi_j^{\varepsilon'} - \psi_j^\varepsilon). \end{aligned}$$

The mean value inequality then yields:

$$\|\psi_{j+1}^{\varepsilon'} - \psi_{j+1}^\varepsilon\|_{L^2(\Omega)} \leq \Delta T \|\mu\|_* |\varepsilon'_j - \varepsilon_j| + \|\psi_j^{\varepsilon'} - \psi_j^\varepsilon\|_{L^2(\Omega)}.$$

Hence:

$$\|\psi_j^{\varepsilon'} - \psi_j^\varepsilon\|_{L^2(\Omega)} \leq \Delta T \|\mu\|_* \sum_{l=0}^{j-1} |\varepsilon'_l - \varepsilon_l| \leq \|\mu\|_* \|\varepsilon' - \varepsilon\|_1.$$

According to a similar argument:

$$\|\chi_j^{\varepsilon'} - \chi_j^\varepsilon\|_{L^2(\Omega)} \leq \Delta T \|\mu\|_* |\varepsilon'_j - \varepsilon_j| + \|\chi_{j+1}^{\varepsilon'} - \chi_{j+1}^\varepsilon\|_{L^2(\Omega)},$$

and consequently:

$$\begin{aligned} \|\chi_j^{\varepsilon'} - \chi_j^\varepsilon\|_{L^2(\Omega)} &\leq \Delta T \|\mu\|_* \sum_{l=j}^{N-1} |\varepsilon'_l - \varepsilon_l| + \|O\|_* \|\psi_N^{\varepsilon'} - \psi_N^\varepsilon\|_{L^2(\Omega)} \\ &\leq \|\mu\|_* \|\varepsilon' - \varepsilon\|_1 + \|O\|_* \|\psi_N^{\varepsilon'} - \psi_N^\varepsilon\|_{L^2(\Omega)} \\ &\leq \|\mu\|_* (1 + \|O\|_*) \|\varepsilon' - \varepsilon\|_1. \end{aligned}$$

Remark 2.2. : For algorithmic reasons, the adjoint state may be propagated with a field $\tilde{\varepsilon}$ that does not coincide with ε (see (6)), the field bringing about the final condition $\chi_N^{\tilde{\varepsilon}} = O\psi_N^\varepsilon$. However, the previous estimate still holds insofar as we have:

$$\begin{aligned} \|\chi_j^{\tilde{\varepsilon}} - \chi_j^\varepsilon\|_{L^2(\Omega)} &\leq \|\mu\|_* \|\tilde{\varepsilon}' - \tilde{\varepsilon}\|_1 + \|O\|_* \|\psi_N^{\tilde{\varepsilon}} - \psi_N^\varepsilon\|_{L^2(\Omega)} \\ &\leq \|\mu\|_* (\|\tilde{\varepsilon}' - \tilde{\varepsilon}\|_1 + \|O\|_* \|\varepsilon' - \varepsilon\|_1). \end{aligned} \tag{14}$$

3. IMPLICIT DISCRETE MONOTONIC SCHEMES

This section aims at recalling the definition of the implicit discrete monotonic schemes and presenting some of their proprieties.

3.1. Definition of the schemes

Consider two real numbers $\delta, \eta \in [0, 2[$ and the operator $\mu^*(h)$ defined by:

$$\mu^*(h) = \frac{e^{-i\mu h \Delta T} - Id}{-ih \Delta T}. \tag{15}$$

This function is an approximation of μ inasmuch as:

$$\|\mu^*(h) - \mu\|_* \leq \Delta T \|\mu\|_*^2 |h|, \quad (16)$$

which can be obtained by the mean value inequality, since $\|\frac{d\mu^*(h)}{dh}\|_* \leq \Delta T \|\mu\|_*^2$.

Given initial control fields $\varepsilon^0, \tilde{\varepsilon}^0$ and their associated state ψ^0 and adjoint state χ^0 , suppose that for some $k \geq 1$, $\psi^{k-1}, \chi^{k-1}, \varepsilon^{k-1}, \tilde{\varepsilon}^{k-1}$ are known. The computation of $\psi^k, \chi^k, \varepsilon^k, \tilde{\varepsilon}^k$ is achieved as follows:

$$\begin{cases} \psi_{j+1}^k &= e^{\frac{H_0 \Delta T}{2i}} e^{\frac{V - \mu \varepsilon_j^k}{i} \Delta T} e^{-\frac{H_0 \Delta T}{2i}} \psi_j^k \\ \varepsilon_j^k &= (1 - \delta) \tilde{\varepsilon}_j^{k-1} - \frac{\delta}{\alpha} Im \langle \tilde{\chi}_j^{k-1} | \mu^*(\tilde{\varepsilon}_j^{k-1} - \varepsilon_j^k) | \tilde{\psi}_j^k \rangle \\ \psi_0^k &= \psi_{init}, \end{cases} \quad (17)$$

$$\begin{cases} \chi_j^k &= e^{-\frac{H_0 \Delta T}{2i}} e^{\frac{-V + \mu \varepsilon_j^k}{i} \Delta T} e^{-\frac{H_0 \Delta T}{2i}} \chi_{j+1}^k \\ \tilde{\varepsilon}_j^k &= (1 - \eta) \varepsilon_j^k - \frac{\eta}{\alpha} Im \langle \tilde{\chi}_j^k | \mu^*(\varepsilon_j^k - \tilde{\varepsilon}_j^k) | \tilde{\psi}_{j+1}^k \rangle \\ \chi_N^k &= O \psi_N^k, \end{cases} \quad (18)$$

where:

$$\tilde{\chi}_j^\varepsilon = e^{-\frac{H_0 \Delta T}{2i}} \chi_j^\varepsilon, \tilde{\psi}_j^\varepsilon = e^{-\frac{H_0 \Delta T}{2i}} \psi_j^\varepsilon.$$

Subsequently, the initial value ε^0 of the monotonic schemes is considered fixed.

3.2. Proprieties of sequence $(\varepsilon^k)_{k \in \mathbb{N}}$

3.2.1. Upper bound

A first propriety of $(\varepsilon^k)_{k \in \mathbb{N}}$ and $(\tilde{\varepsilon}^k)_{k \in \mathbb{N}}$ defined in (17) and (18) is that these sequences are bounded. Indeed, the following result can be proved by induction (see [12]).

Lemma 3.1. *Given an initial field ε^0 , let us defined M by:*

$$M = \max(\|\varepsilon^0\|_\infty, \max(1, \frac{\delta}{2 - \delta}, \frac{\eta}{2 - \eta}) \frac{\|O\|_* \|\mu\|_*}{\alpha}). \quad (19)$$

The sequences $(\varepsilon^k)_{k \in \mathbb{N}}$ and $(\tilde{\varepsilon}^k)_{k \in \mathbb{N}}$ match the following conditions:

$$\forall k \in \mathbb{N}, \forall j = 0 \dots N - 1, |\varepsilon_j^k| \leq M, |\tilde{\varepsilon}_j^k| \leq M. \quad (20)$$

3.2.2. Monotonic convergence

A computation of the variation in the cost functional values leads to:

$$\begin{aligned} J_{\Delta T}(\varepsilon^{k+1}) - J_{\Delta T}(\varepsilon^k) &= \langle \psi_N^{k+1} - \psi_N^k | O | \psi_N^{k+1} - \psi_N^k \rangle \\ &+ \sum_{j=0}^{N-1} 2Re \langle \tilde{\chi}_{j+1}^k | e^{\frac{\mu(\varepsilon_j^k - \tilde{\varepsilon}_j^k)}{i} \Delta T} - Id | \tilde{\psi}_{j+1}^k \rangle - \alpha \Delta T ((\tilde{\varepsilon}_j^k)^2 - (\varepsilon_j^k)^2) \\ &+ \sum_{j=0}^{N-1} 2Re \langle \tilde{\chi}_j^k | e^{-\frac{\mu(\varepsilon_j^{k+1} - \tilde{\varepsilon}_j^k)}{i} \Delta T} - Id | \tilde{\psi}_j^{k+1} \rangle - \alpha \Delta T ((\varepsilon_j^{k+1})^2 - (\tilde{\varepsilon}_j^k)^2). \end{aligned} \quad (21)$$

Note that this equality holds for any sequence of controls $(\varepsilon^k)_{k \in \mathbb{N}}$ and $(\tilde{\varepsilon}^k)_{k \in \mathbb{N}}$. In the case of the implicit schemes (17)–(18), this expression reads:

$$\begin{aligned}
J_{\Delta T}(\varepsilon^{k+1}) - J_{\Delta T}(\varepsilon^k) &= \langle \psi_N^{k+1} - \psi_N^k | O | \psi_N^{k+1} - \psi_N^k \rangle \\
&\quad + \alpha \Delta T \sum_{j=0}^{N-1} \left(\frac{2}{\delta} - 1 \right) (\tilde{\varepsilon}_j^k - \varepsilon_j^{k+1})^2 + \left(\frac{2}{\eta} - 1 \right) (\varepsilon_j^k - \tilde{\varepsilon}_j^k)^2 \\
&= \langle \psi_N^{k+1} - \psi_N^k | O | \psi_N^{k+1} - \psi_N^k \rangle \\
&\quad + \alpha \left(\frac{2}{\delta} - 1 \right) \|\tilde{\varepsilon}^k - \varepsilon^{k+1}\|_2^2 + \alpha \left(\frac{2}{\eta} - 1 \right) \|\varepsilon^k - \tilde{\varepsilon}^k\|_2^2.
\end{aligned} \tag{22}$$

This result, combined with the bounded character of $(\varepsilon^k)_{k \in \mathbb{N}}$ leads to the following theorem.

Theorem 3.2. *The implicit schemes (17)–(18) ensure the monotonic convergence of the cost functional $J_{\Delta T}$ insofar as:*

$$J_{\Delta T}(\varepsilon^k) \leq J_{\Delta T}(\varepsilon^{k+1}). \tag{23}$$

Furthermore there exists l_{ε^0} such that:

$$\lim_{k \rightarrow +\infty} J_{\Delta T}(\varepsilon^k) = l_{\varepsilon^0}.$$

Proof. : Inequality (23) is a trivial consequence of (22), since O is a positive operator. By means of (20), we know that:

$$\forall k \in \mathbb{N}, \quad J_{\Delta T}(\varepsilon^k) \leq \|O\|_*,$$

hence the existence of l_{ε^0} . □

We keep the notation l_{ε^0} in the sequel.

3.2.3. Limit points of $(\varepsilon^k)_{k \in \mathbb{N}}$

Having reached these preliminary results, we are now in a position to describe the limit points set C_{ε^0} of sequence $(\varepsilon^k)_{k \in \mathbb{N}}$.

Lemma 3.3. *Keeping the previous notations:*

$$C_{\varepsilon^0} \subset C,$$

where C is the set of critical points, defined by (12).

Proof. : Consider a convergent subsequence $(\varepsilon^{k_n})_{n \in \mathbb{N}}$ of $(\varepsilon^k)_{k \in \mathbb{N}}$ and its limit ε^∞ . By means of continuity and since $\|\varepsilon^{k_n} - \tilde{\varepsilon}^{k_n-1}\|_2 \rightarrow 0$ (see (22)), we find the following limits:

$$\begin{aligned}
\tilde{\varepsilon}^{k_n-1} &\rightarrow \varepsilon^\infty, \\
\mu^*(\varepsilon_j^k - \tilde{\varepsilon}_j^{k-1}) &\rightarrow \mu, \\
\psi^{k_n} &\rightarrow \psi^{\varepsilon^\infty}, \\
\chi^{k_n-1} &\rightarrow \chi^{\varepsilon^\infty}.
\end{aligned}$$

When n tends to $+\infty$, Equation (17) becomes:

$$\forall j = 0 \dots N-1, \quad \varepsilon_j^\infty = -\frac{1}{\alpha} \text{Im} \langle \tilde{\chi}_j^{\varepsilon^\infty} | \mu | \check{\psi}_j^{\varepsilon^\infty} \rangle,$$

which is the desired conclusion. □

Thanks to (20), a standard argument of compactness shows that:

$$d(\varepsilon^k, C_{\varepsilon^0}) \rightarrow 0, \quad (24)$$

where $d(\varepsilon^k, C_{\varepsilon^0})$ is the distance associated to $\|\cdot\|_2$ between ε^k and set C_{ε^0} . Furthermore, Inequality (23) then implies:

$$J_{\Delta T}(C_{\varepsilon^0}) = l_{\varepsilon^0}. \quad (25)$$

Finally, note that since C is compact (see (12)), C_{ε^0} is also compact.

3.3. Estimates of the gradient

This section introduces an estimate of the norm of the gradient in the points of the monotonic schemes. Let us recall that according to (11), we know that:

$$\|\nabla J_{\Delta T}(\varepsilon^k)\|_1 = 2\Delta T \sum_{j=0}^{N-1} |Im \langle \tilde{\chi}_j^{\varepsilon^k} | \mu | \check{\psi}_j^k \rangle + \alpha \varepsilon_j^k|.$$

Lemma 3.4. *There exists $\lambda \geq 0$ such that:*

$$\|\nabla J_{\Delta T}(\varepsilon^k)\|_1 \leq \lambda(\|\varepsilon^k - \tilde{\varepsilon}^{k-1}\|_2 + \|\tilde{\varepsilon}^{k-1} - \varepsilon^{k-1}\|_2). \quad (26)$$

Proof. : If we focus on one coefficient of $J_{\Delta T}(\varepsilon^k)$, we find:

$$\begin{aligned} Im \langle \tilde{\chi}_j^{\varepsilon^k} | \mu | \check{\psi}_j^k \rangle + \alpha \varepsilon_j^k &= Im \langle \tilde{\chi}_j^{k-1} | \mu^* (\tilde{\varepsilon}_j^{k-1} - \varepsilon_j^k) | \check{\psi}_j^k \rangle + \alpha \varepsilon_j^k \\ &\quad + Im \langle \tilde{\chi}_j^{k-1} | \mu - \mu^* (\tilde{\varepsilon}_j^{k-1} - \varepsilon_j^k) | \check{\psi}_j^k \rangle \\ &\quad + Im \langle \tilde{\chi}_j^{\varepsilon^k} - \tilde{\chi}_j^{k-1} | \mu | \check{\psi}_j^k \rangle. \end{aligned} \quad (27)$$

Let us estimate each term of this decomposition. Definition (17) of the algorithm implies that:

$$Im \langle \tilde{\chi}_j^{k-1} | \mu^* (\tilde{\varepsilon}_j^{k-1} - \varepsilon_j^k) | \check{\psi}_j^k \rangle + \alpha \varepsilon_j^k = \frac{\alpha}{\delta} (\tilde{\varepsilon}_j^{k-1} - \varepsilon_j^k). \quad (28)$$

Then, thanks to (16), we obtain:

$$|Im \langle \tilde{\chi}_j^k | \mu - \mu^* (\tilde{\varepsilon}_j^{k-1} - \varepsilon_j^k) | \check{\psi}_j^k \rangle| \leq \Delta T \|\mu\|_*^2 \|O\|_* |\varepsilon_j^k - \tilde{\varepsilon}_j^{k-1}|. \quad (29)$$

Lastly, Inequality (14) (see Remark 2.2) yields:

$$|Im \langle \tilde{\chi}_j^{\varepsilon^k} - \tilde{\chi}_j^{k-1} | \mu | \check{\psi}_j^k \rangle| \leq \|\mu\|_*^2 (\|\varepsilon^k - \tilde{\varepsilon}^{k-1}\|_1 + \|O\|_* \|\varepsilon^k - \varepsilon^{k-1}\|_1). \quad (30)$$

Combining (28)–(30) with (27), we come to Equation (26) where

$$\lambda = 2\sqrt{T} \left(\frac{\alpha}{\delta} + (T + \Delta T) \|\mu\|_*^2 (1 + \|O\|_*) \right).$$

□

4. CONVERGENCE OF THE IMPLICIT SCHEMES

The above mentioned results enable us to prove the convergence of the schemes. First we will present a general inequality disclosed by Lojasiewicz [9, 10] (see also [3]), and use it to prove that $(\varepsilon^k)_{k \in \mathbb{N}}$ defined by (17)–(18) is Cauchy.

4.1. Lojasiewicz inequality

The Lojasiewicz inequality enables us to estimate the variation in an analytic function by its gradient. This result is detailed in the next theorem.

Theorem 4.1 (Lojasiewicz inequality). *Let $\Gamma : \mathbb{R}^n \rightarrow \mathbb{R}$ be an analytic function in a neighborhood of a point a in \mathbb{R}^n . Then there exists $\sigma > 0$ and $0 < \theta \leq \frac{1}{2}$ such that:*

$$\forall x \in \mathbb{R}^n, x \in B(a, \sigma) \quad \|\nabla \Gamma(x)\| \geq |\Gamma(x) - \Gamma(a)|^{1-\theta},$$

where $B(a, \sigma)$ denotes the ball centered in a with a radius equal to σ , $\|\cdot\|$ is a norm on \mathbb{R}^n .

The real number θ is called a Lojasiewicz exponent of a . A more precise result can be obtained if the Hessian matrix of Γ , denoted by $H_\Gamma(a)$, is invertible (see, e.g. [5]).

Lemma 4.2. *Suppose that $H_\Gamma(a)$ is invertible, then there exists $\sigma > 0$ and $\kappa > 0$ such that:*

$$\forall x \in \mathbb{R}^n, x \in B(a, \sigma) \quad \|\nabla \Gamma(x)\| \geq \kappa |\Gamma(x) - \Gamma(a)|^{\frac{1}{2}}.$$

In order to apply these results to our problem, let us define the shifted cost functional:

$$\tilde{J}_{\Delta T}(\varepsilon) = l_{\varepsilon^0} - J_{\Delta T}(\varepsilon).$$

It is easy to check that $\tilde{J}_{\Delta T}$ is analytic. Now, consider a in C_{ε^0} . By means of (25), we find that $\tilde{J}_{\Delta T}(a) = 0$. Consequently, Theorem 4.1 ensures that there exist $0 < \theta_a \leq 1/2$ and $\sigma_a > 0$ such that:

$$\forall \varepsilon \in \mathbb{R}^N, \|\varepsilon - a\|_1 < \sigma_a \quad \|\nabla J_{\Delta T}(\varepsilon)\|_1 \geq |\tilde{J}_{\Delta T}(\varepsilon)|^{1-\theta_a}.$$

The compactness of C_{ε^0} enables us to extract from the set $\{B(a, \frac{\sigma_a}{2}), a \in C_{\varepsilon^0}\}$ a family $F_{\varepsilon^0} = \{B(a_i, \frac{\sigma_{a_i}}{2})\}_{i \in I}$, where I is a finite set of indexes such that:

$$C_{\varepsilon^0} \subset F_{\varepsilon^0}.$$

Let us denote by $\theta' \in]0, 1/2]$, the lower bound of $\{\theta_{a_i}\}_{i \in I}$ and by σ' , the lower bound of $\{\frac{\sigma_{a_i}}{2}\}_{i \in I}$. Given ε such that $d(\varepsilon, C_{\varepsilon^0}) < \sigma'$, there exists i_ε such that $\varepsilon \in B(a_{i_\varepsilon}, \sigma_{a_{i_\varepsilon}})$ and we come to the following version of Theorem 4.1:

Lemma 4.3. *Keeping the above notations:*

$$\forall \varepsilon \in \mathbb{R}^N, d(\varepsilon, C_{\varepsilon^0}) < \sigma', \quad \|\nabla J_{\Delta T}(\varepsilon)\|_1 \geq |\tilde{J}_{\Delta T}(\varepsilon)|^{1-\theta'}.$$

In case $H_{J_{\Delta T}}$ is invertible on C_{ε^0} , a similar analysis can be led to obtain the corresponding version of Lemma 4.2.

Lemma 4.4. *Suppose that $H_{J_{\Delta T}}(\varepsilon)$ is invertible for all $\varepsilon \in C_{\varepsilon^0}$,*

$$\exists \sigma'' > 0, \exists \kappa' > 0, \forall \varepsilon \in \mathbb{R}^N, d(\varepsilon, C_{\varepsilon^0}) < \sigma'', \quad \|\nabla J_{\Delta T}(\varepsilon)\|_1 \geq \kappa' |\tilde{J}_{\Delta T}(\varepsilon)|^{\frac{1}{2}}.$$

Summarizing the above mentioned results, we have obtained that there exist $\tilde{\sigma} > 0$, $\tilde{\kappa} > 0$ and $\tilde{\theta} \in]0, \frac{1}{2}]$ such that:

$$d(\varepsilon, C_{\varepsilon^0}) < \tilde{\sigma}, \quad \|\nabla J_{\Delta T}(\varepsilon)\|_1 \geq \tilde{\kappa} |\tilde{J}_{\Delta T}(\varepsilon)|^{1-\tilde{\theta}}, \quad (31)$$

with $\tilde{\theta} = 1/2$ when $H_{J_{\Delta T}}(\varepsilon)$ is invertible.

4.2. Cauchy propriety of the monotonic sequences

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

Theorem 4.5. *Sequence $(\varepsilon^k)_{k \in \mathbb{N}}$ defined by (17)–(18) converges towards a critical point of $J_{\Delta T}$.*

Proof. : First suppose that:

$$\forall k \in \mathbb{N}, \tilde{J}_{\Delta T}(\varepsilon^k) \neq 0.$$

According to (24), there exists k_0 such that (31) holds for all ε^k with $k \geq k_0$, with $\tilde{\theta} = 1/2$ if $H_{J_{\Delta T}}$ is invertible on C_{ε^0} . Consider an integer $k \geq k_0$. Thanks to the results above:

$$\begin{aligned} (\tilde{J}_{\Delta T}(\varepsilon^k))^{\tilde{\theta}} - (\tilde{J}_{\Delta T}(\varepsilon^{k+1}))^{\tilde{\theta}} &\geq \frac{\tilde{\theta}}{(\tilde{J}_{\Delta T}(\varepsilon^{k+1}))^{1-\tilde{\theta}}} (J_{\Delta T}(\varepsilon^{k+1}) - J_{\Delta T}(\varepsilon^k)) \\ &\geq \frac{\tilde{\kappa}\tilde{\theta}}{\|\nabla J_{\Delta T}(\varepsilon^{k+1})\|_1} \left(\left(\frac{2}{\delta} - 1\right) \|\varepsilon^{k+1} - \tilde{\varepsilon}^k\|_2^2 + \left(\frac{2}{\eta} - 1\right) \|\tilde{\varepsilon}^k - \varepsilon^k\|_2^2 \right) \\ &\geq \frac{\tilde{\kappa}\tilde{\theta}a_{(\delta,\eta)}}{\|\nabla J_{\Delta T}(\varepsilon^{k+1})\|_1} \left(\|\varepsilon^{k+1} - \tilde{\varepsilon}^k\|_2 + \|\tilde{\varepsilon}^k - \varepsilon^k\|_2 \right)^2 \\ &\geq \frac{\tilde{\kappa}\tilde{\theta}a_{(\delta,\eta)}}{\lambda} \left(\|\varepsilon^{k+1} - \tilde{\varepsilon}^k\|_2 + \|\tilde{\varepsilon}^k - \varepsilon^k\|_2 \right) \end{aligned} \quad (32)$$

$$\geq \frac{\tilde{\kappa}\tilde{\theta}a_{(\delta,\eta)}}{\lambda} \|\varepsilon^{k+1} - \varepsilon^k\|_2 \quad (33)$$

where $a_{(\delta,\eta)} = \frac{1}{\max(\delta,\eta)} - \frac{1}{2}$. Given $q \in \mathbb{N}$, Inequality (33) leads to:

$$\begin{aligned} (\tilde{J}_{\Delta T}(\varepsilon^k))^{\tilde{\theta}} - (\tilde{J}_{\Delta T}(\varepsilon^{k+q}))^{\tilde{\theta}} &\geq \frac{\tilde{\kappa}\tilde{\theta}a_{(\delta,\eta)}}{\lambda} \sum_{l=k}^{k+q-1} \|\varepsilon^{l+1} - \varepsilon^l\|_2 \\ &\geq \frac{\tilde{\kappa}\tilde{\theta}a_{(\delta,\eta)}}{\lambda} \|\varepsilon^{k+q} - \varepsilon^k\|_2. \end{aligned}$$

Since $((\tilde{J}_{\Delta T}(\varepsilon^k))^{\tilde{\theta}})_{k \in \mathbb{N}}$ is a Cauchy sequence, we conclude that the sequence $(\varepsilon^k)_{k \in \mathbb{N}}$ is also Cauchy.

In case there exists k_1 such that $\tilde{J}_{\Delta T}(\varepsilon^{k_1}) = 0$, the monotonicity of the algorithm implies that $J_{\Delta T}(\varepsilon^{k_1}) = J_{\Delta T}(\varepsilon^{k_1+1}) = J_{\Delta T}(\varepsilon^{k_1+2}) = \dots$ and according to (22) the sequence $(\varepsilon^k)_{k \in \mathbb{N}}$ is constant for $k \geq k_1$.

Lastly, the limit that has been reached belongs to C according to Lemma 3.3. \square

Remark 4.6. : *A similar proof can be developed when $\delta = 0, \eta \neq 0$ and $\delta \neq 0, \eta = 0$. In case $\delta = 0, \eta = 0$, the convergence is trivial.*

5. RATE OF CONVERGENCE

In this section, we will present both theoretical and numerical results regarding the rate of convergence of the discrete monotonic schemes.

5.1. Theoretical results

The rate of convergence can be evaluated by a making a second use of Łojasiewicz inequality. The result is summarized in the next theorem.

Theorem 5.1. *Let us denote by ε^∞ the limit of $(\varepsilon^k)_{k \in \mathbb{N}}$ defined by (17)–(18) and by $\tilde{\theta}$ and $\tilde{\kappa}$ the real numbers appearing in (31), where $C_{\varepsilon^0} = \{\varepsilon^\infty\}$.*

If $\tilde{\theta} < \frac{1}{2}$, then there exists $c > 0$ such that:

$$\|\varepsilon^k - \varepsilon^\infty\|_2 \leq ck^{-\frac{\tilde{\theta}}{1-2\tilde{\theta}}}. \quad (34)$$

If $\tilde{\theta} = \frac{1}{2}$, then there exist c' and τ such that:

$$\|\varepsilon^k - \varepsilon^\infty\|_2 \leq c'e^{-\tau k}. \quad (35)$$

Proof. : As in the proof of Theorem 4.5, let be $k_0 \geq 0$ such that

$$\forall l \geq k_0 \quad \|\nabla J_{\Delta T}(\varepsilon^l)\|_1 \geq \tilde{\kappa} |\tilde{J}_{\Delta T}(\varepsilon^l)|^{1-\tilde{\theta}}. \quad (36)$$

Let us fix $k \geq k_0$ and introduce Δ^k defined by:

$$\Delta^k = \sum_{l=k}^{\infty} \|\varepsilon^{l+1} - \varepsilon^l\|_2 + \|\varepsilon^l - \varepsilon^l\|_2.$$

Sticking to a general way of reasoning, we may assume that $\Delta^k > 0$ for any $k \geq k_0$. By summing (32) between k and $+\infty$, we obtain:

$$(\tilde{J}_{\Delta T}(\varepsilon^k))^{\tilde{\theta}} \geq \frac{\tilde{\kappa}\tilde{\theta}a_{(\delta,\eta)}}{\lambda} \Delta^k.$$

This estimate, combined with (36), yields:

$$\|\nabla J_{\Delta T}(\varepsilon^k)\|_1 \geq \tilde{\kappa} \left(\frac{\tilde{\kappa}\tilde{\theta}a_{(\delta,\eta)}}{\lambda} \Delta^k \right)^{\frac{1-\tilde{\theta}}{\tilde{\theta}}}.$$

From Lemma 3.4, we get:

$$\lambda(\Delta^{k-1} - \Delta^k) \geq \tilde{\kappa} \left(\frac{\tilde{\kappa}\tilde{\theta}a_{(\delta,\eta)}}{\lambda} \Delta^k \right)^{\frac{1-\tilde{\theta}}{\tilde{\theta}}},$$

which can be rewritten as follows:

$$\frac{\Delta^{k-1} - \Delta^k}{(\Delta^k)^\beta} \geq \nu, \quad (37)$$

with $\nu > 0$ and $\beta = \frac{1-\tilde{\theta}}{\tilde{\theta}}$.

Suppose that $\tilde{\theta} = \frac{1}{2}$, i.e., $\beta = 1$. Equation (37) reads:

$$(1 + \nu)^{k_0} \Delta^{k_0} \left(\frac{1}{1 + \nu} \right)^k \geq \Delta^k,$$

and (35) is proved with $c' = (1 + \nu)^{k_0} \Delta^{k_0}$ and $\tau = \ln(1 + \nu)$.

Now let us consider the case in which $\tilde{\theta} < \frac{1}{2}$. Let $r \in]0, 1[$, and first suppose that:

$$(\Delta^k)^\beta \geq r(\Delta^{k-1})^\beta.$$

Since $1 - \beta < 0$, the function $s \mapsto s^{1-\beta}$ is convex and consequently:

$$\begin{aligned} (\Delta^k)^{1-\beta} - (\Delta^{k-1})^{1-\beta} &\geq (\beta - 1) \frac{\Delta^{k-1} - \Delta^k}{(\Delta^{k-1})^\beta} \\ &\geq (\beta - 1)r \frac{\Delta^{k-1} - \Delta^k}{(\Delta^k)^\beta} \\ &\geq (\beta - 1)r\nu. \end{aligned}$$

In the other case:

$$(\Delta^k)^\beta \leq r(\Delta^{k-1})^\beta,$$

and consequently:

$$(\Delta^k)^{1-\beta} - (\Delta^{k-1})^{1-\beta} \geq (\Delta^k)^{1-\beta} - (r^{\frac{1}{\beta}} \Delta^k)^{1-\beta} = (1 - r^{\frac{1-\beta}{\beta}})(\Delta^k)^{1-\beta} \geq (1 - r^{\frac{1-\beta}{\beta}})(\Delta^{k_0})^{1-\beta}.$$

Thus, in any case, there exists $\nu' \geq 0$ such that:

$$(\Delta^k)^{1-\beta} - (\Delta^{k-1})^{1-\beta} \geq \nu'. \quad (38)$$

Consider now $k' > k$. Inequality (38) implies that for small enough a c , we get:

$$\Delta^{k'} \leq \left(\nu'(k' - k) + (\Delta^k)^{2 - \frac{1}{\theta}} \right)^{-\frac{\theta}{1-2\theta}} \leq ck'^{-\frac{\theta}{1-2\theta}},$$

and (34) follows. \square

Remark 5.2. : *Thanks to Lemma 2.1, we have thus obtained that if:*

$$\alpha > 2\|\mu\|_*^2 \|O\|_* T, \quad (39)$$

the convergence of the schemes is at least linear.

5.2. Numerical results

In order to test the performance of the algorithm we have chosen a case already treated in the literature. The system under consideration is the $O - H$ bond that vibrates in a Morse type potential. We refer to [20] for the numerical details concerning this system. The objective is to localize the wavefunction at a given location x' ; this is expressed through the requirement that $\langle \psi(T) | O | \psi(T) \rangle$ is maximized, where the observable O is defined by $O(x) = \frac{\gamma_0}{\sqrt{\pi}} e^{-\gamma_0^2(x-x')^2}$. In our test, $\beta = 1$, $\|\mu\|_* = 0.68151$, $\|O\|_* = 12.375$ and $T = 131000$. Numerical tests carried out on this example show that though (39) is not true at all, the convergence of the algorithm is linear, as it appears on Figure 1. Therefore some further analysis has to be done to improve Lemma 2.1 and the results of Section 5.1.

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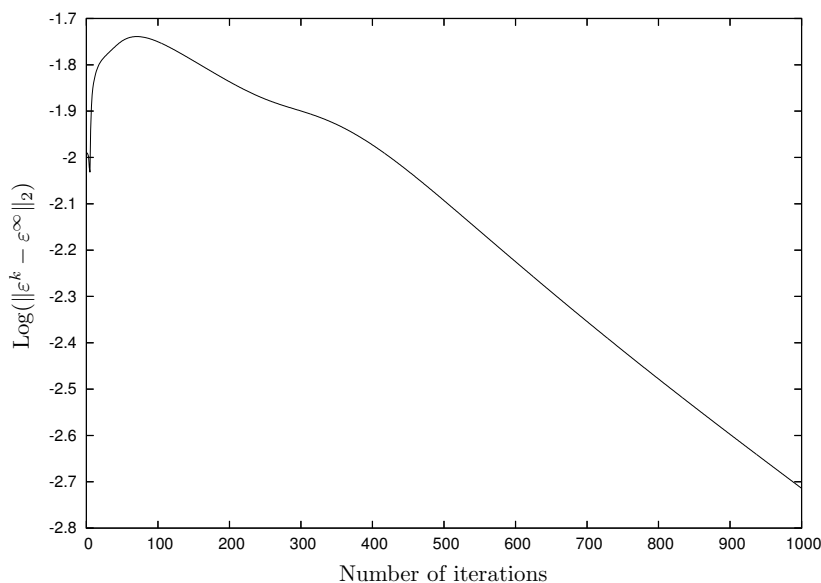


FIGURE 1. The rate of convergence is linear after the 500-th iteration.

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APPENDIX: CONVERGENCE OF THE EXPLICIT DISCRETE MONOTONIC SCHEME

In [12], an explicit scheme has also been presented. The proof of convergence of this scheme, although analogous to that of the implicit scheme, is slightly more elaborate. We briefly introduce here a sufficient condition for a convergence.

1. Definition of the scheme

Given the initial control amplitudes ε^0 , $\tilde{\varepsilon}^0$ and their associated state ψ^0 and adjoint state χ^0 , suppose that for some $k \geq 1$, ψ^{k-1} , χ^{k-1} , ε^{k-1} , $\tilde{\varepsilon}^{k-1}$ have already been computed. The iterated quantities of ψ^k , χ^k , ε^k , $\tilde{\varepsilon}^k$ are defined as follows:

$$\left\{ \begin{array}{l} \psi_{j+1}^k = e^{-\frac{H_0 \Delta T}{2i}} e^{\frac{V - \mu \varepsilon_j^k}{i} \Delta T} e^{-\frac{H_0 \Delta T}{2i}} \psi_j^k \\ \varepsilon_j^k = (1 - \delta_j^k) \varepsilon_j^{k-1} - \frac{\delta_j^k}{\alpha} \text{Im} \langle \tilde{\chi}_j^{k-1} | \mu | \psi_j^k \rangle \\ \psi_0^k = \psi_{init}, \end{array} \right. \quad (40)$$

$$\left\{ \begin{array}{l} \chi_j^k = e^{-\frac{H_0 \Delta T}{2i}} e^{\frac{-V + \mu \tilde{\varepsilon}_j^k}{i} \Delta T} e^{-\frac{H_0 \Delta T}{2i}} \chi_{j+1}^k \\ \tilde{\varepsilon}_j^k = (1 - \eta_j^k) \tilde{\varepsilon}_j^{k-1} - \frac{\eta_j^k}{\alpha} \text{Im} \langle \tilde{\chi}_{j+1}^k | \mu | \tilde{\psi}_{j+1}^k \rangle \\ \chi_N^k = O \psi_N^k, \end{array} \right. \quad (41)$$

where:

$$\delta_j^k = \frac{\alpha}{\alpha + \Delta T \text{Re} \langle \tilde{\chi}_j^{k-1} | \mu^2 | \psi_j^k \rangle},$$

and:

$$\eta_j^k = \frac{\alpha}{\alpha + \Delta T \text{Re} \langle \tilde{\chi}_{j+1}^k | \mu^2 | \tilde{\psi}_{j+1}^k \rangle}.$$

2. Proprieties of sequence $(\varepsilon^k)_{k \in \mathbb{N}}$

2.1 Upper bound

The first step of the convergence analysis is to obtain an upper bound for the fields. Suppose that:

$$\alpha > 2\Delta T \|\mu\|_*^2 \|O\|_*. \quad (42)$$

This condition ensures that:

$$\forall k \in \mathbb{N}, \forall j = 0 \dots N-1, \delta_j^{k+1} \in [0, 2\frac{\alpha}{\alpha+e}], \eta_j^{k+1} \in [0, 2\frac{\alpha}{\alpha+e}],$$

where $e = \alpha - 2\Delta T \|\mu\|_*^2 \|O\|_*$. An analysis similar to that in the proof of Lemma 3.1 (see [12]) gives the following result:

Lemma 5.3. *Suppose that (42) is fulfilled. Given an initial field ε^0 , let us define M by:*

$$M = \max(\|\varepsilon^0\|_\infty, \max(1, \frac{1}{e})\|O\|_* \|\mu\|_*). \quad (43)$$

The sequences $(\varepsilon^k)_{k \in \mathbb{N}}$ and $(\tilde{\varepsilon}^k)_{k \in \mathbb{N}}$ meet the requirements:

$$\forall k \in \mathbb{N}, \forall j = 0 \dots N-1, |\varepsilon_j^k| \leq M, |\tilde{\varepsilon}_j^k| \leq M.$$

2.2 Monotonic convergence

In the case of the explicit scheme, Equation (21) cannot be explicitly simplified as was the case for the implicit schemes. However, the Taylor-Lagrange formula stipulates the existence of two real numbers x_j^k and y_j^k in $[-M, M]$ such that:

$$\begin{aligned} \operatorname{Re} \langle \check{\chi}_{j+1}^k | e^{\frac{\mu(\varepsilon_j^k - \tilde{\varepsilon}_j^k)}{i} \Delta T} - \operatorname{Id} | \tilde{\psi}_{j+1}^k \rangle &= \operatorname{Im} \langle \check{\chi}_{j+1}^k | \mu | \tilde{\psi}_{j+1}^k \rangle (\varepsilon_j^k - \tilde{\varepsilon}_j^k) \Delta T \\ &\quad - \operatorname{Re} \langle \check{\chi}_{j+1}^k | \mu^2 e^{-i\mu x_j^k \Delta T} | \tilde{\psi}_{j+1}^k \rangle > \frac{(\varepsilon_j^k - \tilde{\varepsilon}_j^k)^2 \Delta T^2}{2}, \end{aligned} \quad (44)$$

and:

$$\begin{aligned} \operatorname{Re} \langle \tilde{\chi}_j^k | e^{i\mu(\varepsilon_j^{k+1} - \tilde{\varepsilon}_j^k) \Delta T} - \operatorname{Id} | \check{\psi}_j^{k+1} \rangle &= -\operatorname{Im} \langle \tilde{\chi}_j^k | \mu | \check{\psi}_j^{k+1} \rangle (\varepsilon_j^{k+1} - \tilde{\varepsilon}_j^k) \Delta T \\ &\quad + \operatorname{Re} \langle \tilde{\chi}_j^k | \mu^2 e^{i\mu y_j^k \Delta T} | \check{\psi}_j^{k+1} \rangle > \frac{(\varepsilon_j^{k+1} - \tilde{\varepsilon}_j^k)^2 \Delta T^2}{2}. \end{aligned} \quad (45)$$

Combining (44) and (45) with the definitions of ε_j^k and $\tilde{\varepsilon}_j^k$ given by (40)–(41), we can conclude that (21) can be written as follows:

$$\begin{aligned} J_{\Delta T}(\varepsilon^{k+1}) - J_{\Delta T}(\varepsilon^k) &= \langle \psi_N^{k+1} - \psi_N^k | O | \psi_N^{k+1} - \psi_N^k \rangle \\ &\quad + \Delta T \sum_{j=0}^{N-1} (\varepsilon_j^k - \tilde{\varepsilon}_j^k)^2 [\alpha + \Delta T \operatorname{Re} \langle \check{\chi}_{j+1}^k | \mu^2 | \tilde{\psi}_{j+1}^k \rangle \\ &\quad \quad \quad + \Delta T \operatorname{Re} \langle \check{\chi}_{j+1}^k | \mu^2 (\operatorname{Id} - e^{-i\mu x_j^k \Delta T}) | \tilde{\psi}_{j+1}^k \rangle] \\ &\quad + \Delta T \sum_{j=0}^{N-1} (\tilde{\varepsilon}_j^k - \varepsilon_j^{k+1})^2 [\alpha + \Delta T \operatorname{Re} \langle \tilde{\chi}_j^k | \mu^2 | \check{\psi}_j^{k+1} \rangle \\ &\quad \quad \quad + \Delta T \operatorname{Re} \langle \tilde{\chi}_j^k | \mu^2 (\operatorname{Id} - e^{i\mu y_j^k \Delta T}) | \check{\psi}_j^{k+1} \rangle]. \end{aligned}$$

We are now in a position to claim the following result, which is the equivalent of formula (22) associated with the implicit schemes.

Lemma 5.4. *Suppose that the real number $\gamma = \alpha - 3\Delta T \|\mu\|_*^2 \|O\|_*$ is strictly positive. Then the explicit scheme is monotonic and:*

$$J_{\Delta T}(\varepsilon^{k+1}) - J_{\Delta T}(\varepsilon^k) \geq \gamma [\|\varepsilon_j^k - \tilde{\varepsilon}_j^k\|_2^2 + \|\tilde{\varepsilon}_j^k - \varepsilon_j^{k+1}\|_2^2].$$

3. Convergence

The end of the proof of convergence of the explicit scheme can then be done in a similar way as for implicit schemes (in particular, the proof of Lemma 3.4 can be easily adapted). The next theorem summarizes the result reached.

Theorem 5.5. *Suppose that:*

$$\alpha > 3\Delta T \|\mu\|_*^2 \|O\|_*.$$

Then the sequence $(\varepsilon^k)_{k \in \mathbb{N}}$ defined by (40)–(41) converges towards a critical point of $J_{\Delta T}$.