

QUADRATURE METHOD FOR EQUATIONS WITH NONLINEAR BOUNDARY CONDITIONS ARISING IN A THERMAL EXPLOSION THEORY

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ABSTRACT. We consider a 1-dimensional reaction diffusion equation with the following boundary conditions arising in a theory of the thermal explosion

$$\begin{cases} -u''(t) = \lambda f(u(t)), & t \in (0, l), \\ -u'(0) + C(0)u(0) = 0, \\ u'(l) + C(l)u(l) = 0, \end{cases}$$

where $C : [0, \infty) \rightarrow (0, \infty)$ is a continuous and nondecreasing function, $\lambda > 0$ is a parameter and $f : [0, \infty) \rightarrow (0, \infty)$ is a continuous function. We establish the extension of Quadrature method introduced in [8]. Using this extension, we provide numerical results for models with a typical function of f and C in a thermal explosion theory, which verify the existence, uniqueness and multiplicity results proved in [6].

1. Introduction

A typical model in combustion theory is the problem of thermal explosion which is spontaneous ignition of a rapid combustion process. The model reads as:

$$\begin{cases} T_t - \Delta T = \lambda f(T), & (t, x) \in (0, \infty) \times \Omega, \\ \mathbf{n} \cdot \nabla T + C(T)T = 0 & (t, x) \in (0, \infty) \times \partial\Omega, \\ T(0, x) = 0, & x \in \partial\Omega. \end{cases} \quad (1)$$

Here, T is an appropriately normalized temperature distribution in a bounded domain $\Omega \subset \mathbb{R}^n, n \geq 1$. The most common example of chemical reaction term is Arrhenius law in which case $f(T) = \exp(\frac{\alpha T}{\alpha + T})$, where the parameter $\alpha > 0$ (usually large) is a scaled activation energy. The parameter $\lambda > 0$ is a scaling parameter and can be associated with the size of the domain Ω which grows

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as λ increases. The heat-loss conditions are imposed on a boundary $\partial\Omega$ with outward normal \mathbf{n} , where the heat loss parameter $C(T)$ is assumed that $C : [0, \infty) \rightarrow (0, \infty)$ is a continuous and non decreasing function. Physically this assumption means that the heat loss through the boundary is always present and increases for higher temperatures. Further, initial normalized temperature is assumed to be equal to the one of the surrounding which is set to be equal to zero. It is well known the long time behavior of solutions for the problem (1) is fully determined by its stationary solutions, which is solutions of the following problem

$$\begin{cases} -\Delta u = \lambda f(u), & x \in \Omega, \\ \mathbf{n} \cdot \nabla u + C(u)u = 0, & x \in \partial\Omega. \end{cases} \tag{2}$$

In the literature, existence, uniqueness and multiplicity of reaction diffusion equations with various reaction term f were studied quite extensively (see [1]-[5],[7]-[11]) under either Dirichlet boundary condition or nonlinear boundary condition.

In this paper, we consider the following one-dimensional model of (2):

$$\begin{cases} -u''(t) = \lambda f(u(t)), & t \in (0, l), \\ -u'(0) + C(0)u(0) = 0, \\ u'(l) + C(l)u(l) = 0, \end{cases} \tag{3}$$

where λ is a positive parameter, l is a positive constant, $C : [0, \infty) \rightarrow (0, \infty)$ is a continuous and nondecreasing function and $f : [0, \infty) \rightarrow (0, \infty)$ is a continuous function. To investigate bifurcation diagrams of problems with nonlinear boundary conditions like (3), we first establish an extension of the Quadrature method introduced in [8]. To state our main result, we define $F(u) = \int_0^u f(s) ds$.

Theorem 1.1. *If u_λ is a positive solution of (3) with $\|u_\lambda\|_\infty = \rho$, then*

$$\sqrt{\lambda} = \frac{\sqrt{2}}{l} \int_{m_\rho}^\rho \frac{ds}{\sqrt{F(\rho) - F(s)}}, \tag{4}$$

where for each $\rho \in (0, \infty)$, $m_\rho \in (0, \rho)$ is the unique solution of

$$\frac{C(m)m}{\sqrt{2(F(\rho) - F(m))}} = \frac{\sqrt{2}}{l} \int_m^\rho \frac{ds}{\sqrt{F(\rho) - F(s)}}. \tag{5}$$

Conversely, if for each $\rho > 0$ there exist $\lambda > 0$ and $m_\rho \in (0, \rho)$ satisfying (4) and (5), then (3) has a positive solution u_λ with $\|u_\lambda\|_\infty = \rho$ and $u_\lambda(0) = m_\rho = u_\lambda(l)$.

This paper is organized as follows: Section 2 is devoted to the proof of Theorem 1.1. In Section 3, we recall some existence, uniqueness and multiplicity results of (2) related to our problem (3). In Section 4, we provide numerical simulations of the bifurcation diagram for the problem when $f(u) = e^{\frac{\alpha u}{\alpha+u}}$ and $C(u) = \frac{1-a}{a} + \frac{1}{a}u$. This verifies numerically the results introduced in Section 3.

2. Proof of Theorem 1.1

Let u be a positive solution of (3). Now multiplying (3) by u' , we have

$$-u''(t)u'(t) = \lambda f(u(t))u'(t), \quad t \in (0, l),$$

and so

$$\frac{d}{dt} \left[\frac{1}{2}u'(t)^2 + \lambda F(u(t)) \right] = 0, \quad t \in (0, l).$$

Hence

$$\frac{1}{2}u'(t)^2 + \lambda F(u(t)) = \text{constant}, \quad t \in [0, l].$$

Since $u''(t) < 0$ in $(0, l)$, there exists a unique $t_0 \in (0, l)$ such that $u'(t) > 0$ in $[0, t_0)$, $u'(t) < 0$ in $(t_0, l]$ and $u'(t_0) = 0$. Since $u'(t_0) = 0$, the constant is determined by $\lambda F(\rho)$. Hence, we have

$$u'(t)^2 = 2\lambda(F(\rho) - F(u(t))), \quad t \in [0, l], \tag{6}$$

where $\rho := \|u\|_\infty = u(t_0)$. We first claim that $t_0 = \frac{l}{2}$. Since the differential equation in (3) is autonomous, the solution has to be symmetric about t_0 . Hence, it is sufficient to show that $u(0) = u(l)$. From (6) and the boundary conditions in (3), we easily see that $u(0)$ and $u(l)$ are zeros of the function

$$g(x) := C(x)^2x^2 - 2\lambda(F(\rho) - F(x)).$$

But the function $g(x)$ is increasing for $x \geq 0$, and hence we have $u(0) = u(l)$. Thus, u is symmetric about $t = \frac{l}{2}$, $u'(t) > 0$ in $[0, \frac{l}{2})$, $u'(t) < 0$ in $(\frac{l}{2}, l]$ and $u'(\frac{l}{2}) = 0$. Now let $m := u(0) = u(l)$ and we rewrite (6) as follows:

$$\sqrt{\lambda} = \frac{u'(t)}{\sqrt{2(F(\rho) - F(u(t)))}}, \quad t \in [0, \frac{l}{2}]. \tag{7}$$

Applying the boundary condition at $t = 0$ to (7), we obtain

$$\sqrt{\lambda} = \frac{C(m)m}{\sqrt{2(F(\rho) - F(m))}}$$

and integrating (7) from 0 to $\frac{l}{2}$, we have

$$\sqrt{\lambda} = \frac{\sqrt{2}}{l} \int_m^\rho \frac{ds}{\sqrt{F(\rho) - F(s)}}. \tag{8}$$

Hence we see that m and ρ must be related by

$$H(m) := \frac{C(m)m}{\sqrt{2(F(\rho) - F(m))}} = \frac{\sqrt{2}}{l} \int_m^\rho \frac{ds}{\sqrt{F(\rho) - F(s)}} := G(m). \tag{9}$$

It is easy to see that H increases from 0 to ∞ while G decreases from a positive value to zero as m increases from 0 to ρ . This means that for each $\rho \in (0, \infty)$ there exists a unique $m_\rho \in (0, \rho)$ which satisfies (9) (see Figure 1). Now using

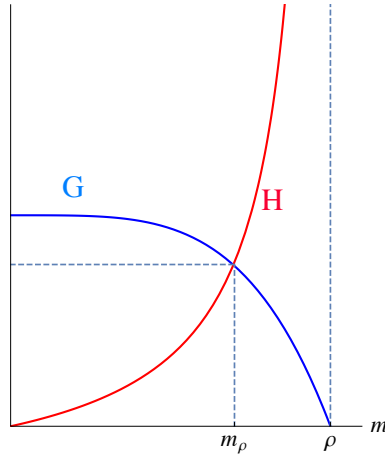


FIGURE 1. $H(m)$ increases in $[0, \rho]$ and $G(m)$ decreases in $[0, \rho]$

this $m_\rho \in (0, \rho)$, we obtain from (8) the relation:

$$\sqrt{\lambda} = \frac{\sqrt{2}}{l} \int_{m_\rho}^\rho \frac{ds}{\sqrt{F(\rho) - F(s)}}.$$

Conversely, for each given $\rho > 0$, if there exists $\lambda > 0$ that satisfies (4) and (5), one can backtrack to show that (3) has a positive solution u_λ of the form in Figure 2. Let $\rho \in (0, \infty)$ be fixed arbitrarily. Then there exists a

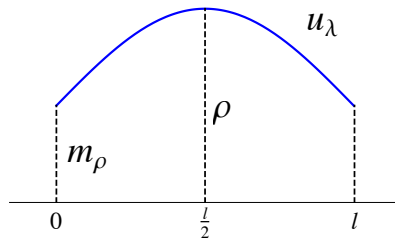


FIGURE 2. Positive solution of (3)

unique $m_\rho \in (0, \rho)$ satisfying (5). For such a $m_\rho (= m)$ we define a function $L : [m, \rho] \rightarrow \mathbb{R}$ by

$$L(u) = \int_m^u \frac{ds}{\sqrt{F(\rho) - F(s)}}.$$

Note that $L(u)$ is increasing on (m, ρ) as $L'(u) = \frac{1}{\sqrt{F(\rho)-F(u)}} > 0$ in (m, ρ) . Hence, the minimum of $L(u)$ is $L(m) = 0$ and the maximum is $L(\rho)$. Here we see that

$$L(\rho) = \int_m^\rho \frac{ds}{\sqrt{F(\rho)-F(s)}} = l\sqrt{\frac{\lambda}{2}} \tag{10}$$

by (4). Now, we claim that there exists a unique function $u : [0, \frac{l}{2}) \rightarrow [m, \rho)$ such that

$$L(u(x)) := \int_m^{u(x)} \frac{ds}{\sqrt{F(\rho)-F(s)}} = \sqrt{2\lambda}x.$$

Let us define $J : [0, \frac{l}{2}) \times [m, \rho) \rightarrow \mathbb{R}$ by

$$J(x, u) = \int_m^u \frac{ds}{\sqrt{F(\rho)-F(s)}} - \sqrt{2\lambda}x. \tag{11}$$

Then, there exists $(x_0, u_0) := (0, m) \in [0, \frac{l}{2}) \times [m, \rho)$ such that $J(x_0, u_0) = 0$. Note that $J \in C^1$ and $J_u(x_0, u_0) \neq 0$ as $J_u = \frac{1}{\sqrt{F(\rho)-F(u)}} > 0$. Hence, Implicit Function Theorem yields that there exists a unique $u \in C^1$ function such that $J(x, u(x)) = 0$ for $x \in [0, \frac{l}{2})$ with $u(0) = m$. From (10), we define $u(\frac{l}{2}) = \rho$. Now, we rewrite (11) as

$$\int_m^{u(x)} \frac{ds}{\sqrt{F(\rho)-F(s)}} = \sqrt{2\lambda}x, \quad x \in [0, \frac{l}{2}). \tag{12}$$

Differentiating (12) with respect to x , we have

$$\frac{u'(x)}{\sqrt{2(F(\rho)-F(u(x)))}} = \sqrt{\lambda}, \quad x \in [0, \frac{l}{2}), \tag{13}$$

which is written as

$$u'(x) = \sqrt{2\lambda(F(\rho)-F(u(x)))}, \quad x \in [0, \frac{l}{2}). \tag{14}$$

Differentiating it again, it follows that

$$-u''(x) = \lambda f(u(x)), \quad x \in [0, \frac{l}{2}).$$

Next, from (4), (5) and (13) with $x = 0$, we obtain that

$$\frac{C(m)m}{\sqrt{2(F(\rho)-F(m))}} = \frac{u'(0)}{\sqrt{2(F(\rho)-F(u(0)))}},$$

which implies that the boundary condition $-u'(0) + C(u(0))u(0) = 0$ is satisfied. Since $u'(x) = \sqrt{2\lambda(F(\rho)-F(u(x)))} > 0$ in (14), u is increasing on $[0, \frac{l}{2})$. From $u(\frac{l}{2}) = \rho$ and (14), we define $u'(\frac{l}{2}) = 0$. Note that the solution of (3) is symmetric about $x = \frac{l}{2}$. Now, we define $u(x)$ in $(\frac{l}{2}, l]$ such that $u(x) = u(l-x)$ for all $x \in (\frac{l}{2}, l]$. Then, there exists a positive solution u_λ with $\|u\|_\infty = \rho$ of (3) satisfying (4) and (5).

3. Known results

In this section, we recall some results concerning existence, uniqueness and multiplicity of solutions for the problem (2) established in [6].

Theorem 3.1. *The boundary value problem (2) has a positive solution for all $\lambda > 0$. Moreover, if $\frac{s}{f(s)}$ is increasing on $[0, \infty)$, then this solution is unique for any $\lambda > 0$.*

Let $e \in C^2(\bar{\Omega})$ be the unique solution of the following linear elliptic problem

$$\begin{cases} -\Delta e = 1, & x \in \Omega, \\ \mathbf{n} \cdot \nabla e + c_0 e = 0, & x \in \partial\Omega, \end{cases}$$

where $c_0 = C(0)$. Let us denote $Q(p, q) := \frac{pf(q)}{qf(p)}$ for any $0 < p < q$.

Theorem 3.2. *Assume that there exist $0 < p^* < q^*$ such that*

$$Q(p^*, q^*) > \frac{(N + 1)^{N+1} \|e\|_\infty}{N^{N-1} R^2},$$

where R is the radius of largest ball inscribed in Ω in \mathbb{R}^N . Then, (2) has at least three positive solutions provided $\lambda_1 < \lambda < \lambda_2$ where

$$\lambda_1 = \frac{q^* (N + 1)^{N+1}}{f(q^*) R^2 N^{N-1}}, \quad \lambda_2 = \frac{p^*}{f(p^*) \|e\|_\infty}.$$

Remark 1. In the case when $f(s) = e^{\frac{\alpha s}{\alpha+s}}$, if choosing $p^* = 1$ and $q^* = \alpha$, we have

$$Q(p^*, q^*) = \frac{1}{\alpha} \exp\left(\frac{\alpha^2}{2(\alpha + 2)}\right) \tag{15}$$

and therefore $Q(p^*, q^*)$ can be arbitrary large for large enough α .

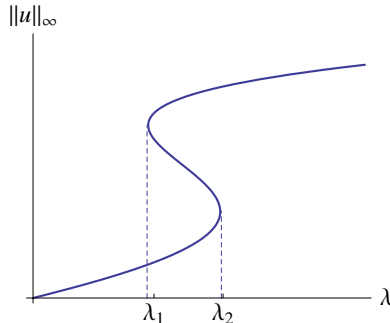


FIGURE 3. S-shaped bifurcation diagram for (2) showing the results of Theorem 3.1 and 3.2

4. Computational results

Here we consider a 1-dimensional thermal explosion model when $\Omega = (0, \lambda^2)$, $f(u) = \exp(\frac{\alpha u}{\alpha+u})$ and $C(u) = \frac{1-a}{a} + \frac{1}{a}u$, where $\alpha > 0$ and $0 < a < 1$. In particular, we study the boundary value problem

$$\begin{cases} -u''(t) = \lambda \exp\left(\frac{\alpha u}{\alpha+u}\right), & t \in (0, \lambda^2), \\ -u'(0) + \left(\frac{1-a}{a} + \frac{1}{a}u(0)\right) u(0) = 0, \\ u'(\lambda^2) + \left(\frac{1-a}{a} + \frac{1}{a}u(\lambda^2)\right) u(\lambda^2) = 0, \end{cases} \tag{16}$$

where $\lambda > 0$ is a positive parameter.

Now we provide numerical results of bifurcation diagram which show the existence, uniqueness and multiplicity when the parameter λ changes. Here we plot bifurcation curves via Quadrature method obtained in Theorem 1.1 using Mathematica. We consider the bifurcation diagrams for the case when $f(u) = \exp(\frac{\alpha u}{\alpha+u})$ for various values of α . Figure 4 shows that λ is an increasing function of ρ when $0 < \alpha < 4$ and $0 < a < 1$. This is expected since if $0 < \alpha < 4$, then $\frac{u}{f(u)} = \frac{u}{\exp[\frac{\alpha u}{\alpha+u}]}$ is increasing for all $u \geq 0$, and by Theorem 3.1, (16) has a unique solution for all $\lambda > 0$.

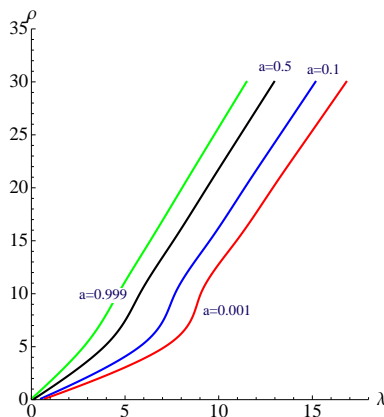


FIGURE 4. Bifurcation curve for certain values of $a \in (0, 1)$ when $\alpha = 3$

In Figure 5, bifurcation diagrams are provided when $4 \leq \alpha \leq 6$. For $4 \leq \alpha \leq 5.2$, the bifurcation curve of (16) is S -shaped for $a \approx 0$, while λ is an increasing function of ρ for $a \approx 1$. However, when $\alpha = 6$, we see that the bifurcation curves of (16) are S -shaped for all values of $a \in (0, 1)$ as in Remark 1.

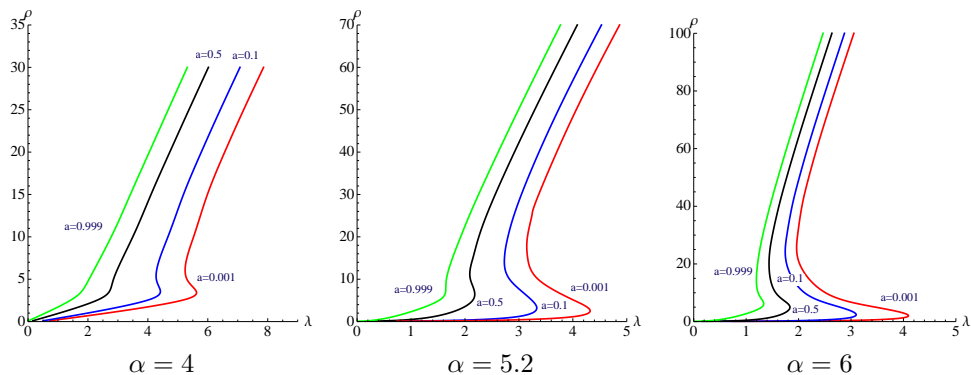


FIGURE 5. The critical value of λ corresponding to the case with the heat loss ($a \approx 1$) is significantly lower than those corresponding to cold boundary condition ($a \approx 0$).

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