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MAT

SERIE A : CONFERENCIAS, SEMINARIOS Y TRABAJOS DE MATEMÁTICA

No. 3

VI SEMINARIO SOBRE PROBLEMAS DE FRONTERA LIBRE Y SUS APLICACIONES

Primera Parte

Domingo A. Tarzia (Ed.)

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Rosario, Agosto 2001

El VI Seminario sobre Problemas de Frontera Libre y sus Aplicaciones tuvo lugar en el Departamento de Matemática de la FCE de la Universidad Austral, en Rosario, del 16 al 18 de Diciembre de 1998. Fue realizado con el apoyo del Proyecto de Investigación Plurianual del CONICET “Problemas de Frontera Libre para la Ecuación del Calor-Difusión” y gracias a un subsidio otorgado por el CONICET.

Los problemas de frontera libre son aquellos problemas de contorno donde interviene además, una superficie incógnita (la “frontera libre”) que separa dos o más regiones, sobre la cual se conocen datos que dependen del modelo analizado. Según el número de dimensiones del espacio, en lugar de una superficie de separación se podrá tener una curva o un número finito de puntos.

El avance considerable que se ha obtenido en el desarrollo teórico de estos temas a nivel nacional y sus potenciales aplicaciones a la industria (electropintura, envenenamiento y regeneración de catalizadores; combustión de sólidos; solidificación de aleaciones binarias; soldadura de metales; colada continua del acero; congelación de alimentos en la industria frigorífica; almacenamiento de energía térmica de origen solar por cambio de fase; oxidación del zirconio y fusión del dióxido de uranio en reactores nucleares, en caso de accidentes; procesos de ablación térmica; difusión-consumo de oxígeno en tejidos vivos, para el tratamiento médico de tumores mediante la aplicación de radiaciones; problemas de control óptimo ligados a procesos con cambio de fase; solidificación de suelos húmedos; derretimiento de glaciares; crecimiento de raíces de cultivo; precio en las opciones americanas; etc.) impulsaron su realización, prosiguiendo la línea de los Seminarios anteriores, con el objetivo de facilitar la interacción entre las personas y grupos de investigación que trabajan en dichos problemas y en temas conexos, y de despertar el interés y promover el acercamiento de jóvenes graduados.

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Esta primera parte contiene cinco de las conferencias y comunicaciones presentadas. La nómina general se incluye, en orden cronológico, en la página 42.

Los manuscritos fueron recibidos y aceptados en marzo de 2001.

**CONDITIONS TO OBTAIN A WAITING TIME FOR A
DISCRETE TWO-PHASE STEFAN PROBLEM**

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RESUMEN

En este trabajo se considera un problema unidimensional de conducción de calor no-estacionario, con condiciones de borde mixtas. Con un esquema en diferencias finitas implícito se obtienen condiciones suficientes para asegurar que la solución será positiva en un paso de tiempo, si es positiva en el paso de tiempo anterior. También se deduce, empleando un esquema en diferencias finitas explícito, la expresión de la temperatura en cada paso de tiempo, como un polinomio en la variable $\lambda = \alpha \frac{\Delta t}{\Delta x^2}$, con coeficientes dados como una función de los datos del problema. Se pueden así establecer condiciones suficientes sobre los datos que aseguran la existencia de un tiempo de espera, a partir del cual comienza el cambio de fase.

PALABRAS CLAVE

Conducción del calor, Cambio de fase, Problema de Stefan, Análisis Numérico, Frontera Libre.

ABSTRACT

In this paper we consider a one-dimensional non-stationary heat conduction problem, with initial datum and with mixed boundary conditions. We obtain, with an implicit finite difference scheme, some sufficient conditions, so that the discrete solution is positive at any moment if it is positive at the previous time step. We also deduce, with an explicit finite difference scheme, the discrete expression of the temperature at each time step, as a polynomial in the variable $\lambda = \alpha \frac{\Delta t}{\Delta x^2}$, with coefficients given as function of the problem dates. So we can establish some sufficient conditions on the data in order to obtain the existence of a waiting time at wich a phase-change begins.

KEYWORDS

Heat Conduction, Phase-change, Stefan Problem, Numerical Analysis, Free-Boundary.

AMS subject classification: 65M06, 80A22

1.- INTRODUCTION

In this paper we consider a one-dimensional heat conduction problem in a finite (or semi-infinite) slab of a material that is initially in the liquid phase, at a temperature $\theta_o(x)$ greater than the phase change temperature, having a heat flux $q(t)$ on the left face $x = 0$ and a temperature condition on the right face $x = x_o$.

We can state the problem through the following equations ($0 < x_0 \leq +\infty$):

$$\rho c \frac{\partial \theta}{\partial t} - k \frac{\partial^2 \theta}{\partial x^2} = 0, \quad 0 < x < x_0, \quad t > 0, \quad (1.1)$$

$$\theta(x,0) = \theta_0(x) > 0, \quad 0 \leq x \leq x_0, \quad (1.2)$$

$$k \frac{\partial \theta}{\partial x}(0,t) = q(t) > 0, \quad t > 0, \quad (1.3)$$

$$\theta(x_0,t) = b(t), \quad t > 0, \quad (1.4)$$

The constants ρ , c and k represent the mass density, the specific heat and the thermal conductivity respectively. For the case $x_0 = +\infty$ we change the condition (1.4) by $\theta(+\infty,t) = \theta_0(+\infty) > 0$, for $t > 0$.

Without loss of generality we assume that the phase-change temperature of the material is 0°C . In accordance with the data θ_0 , q and b , it can happen that [6]:

(a) the heat conduction problem is defined for all time $t > 0$.

(b) there exists a waiting time $t^* < +\infty$ such that another phase (i.e. the solid phase) appears for $t \geq t^*$ and then we have a two-phase Stefan problem. In this case, there exists a free boundary $x = s(t)$, which separates the liquid and solid phases, with $s(t^*) = 0$.

If the temperature on the right face $x = x_0$ is a constant $b(t) = b > 0$, and the flux on the left face $x = 0$ is $q(t) = q > 0$, also a constant, then the stationary solution is given by:

$$\theta_\infty(x) = \frac{q}{k} (x - x_0) + b.$$

In this case a necessary condition to obtain a stationary two-phase Stefan problem is given by [5]:

$$q > \frac{kb}{x_0}.$$

Taking into account that the solution of problem (1.1) – (1.4) with data $b > 0$ and $q > 0$ tends to $\theta_\infty = \theta_\infty(x)$ when t goes to infinity [2], in [6] was considered the problem of finding the relation between the heat flux $q > 0$ on $x = 0$ and a time t_1 such that another phase appears for $t \geq t_1$. The following results were obtained:

Theorem 1: [1]

Suppose the initial temperature verifies the conditions $b \geq \theta_0 \geq 0$ in $[0, x_0]$ and $\theta_0(x_0) = b$. If we consider the t, q plane and we define the following set:

$$Q = \left\{ (t, q) / q > f(t), t > 0 \right\},$$

where

$$f(t) = \frac{bk}{x_0 [1 - \exp(-\frac{\alpha \pi^2 t}{4x_0^2})]} , \alpha = \frac{k}{\rho c} \tag{1.5}$$

then we have a two-phase problem for all $(t, q) \in Q$.

The goal of this paper is to obtain a discrete expression for the inequation $q > f(t)$, obtained in the above theorem.

In section 2 we get some conditions on the data which guarantees the positivity of the discrete solution, i.e. no phase-change occurs.

In section 3, we express the discrete temperature at the face $x = 0$ as a polynomial in the variable $\lambda = \alpha \frac{\Delta t}{\Delta x^2}$ (with Δt the temporal step and Δx the spatial step) and we obtain an inequality for the heat flux q , as a function of data coefficients θ_0 , k and α . In other words, we can determine if there exists a waiting time from which the other phase, the solid phase, appears .

2. AN APPROXIMATION WITH AN IMPLICIT FINITE DIFFERENCE METHOD

We set up a mesh with step $\Delta x = \frac{x_0}{N}$ (N is a natural number) for the spatial variable x and with step Δt for the temporal variable t . We note with U_i^j an approximate value of the temperature θ at the point $(x, t) = (i\Delta x, j\Delta t)$ for $i = 0, 1, \dots, N$ and $j = 1, 2, 3, \dots$, that is $U_i^j \approx \theta(x_i, t_j)$.

We use an implicit finite difference schema, so we can state problem (1.1) – (1.4) in a matrix form :

$$\mathbf{A} \mathbf{U}^j = \mathbf{U}^{j-1} + \mathbf{c}^j \tag{2.1}$$

where \mathbf{A} is the following $N-1$ -dimensional square matrix

$$\mathbf{A} = \begin{pmatrix} 1 + \lambda & -\lambda & 0 & : & : & 0 \\ -\lambda & 1 + 2\lambda & -\lambda & 0 & : & 0 \\ 0 & -\lambda & : & : & : & 0 \\ 0 & : & : & : & : & 0 \\ : & & & & : & -\lambda \\ 0 & 0 & 0 & : & -\lambda & 1 + 2\lambda \end{pmatrix} \tag{2.2}$$

$\lambda = \alpha \frac{\Delta t}{\Delta x^2}$ is a parameter, $\mathbf{U}^j = (U_1^j, U_2^j, \dots, U_{N-1}^j)^t$ is a $N-1$ -dimensional vector and \mathbf{c}^j is the $N-1$ -dimensional vector

$$\mathbf{c}^j = (-\lambda \frac{\Delta x}{k} q(t_j), 0, \dots, 0, \lambda b(t_j))^t \tag{2.3}$$

This regressive finite difference schema is unconditionally stable and it converges to the solution of the continuous problem with a rate of convergence $O(\Delta t + \Delta x^2)$ [3].

We are interested in the relationship between the data, so that if the discrete temperature U_i^j is positive ($i = 0, 1, \dots, N$), then the discrete temperature U_i^{j+1} in the next time step is also positive.

We will see some definitions which will be useful in the sequel:

Definition:

- i) A matrix $\mathbf{M} = (m_{ij})$ is said to be **positive** if all of its elements m_{ij} are non-negatives ($m_{ij} \geq 0 \ \forall i, j$). In particular, a vector $\mathbf{v} = (v_i)$ is said to be **positive** if $v_i \geq 0, \forall i$.
- ii) A square real matrix \mathbf{M} is said to be **monotone** if it is invertible and its inverse is positive.

Moreover (see [1]):

$$\mathbf{M} \text{ is monotone} \Leftrightarrow \{\mathbf{v} \in \mathbb{R}^n: \mathbf{M}\mathbf{v} \geq 0\} \subset \{\mathbf{v} \in \mathbb{R}^n: \mathbf{v} \geq 0\} \quad (2.4)$$

Taking into account the above equivalence, we can prove the following properties [4]:

Theorem 2:

- i) The matrix \mathbf{A} , defined in (2.2), is monotone.
- ii) The inverse matrix \mathbf{A}^{-1} is positive.

Theorem 3:

Let q, θ_0 and b be positive constants ($\theta_0 = b, \mathbf{c}^j = \mathbf{c}, \forall j$) and $\mathbf{U}^j = (U_1^j, U_2^j, \dots, U_{N-1}^j)^t$ which satisfies the schema (2.1) for $j = 1, 2, \dots$. Then, if at the time $t_j = j\Delta t, \mathbf{U}^j$ is positive and the inequality

$$q < \frac{\rho c U_1^j \Delta x}{\Delta t} \quad j = 1, 2, \dots \quad (2.5)$$

holds, then \mathbf{U}^{j+1} is also positive.

3. SOME CONDITIONS TO OBTAIN A WAITING TIME FOR THE DISCRETE PROBLEM

If we use an explicit finite difference schema we get that the discrete temperature U_i^j which approximates $\theta(x_i, t_j)$ satisfies:

$$U_i^j = U_i^{j-1} + \lambda(U_{i+1}^{j-1} - 2U_i^{j-1} + U_{i-1}^{j-1}) \quad i = 1, \dots, N-1, j = 1, 2, 3, \dots \quad (3.1)$$

$$U_i^0 = \theta_0(x_i) \quad i = 0, 1, \dots, N \quad (3.2)$$

$$U_0^j = U_1^j - \frac{\Delta x}{k} q(t_j) \quad j = 1, 2, 3, \dots \quad (3.3)$$

$$U_N^j = b(t_j) \quad j = 1, 2, 3, \dots \quad (3.4)$$

This method is not as efficient as that consider in the above section, because it is conditionally stable and it converges to the solution of problem (1.1) – (1.4) with a convergence rate $O(\Delta t + \Delta x^2)$ only if [3]:

$$\lambda \leq \frac{1}{2} \tag{3.5}$$

Nevertheless we use here this method, because in this way it is possible to obtain an explicit expression for the discrete temperature at the left face $x = 0$ for all time step $j\Delta t$, as a function of the initial and the boundary dates. So we can establish sufficient conditions in order to obtain a waiting time in the discrete problem. We have [4]:

Theorem 4:

If the data b, q and θ_0 are constants, $b = \theta_0$ and (3.5) holds, then, when we consider the scheme (3.1) – (3.4), the values U_i^m of the discrete temperature obtained, verify the following properties:

$$i) U_i^m \leq U_{i+1}^m \quad i = 1, \dots, N-1, m = 0, 1, 2, 3, \dots \tag{3.6}$$

$$ii) U_i^m \geq U_i^{m+1} \quad i = 1, \dots, N, m = 0, 1, 2, 3, \dots \tag{3.7}$$

As a consequence of the above theorem, in order to determine the moment from which the solid phase appears in the discrete problem, it suffices to find the value of j such that $U_0^j < 0$.

In the following theorem, we express the discrete temperature as a polynomial in the variable λ [4]:

Theorem 5:

Under the hypothesis of Theorem 4 it results

$$U_i^1 = \theta_0 \quad i = 1, 2, \dots, N - 1 \tag{3.8}$$

$$U_i^j = \theta_0 - q \frac{\Delta x}{k} P_i^j(\lambda) \quad i = 1, 2, \dots, j - 1 \quad j = 2, 3, \dots \tag{3.9}$$

$$U_i^j = \theta_0 \quad i = j, j + 1, \dots, N-1 \quad j = 2, 3, \dots \tag{3.10}$$

where

$$P_i^j(x) = \sum_{m=i}^{j-1} a_m(i,j) x^m \quad \text{and} \quad a_m(i,j) = (-1)^{m+i} b_m c_{im} d_{jm} \tag{3.11}$$

with

$$b_1 = 1 \quad b_m = \frac{(2m-3)!! 2^{m-1}}{m} \quad m = 2, 3, \dots$$

$$c_{im} = \frac{(2i-1)}{(m-i)! (m+(i-1))!} \quad m = i, i + 1, \dots, j - 1 \tag{3.12}$$

$$d_{jm} = \frac{(j-1)!}{(j-(m+1))!} \quad m = i, i + 1, \dots, j - 1$$

Theorem 6:

Under the hypothesis of Theorem 4 it results

$$U_o^j = \theta_o - q \frac{\Delta x}{k} P_o^j(\lambda) \quad j = 1, 2, \dots \quad (3.13)$$

where the polynomial P_o^j is given by:

$$P_o^j(x) = \sum_{m=0}^{j-1} a_m(j) x^m \quad (3.14)$$

with $a_o(j) = 1$ $a_1(j) = j - 1$ (3.15)

$$a_m(j) = \frac{(-1)^{m+1} 2^{m-1} (2m-3)!! (j-1)!}{(m!)^2 (j-(m+1))!} \quad m = 2, \dots, j-1$$

Corollary 7:

If $q > \frac{\theta_o k}{\Delta x P_o^j(\lambda)}$ then there exists a waiting time $t_j = j\Delta t$ such that the problem (3.1) – (3.4) is a two-phase problem for all $t > t_j$.

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ON SIMILARITY SOLUTIONS FOR THAWING PROCESSES*

Ariel L. LOMBARDI and Domingo A. TARZIA

Abstract

We review some recent results for a mathematical model for thawing in a saturated semi-infinite porous medium when change of phase induces a density jump and a heat flux condition of the type $-q_0 t^{-\frac{1}{2}}$ is imposed on the fixed face $x=0$. Different cases depending on physical parameters are analysed and the explicit solution of the similarity type is obtained when a given condition for the thermal coefficient q_0 is verified.

Key words. Stefan problem, free boundary problems, phase change process, similarity solution, density jump, thawing processes, freezing, solidification.

Resumen. Se realiza una revisión de recientes resultados sobre un modelo matemático de descongelación en un medio poroso semi-infinito saturado cuando un cambio de fase induce un salto de densidad y cuando se impone una condición de flujo de calor del tipo $-q_0 t^{-\frac{1}{2}}$ en el borde fijo $x=0$. Se analizan diferentes casos que dependen de diversos parámetros físicos y se obtiene la solución explícita de tipo similitud cuando una cierta condición sobre el coeficiente térmico q_0 es satisfecha.

Palabras Claves. Problema de Stefan, problemas de frontera libre, procesos de cambio de fase, solución de similitud, salto de densidad, procesos de descongelación, congelación, solidificación.

AMS subject classification. 35R35, 80A22, 35C05.

1 Introduction

Phase-change problems appear frequently in industrial processes and other problems of technological interest [8]. A large bibliography on the subject was given in [11]. In this paper, we consider the problem of thawing of a partially frozen porous media, saturated with an incompressible liquid, with the aim of constructing similarity solutions.

We have in mind the following physical assumptions (see [2], [4], [5]):

1. A sharp interface between the frozen part and the unfrozen part of the domain exists (sharp, in the macroscopic sense).
2. The frozen part is at rest with respect to the porous skeleton, which will be considered to be indeformable.
3. Due to density jump between the liquid and solid phase, thawing can induce either desaturation or water movement in the unfrozen region. We will consider the latter situation assuming that liquid is continuously supplied to keep the medium saturated.

Although thawing has received less attention than freezing, our investigation is in the same spirit as [3], and [9], with the simplification due to the absence of ice lenses and frozen fringes.

We will study a one-dimensional model of the problem, using the following notation:

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$\varepsilon > 0$:	porosity,
$\rho > 0$:	density; ρ_w and ρ_I : density of water and ice (g/cm^3)
$c > 0$:	specific heat at constant density ($\frac{\text{cal}}{\text{g}^\circ\text{C}}$)
$k > 0$:	conductivity ($\frac{\text{cal}}{\text{s cm}^\circ\text{C}}$)
u	:	temperature of unfrozen zone ($^\circ\text{C}$)
v	:	temperature of frozen zone ($^\circ\text{C}$)
$u = v = 0$:	being the melting point at atmospheric pressure
$\lambda > 0$:	latent heat at $u = 0$ (cal/g)
γ	:	coefficient in the Clausius-Clapeyron law ($\text{s}^2\text{cm}^\circ\text{C/g}$)
$\mu > 0$:	viscosity of liquid (g/cm^3)

and subscripts F, U, I and W refer to the frozen medium, unfrozen medium, pure ice and pure water, respectively, while S refers to the porous skeleton.

The unknowns of the problem are a function $x = s(t)$, representing the free boundary separating $Q_1 = \{(x, t) : 0 < x < s(t), t > 0\}$ and $Q_2 = \{(x, t) : s(t) < x, t > 0\}$, and the two functions $u(x, t)$ and $v(x, t)$ defined in Q_1 and Q_2 , respectively. Besides standard requirements, $s(t)$, $u(x, t)$ and $v(x, t)$ fulfil the following conditions (we refer to [4] for a detailed explanation of the model):

$$u_t = a_1 u_{xx} - b\rho\dot{s}(t)u_x, \quad \text{in } Q_1 \quad (1)$$

$$v_t = a_2 v_{xx}, \quad \text{in } Q_2 \quad (2)$$

$$u(s(t), t) = v(s(t), t) = d\rho\dot{s}(t), \quad t > 0 \quad (3)$$

$$k_F v_x(s(t), t) - k_U u_x(s(t), t) = \alpha\dot{s}(t) + \beta\rho\dot{s}(t)\dot{s}^2(t), \quad t > 0 \quad (4)$$

$$v(x, 0) = v(+\infty, t) = -A < 0, \quad x, t > 0 \quad (5)$$

$$s(0) = 0 \quad (6)$$

$$k_U u_x(0, t) = -\frac{q_0}{\sqrt{t}}, \quad t > 0 \quad (7)$$

with

$$a_1 = \alpha_1^2 = \frac{k_U}{\rho_U c_U}, \quad a_2 = \alpha_2^2 = \frac{k_F}{\rho_F c_F}, \quad b = \frac{\varepsilon\rho_W c_W}{\rho_U c_U},$$

$$d = \frac{\varepsilon\gamma\mu}{K}, \quad \rho = \frac{\rho_W - \rho_I}{\rho_W}, \quad \alpha = \varepsilon\rho_I\lambda,$$

$$\beta = \frac{\varepsilon^2\rho_I(c_W - c_I)\gamma\mu}{K} = \varepsilon d\rho_I(c_W - c_I).$$

Problem I consists of equations (1)-(7), while by problem II we mean the system and (1)-(6) and (8) respectively, where

$$u(0, t) = B > 0, \quad t > 0. \quad (8)$$

Problem II was previously studied in [5].

We will look for similarity solutions of Problem I in different cases according to the value of parameters ρ, β y d , following the methods introduced in [5],[10].

First of all, we note that the function $u(x, t) = \Phi(\eta)$, with $\eta = \frac{x}{2\alpha_1\sqrt{t}}$, is a solution of (1) if and only if Φ satisfies the following equation

$$\frac{1}{2}\Phi''(\eta) + \left(\eta - \frac{b\rho}{\alpha_1}\sqrt{t}\dot{s}(t)\right)\Phi'(\eta) = 0$$

and similarly, the function $v(x, t) = \Psi(\eta)$ is solution of (2) if and only if Ψ satisfies the equation

$$\frac{1}{2}\Psi''(\eta) + \eta\Psi'(\eta) = 0.$$

Therefore, we obtain the following result

Theorem 1 *The free boundary problem I has the similarity solutions*

$$\begin{aligned}
 s(t) &= 2\xi\alpha_1\sqrt{t} \\
 u(x,t) &= m\xi^2 + \frac{2q_0\alpha_1}{K_U}g(p,\xi) - \frac{2q_0\alpha_1}{K_U} \int_0^{\frac{x}{2\alpha_1\sqrt{t}}} \exp(pyr - r^2) dr \\
 v(x,t) &= \frac{m\xi^2 + A \operatorname{erf}(\gamma_0\xi)}{\operatorname{erfc}(\gamma_0\xi)} - \frac{m\xi^2}{\operatorname{erfc}(\gamma_0\xi)} \operatorname{erf}\left(\frac{x}{2\alpha_1\sqrt{t}}\right)
 \end{aligned} \tag{9}$$

if and only if the coefficient ξ satisfies the equation

$$q_0 \exp((p-1)y^2) - K_2 F(m,y) = \delta y + \nu y^3, \quad y > 0 \tag{10}$$

where

$$F(m,y) = (A + my^2) \frac{\exp(-\gamma_0^2 y^2)}{\operatorname{erfc}(\gamma_0 y)}, \quad g(p,\xi) = \int_0^y \exp(pyr - r^2) dr \tag{11}$$

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-r^2) dr, \quad \operatorname{erfc}(x) = 1 - \operatorname{erf}(x),$$

and the constants $K_2, m, \delta, \nu, \gamma_0$ are defined as follows

$$\begin{aligned}
 K_2 &= \frac{K_F}{\alpha_2\sqrt{\pi}} & m &= 2d\rho\alpha_1^2 & \gamma_0 &= \frac{\alpha_1}{\alpha_2} > 0 \\
 \delta &= \alpha\alpha_1 > 0 & \nu &= 2\beta\rho\alpha_1^3 & p &= 2b\rho.
 \end{aligned} \tag{12}$$

In order to analyze (10) we need some preliminary results.

Lemma 2 (a) *If $m > 0$, then F grows from A to $+\infty$, when y grows from 0 to $+\infty$. If $m < 0$, then F has a unique positive maximum, from which it decreases to $-\infty$. In both cases, $F(m,y) \sim \sqrt{\pi}\gamma_0 my^3$ when $y \rightarrow +\infty$.*

(b) *For all $p > 0$, we have*

- (i) $g(p,y) \geq \frac{1}{py} (\exp((p-1)y^2) - \exp(-y^2)), \quad y > 0$
- (ii) $g_y(p,y) \geq \exp((p-1)y^2) + \frac{p}{2} (1 - \exp(-y^2)) > 0, \quad y > 0$
- (iii) $g(p,0) = 0, \quad g_y(p,0) = 1, \quad g(p,+\infty) = +\infty.$
- (iv) $\lim_{y \rightarrow +\infty} \frac{g(p,y)}{y^2} = 0$ if $p \leq 0$ and $\lim_{y \rightarrow +\infty} \frac{g(p,y)}{y^2} = +\infty$ if $p > 0$.
- (v) $\lim_{y \rightarrow +\infty} \frac{y g(p,y)}{\exp((p-1)y^2)} = \begin{cases} \frac{1}{p-2} & \text{if } p > 2 \\ +\infty & \text{if } p \leq 2 \end{cases}$

(c) *If $m > 0$ and $\nu \geq -m\sqrt{\pi}\gamma_0 K_2$, then the function*

$$H(y) = F(m,y) + \frac{\nu}{K_2} y^3$$

is strictly increasing.

Proof. The assertions (a) and (b) (i)-(iii) were proved in [5], and (b) (iv) and (v) easily follow from the identity (see [1])

$$\frac{2}{\sqrt{\pi}} g(p,y) = \exp\left(\frac{p^2 y^2}{4}\right) \left(\operatorname{erf}\left(\frac{py}{2}\right) + \operatorname{erf}\left(\frac{(2-p)y}{2}\right) \right).$$

Owing to function

$$\Phi_2(y) = \frac{y \exp(-y^2)}{\sqrt{\pi} \operatorname{erfc}(y)} - y^2$$

is increasing (see [6],[7]) the assertion (c) holds. ■

In Section 2 we prove the existence and the uniqueness of the similarity solution for different values of the physical parameters ρ, β and d . In Section 3, we discuss the equivalence of the problems I and II, and we extend some existence results for problem II obtained in [5].

2 Existence and Uniqueness of Similarity Solutions

In order to solve equation (10) we introduce the following function

$$Q_0(y) = \frac{\delta y + \nu y^3 + K_2 F(m, y)}{\exp((p-1)y^2)} \quad (13)$$

defined for $y > 0$ which verifies $Q_0(0) = K_2 A > 0$.

Theorem 3 *Let m be a positive real number. We define the following sets in the plane ν, p :*

$$R_1 = \{(\nu, p) \in \mathbb{R}^2 : -\sqrt{\pi} K_2 \gamma_0 m \leq \nu, p \leq 1\}, \quad R_2 = \mathbb{R}^2 - R_1.$$

We have:

- (a) *If $(\nu, p) \in R_1$ then the problem I has a unique similarity solution if and only if $q_0 > \frac{K_F}{\alpha_2 \sqrt{\pi}} A$.*
 (b) *If $(\nu, p) \in R_2$ then the problem I has a similarity solution if and only if $0 < q_0 \leq \max_{y \geq 0} Q_0(y)$.*

Proof. To prove the existence (and uniqueness) of similarity solution to problem I, it is necessary and sufficient to verify that the equation (10) has a (unique) solution. The equation (10) has a solution ξ if and only if $q_0 = Q_0(\xi)$. The proof is splitted in four cases [7]:

- (i) $m > 0, \nu \geq 0$ and $p \leq 1$; (ii) $m > 0, \nu \geq 0$ and $p > 1$;
 (iii) $\nu < -\sqrt{\pi} K_2 \gamma_0 m$; (iv) $m > 0, -\sqrt{\pi} K_2 \gamma_0 m \leq \nu < 0$ and $p \leq 1$. ■

Remark 4 *For $m = 0$, i.e. $d\rho = 0$, there exist a unique solution of equation (10) if and only if the inequality $q_0 > K_2 A$ is verified. This result has already been found in [10].*

Remark 5 *We note that in the case $p > 1$, if $\max_{y \geq 0} Q_0(y) > q_0 > K_2 A$ there exist at least two solutions. On the other hand, if q_0 is sufficiently small, then there exists a unique solution. The situation is a bit different in the problem II, studied in [5], where it was proved the existence and uniqueness of similarity solutions in the case $m > 0, \nu \geq 0, p \leq 2$.*

Similarly, we can obtain the following results.

Theorem 6 *Let $m < 0$. We define the sets*

$$R_3 = \{(\nu, p) \in \mathbb{R}^2 : \nu > -\sqrt{\pi} K_2 \gamma_0 m, p \leq 1\}, \quad R_4 = \mathbb{R}^2 - R_3.$$

Then

- (a) *If $(\nu, p) \in R_3$, there exists a solution when $q_0 > K_2 A$.*
 (b) *If $(\nu, p) \in R_4$, there exists a solution when $0 < q_0 \leq \max_{y > 0} Q_0(y)$.*

Proof. By using Proposition 2 we have, $\delta y + \nu y^3 + K_2 F(m, y) \sim \nu + K_2 \sqrt{\pi} \gamma_0 m y^3$ when $y \rightarrow +\infty$ and it follows that if $(\nu, p) \in R_3$ then $\lim_{y \rightarrow +\infty} Q_0(y) = +\infty$, from which we have $[K_2 A, +\infty) \subset \text{Range}(Q_0)$. This proves part (a).

If $(\nu, p) \in R_4$, it is easy to see that the function Q_0 has a positive finite maximum, and then the second part is also proved. ■

Remark 7 *In [7] it was studied the physical acceptability of the similarity solution as a function of the thermal coefficients.*

3 Relationship between Problems I and II

Let (s, u, v) be given by (9), for some constant $\xi > 0$. Then $u(0, t)$ is a constant given by

$$u(0, t) = m\xi^2 + \frac{2q_0}{K_U}g(p, \xi) > 0. \tag{14}$$

Then, we can consider the problem II, by imposing this new temperature as $u(0, t)$ at the fixed face $x = 0$.

Theorem 8 *Let $m > 0$, $\nu > 0$, $p \leq 1$ and $q_0 > K_2A$. If (s, u, v) is the unique similarity solution of Problem I, then (s, u, v) is the unique similarity solution of Problem II, provided the constant B in the condition (8) is given by*

$$B = m\xi^2 + \frac{2q_0\alpha_1}{K_U}g(p, \xi) \tag{15}$$

where ξ is the unique solution of equation (10).

Proof. We know that (s, u, v) is given by (9) where ξ is the unique solution of (10), which can be written as

$$Q_0(y) = q_0, \quad y > 0 \tag{16}$$

By the results obtained in [5], there exists a unique solution to Problem II, with B defined by (15), given by

$$\begin{aligned} \bar{s}(t) &= 2\bar{\xi}\alpha_1\sqrt{t} \\ \bar{u}(x, t) &= B - \frac{m\bar{\xi} - B}{g(p, \bar{\xi})} \int_0^{\frac{x}{2\alpha_1\sqrt{t}}} \exp(p\bar{\xi}r - r^2) dr \\ \bar{v}(x, t) &= \frac{m\bar{\xi}^2 \operatorname{erfc}\left(\frac{x}{2\alpha_2\sqrt{t}}\right) + A \left(\operatorname{erf}(\gamma_0\bar{\xi}) - \operatorname{erf}\left(\frac{x}{2\alpha_2\sqrt{t}}\right) \right)}{\operatorname{erfc}(\gamma_0\bar{\xi})} \end{aligned} \tag{17}$$

where $\bar{\xi}$ is the unique solution of the equation

$$\frac{\sqrt{\pi}}{2}K_1(B - my^2) \frac{\exp((p-1)y^2)}{g(p, y)} - K_2F(m, y) = \delta y + \nu y^3, \quad y > 0 \tag{18}$$

and $K_1 = \frac{K_U}{\alpha_1\pi}$. It is easy to see that the solutions given by (9) and (17) are coincident if and only if $\xi = \bar{\xi}$. Then, it is sufficient to see that ξ is a solution of (18) [7]. ■

Suppose that (s, u, v) is a solution to problem I, with the boundary condition (7). By the results of Section 1, we know that (s, u, v) are given by (9), where ξ must satisfy the equation (10). For this solution, the temperature in the fixed boundary is constant and equal to $B = u(0, t) = T_0(q_0, \xi)$, where T_0 is the real function defined by

$$T_0(q, y) = my^2 + \frac{2}{\sqrt{\pi}}\frac{q}{K_1}g(p, y), \quad q > 0, y > 0. \tag{19}$$

Assuming that $q > 0$, we will describe some properties of function T_0 . First of all, we note that $T_0(q, 0) = 0$. Besides, it follows from the proposition 2 that if $m > 0$ and $p > 0$, then $T_0(q, y)$ is an increasing function in both of its arguments, with $T_0(q, +\infty) = +\infty$. If $m < 0$ and $p > 0$, then $T_0(q, +\infty) = +\infty$, and if $m < 0$ and $p \leq 0$, then $T_0(q, +\infty) = -\infty$. Finally, if $m > 0$ and $p < 0$ then $T_0(q, +\infty) = +\infty$.

Suppose that $m > 0$. For each $\bar{\xi} > 0$ let

$$\bar{q}_0 = Q_0(\bar{\xi}) \tag{20}$$

where Q_0 is the function defined by (13). Let $\bar{B} = T_0(\bar{q}_0, \bar{\xi}) = m\bar{\xi}^2 + \frac{2}{\sqrt{\pi}}\frac{\bar{q}_0}{K_1}g(p, \bar{\xi})$, then a solution to problem I with $q_0 = \bar{q}_0$, which is given by (9) with $\xi = \bar{\xi}$ because of (20), corresponds to a solution to Problem II with $B = \bar{B}$. Then, given $B > 0$, we can show the existence of solution to Problem II, by proving that B belongs to the image set of the function $J(\cdot) = T_0(Q_0(\cdot), \cdot)$. For different values of the physical parameters, we study function J and we obtain the following results [7].

Theorem 9 Let $m > 0$. If $\nu \geq -\sqrt{\pi}K_2m\gamma_0$, then there exists a similarity solution to Problem II. If, in addition, $0 \leq p \leq 1$, then the similarity solution is unique. For the case $\nu < -\sqrt{\pi}K_2m\gamma_0$, a sufficient condition in order to have the existence of a solution to Problem II, is that B verifies the inequality

$$B < m \frac{\delta}{|\nu|} + \frac{2}{\sqrt{\pi}} \frac{M}{K_1} g \left(p, \sqrt{\frac{\delta}{|\nu|}} \right).$$

Remark 10 The last Theorem, extends a result of [5], where it was proved that if $m > 0, \nu < 0$, then there exists a solution to Problem II when

$$B < \frac{m\delta}{|\nu|}.$$

Proposition 11 Suppose $m < 0$ and $\nu > \sqrt{\pi}K_2|m|\gamma_0$, then:

(a) If $p \leq 2$ the problem II has a similarity solution if

$$B > \max(0, J(y_0)) \quad (21)$$

(b) If $p > 2$ the problem II has a similarity solution if $m + \frac{2(\nu + \sqrt{p^2 K_2 m \gamma_0})}{\sqrt{p^2 K_1 (p-2)}} > 0$ and (21) are verified.

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DIRECT AND INVERSE SCATTERING FOR THE NONLINEAR SCHRÖDINGER EQUATION WITH A POTENTIAL*

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Resumen

En este artículo se presenta una reseña de resultados recientes en la teoría de dispersión para la ecuación de Schrödinger no lineal en una dimensión y con un potencial. En particular, en la construcción del operador de dispersión para energías pequeñas y en la resolución del problema inverso. Específicamente, damos condiciones en el potencial y en la no linealidad tales que el operador de dispersión para energías pequeñas determina unívocamente el potencial y la no linealidad, y damos un método para la reconstrucción de ambos. Estos resultados están basados en la estimación $L^1 - L^\infty$ que demostramos en [10].

Palabras claves: dispersión inversa, ecuación de Schrödinger no lineal.

Abstract

In this paper we review recent results on the scattering theory for the nonlinear Schrödinger equation with a potential on the line. In particular, on the construction of the low-energy scattering operator and on the solution of the inverse scattering problem. Namely, we give conditions on the potential and on the nonlinearity such that the low-energy scattering operator determines uniquely the potential and the nonlinearity, and we give a method for the reconstruction of both. These results are based on the $L^1 - L^\infty$ estimate that we proved in [10].

Key words: inverse scattering, nonlinear Schrödinger equation.

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1 Introduction

In this paper I wish to discuss some recent results in the scattering theory of nonlinear evolution equations of dispersive type. We will consider in particular the nonlinear Schrödinger equation. This is one of the main equations of mathematical physics and it is a typical case that shows many of the main features of other equations. The aim of direct scattering theory is to study the behavior for large times of the solutions, and in particular to prove that -under appropriate conditions- the solutions are asymptotic as $t \rightarrow \pm\infty$ to solutions of a simpler, linear equation with constant coefficients. Since the solutions of the later equation are obtained by Fourier transform, direct scattering theory allows us to describe the asymptotic behavior of the solutions to our nonlinear evolution equation in a simple way. Of course, this situation excludes the case of nonlinear bound-states, that are solutions periodic in time. This requires either that the initial data is small or that the interaction is repulsive in a appropriate sense. The operator that to the initial data of the asymptotic solution as $t \rightarrow -\infty$ assigns the initial data of the asymptotic solution as $t \rightarrow \infty$ is the scattering operator. The purpose of inverse scattering theory is to obtain information on the potential and the nonlinearity, from the scattering operator. In other words, we wish to obtain as much information as possible on the potential and the nonlinearity, from the asymptotic behavior of the solutions; more precisely, from the relation of the asymptotic behaviors as $t \rightarrow \pm\infty$. Some of the main problems are uniqueness: does the scattering operator uniquely determines the potential and the nonlinearity?, and reconstruction: to obtain formulae that allow to reconstruct the potential and the nonlinearity from the scattering operator.

We will discuss the following nonlinear Schrödinger equation with a potential,

$$i\frac{\partial}{\partial t}u(t, x) = -\frac{d^2}{dx^2}u(t, x) + V_0(x)u(t, x) + F(x, u), u(0, x) = \phi(x), \quad (1.1)$$

where $t, x \in \mathbf{R}$, the potential, V_0 , is a real-valued function and $F(x, u)$ is a complex-valued function. In the case where the potential is zero, $V_0 \equiv 0$, there is a very large literature on the direct scattering problem . See for example [1], [2], [3],[4] [5], [7] and [8]. When $V_0 \equiv 0$ the linearized equation is the free Schrödinger equation,

$$i\frac{\partial}{\partial t}u(t, x) = -\frac{d^2}{dx^2}u(t, x), u(0, x) = \phi(x). \quad (1.2)$$

Let us denote by H_0 the self-adjoint realization of $-\frac{d^2}{dx^2}$ in L^2 with domain the Sobolev space $W_{2,2}$ and let us define e^{-itH_0} by functional calculus. The solution to (1.2) is given

by, $e^{-itH_0}\phi$. It follows immediately from the explicit formula for the kernel of e^{-itH_0} that the following $L^1 - L^\infty$ estimate holds,

$$\|e^{-itH_0}\phi\|_{L^\infty} \leq C \frac{1}{\sqrt{|t|}} \|\phi\|_{L^1}. \quad (1.3)$$

The estimate (1.3) expresses in a quantitative way a important property of the solutions to (1.2). Namely, that as $t \rightarrow \pm\infty$ the solutions not only propagate to spacial infinity, but they also *spread* uniformly in space. This is known in the physics literature as *wave packet spreading*. This spreading is essential in the study of the nonlinear Schrödinger equation. This can be seen as follows. For simplicity, suppose that $\phi \in L^1 \cap W_{1,2}$. Then, we have that,

$$\|e^{-itH_0}\phi\|_{L^\infty} \leq C \frac{1}{\sqrt{1+|t|}} (\|\phi\|_{L^1} + \|\phi\|_{W_{1,2}}).$$

Suppose moreover, that $F(x, u) = \lambda|u|^{(p-1)}u$, for some constant λ and some large positive p . Then, if ϕ is small enough; initially F will be small and the solution to (1.1) with $V_0 \equiv 0$ will propagate for small times essentially like a solution to the free Schrödinger equation (1.2). Moreover, because of the *spreading* the solution will be even smaller as t increases, and this will give the nonlinear term no chance to become very big and to make the solution blow-up in a finite time. If the initial data is not small, but the nonlinearity is repulsive -in a proper sense- a similar phenomenon takes place. In both cases there is a balance within the linear and the nonlinear terms that makes possible the existence of solutions global in time, and that permits the analysis of the large time asymptotics of the solutions in terms of the solutions to the free Schrödinger equation (1.2), i.e., scattering takes place. But what happens when the the potential V_0 is not identically zero? In this case the linearized equation is the following Schrödinger equation with a potential,

$$i \frac{\partial}{\partial t} u(t, x) = -\frac{d^2}{dx^2} u(t, x) + V_0(x)u(t, x), u(0, x) = \phi(x), \quad (1.4)$$

and we would need that an estimate as (1.3) holds with H_0 replaced with the perturbed Hamiltonian, $H := H_0 + V_0$. The problem is that such an estimate is at worst not true and at best quite hard to come by. Suppose for example that H has an eigenvalue, E , with eigenvector ϕ , i.e., that $H\phi = E\phi$. Then, $e^{-itH}\phi = e^{-itE}\phi$. This solution is periodic in time and it does not spreads at all; $\|e^{-itH}\phi\|_{L^\infty} = \|\phi\|_{L^\infty}$. However, we can hope that an estimate as (1.3) holds for initial data in \mathcal{H}_c , where \mathcal{H}_c is the subspace of continuity for H , that is to say, the orthogonal complement of the subspace spanned by all eigenvectors of

H . In one dimension this is rather delicate estimate-due to the singularity at low energy-that has been proved only recently in [10]. We give this result below, but first we state some standard notations and definitions. For any $\gamma \in \mathbf{R}$, let us denote by L_γ^1 the Banach space of all complex-valued measurable functions, ϕ , defined on \mathbf{R} and such that

$$\|\phi\|_{L_\gamma^1} := \int |\phi(x)|(1+|x|)^\gamma dx < \infty.$$

We say that $V_0 \in L_1^1$ is *generic* if the Jost solutions to the stationary Schrödinger equation at zero energy are linearly independent, and we say that V_0 is *exceptional* if they are linearly dependent. See [10] for details. We denote by P_c the orthogonal projector in L^2 onto \mathcal{H}_c .

THEOREM 1.1. *(The $L^1 - L^\infty$ estimate [10]). Suppose that $V \in L_\gamma^1$ where in the generic case $\gamma > 3/2$ and in the exceptional case $\gamma > 5/2$. Then for some constant C ,*

$$\|e^{-itH} P_c\|_{\mathcal{B}(L^1, L^\infty)} \leq \frac{C}{\sqrt{|t|}}. \quad (1.5)$$

COROLLARY 1.2. *(The $L^p - L^{\dot{p}}$ estimate [10]). Suppose that the conditions of Theorem 1.1 are satisfied. Then for $1 \leq p \leq 2$ and $\frac{1}{p} + \frac{1}{\dot{p}} = 1$,*

$$\|e^{-itH} P_c\|_{\mathcal{B}(L^p, L^{\dot{p}})} \leq \frac{C}{|t|^{\left(\frac{1}{p} - \frac{1}{2}\right)}}. \quad (1.6)$$

The $L^1 - L^\infty$ estimates have many applications. See for example [1]. In fact, in page 27 of [1] the problem of proving estimate (1.5) was posed as an interesting open problem of independent importance, but actually [10] already existed in preprint form when [1] was published. Corollary 1.2 follows from Theorem 1.1 using the fact that e^{-itH} is unitary in L^2 and by interpolation. The proof of (1.5) given in [10] is based in a careful analysis of the low energy behavior of the Jost solutions that uses the fact that the Jost solutions are obtained as solutions of integral equations of Volterra type and techniques of ordinary differential equations. The $L^1 - L^\infty$ estimate (1.5) is the key to the solution of the low-energy direct scattering problem and of the inverse scattering problem in [10] and [13]. We state the results below after we introduce some more standard notations. As usual, we say that $F(x, u)$ is a C^k function of u in the real sense if for each $x \in \mathbf{R}$, $\Re F$ and $\Im F$ are C^k functions with respect to the real and imaginary parts of u . We assume that F is C^2 in the real sense and that $\left(\frac{\partial}{\partial x} F\right)(x, u)$ is C^1 in the real sense. If $F = F_1 + iF_2$ with F_1, F_2 real-valued, and $u = r + is, r, s \in \mathbf{R}$ we denote,

$$F^{(2)}(x, u) := \sum_{j=1}^2 \left[\left| \frac{\partial^2}{\partial r^2} F_j(x, u) \right| + \left| \frac{\partial^2}{\partial r \partial s} F_j(x, u) \right| + \left| \frac{\partial^2}{\partial s^2} F_j(x, u) \right| \right],$$

$$\left(\frac{\partial}{\partial x} F \right)^{(1)}(x, u) := \sum_{j=1}^2 \left[\left| \frac{\partial}{\partial r} \left(\frac{\partial}{\partial x} F_j \right) (x, u) \right| + \left| \frac{\partial}{\partial s} \left(\frac{\partial}{\partial x} F_j \right) (x, u) \right| \right]$$

Let us define,

$$M := \left\{ u \in C(\mathbf{R}, W_{1,p+1}) : \sup_{t \in \mathbf{R}} (1 + |t|)^d \|u\|_{W_{1,p+1}} < \infty \right\},$$

with norm

$$\|u\|_M := \sup_{t \in \mathbf{R}} (1 + |t|)^d \|u\|_{W_{1,p+1}},$$

where $p \geq 1$, and $d := \frac{1}{2} \frac{p-1}{p+1}$. For functions $u(t, x)$ defined in \mathbf{R}^2 we denote $u(t)$, for $u(t, \cdot)$.

THEOREM 1.3. *(The low-energy scattering operator [13]) Suppose that $V_0 \in L^1_\gamma$, where in the generic case $\gamma > 3/2$ and in the exceptional case $\gamma > 5/2$, that H has no eigenvalues, and that*

$$N(V_0) := \sup_{x \in \mathbf{R}} \int_x^{x+1} |V_0(y)|^2 dy < \infty.$$

Furthermore, assume that F is C^2 in the real sense, that $F(x, 0) = 0$, and that for each fixed $x \in \mathbf{R}$ all the first order derivatives, in the real sense, of F vanish at zero. Moreover, suppose that $\frac{\partial}{\partial x} F$ is $C^{(1)}$ in the real sense. We assume that the following estimates hold:

$$F^{(2)}(x, u) = O(|u|^{p-2}), \quad \left(\frac{\partial}{\partial x} F \right)^{(1)}(x, u) = O(|u|^{p-1}), \quad u \rightarrow 0, \quad \text{uniformly for } x \in \mathbf{R},$$

for some $\rho < p < \infty$, and where ρ is the positive root of $\frac{1}{2} \frac{\rho-1}{\rho+1} = \frac{1}{\rho}$. Then, there is a $\delta > 0$ such that for all $\phi_- \in W_{2,2} \cap W_{1,1+\frac{1}{\rho}}$ with $\|\phi_-\|_{W_{2,2}} + \|\phi_-\|_{W_{1,1+\frac{1}{\rho}}} \leq \delta$, there is a unique solution, u , to (1.1) such that $u \in C(\mathbf{R}, W_{1,2}) \cap M$ and,

$$\lim_{t \rightarrow -\infty} \|u(t) - e^{-itH} \phi_-\|_{W_{1,2}} = 0.$$

Moreover, there is a unique $\phi_+ \in W_{1,2}$ such that

$$\lim_{t \rightarrow \infty} \|u(t) - e^{-itH} \phi_+\|_{W_{1,2}} = 0.$$

Furthermore, $e^{-itH} \phi_\pm \in M$ and

$$\|u - e^{-itH} \phi_\pm\|_M \leq C \|e^{-itH} \phi_\pm\|_M^p,$$

$$\|\phi_+ - \phi_-\|_{W_{1,2}} \leq C \left[\|\phi_-\|_{W_{2,2}} + \|\phi_-\|_{W_{1,1+\frac{1}{p}}} \right]^p.$$

The scattering operator, $S_{V_0} : \phi_- \mapsto \phi_+$ is injective on $W_{1,1+\frac{1}{p}} \cap W_{2,2}$.

Note that, $\rho \approx 3.56$.

The wave operators for the linear scattering problem corresponding to equation (1.1) with $F \equiv 0$ and equation (1.2) are given by:

$$W_{\pm} := s - \lim_{t \rightarrow \pm\infty} e^{itH} e^{-itH_0}.$$

It is proven in [6] that the limits above exist in the strong topology in L^2 and that $\text{Range} W_{\pm} = \mathcal{H}_c$. The corresponding scattering operator is given by,

$$S_L := W_+^* W_-.$$

The scattering operator below relates asymptotic states that are solutions to the linear Schrödinger equation and it is the appropriate one for the reconstruction of V_0 .

$$S := W_+^* S_{V_0} W_- . \tag{1.7}$$

In the following theorem we reconstruct S_L from S .

THEOREM 1.4. ([13]) *Suppose that the assumptions of Theorem 1.3 are satisfied. Then for every $\phi_- \in W_{2,2} \cap W_{1,1+\frac{1}{p}}$*

$$\left. \frac{d}{d\epsilon} S(\epsilon\phi) \right|_{\epsilon=0} = S_L \phi, \tag{1.8}$$

where the derivative in the left-hand side of (1.8) exists in the strong convergence in $W_{1,2}$.

COROLLARY 1.5. ([13]) *Under the conditions of Theorem 1.3 the scattering operator, S , determines uniquely the potential V_0 .*

■

In the case where $F(x, u) = \sum_{j=1}^{\infty} V_j(x) |u|^{2(j_0+j)} u$ we can also reconstruct the $V_j, j = 1, 2, \dots$.

LEMMA 1.6. ([13]) *Suppose that the conditions of Theorem 1.3 are satisfied, and moreover, that $F(x, u) = \sum_{j=1}^{\infty} V_j(x)|u|^{2(j_0+j)}u$, where j_0 is an integer such that, $j_0 \geq (p-3)/2$, for $|u| \leq \eta$, for some $\eta > 0$, and where $V_j \in W_{1,\infty}$ with $\|V_j\|_{W_{1,\infty}} \leq C^j$, $j = 1, 2, \dots$, for some constant C . Then, for any $\phi \in W_{2,2} \cap W_{1,1+\frac{1}{p}}$ there is an $\epsilon_0 > 0$ such that for all $0 < \epsilon < \epsilon_0$:*

$$i((S_V - I)(\epsilon\phi), \phi)_{L^2} = \sum_{j=1}^{\infty} \epsilon^{2(j_0+j)+1} \left[\int \int dt dx V_j(x) |e^{-itH} \phi|^{2(j_0+j+1)} + Q_j \right], \quad (1.9)$$

where $Q_1 = 0$ and $Q_j, j > 1$, depends only on ϕ and on V_k with $k < j$. Moreover, for any $\acute{x} \in \mathbf{R}$, and any $\lambda > 0$, we denote, $\phi_\lambda(x) := \phi(\lambda(x - \acute{x}))$. Then, if $\phi \neq 0$:

$$V_j(\acute{x}) = \frac{\lim_{\lambda \rightarrow \infty} \lambda^3 \int \int dt dx V_j(x) |e^{-itH} \phi_\lambda|^{2(j_0+j+1)}}{\int \int dt dx |e^{-itH_0} \phi|^{2(j_0+j+1)}}. \quad (1.10)$$

COROLLARY 1.7. ([13]) *Under the conditions of Lemma 1.6 the scattering operator, S , determines uniquely the potentials $V_j, j = 0, 1, \dots$.*

The method to reconstruct the potentials $V_j, j = 0, 1, \dots$, is as follows. First S_L is obtained from S using (1.8). By any standard method for inverse scattering for the linear Schrödinger equation on the line (recall that H has no eigenvalues) we reconstruct V_0 . We then reconstruct S_{V_0} from S using (1.7). Finally (1.9) and (1.10) give us, recursively, $V_j, j = 1, 2, \dots$.

For the proof of these results, the extension to the multidimensional case and to the nonlinear Klein-Gordon equation see [9], [10], [11], [12], [13], [14] and [15]. In these papers also a discussion of the literature is given.

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A STEFAN PROBLEM FOR A NON-CLASSICAL HEAT EQUATION*

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Abstract

We review some recent results concerning to the heat equation with a heat source depending on the heat flux occurring at the fixed $x=0$ of a semi-infinite material. We also present a new free boundary problem (one-phase Stefan-like problem) for a non-classical heat equation, and we obtain the temperature and the free boundary (the phase-change interface) through the solution of a system of two Volterra integral equations.

Resumen: Se da una revisión de algunos recientes resultados concernientes a la ecuación del calor con una fuente que depende del flujo de calor que ocurre en la frontera fija $x=0$ de un cuerpo semi-infinito. También se presenta un nuevo problema de frontera libre (problema de tipo Stefan a una fase) para una ecuación no clásica para la cual se obtiene la temperatura y la frontera libre (la frontera de cambio de fase) a través de la solución de un sistema de dos ecuaciones integrales de Volterra.

Key words: Non-classical heat equation, asymptotic behavior, Stefan problem, phase-change problem, free boundary problem, Volterra integral equation.

Palabras claves: Ecuación del calor no-clásico, comportamiento asintótico, problema de Stefan, problema de cambio de fase, problemas de frontera libre, ecuación integral de Volterra.

AMS Subject classification: 35R35, 80A22, 35K05, 45D05, 35B40.

1 Introduction

The following non-classical heat conduction problem for a semi-infinite material was studied in [17]

$$\begin{cases} u_t(x, t) - u_{xx}(x, t) = \Phi(x)F(u_x(0, t)), & x > 0, \quad t > 0, \\ u(0, t) = g(t), & t > 0, \\ u(x, 0) = h(x), & x > 0, \end{cases} \quad (1)$$

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where Φ , g , h are real functions defined on \mathbb{R}^+ and F is defined on $\mathbb{R}^+ \times \mathbb{R}$ which depends on the heat flux at the extremum $x = 0$. Non-classical problems like (1) are motivated by the modelling of a system of temperature regulation in isotropic media and the source term $\Phi(x) F(u_x(0, t))$ describes a cooling or heating effect depending on the properties of F which are related to the evolution of the heat flux $u_x(0, t)$. It is called the thermostat problem. Related problems are considered in [4],[6],[9]. Under suitable assumptions on data, existence, uniqueness and monotone-continuous dependence on the data are established in [17] for problem (1).

It was consider in [2] the simple instance of problem (1) given by

$$\begin{cases} u_t - u_{xx} = -F(u_x(0, t)), & x > 0, \quad t > 0, \\ u(0, t) = 0, & t > 0, \\ u(x, 0) = h(x), & x > 0, \end{cases} \quad (2)$$

where $h(x)$, $x > 0$, and $F(v)$, $v \in \mathbb{R}$, are continuous functions. The function F , referred as *control function*, was assumed to fulfill the following condition:

A) $v F(v) \geq 0, F(0) = 0$,

which intuitively means that the control attempts to stabilize the process at every time.

As it is shown in [18] (see also [17]), the solution to problem (2) can be represented by

$$u(x, t) = u_0(x, t) - \int_0^t \operatorname{erf}\left(\frac{x}{2\sqrt{t-\tau}}\right) F(V(\tau)) d\tau, \quad (3)$$

where $u_0 = u_0(x, t)$, defined by

$$u_0(x, t) = \int_0^{+\infty} G(x, t; \xi, 0) h(\xi) d\xi, \quad (4)$$

is the solution to problem (2) with null source term $F = 0$. Function $V = V(t)$ in (3) represents the heat flux at the extremum of the slab, i.e.

$$V(t) = u_x(0, t), \quad t > 0, \quad (5)$$

and it satisfies the following Volterra integral equation

$$V(t) = V_0(t) - \int_0^t \frac{F(V(\tau))}{\sqrt{\pi(t-\tau)}} d\tau, \quad (6)$$

where the forcing function $V_0(t)$ is given by

$$V_0(t) = \frac{1}{2\sqrt{\pi t^{\frac{3}{2}}}} \int_0^{+\infty} \xi \exp\left(-\frac{\xi^2}{4t}\right) h(\xi) d\xi, \quad t > 0. \quad (7)$$

Function G in (4) denotes the Green function of the heat equation in the quarter plane and, as it is well-known, it can be written as $G(x, t; \xi, \tau) = K(x, t; \xi, \tau) - K(-x, t; \xi, \tau)$, $x, \xi > 0$, $t > \tau > 0$, where

$$K(x, t; \xi, \tau) = \frac{1}{\sqrt{4\pi(t-\tau)}} \exp\left(-\frac{(x-\xi)^2}{4(t-\tau)}\right),$$

is the one-dimensional heat kernel. Moreover, we also define the Neumann function of the heat equation in the quarter plane as $N(x, t; \xi, \tau) = K(x, t; \xi, \tau) + K(-x, t; \xi, \tau)$, $x, \xi > 0$, $t > \tau > 0$.

From now on, we suppose that h is a non-negative and non-identically null function which, in view of (7), implies $V_0(t) > 0$, $t > 0$. When the control function F satisfies condition (A) and, moreover, the initial temperature h is non-negative, then the solution $u(x, t)$ to problem (2) tends to zero when $t \rightarrow +\infty$ (see [17], [18]). In [2] was studied the problem of "controlling" problem (2) through F so that, by the stabilizing effect of the control, its solution should converge to zero (when the time goes to infinity) faster than that corresponding to problem (2) in absence of control; i.e. $\lim_{t \rightarrow +\infty} u(x, t)/u_0(x, t) = 0$. The heat flux $w(x, t) = u_x(x, t)$ satisfies a classical heat conduction problem with a nonlinear convective condition at $x = 0$. The first papers in this direction are [10] and [13]. Other related problems are considered in [1], [8] and [12]. In [2], a general study of the above stated control problem for (2) was done finding spatially uniform bounds for the quotient $u(x, t)/u_0(x, t)$ which depend on the solution $V(t)$ to integral equation (6), from which becomes apparent that condition (A) is not sufficient to attain the objective of the control; i.e., to obtain $\lim_{t \rightarrow +\infty} u(x, t)/u_0(x, t) = 0$. In Section 2, for linear control functions $F(v) = \lambda v$, we give an example to illustrate that there exists an exact solution to problem (6) providing $u(x, t)/u_0(x, t) \cong 1/(2\lambda^2 t)$, $t \rightarrow +\infty$. In Section 3, we present a one-phase Stefan problem for a semi-infinite material for a non-classical heat equation with a source term F which depends of the evolution of the heat flux at the extremum $x = 0$. Its solution is given by the solution of a system of two Volterra integral equations [3],[7],[11].

2 Constant initial temperature and their control function

We shall consider the instance of problem (2) corresponding to a constant initial temperature $h(x) = h_0 > 0$, $x \geq 0$. The solution to problem (2) is represented by (3) with

$$u_0(x, t) = h_0 \operatorname{erf}\left(\frac{x}{2\sqrt{t}}\right), \quad x > 0, \quad t > 0, \quad (8)$$

while $V = V(t)$ becomes the solution to the Volterra integral equation

$$V(t) = \frac{h_0}{\sqrt{\pi t}} - \int_0^t \frac{F(V(\tau))}{\sqrt{\pi(t-\tau)}} d\tau, \quad t > 0. \quad (9)$$

Therefore, the following inequalities

$$\frac{\sqrt{\pi t}}{h_0} V(t) \leq \frac{u(x, t)}{u_0(x, t)} \leq \frac{1}{h_0} \int_0^t \frac{V(\tau)}{\sqrt{\pi(t-\tau)}} d\tau = 1 - \frac{1}{h_0} \int_0^t F(V(\tau)) d\tau, \quad (10)$$

hold for $x > 0$, $t > 0$ [2].

From now on we suppose the case of linear controls: i.e.,

$$F(v) = \lambda v, \quad (\lambda > 0), \quad (11)$$

and in order to obtain the explicit solutions u and V of the problems (2) and (9) respectively, we define the real function $Q(x) = \sqrt{\pi} x \exp(x^2) \operatorname{erfc}(x)$, defined for $x > 0$ [15] which satisfies the following properties: $Q(0) = 0$, $Q(+\infty) = 1$, $Q'(x) > 0$, $x > 0$. The most important facts on the behavior of the solution $V(t)$ to equation (9) corresponding to a linear control (11) are collected in the following result (See [2]).

Lemma 1 *If F is given by (11), then we have*

$$0 < V(t) = \frac{h_0}{\sqrt{\pi t}} \left[1 - Q(\lambda\sqrt{t}) \right] < \frac{h_0}{\sqrt{\pi t}}, \quad (12)$$

$$1 - \frac{1}{h_0} \int_0^t F(V(\tau)) d\tau = \exp(\lambda^2 t) \operatorname{erfc}(\lambda\sqrt{t}), \quad (13)$$

for all $t > 0$ and $\lim_{t \rightarrow +\infty} u(x, t)/u_0(x, t) = 0$, uniformly in $x > 0$. Furthermore, we have the estimates

$$\frac{1}{\pi\lambda^2 t} \leq \frac{u(x, t)}{u_0(x, t)} \leq \frac{1}{\lambda\sqrt{\pi t}}, \quad (14)$$

as $t \rightarrow +\infty$. Moreover, the temperature u is given by

$$u(x, t) = h_0 \exp(\lambda^2 t) \left[\operatorname{erfc}(\lambda\sqrt{t}) - \exp(\lambda x) \operatorname{erfc}\left(\lambda\sqrt{t} + \frac{x}{2\sqrt{t}}\right) \right], \quad (15)$$

and a more accurate estimation $\frac{u(x, t)}{u_0(x, t)} \sim 1/(2\lambda t^2)$, when $t \rightarrow +\infty$, uniformly in $x > 0$ is also obtained.

3 A Stefan problem for a non-classical heat equation.

We consider the following free boundary problem (one-phase Stefan problem) for the temperature $u = u(x, t)$ and the free boundary $x = s(t)$ (see [16]) with a control function F which depends on the evolution of the heat flux at the extremum $x = 0$ given by the following conditions:

$$\begin{cases} u_t - u_{xx} = -F(u_x(0, t)), & 0 < x < s(t), 0 < t < T, \\ u(0, t) = f(t) \geq 0, & 0 < t < T, \\ u(s(t), t) = 0, u_x(s(t), t) = -\dot{s}(t), & 0 < t < T, \\ u(x, 0) = h(x), & 0 \leq x \leq b = s(0). \end{cases} \quad (16)$$

Theorem 2 *The solution of the free boundary problem (16) is given by*

$$\begin{aligned} u(x,t) &= \int_0^b G(x,t;\xi,0)h(\xi)d\xi + \int_0^t G_\xi(x,t;0,\tau)f(\tau)d\tau + \int_0^t G_\xi(x,t;s(\tau),\tau)v(\tau)d\tau \\ &\quad - \iint_{D(t)} G(x,t;\xi,\tau)F(V(\tau))d\xi d\tau, \\ s(t) &= b - \int_0^t v(\tau)d\tau \end{aligned}$$

where $D(t) = \{(x,\tau) / 0 < x < s(\tau), 0 < \tau < t\}$, and $v(t) = u_x(s(t),t) = -\dot{s}(t)$ and $V(t) = u_x(0,t)$ must satisfy the following system of two Volterra integral equations

$$\begin{aligned} v(t) &= 2[h(0) - f(0)]N(s(t),t;0,0) + \int_0^b N(s(t),t;\xi,0)h'(\xi)d\xi \\ &\quad - 2 \int_0^t N(s(t),t;0,\tau)\dot{f}(\tau)d\tau + 2 \int_0^t G_x(s(t),t;s(\tau),\tau)v(\tau)d\tau \\ &\quad + 2 \int_0^t [N(s(t),t;s(\tau),\tau) - N(s(t),t;0,\tau)]F(V(\tau))d\tau, \\ V(t) &= [h(0) - f(0)]N(0,t;0,0) + \int_0^b N(0,t;\xi,0)h'(\xi)d\xi - \int_0^t N(0,t;0,\tau)\dot{f}(\tau)d\tau \\ &\quad + \int_0^t G_x(0,t;s(\tau),\tau)v(\tau)d\tau + \int_0^t [N(0,t;s(\tau),\tau) - N(0,t;0,\tau)]F(V(\tau))d\tau, \end{aligned}$$

where G and N are the Green and Neumann functions of the heat equation in the quarter plane, defined previously in Section 1.

Proof. We compute $u_x(x,t)$, and their corresponding limits as $x \rightarrow 0^+$ and $x \rightarrow s(t)^-$. By using the jump relations [5], [14] the system of two Volterra integral equations holds.

The corresponding study of the existence and uniqueness of the solution will be given in a forthcoming paper.

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A Quasilinearization Approach for Parameter Identification in Nonlinear Abstract Cauchy Problems

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Abstract: A quasilinearization approach for parameter identification in nonlinear abstract Cauchy problems in which the parameter appears in the nonlinear term, is presented. This approach has two main advantages over the classical one: it is much more intuitive and the derivation of the algorithm is done without need of the sensitivity equations on which classical quasilinearization is based. Sufficient conditions for the convergence of the algorithm are derived in terms of the regularity of the solutions with respect to the parameters. A comparison with the standard approach is presented and an application is included in which the non-physical parameters in a mathematical model for shape memory alloys are estimated.

Key Words: Abstract Cauchy problem, quasilinearization, parameter identification, semigroup, shape memory alloy.

Resumen: Se presenta un método para la identificación de parámetros basado en cuasi-linealización para problemas de Cauchy abstractos no lineales en los que el parámetro aparece en el término no lineal. Este método tiene dos ventajas principales sobre el método clásico: es mucho más intuitivo y el algoritmo se obtiene sin utilizar las ecuaciones de sensibilidad en las cuales se basan los métodos clásicos de cuasi-linealización. Se derivan condiciones suficientes para la convergencia del algoritmo en términos de la regularidad de las soluciones con respecto a los parámetros. Se presenta una comparación con el método clásico y una aplicación en la que se estiman los parámetros no físicos en un modelo matemático para materiales con memoria de forma.

Palabras clave: Problemas de Cauchy abstractos, cuasi-linealización, identificación de parámetros, semigrupo, materiales con memoria de forma.

AMS Subject Classification: 34K30, 34G20, 35R30.

1. Introduction

Let Z be a Banach space, A the infinitesimal generator of an analytic semigroup $T(t)$ on Z , D a subset of Z , \tilde{Q} a separable Hilbert space, Q a subset of \tilde{Q} and F be a mapping, $F : Q \times [0, T] \times D \rightarrow Z$. We shall consider the following nonlinear Cauchy problem in Z :

$$(P)_q \begin{cases} \dot{z}(t) = Az(t) + F(q, t, z(t)), & t \in (0, T) \\ z(0) = z_0. \end{cases}$$

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The spaces Z and \tilde{Q} will be referred to as the *state-space* and the *parameter space*, respectively, while \mathcal{Q} will be called the *admissible parameter set*.

Let Y be a real Hilbert space and \mathcal{C} a bounded linear operator from Z into Y , $\mathcal{C} \in \mathcal{L}(Z, Y)$. We shall refer to Y and \mathcal{C} as the *observation space* and *observation operator*, respectively. Let $\hat{z}_i \in Y$, be “observations” at times t_i , $0 \leq t_i \leq T$, $i = 1, 2, \dots, m$ of the process described by the IVP $(P)_q$. The “parameter identification problem” (ID problem in the sequel) associated to $(P)_q$ and the observations $\{\hat{z}_i\}_{i=1}^m$ is:

(ID) : find $q \in \mathcal{Q}$ that minimizes the error criterion

$$J(q) \doteq \frac{1}{2} \sum_{i=1}^m \|\mathcal{C}z(t_i; q) - \hat{z}_i\|_Y^2 \quad (1.1)$$

where $z(t; q)$ denotes the unique solution of $(P)_q$ in the interval $[0, T)$. In the next section we will provide sufficient conditions for the existence and uniqueness of solutions.

There are two general approaches to ID problems. The first one, frequently used in linear problems, is the so called *indirect approach*. Here, the identification algorithm starts with a finite dimensional approximation of the infinite dimensional problem, after which an optimization algorithm based on these approximations is implemented. The second approach, called the *direct approach*, consists of applying an optimization algorithm to the infinite dimensional problem $(P)_q$ and using finite dimensional approximations when needed to solve the resulting infinite dimensional subproblems. Depending on the problem being considered, one method can be more efficient than the other. Methods based on the indirect approach are usually easier to implement computationally, however in general they require that the dynamic equations be solved a greater number of times than direct methods do. For this reason, in practical problems the use of indirect methods is mainly restricted to linear problems. Also, for indirect methods, no more than subsequential convergence can be obtained while “full” convergence can be proved for certain direct methods.

The convergence issue in ID problems is very important. Although direct methods usually generate much more efficient algorithms and quite often full convergence can be shown, they have the drawback that they require the solution of the system to be smooth with respect to the parameters. In many cases this smoothness does not exist or it may be difficult to prove.

Identification problems arise often in many physical, geological, chemical and biological systems. It is for that reason that a great amount of attention has been devoted to the study of identification methods for linear and nonlinear distributed parameter systems. In particular, the quasilinearization approach to ID problems has been studied by several authors for different types of problems. Brewer, Burns and Cliff [5] have worked on many identification issues that arise in the study and application of quasilinearization methods for nonhomogeneous linear systems of the type $\dot{z}(t) = A(q)z(t) + u(t)$, where the dependence on the unknown parameter q comes through the linear operator $A(q)$. Hammer [8] applied these tools to nonlinear problems of the type $\dot{z}(t) = A(q)z(t) + f(t, z)$, where $f(t, z)$ is nonlinear in z but it does not depend on the unknown parameter q . Banks and Groome [2] considered a quasilinearization approach for ID problems arising in the study of general nonlinear problems of the type $\dot{z}(t) = g(t, z(t), q)$, but their work is valid in finite dimensional state spaces only, i.e., $z(t) \in \mathbb{R}^n$ and it does not extend to the associated infinite dimensional case. To our knowledge, ID problems for systems of the type $(P)_q$ have never been studied previously.

The organization of this article is as follows. In Section 2 the quasilinearization algorithm for parameter identification in an abstract context is derived. In Section 3 sufficient conditions for the convergence of the algorithm are given. In Section 4 a comparison is made between the approach presented here and the standard approach to quasilinearization. In Section 5 an application is presented in which the parameters that define the free energy in a model for Shape Memory Alloys are identified.

2. Quasilinearization Algorithm

In this section we will introduce the algorithm, but first we need to recall some properties of analytic semigroups and make some assumptions on the nonlinear part of the equation.

Let $\rho(A)$ and $\sigma(A)$ denote the resolvent and spectrum of A , respectively. Since A generates an analytic semigroup, $\omega \doteq \sup \{ \operatorname{Re}(\lambda) : \lambda \in \sigma(A) \}$ is finite and for any complex λ with $\operatorname{Re}(\lambda) > \omega$ the fractional powers $(\lambda I - A)^\delta$ of $\lambda I - A$ are closed, linear and invertible operators in Z , for any $\delta \in [0, 1]$ (see [11]). From this point on, λ will be fixed with $\operatorname{Re}(\lambda) > \omega$, Z_δ shall denote the space $\operatorname{Dom}((\lambda I - A)^\delta)$ imbedded with the norm of the graph of $(\lambda I - A)^\delta$. Due to the fact that $\operatorname{Re}(\lambda) > \omega$, one has $\lambda \in \rho(A)$ and this norm is equivalent to the norm $\|z\|_\delta \doteq \|(\lambda I - A)^\delta z\|_Z$.

Consider the following standing hypothesis.

(H1). *There exists $\delta \in (0, 1)$ such that $Z_\delta \subset D$ and $F : \mathcal{Q} \times [0, T] \times Z_\delta \rightarrow Z$ is locally Lipschitz continuous in t and z , i.e., for any $q \in \mathcal{Q}$ and any bounded subset U of $[0, T] \times Z_\delta$ there exists a constant $L = L(q, U)$ such that*

$$\|F(q, t_1, z_1) - F(q, t_2, z_2)\|_Z \leq L(|t_1 - t_2| + \|z_1 - z_2\|_\delta), \quad \forall (t_i, z_i) \in U, \quad i = 1, 2.$$

where the constant L can be chosen independent of q on any compact subset \mathcal{Q}_C of \mathcal{Q} .

The following theorem follows immediately from Theorem 6.3.1 in [11].

THEOREM 1. *Let $q \in \mathcal{Q}$ and $z_0 \in Z_\delta$. If F satisfies (H1), then there exists $t_1 = t_1(q, z_0) > 0$ such that $(P)_q$ has a unique classical solution on $[0, t_1)$. i.e., there exists a function $z(\cdot) \in C^0([0, t_1) : Z_\delta) \cap C^1((0, t_1) : Z)$ such that $\dot{z}(t) = Az(t) + F(q, t, z(t))$ for all $t \in (0, t_1)$ and $z(0) = z_0$. The function $z(t)$ satisfies the integral equation*

$$z(t) = T(t)z_0 + \int_0^t T(t-s)F(q, s, z(s)) ds, \quad \forall t \in [0, t_1).$$

Also, $t_1(q, z_0) > 0$ can be chosen independent of q on compact subsets of \mathcal{Q} .

Let us denote by $z(t; q)$ the local solution $z(t)$ of $(P)_q$. Consider now the parameter estimation problem (ID). We shall assume from now on that for each fixed $t \in [0, t_1)$ the mapping $q \rightarrow z(t; q)$ is Fréchet differentiable. Sufficient conditions on F that guarantee this assumption are given in the next theorem. A proof can be found in [6, Theorem 2.3].

THEOREM 2. *Assume (H1) holds for some $\delta \in (0, 1)$ and the mapping $(q, z(\cdot)) \rightarrow F(q, \cdot, z(\cdot))$ from $\mathcal{Q} \times L^\infty(0, T : Z_\delta)$ into $L^\infty(0, T : Z)$ is Fréchet differentiable in both variables. Assume also that the mapping $(q, z(\cdot)) \rightarrow F_q(q, \cdot, z(\cdot))$ from $\mathcal{Q} \times L^\infty(0, T : Z_\delta)$ into $L^\infty(0, T : \mathcal{L}(\tilde{\mathcal{Q}}, Z))$ is locally Lipschitz continuous with respect to q and z . Then the mapping $q \rightarrow z(\cdot; q)$ is Fréchet differentiable from $\mathcal{Q} \rightarrow L^\infty(0, T : Z_\delta)$ and for any $h \in \tilde{\mathcal{Q}}$, $z_q(t; q)h$ is the solution $v_h(t)$ of the linear IVP*

$$\begin{cases} \dot{v}_h(t) = Av_h(t) + F_z(q, t, z(t; q))v_h(t) + F_q(q, t, z(t; q))h, & t \in (0, T) \\ v_h(0) = 0. \end{cases}$$

Here F_q and F_z denote the Fréchet derivatives of F with respect to q and z , respectively.

We shall assume that there exists a minimizer $q^* \in \mathcal{Q}$ of $J(q)$, given in (ID). Although at a first glance this assumption may look too restrictive, it reflects the fact that we are only interested in finding minimizers that are admissible. In practical problems admissibility reflects the physical restrictions on the parameters.

The following algorithm is proposed. Start with an initial guess parameter q^0 of q^* .

Step 1: Given an estimate q^k of q^* , $k \geq 0$, approximate $z(t; q)$ by its first order Taylor expansion around q^k , i.e., let $z^{k+1}(t; q) \doteq z(t; q^k) + z_q(t; q^k)(q - q^k)$ where $z_q(t; q^k)$ denotes the Fréchet derivative of $z(t; q)$ with respect to q , evaluated at q^k .

Step 2: Define the modified error criterion $J^k : \tilde{\mathcal{Q}} \rightarrow \mathbb{R}_0^+$ by

$$\begin{aligned} J^k(q) &\doteq \frac{1}{2} \sum_{i=1}^m \|\mathcal{C}z^{k+1}(t_i; q) - \hat{z}_i\|_Y^2 \\ &= \frac{1}{2} \sum_{i=1}^m \|\mathcal{C}[z(t_i; q^k) + z_q(t_i; q^k)(q - q^k)] - \hat{z}_i\|_Y^2. \end{aligned}$$

Step 3: Next, define q^{k+1} to be a minimizer of the modified error criterion $J^k(q)$. In order to find q^{k+1} , differentiate $J^k(q)$, set the result equal to zero and solve for q . Finally, call this solution q^{k+1} , replace k with $k+1$ and repeat Step 1.

It is important to mention here that our minimization problem is a constrained problem since we seek a minimizer $q^* \in \mathcal{Q}$. However, we have treated the problem as being unconstrained and therefore there is no a priori guarantee that if q^k is in \mathcal{Q} then q^{k+1} will be in \mathcal{Q} . We shall overcome this difficulty by assuming that q^* is an interior point of \mathcal{Q} . Under this additional hypothesis we will prove (in Theorems 7 and 8) that if the initial guess q^0 is sufficiently close to q^* , then all the iterates q^k are also in \mathcal{Q} .

Observe that, unless $z_q(t_i; q^k) = 0$, for all $i = 1, 2, \dots, m$, the functional $J^k(q)$ is strictly convex and there exists only one solution of $D_q(J^k(q)) = 0$. This solution is a minimizer. Also, the condition $D_q(J^k(q)) = 0$ is satisfied if and only if

$$\sum_{i=1}^m \langle \mathcal{C}z_q(t_i; q^k)h, \mathcal{C}z_q(t_i; q^k)(q - q^k) \rangle_Y = - \sum_{i=1}^m \langle \mathcal{C}z_q(t_i; q^k)h, \mathcal{C}z(t_i; q^k) - \hat{z}_i \rangle_Y$$

for every $h \in \tilde{\mathcal{Q}}$.

Let $\{g_j : j = 1, 2, \dots\}$ be an orthonormal basis of $\tilde{\mathcal{Q}}$. Then, the equation above is equivalent to

$$\sum_{i=1}^m \langle \mathcal{C}z_q(t_i; q^k)g_j, \mathcal{C}z_q(t_i; q^k)(q - q^k) \rangle_Y = - \sum_{i=1}^m \langle \mathcal{C}z_q(t_i; q^k)g_j, \mathcal{C}z(t_i; q^k) - \hat{z}_i \rangle_Y, \quad (2.1)$$

for $j = 1, 2, \dots$. Since $\{g_j\}$ is an orthonormal basis, $q \in \tilde{\mathcal{Q}}$ iff there exists a unique $\alpha = (\alpha_1, \alpha_2, \dots) \in \ell^2$ such that $q = \sum_{j=1}^{\infty} \alpha_j g_j$ and $\|q\|_{\tilde{\mathcal{Q}}} = \|\alpha\|_{\ell^2}$. Therefore the parameter identification problem can be reformulated in terms of the coefficients of q as follows. Define $\ell^2(\mathcal{Q}) = \{\alpha \in \ell^2 : q_\alpha = \sum_{j=1}^{\infty} \alpha_j g_j \in \mathcal{Q}\}$. Given $\alpha^k \in \ell^2(\mathcal{Q})$ ($q^k \in \mathcal{Q}$) determine $\alpha^{k+1} \in \ell^2(\mathcal{Q})$ by solving equations (2.1) for q .

More precisely, for each $\alpha \in \ell^2$, let q_α denote the expression $\sum_{j=1}^{\infty} \alpha_j g_j$, and define

$$P(\alpha)\gamma \doteq \sum_{i=1}^m M(t_i; q_\alpha)^* [M(t_i; q_\alpha)\gamma], \quad \gamma \in \ell^2,$$

where for each $q \in \tilde{\mathcal{Q}}$, $t \in [0, T]$, $M(t; q) : \ell^2 \rightarrow Y$ is defined by

$$M(t; q)\alpha = [\mathcal{C}z_q(t; q)g_1 \quad \mathcal{C}z_q(t; q)g_2 \quad \dots] \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \end{bmatrix} = \mathcal{C}z_q(t; q)q_\alpha$$

and $M(t; q)^* : Y \rightarrow \ell^2$ denotes the adjoint of the operator $M(t; q)$. With this notation α^{k+1} can be computed as

$$\begin{aligned} \alpha^{k+1} &= \alpha^k - [P(\alpha^k)]^{-1} \sum_{i=1}^m M(t_i; q_{\alpha^k})^* [\mathcal{C}z(t_i; q_{\alpha^k}) - \hat{z}_i] \\ &\doteq E(\alpha^k) \end{aligned} \quad (2.2)$$

whenever $[P(\alpha^k)]^{-1}$ exists.

Although the above steps completely define the quasilinearization algorithm, it is important to mention that in the present form it cannot be implemented computationally due to the fact that $\tilde{\mathcal{Q}}$ can be infinite dimensional. However, if it is known that q^* belongs to a finite dimensional subspace $\tilde{\mathcal{Q}}^s$ of $\tilde{\mathcal{Q}}$, or if we want to determine the parameter q^{s*} that minimizes $J(q)$ over some finite dimensional subspace $\tilde{\mathcal{Q}}^s$ of $\tilde{\mathcal{Q}}$, the algorithm can be properly modified to be computationally implementable.

3. Convergence of the quasilinearization algorithm

In this section we shall deal with convergence issues related to the algorithm introduced in the previous section. Sufficient conditions for the convergence of the algorithm will be presented. Two preliminary lemmas will be needed.

LEMMA 3. Let $t \in [0, T]$ be fixed and $M(t; q)$ as defined above. If the mapping $q \rightarrow z(t; q)$ from $\mathcal{Q} \rightarrow Z_\delta$ has a locally Lipschitz continuous Fréchet derivative, then the mapping $\alpha \rightarrow M(t; q_\alpha)$ is continuous from $\ell^2(\mathcal{Q}) \rightarrow \mathcal{L}(\ell^2, Y)$. Moreover, for any $\alpha \in \ell^2(\mathcal{Q})$, there exist positive constants η_α and \mathcal{L}_α depending on t such that

$$\|M(t; q_\alpha) - M(t; q_{\tilde{\alpha}})\|_{\mathcal{L}(\ell^2, Y)} \leq \mathcal{L}_\alpha |\alpha - \tilde{\alpha}|_{\ell^2}, \quad \forall \tilde{\alpha} \in B_{\eta_\alpha}(\alpha),$$

where $B_{\eta_\alpha}(\alpha)$ denotes the open ball in ℓ^2 of radius η_α centered at α . The same result holds for the mapping $\alpha \rightarrow M(t; q_\alpha)^*$.

PROOF. Let $t \in [0, T]$ be fixed. By hypothesis, for each $\alpha \in \ell^2(\mathcal{Q})$ there exist positive constants η_α and L_α such that $\|z_q(t; q_\alpha) - z_q(t; q_{\tilde{\alpha}})\|_{\mathcal{L}(\tilde{\mathcal{Q}}, Z)} < L_\alpha \|q_\alpha - q_{\tilde{\alpha}}\|$ for every $\tilde{\alpha} \in B_{\eta_\alpha}(\alpha)$. It then follows that

$$\begin{aligned} \|M(t; q_\alpha) - M(t; q_{\tilde{\alpha}})\|_{\mathcal{L}(\ell^2, Y)} &= \sup_{\gamma \in \ell^2, |\gamma|=1} \|[M(t; q_\alpha) - M(t; q_{\tilde{\alpha}})]\gamma\|_Y \\ &= \sup_{\gamma \in \ell^2, |\gamma|=1} \|\mathcal{C}z_q(t; q_\alpha) - \mathcal{C}z_q(t; q_{\tilde{\alpha}})\|_Y \|\gamma\|_Y \\ &\leq \|\mathcal{C}\|_{\mathcal{L}(Z, Y)} \sup_{\gamma \in \ell^2, |\gamma|=1} \left\{ \|z_q(t; q_\alpha) - z_q(t; q_{\tilde{\alpha}})\|_{\mathcal{L}(\tilde{\mathcal{Q}}, Z)} \|\gamma\|_{\tilde{\mathcal{Q}}} \right\} \\ &\leq \|\mathcal{C}\|_{\mathcal{L}(Z, Y)} L_\alpha \|q_\alpha - q_{\tilde{\alpha}}\|_{\tilde{\mathcal{Q}}} \\ &= \|\mathcal{C}\|_{\mathcal{L}(Z, Y)} L_\alpha |\alpha - \tilde{\alpha}| \doteq \mathcal{L}_\alpha |\alpha - \tilde{\alpha}| \end{aligned}$$

provided $\tilde{\alpha} \in B_{\eta_\alpha}(\alpha)$. ■

LEMMA 4. Under the same hypothesis of Lemma 3, the mapping $\alpha \rightarrow P(\alpha)$ is locally Lipschitz continuous from $\ell^2(\mathcal{Q}) \rightarrow \mathcal{L}(\ell^2, \ell^2)$.

PROOF. The result follows immediately from Lemma 3. In fact, observe that

$$\begin{aligned} [P(\alpha) - P(\tilde{\alpha})]\gamma &= \sum_{i=1}^m M(t_i; q_\alpha)^* M(t_i; q_\alpha)\gamma - \sum_{i=1}^m M(t_i; q_{\tilde{\alpha}})^* M(t_i; q_{\tilde{\alpha}})\gamma \\ &= \sum_{i=1}^m M(t_i; q_\alpha)^* [M(t_i; q_\alpha) - M(t_i; q_{\tilde{\alpha}})]\gamma \\ &\quad + \sum_{i=1}^m [M(t_i; q_\alpha)^* - M(t_i; q_{\tilde{\alpha}})^*] M(t_i; q_{\tilde{\alpha}})\gamma. \quad \blacksquare \end{aligned}$$

Before stating the main results concerning the convergence of the quasilinearization algorithm (QA), we will first need to recall the concept of a *point of attraction*. Sufficient conditions for an iteration mapping on a Banach space to have a point of attraction are given in Lemma 6.

DEFINITION 5. Let U be an open subset of a Banach space X and $E : U \subset X \rightarrow X$. We say that x^* is a point of attraction of the iteration $x^{k+1} = E(x^k)$ if there exists an open neighborhood S of x^* such that $S \subset U$ and for any $x^0 \in S$, the iterates $x^k \in U$, for all $k \geq 1$ and $x^k \rightarrow x^*$ as $k \rightarrow \infty$.

LEMMA 6. Let U be an open subset of a Banach space X , $E : U \subset X \rightarrow X$, $x^* \in U$ and suppose there is a ball $B = B_\eta(x^*) \subset U$ and $\alpha \in (0, 1)$ such that

$$\|E(x) - x^*\| \leq \alpha \|x - x^*\|, \quad \forall x \in B.$$

Then x^* is a point of attraction of the iteration $x^{k+1} = E(x^k)$.

PROOF. Whenever $x^0 \in B$, we have that $\|x^1 - x^*\| = \|E(x^0) - x^*\| \leq \alpha \|x^0 - x^*\| < \alpha\eta < \eta$, and therefore $x^1 \in B$. By induction $\|x^{k+1} - x^*\| = \|E(x^k) - x^*\| \leq \alpha \|x^k - x^*\| \leq \alpha^{k+1} \|x^0 - x^*\| \rightarrow 0$ as $k \rightarrow \infty$. Hence $x^k \in B \forall k$ and $x^k \rightarrow x^*$ as $k \rightarrow \infty$. ■

THEOREM 7. (LOCAL CONVERGENCE OF THE QA UNDER EXACT FIT-TO-DATA ASSUMPTION). *Assume the hypothesis of Lemma 3 holds. Assume also that there exist an open set $U \subset \ell^2(Q)$ and $\alpha^* \in U$ such that $[P(\alpha^*)]^{-1}$ exists and $J(q_{\alpha^*}) = 0$. Let E be the iteration mapping defined by (2.2). Then, for every $\epsilon > 0$, there exists a constant $\delta > 0$ so that $|\alpha - \alpha^*| < \delta$ implies*

$$|E(\alpha) - \alpha^*| \leq K|\alpha - \alpha^*|^2 + \epsilon|\alpha - \alpha^*|$$

where K is a constant depending only on α^* (not on ϵ). In particular, α^* is a point of attraction of the iteration $\alpha^{k+1} = E(\alpha^k)$.

PROOF. By definition

$$E(\alpha) = \alpha - [P(\alpha)]^{-1} \left\{ \sum_{i=1}^m M(t_i; q_\alpha)^* (\mathcal{C}z(t_i; q_\alpha) - \hat{z}_i) \right\}$$

whenever $[P(\alpha)]^{-1}$ exists. Hence,

$$\begin{aligned} E(\alpha) - \alpha^* &= \alpha - [P(\alpha)]^{-1} \left\{ \sum_{i=1}^m M(t_i; q_\alpha)^* (\mathcal{C}z(t_i; q_\alpha) - \hat{z}_i) \right\} - \alpha^* \\ &= [P(\alpha)]^{-1} \left\{ P(\alpha) (\alpha - \alpha^*) - \sum_{i=1}^m M(t_i; q_\alpha)^* (\mathcal{C}z(t_i; q_\alpha) - \hat{z}_i) \right\} \\ &= [P(\alpha)]^{-1} \left\{ \sum_{i=1}^m M(t_i; q_\alpha)^* [M(t_i; q_\alpha) (\alpha - \alpha^*) - \mathcal{C}z(t_i; q_\alpha) + \hat{z}_i] \right\} \\ &= [P(\alpha)]^{-1} \left\{ \sum_{i=1}^m M(t_i; q_\alpha)^* [M(t_i; q_\alpha) - M(t_i; q_{\alpha^*})] (\alpha - \alpha^*) \right\} \\ &\quad - [P(\alpha)]^{-1} \left\{ \sum_{i=1}^m M(t_i; q_\alpha)^* [\mathcal{C}z(t_i; q_\alpha) - \mathcal{C}z(t_i; q_{\alpha^*}) - M(t_i; q_{\alpha^*}) (\alpha - \alpha^*)] \right\} \\ &\quad - [P(\alpha)]^{-1} \left\{ \sum_{i=1}^m M(t_i; q_\alpha)^* [\mathcal{C}z(t_i; q_{\alpha^*}) - \hat{z}_i] \right\}. \end{aligned}$$

Since $J(q_{\alpha^*}) = 0$, the third term on the right hand side equals zero. Also, since $[P(\alpha^*)]^{-1}$ exists, by continuity there exist positive constants δ_1 and K_P such that $\| [P(\alpha)]^{-1} \|_{\mathcal{L}(\ell^2, \ell^2)} \leq K_P$ whenever $|\alpha - \alpha^*| < \delta_1$. Also, from Lemma 3 there exists $M > 0$ such that $\|M(t_i; q_\alpha)^*\| \leq M$ for $i = 1, 2, \dots, m$, provided $|\alpha - \alpha^*| < \delta_1$.

Consequently, for $|\alpha - \alpha^*| < \delta_1$ one has

$$\begin{aligned} |E(\alpha) - \alpha^*| &\leq K_P M \sum_{i=1}^m \| [M(t_i; q_\alpha) - M(t_i; q_{\alpha^*})] (\alpha - \alpha^*) \| \\ &\quad + K_P M \sum_{i=1}^m \| \mathcal{C}z(t_i; q_\alpha) - \mathcal{C}z(t_i; q_{\alpha^*}) - M(t_i; q_{\alpha^*}) (\alpha - \alpha^*) \| \\ &\doteq A + B. \end{aligned}$$

Now, by Lemma 3, if $|\alpha - \alpha^*| < \eta_{\alpha^*}$, then $A \leq K_P M m \mathcal{L}_{\alpha^*} |\alpha - \alpha^*|^2$. Also, since

$$M(t_i; q_{\alpha^*}) (\alpha - \alpha^*) = \mathcal{C}z_q(t_i; q_{\alpha^*}) (q_\alpha - q_{\alpha^*}),$$

we have from the definition of the Fréchet derivative $z_q(t; q)$ that given $\epsilon > 0$ there exists $\delta_2 = \delta_2(\epsilon, \alpha^*) > 0$ such that $|\alpha - \alpha^*| < \delta_2$ implies

$$\| \mathcal{C}z(t_i; q_\alpha) - \mathcal{C}z(t_i; q_{\alpha^*}) - M(t_i; q_{\alpha^*}) (\alpha - \alpha^*) \| \leq \epsilon \|q_\alpha - q_{\alpha^*}\| = \epsilon |\alpha - \alpha^*|,$$

for all $i = 1, 2, \dots, m$. Finally for any α such that $|\alpha - \alpha^*| < \delta^* \doteq \min \{\delta_1, \delta_2, \eta_{\alpha^*}\}$ one has

$$|E(\alpha) - \alpha^*| \leq K_P M m \left[\mathcal{L}_{\alpha^*} |\alpha - \alpha^*|^2 + \epsilon |\alpha - \alpha^*| \right]$$

and the desired result follows. By Lemma 6, α^* is a point of attraction of the iteration $\alpha^{k+1} = E(\alpha^k)$. ■

It is important to note that in Theorem 7 we have assumed an exact fit-to-data at the minimizer α^* . In practice, when working with real parameter identification problems, this is not a realistic assumption due to possible observation, measuring and modeling errors. In the next theorem we weaken this exact fit-to-data assumption.

THEOREM 8. (LOCAL CONVERGENCE OF THE QA WITH NOISY DATA). *Assume the hypothesis of Lemma 3 holds. Assume also that there exist an open set $U \subset \ell^2(\mathcal{Q})$ and $\alpha^* \in U$ such that $P(\alpha^*)$ is non-singular and α^* is a fixed point of E , i.e. $\alpha^* = E(\alpha^*)$. Let δ_1 and $K_P \doteq \sup \left\{ \|P(\alpha)\|^{-1} : |\alpha - \alpha^*| \leq \delta_1 \right\}$ be as in Theorem 7 and let \mathcal{L} be the smallest constant satisfying*

$$\|M(t_i; q_\alpha)^* - M(t_i; q_{\alpha^*})^*\| \leq \mathcal{L} |\alpha - \alpha^*|, \quad \forall |\alpha - \alpha^*| < \delta_1, \quad i = 1, 2, \dots, m,$$

and suppose that

$$\gamma \doteq K_P \mathcal{L} \sum_{i=1}^m \|Cz(t_i; q_{\alpha^*}) - \hat{z}_i\| < 1.$$

Then α^* is a point of attraction of the iteration $\alpha^{k+1} = E(\alpha^k)$.

PROOF. Let $\epsilon > 0$ be given. Following the same steps as in the proof of Theorem 7, we find that

$$\begin{aligned} |E(\alpha) - \alpha^*| &\leq K_P M m \left[\mathcal{L} |\alpha - \alpha^*|^2 + \epsilon |\alpha - \alpha^*| \right] \\ &\quad + \left\| [P(\alpha)]^{-1} \sum_{i=1}^m M(t_i; q_\alpha)^* [Cz(t_i; q_{\alpha^*}) - \hat{z}_i] \right\|, \end{aligned} \quad (3.1)$$

provided $|\alpha - \alpha^*| < \delta^*$, where $\delta^* = \min(\delta_1, \delta_2, \eta_{\alpha^*})$ is as in Theorem 7. But,

$$\sum_{i=1}^m M(t_i; q_{\alpha^*})^* [Cz(t_i; q_{\alpha^*}) - \hat{z}_i] = 0, \quad (3.2)$$

since, by assumption, $\alpha^* = E(\alpha^*)$. Combining (3.1) and (3.2) we obtain

$$\begin{aligned} |E(\alpha) - \alpha^*| &\leq K_P M m \left[\mathcal{L} |\alpha - \alpha^*|^2 + \epsilon |\alpha - \alpha^*| \right] \\ &\quad + K_P \left\| \sum_{i=1}^m [M(t_i; q_\alpha)^* - M(t_i; q_{\alpha^*})^*] [Cz(t_i; q_{\alpha^*}) - \hat{z}_i] \right\| \\ &\leq K_P M m \left[\mathcal{L} |\alpha - \alpha^*|^2 + \epsilon |\alpha - \alpha^*| \right] \\ &\quad + K_P \mathcal{L} |\alpha - \alpha^*| \sum_{i=1}^m \|Cz(t_i; q_{\alpha^*}) - \hat{z}_i\| \\ &= K_P M m \left[\mathcal{L} |\alpha - \alpha^*|^2 + \epsilon |\alpha - \alpha^*| \right] + \gamma |\alpha - \alpha^*| \end{aligned}$$

where $\gamma < 1$ by hypothesis. Choosing $\epsilon \leq \frac{1-\gamma}{4K_P M m}$ it follows that $|E(\alpha) - \alpha^*| \leq \frac{1+\gamma}{2} |\alpha - \alpha^*|$ for every α satisfying $|\alpha - \alpha^*| < \min \left(\delta^*, \frac{1-\gamma}{4K_P M m \mathcal{L}} \right)$. This concludes the proof. ■

It is important to note here that in Lemma 3 as well as in Theorems 7 and 8 we have assumed the local Lipschitz continuity of the mapping $q \rightarrow z_q(t; q)$. The following theorem, whose proof can be found in [6, Theorem 3.1] states sufficient conditions on $F(q, t, z)$ under which this assumption is guaranteed.

THEOREM 9. *Let the hypotheses of Theorem 2 hold. Assume also that the mapping $(q, z(\cdot)) \rightarrow F_z(q, \cdot, z(\cdot))$ from $\mathcal{Q} \times L^\infty(0, T : Z_\delta)$ into $L^\infty(0, T : \mathcal{L}(Z_\delta, Z))$ is locally Lipschitz continuous with respect to both variables q and $z(\cdot)$. Then, the mapping $q \rightarrow z_q(\cdot; q)$ from $\mathcal{Q} \rightarrow L^\infty(0, T : \mathcal{L}(\mathcal{Q}, Z))$ is locally Lipschitz continuous.*

4. A comparison with the standard approach to quasilinearization

In the standard literature ([5], [8]) the quasilinearization algorithm is introduced in a rather different manner than the one discussed in the previous sections. For the sake of completeness, we briefly present here this standard, although less intuitive approach. In spite of the fact that at a first glance, the methods look completely dissimilar, we shall show that they both lead to the same iterative process.

Assume that the nonlinear term $F(q, t, z)$ is Fréchet differentiable with respect to q and z . Given an estimate $q^k \in \mathcal{Q}$ of the minimizer $q^* \in \mathcal{Q}$, we define $z^k(t) = z(t; q^k)$ and linearize problem $(P)_q$ about $(q^k, z^k(t))$. This procedure yields the following IVP $(P)_q^k$

$$(P)_q^k \begin{cases} \dot{z}(t) = Az^k(t) + F(q^k, t, z^k(t)) \\ \quad + F_q(q^k, t, z^k(t))(q - q^k) \\ \quad + A(z(t) - z^k(t)) + F_z(q^k, t, z^k(t))(z(t) - z^k(t)) \\ z(0) = z_0. \end{cases}$$

Next, we define $z^{k+1}(t; q)$ to be the solution of $(P)_q^k$ and choose q^{k+1} to be a minimizer of the modified error criterion

$$J^k(q) = \frac{1}{2} \sum_{i=1}^m \|\mathcal{C}z^{k+1}(t_i; q) - \hat{z}_i\|^2.$$

Observing $(P)_q^k$, we see that $v(t) = z^{k+1}(t; q) - z^k(t)$ is a solution of the IVP

$$\begin{cases} \dot{v}(t) = Av(t) + F_q(q^k, t, z(t; q^k))(q - q^k) + F_z(q^k, t, z(t; q^k))v(t), \\ v(0) = 0. \end{cases} \quad (4.1)$$

This system is known as the ‘‘sensitivity equations’’ associated to the ID problem. In view of Theorem 2, $v(t)$ is the Fréchet q -derivative of $z(t; q)$ evaluated at q^k and applied to $(q - q^k)$, i.e. $v(t) = z_q(t; q^k)(q - q^k)$ and therefore

$$z^{k+1}(t; q) = z(t; q^k) + z_q(t; q^k)(q - q^k).$$

Hence,

$$J^k(q) = \frac{1}{2} \sum_{i=1}^m \|\mathcal{C} [z(t_i; q^k) + z_q(t_i; q^k)(q - q^k)] - \hat{z}_i\|_Y^2,$$

which is the same error criterion obtained in Section 2.

As we can see, the classical quasilinearization approach is based upon the *linearization of the initial value problem* around the solution corresponding to the guess parameter. The derivation requires previous knowledge of the sensitivity equations (4.1). On the other hand the method introduced in Section 2 is based simply upon the *linearization of the solution* of the IVP $(P)_q$ around the guess parameter. The derivation of the algorithm does not require the sensitivity equations. We emphasize however that in the computational implementation, both methods make use of the derivatives of the solutions with respect to the unknown parameters and, therefore, of system (4.1).

5. An application example - Numerical results

In this section we consider an example in which the quasilinearization algorithm is used to solve a parameter estimation problem in the following system of nonlinear partial differential equations:

$$\rho u_{tt} - \beta \rho u_{xxt} + \gamma u_{xxx} = f(x, t) + (2\alpha_2(\theta - \theta_1)u_x - 4\alpha_4 u_x^3 + 6\alpha_6 u_x^5)_x, \quad x \in (0, 1), 0 \leq t \leq T \quad (5.1a)$$

$$C_v \theta_t - k \theta_{xx} = g(x, t) + 2\alpha_2 \theta u_x u_{xt} + \beta \rho u_{xt}^2, \quad x \in (0, 1), 0 \leq t \leq T \quad (5.1b)$$

$$u(x, 0) = u_0(x), \quad u_t(x, 0) = v_0(x), \quad \theta(x, 0) = \theta_0(x), \quad x \in (0, 1) \quad (5.1c)$$

$$u(0, t) = u(1, t) = u_{xx}(0, t) = u_{xx}(1, t) = 0, \quad 0 \leq t \leq T \quad (5.1d)$$

$$\theta_x(0, t) = \theta_x(1, t) = 0, \quad 0 \leq t \leq T. \quad (5.1e)$$

These equations arise from the conservation laws of linear momentum and energy in a one-dimensional shape memory beam. The functions u and θ represent displacement and absolute temperature, respectively. The subscripts “ x ” and “ t ” denote partial derivatives and $\rho, C_v, k, \beta, \gamma, \alpha_2, \alpha_4, \alpha_6, \theta_1$ are positive constants depending on the alloy being considered. The functions $f(x, t)$ and $g(x, t)$ denote distributed forces and distributed heat sources. For a detailed explanation of the model and the meaning of the parameters involved we refer the reader to [12] and the references therein.

The semigroup theory (see [11]) provides a powerful tool for treating initial-boundary value problems as ordinary differential equations in abstract spaces. In particular, this approach has been proved to be very useful for showing existence and uniqueness of solutions as well as well-posedness of partial differential equations. Semigroup theory is also very popular in other related areas such as inverse problems associated to certain IBVP, identification and control. The basic theory and a few applications to PDE's can be found in [11] and reference [3] is an excellent source for applications of the theory to more concrete problems.

We are mainly interested in using experimental data to estimate the parameters $\alpha_2, \alpha_4, \alpha_6$ and θ_1 . It is important to note that these are non-physical parameters and therefore they cannot be estimated from laboratory experiments. Next, following the theoretical approach mentioned above, we shall formulate the IBVP (5.1a-e) as an abstract nonlinear Cauchy problem in an appropriate Banach Space. We first define the admissible parameter set as $\mathcal{Q} \doteq \{q = (\alpha_2, \alpha_4, \alpha_6, \theta_1) \mid q \in \mathbb{R}_+^4\}$, and the state space Z as the Hilbert space $H_0^1(0, 1) \cap H^2(0, 1) \times L^2(0, 1) \times L^2(0, 1)$ with the inner product

$$\left\langle \begin{pmatrix} u \\ v \\ \theta \end{pmatrix}, \begin{pmatrix} \tilde{u} \\ \tilde{v} \\ \tilde{\theta} \end{pmatrix} \right\rangle \doteq \gamma \int_0^1 u''(x) \overline{\tilde{u}''(x)} dx + \rho \int_0^1 v(x) \overline{\tilde{v}(x)} dx + \frac{C_v}{k} \int_0^1 \theta(x) \overline{\tilde{\theta}(x)} dx.$$

The operator A on Z is defined by

$$\text{Dom}(A) = \left\{ \begin{pmatrix} u \\ v \\ \theta \end{pmatrix} \in Z \mid \begin{array}{l} u \in H^4(0, 1), u(0) = u(1) = u''(0) = u''(1) = 0 \\ v \in H_0^1(0, 1) \cap H^2(0, 1) \\ \theta \in H^2(0, 1), \theta'(0) = \theta'(1) = 0 \end{array} \right\}$$

and for $z = \begin{pmatrix} u \\ v \\ \theta \end{pmatrix} \in \text{Dom}(A)$,

$$A \begin{pmatrix} u \\ v \\ \theta \end{pmatrix} \doteq \begin{pmatrix} 0 & I & 0 \\ -\frac{\gamma}{\rho} \frac{\partial^4}{\partial x^4} & \beta \frac{\partial^2}{\partial x^2} & 0 \\ 0 & 0 & \frac{k}{C_v} \frac{\partial^2}{\partial x^2} \end{pmatrix} \begin{pmatrix} u \\ v \\ \theta \end{pmatrix}.$$

We also define $z_0(x) = \begin{pmatrix} u_0(x) \\ v_0(x) \\ \theta_0(x) \end{pmatrix}$ and $F(q, t, z) : \mathcal{Q} \times [0, T] \times D \rightarrow Z$ by

$$F(q, t, z) = \begin{pmatrix} 0 \\ f_2(q, t, z) \\ f_3(q, t, z) \end{pmatrix}, \tag{5.2}$$

where

$$\begin{aligned} \rho f_2(q, t, z)(x) &= f(x, t) + (2\alpha_2(\theta - \theta_1)u_x - 4\alpha_4u_x^3 + 6\alpha_6u_x^5)_x, \\ C_v f_3(q, t, z)(x) &= g(x, t) + 2\alpha_2\theta u_x v_x + \beta \rho v_x^2, \end{aligned}$$

and $D \doteq H_0^1(0, 1) \cap H^2(0, 1) \times H^1(0, 1) \times H^1(0, 1)$.

With the above notation, the IBVP (5.1a-e) can be written as the following abstract Cauchy problem in the Hilbert space Z :

$$(\mathcal{P}) \begin{cases} \frac{d}{dt} z(t) = Az(t) + F(q, t, z), & 0 < t < T \\ z(0) = z_0. \end{cases} \tag{5.3}$$

Consider the following standing hypothesis.

(H2). For each fixed $t \geq 0$, the functions $f(\cdot, t)$, $g(\cdot, t)$ belong to $L^2(0, 1)$ and there exist nonnegative functions $K_f(x)$, $K_g(x) \in L^2(0, 1)$ such that

$$|f(x, t_1) - f(x, t_2)| \leq K_f(x)|t_1 - t_2|, \quad |g(x, t_1) - g(x, t_2)| \leq K_g(x)|t_1 - t_2|$$

for all $x \in (0, 1)$, $t_1, t_2 \in [0, T]$.

The following results can be easily derived from theorems 3.7 and 3.11 in [13] with only slight modifications in order to take into account for the different boundary conditions being considered here. Since the modifications needed are trivial and the proof is not important for the goals pursued by this article, we do not give details here.

THEOREM 10. *The operator A defined above generates an analytic semigroup $T(t)$ in Z . Hypothesis (H2) implies that the mapping F as defined by (5.2) satisfies hypothesis (H1) for any $\delta \in (\frac{3}{4}, 1)$.*

The following theorem shows that the operator A and the function F satisfy the regularity conditions required by Theorems 2 and 9 to ensure the existence and Lipschitz continuity of the Fréchet derivative of the mapping $q \rightarrow z(t; q)$. This result, together with Theorems 7 and 8, will yield the local convergence of the quasilinearization algorithm to the optimal parameter.

THEOREM 11. *Let Z , A and $F(q, t, z)$ be as defined above and assume (H2) holds. Then the mapping $(q, z(\cdot)) \rightarrow F(q, \cdot, z(\cdot))$ from $\mathcal{Q} \times L^\infty(0, T : Z_\delta)$ into $L^\infty(0, T : Z)$ is Fréchet differentiable in both variables. Also, the mappings $(q, z(\cdot)) \rightarrow F_q(q, \cdot, z(\cdot))$ and $(q, z(\cdot)) \rightarrow F_z(q, \cdot, z(\cdot))$ are locally Lipschitz continuous from $\mathcal{Q} \times L^\infty(0, T : Z_\delta)$ into $L^\infty(0, T : \mathcal{L}(\tilde{\mathcal{Q}}, Z))$ and from $\mathcal{Q} \times L^\infty(0, T : Z_\delta)$ into $L^\infty(0, T : \mathcal{L}(Z_\delta, Z))$, respectively.*

PROOF. This result follows immediately after observing that $f_2(q, t, z)$ and $f_3(q, t, z)$, as previously defined, are Fréchet differentiable with respect to q and z . Moreover, these derivatives can be computed explicitly and are given by:

$$\begin{aligned} D_z f_2(q, t, \begin{pmatrix} u \\ v \\ \theta \end{pmatrix}) \begin{pmatrix} \tilde{u} \\ \tilde{v} \\ \tilde{\theta} \end{pmatrix} &= f_{2,u} \tilde{u} + f_{2,v} \tilde{v} + f_{2,\theta} \tilde{\theta}, \\ D_z f_3(q, t, \begin{pmatrix} u \\ v \\ \theta \end{pmatrix}) \begin{pmatrix} \tilde{u} \\ \tilde{v} \\ \tilde{\theta} \end{pmatrix} &= f_{3,u} \tilde{u} + f_{3,v} \tilde{v} + f_{3,\theta} \tilde{\theta}, \\ D_q f_2(q, t, \begin{pmatrix} u \\ v \\ \theta \end{pmatrix}) &= \frac{1}{\rho} \left[2\theta' u' + 2(\theta - \theta_1) u'', -12(u')^2 u'', 30(u')^4 u'', -2\alpha_2 u'' \right], \\ D_q f_3(q, t, \begin{pmatrix} u \\ v \\ \theta \end{pmatrix}) &= \frac{1}{C_v} [2\theta u' v', 0, 0, 0], \end{aligned}$$

where the linear operators $f_{i,u}$, $f_{i,v}$ and $f_{i,\theta}$, $i = 2, 3$ are given by

$$\begin{aligned} f_{2,u} &= \frac{1}{\rho} \left\{ 2\alpha_2 \theta' D + 2\alpha_2 (\theta - \theta_1) D^2 - 24\alpha_4 u' u'' D - 12\alpha_4 (u')^2 D^2 \right. \\ &\quad \left. + 120\alpha_6 (u')^3 u'' D + 30\alpha_6 (u')^4 D^2 \right\}, \\ f_{2,v} &= 0 \\ f_{2,\theta} &= \frac{1}{\rho} \{ 2\alpha_2 u' D + 2\alpha_2 u'' \}, \\ f_{3,u} &= \frac{1}{C_v} \{ 2\alpha_2 \theta v' D \} \\ f_{3,v} &= \frac{1}{C_v} \{ 2\alpha_2 \theta u' D + 2\beta \rho v' D \}, \\ f_{3,\theta} &= \frac{1}{C_v} \{ 2\alpha_2 u' v' \}. \quad \blacksquare \end{aligned}$$

In the examples that follow we make use of the parameter values reported by F. Falk in [7] for the alloy $\text{Au}_{23}\text{Cu}_{30}\text{Zn}_{47}$. These values are: $\alpha_2 = 24 \text{ J cm}^{-3} \text{ K}^{-1}$, $\alpha_4 = 1.5 \times 10^5 \text{ J cm}^{-3}$, $\alpha_6 = 7.5 \times 10^6 \text{ J cm}^{-3} \text{ K}^{-1}$, $\theta_1 = 208 \text{ K}$, $C_v = 2.9 \text{ J cm}^{-3} \text{ K}^{-1}$, $k = 1.9 \text{ w cm}^{-1} \text{ K}^{-1}$, $\rho = 11.1 \text{ g cm}^3$, $\beta = 1$ and $\gamma = 10^{-12} \text{ J cm}^{-1}$. We want to estimate $q^* = (\alpha_2, \alpha_4, \alpha_6, \theta_1) = (24, 1.5 \times 10^5, 7.5 \times 10^6, 208)$.

Under certain general conditions, the one-to-oneness of the mapping $q \rightarrow z(t; q)$ in this particular example can be proved (see [10]). The choice of the examples below was made in order to fulfill these conditions.

Example 1: *Exact data.*

For this example we take $u_0 \equiv 0$, $v_0 \equiv 0$, $\theta_0 \equiv 200 \text{ K}$, $g(x, t) \equiv 0$,

$$f(x, t) = \begin{cases} 1 \times 10^5, & \text{if } 0.4 \leq x \leq 0.6, \\ 0, & \text{otherwise} \end{cases}$$

and $T = 0.01$. First, we obtain $u(t, x, q^*)$ and $\theta(t, x, q^*)$ by numerically solving the problem. For this purpose we make use of the spectral method developed in [9]. The observations are then taken to be $\hat{z}_i = \left\{ \begin{pmatrix} u(x_j, t_i; q^*) \\ \theta(x_j, t_i; q^*) \end{pmatrix} \right\}_{j=1}^9$, where $t_i = 0.001 i$, $i = 1, 2, \dots, 10$ and $x_j = 0.01 j$, $j = 1, 2, \dots, 9$. We start with an initial estimate $q^0 = (50, 3 \times 10^5, 15 \times 10^6, 420)$, approximately equal to twice q^* . The results of the iterations produced by the quasilinearization algorithm are shown in Table 1 and Figures 1.a-d. Figure 2a shows a comparison between $u(x, T; q^*)$ and $u(x, T; q^k)$ while in Figure 2b, $\theta(x, T; q^*)$ and $\theta(x, T; q^k)$ are drawn for different values of k .

k	α_2	α_4	α_6	θ_1	$J(q^k)$
0	50.0000	300000	1.50000e+07	420.000	1994.6900
1	16.1807	228111	1.40769e+07	459.904	611.1950
2	26.1790	222964	8.71784e+06	33.096	280.8220
3	25.3531	246241	8.83171e+06	126.468	15.3156
4	24.2770	178223	7.87660e+06	181.091	7.1313
5	24.0166	151184	7.51451e+06	206.550	0.6210
6	24.0012	150073	7.50096e+06	207.927	0.0122
7	24.0001	150006	7.50008e+06	207.994	0.0030
8	24.0001	150002	7.50003e+06	207.998	0.0029
9	24.0000	150002	7.50002e+06	207.998	0.0029
10	24.0000	150002	7.50002e+06	207.998	0.0029

Table 1: Values of the parameters and of the error criterion at different iteration steps.

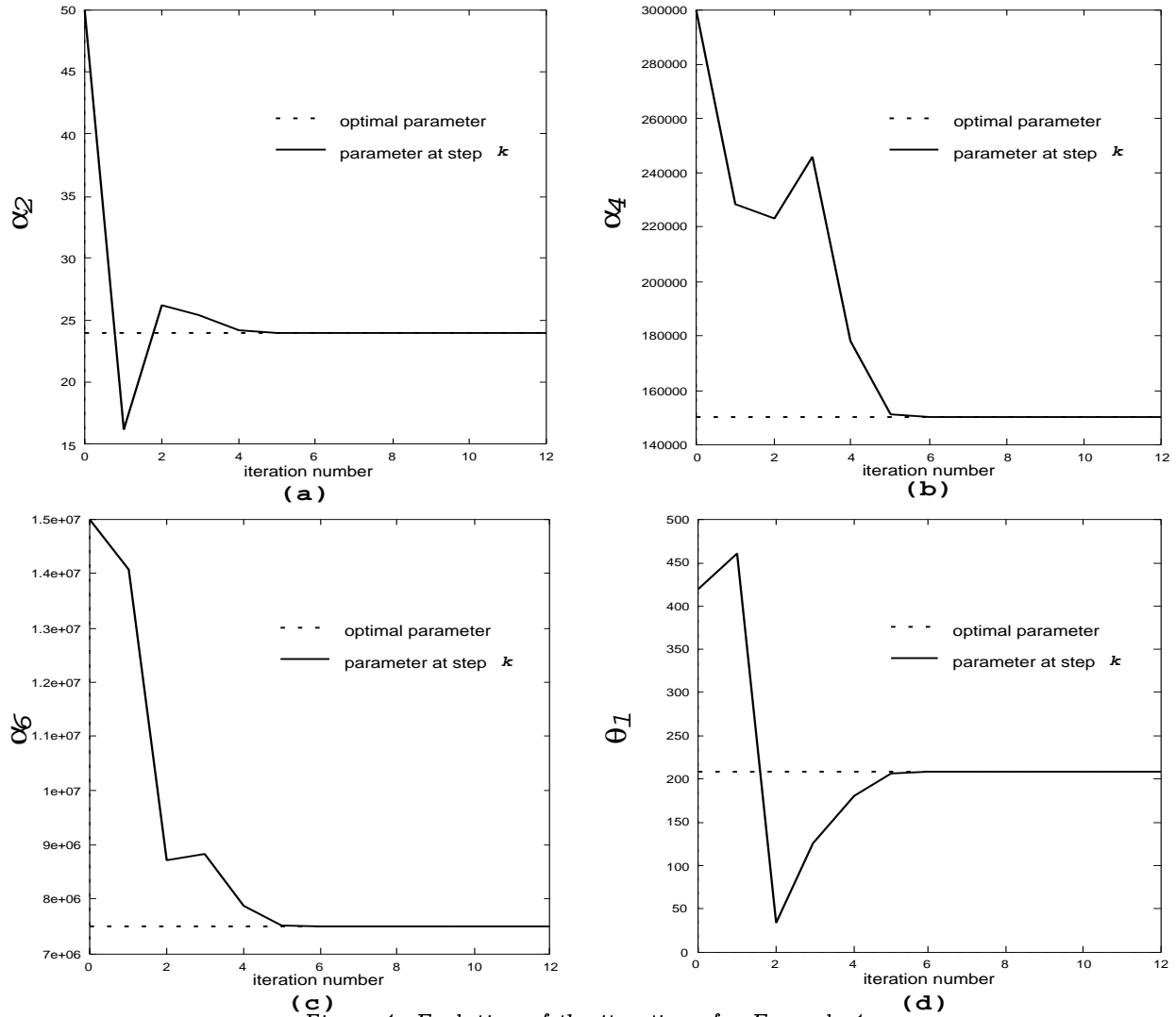


Figure 1: Evolution of the iterations for Example 1.

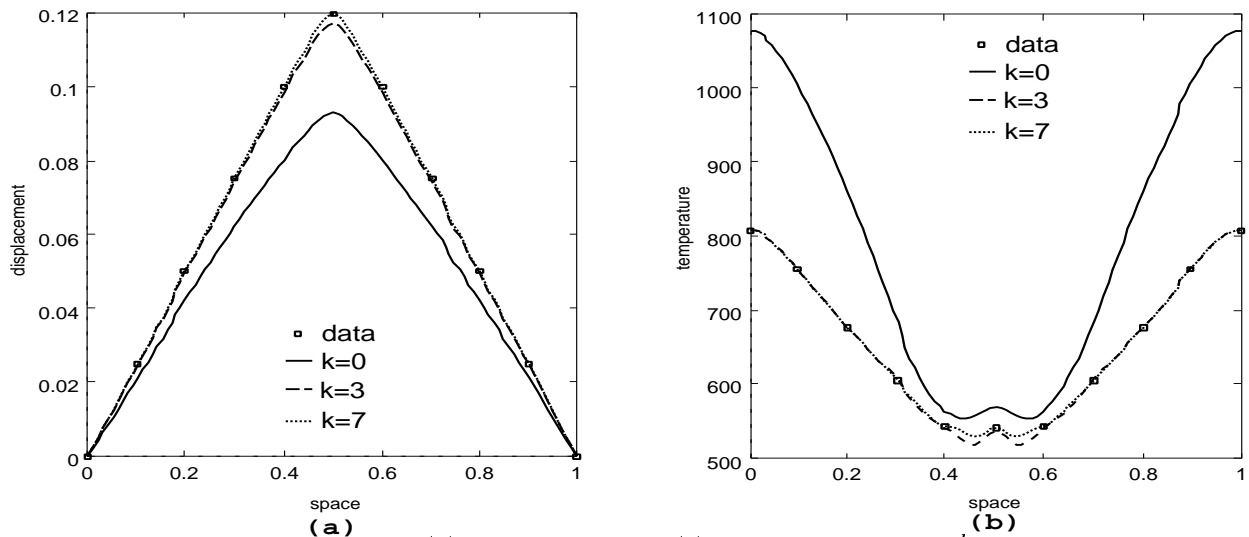


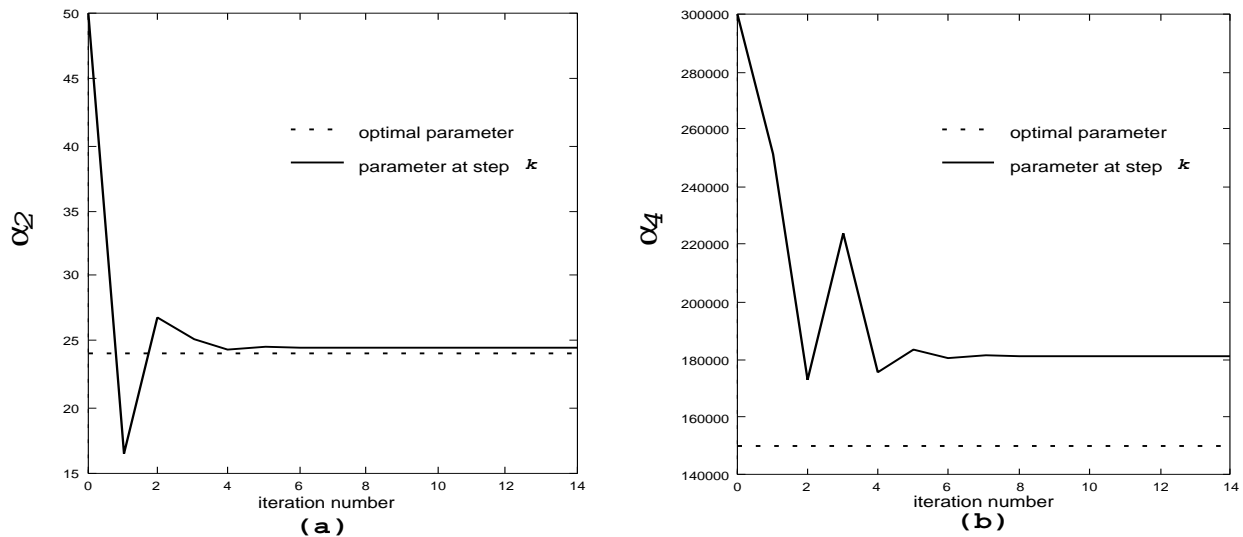
Figure 2: Displacement (a) and Temperature (b) at $T = 0.01$ for $q = q^k$, $k = 0, 3, 7$.

Example 2: *Noisy data.*

This example is analogous to Example 1, except that now we add random noise to the observation data in order to simulate measuring and modeling errors. More precisely, the observations are taken to be $\hat{z}_i = \left\{ \left(\begin{matrix} u(x_j, t_i; q^*) + r_{i,j} \\ \theta(x_j, t_i; q^*) + \tilde{r}_{i,j} \end{matrix} \right) \right\}_{j=1}^9$, where $r_{i,j}$ and $\tilde{r}_{i,j}$ are random numbers uniformly distributed in $(-0.05\bar{u}, 0.05\bar{u})$ and $(-0.05\bar{\theta}, 0.05\bar{\theta})$, respectively, with $\bar{u} = \frac{1}{90} \sum_{i=1}^{10} \sum_{j=1}^9 |u(x_j, t_i; q^*)|$ and $\bar{\theta} = \frac{1}{90} \sum_{i=1}^{10} \sum_{j=1}^9 \theta(x_j, t_i; q^*)$. The initial estimate is again $q^0 = (50, 3 \times 10^5, 15 \times 10^6, 420)$. The results of the iterations are shown in Table 2, and Figure 3. Figure 4a shows a comparison between $u(x, T; q^*)$ and $u(x, T; q^k)$ while in Figure 4b $\theta(x, T; q^*)$ and $\theta(x, T; q^k)$ are drawn for different values of k .

k	α_2	α_4	α_6	θ_1	$J(q^k)$
0	50.0000	300000	1.50000e+07	420.000	1987.240
1	16.5263	251533	1.43413e+07	450.975	604.570
2	26.7351	173032	7.92651e+06	77.3584	261.591
3	25.1282	223785	8.54573e+06	148.386	111.619
4	24.2875	176007	7.84280e+06	189.479	111.030
5	24.4436	183683	7.95702e+06	183.663	110.985
6	24.4070	180771	7.91592e+06	186.193	110.977
7	24.4184	181677	7.92857e+06	185.411	110.979
8	24.4151	181408	7.92483e+06	185.645	110.978
9	24.4161	181487	7.92593e+06	185.576	110.979
10	24.4158	181464	7.92560e+06	185.596	110.978
11	24.4159	181471	7.92570e+06	185.590	110.978
12	24.4159	181469	7.92567e+06	185.592	110.978
13	24.4159	181469	7.92568e+06	185.592	110.978

Table 2: Values of the parameters and of the error criterion at different iteration steps.



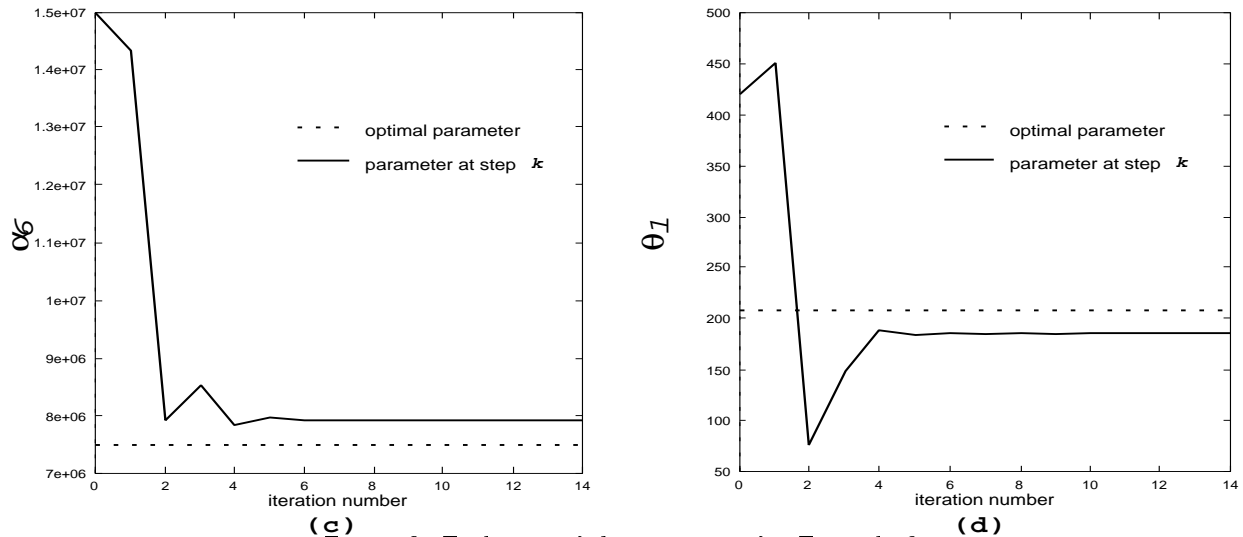


Figure 3: Evolution of the iterations for Example 2.

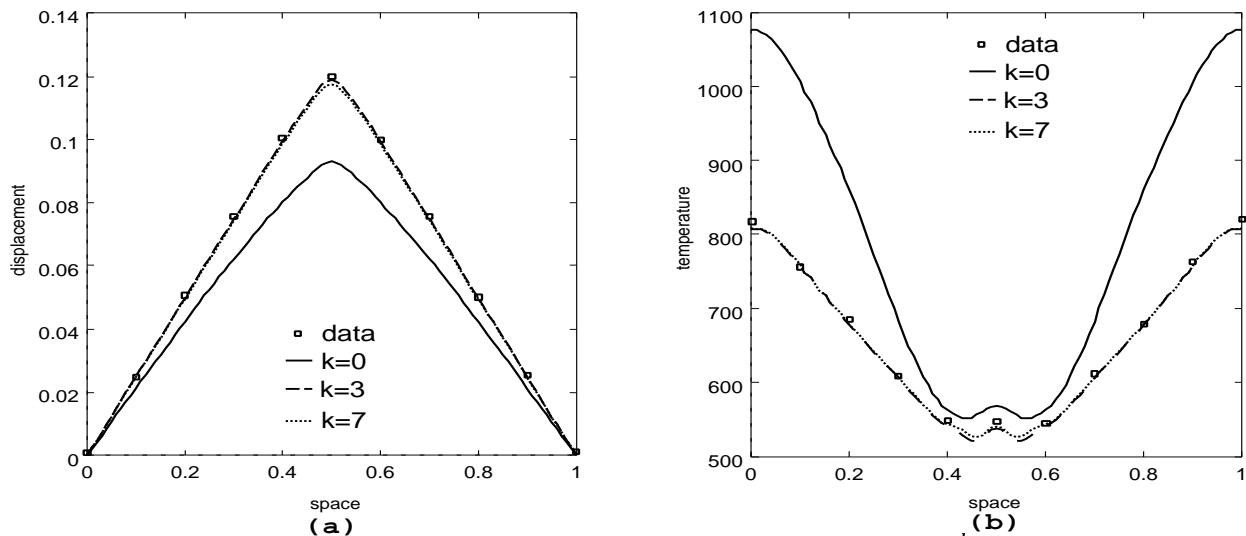


Figure 4: Displacement (a) and Temperature (b) at $T = 0.01$ for $q = q^k$, $k = 0, 3, 7$.

Example 3: *Comparison between direct and indirect methods.*

In this example we solve the ID problem using an indirect method and the algorithm presented in Section 2. The purpose is to illustrate the different convergence rates of the two approaches. We take u_0, v_0, θ_0, f and g as in Example 1.

The indirect method consists of approximating the solution of the dynamic equations using the algorithm proposed in [9] and applying afterwards the optimization algorithm of Hooke and Jeeves [4] to solve the resulting optimization problem. We obtain \hat{z}_i as in Example 1 and start with the initial estimate $q^0 = (25, 2 \times 10^5, 9 \times 10^6, 220)$. The results of the iterations are shown in Table 3.

k	α_2		α_4		α_6		θ_1	
	D	I	D	I	D	I	D	I
0	25	25	200000	200000	9e+06	9e+06	215	215
12	24.004	24.1250	149991	176000	7500020	8865000	207.999	202.1
40	24.004	24.9375	149991	161500	7500020	7537500	207.999	202.1
100	24.004	25.7344	149991	154000	7500020	6907500	207.999	202.1
500	24.004	24.8140	149991	149738	7500020	7333770	207.999	206.564
1000	24.004	24.4651	149991	149967	7500020	7462530	207.999	207.355
2000	24.004	24.1638	149991	150040	7500020	7499950	207.999	207.801
3000	24.004	24.0651	149991	150011	7500020	7500490	207.999	207.924

Table 3: Comparison of the convergence speeds between a direct (D) and an indirect (I) method.

6. Conclusions

A new approach for identifying the unknown parameter q in nonlinear abstract Cauchy problems of the type $\dot{z}(t) = Az(t) + F(q, t, z(t))$ was introduced. This approach has two main advantages over classical methods. First of all it is much more intuitive since it is based upon linearization of the solution about an initial guess parameter rather than on the linearization of the whole problem about a particular solution. Secondly, unlike in the classical setting, the derivation of the algorithm does not rely upon the sensitivity equations. We have included sufficient conditions for the convergence of the algorithm in terms of the regularity of the solutions with respect to the unknown parameter.

Finally, an application was considered in which the nonphysical parameters defining the free energy potential in a mathematical model for shape memory alloys are estimated. Several numerical examples are presented and convergence speeds are compared with those of an indirect method.

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CONFERENCIAS Y COMUNICACIONES DEL VI SEMINARIO SOBRE PROBLEMAS DE FRONTERA LIBRE Y SUS APLICACIONES.

Miércoles 16 de diciembre de 1998

- Domingo A. Tarzia (Rosario), “Introducción a los problemas de frontera libre para la ecuación del calor-difusión. El problema de cambio de fase y las soluciones exactas de Lamé-Clapeyron y de Neumann”. Actividad dirigida principalmente a los que se inician en el tema del Seminario.
- Carmen Cortázar (Santiago de Chile), “El fenómeno de blow-up en un problema de reacción-difusión”.
- Cristina Turner (Córdoba), “Modelos matemáticos para el fluido de Bingham”.
- Mario Storti (Santa Fe), “Problema de superficie libre en hidrodinámica naval”.
- Juan Carlos Reginato (Río Cuarto), “Cálculo de toma de nutrientes por raíces de cultivos mediante un modelo de frontera móvil”.
- Rodolfo Mascheroni (La Plata), “Modelo de deshidratación osmótica de elementos vegetales”.

Jueves 17 de diciembre de 1998

- Manuel Elgueta (Santiago de Chile), “Unicidad vs. No unicidad para un problema de medios porosos”.
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- Domingo A. Tarzia (Rosario), “Problemas de conducción del calor no clásicos para un material semi-infinito”.

Viernes 18 de diciembre de 1998

- Luis T. Villa (Salta), “Problema de frontera libre en procesos de transferencia de materia y energía con reacción química”.
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[1] CAFFARELLI L. A. & VAZQUEZ J.L., *A free-boundary problem for the heat equation arising in flame propagation*, Trans. Amer. Math. Soc., 347 (1995), pp. 411-441.

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