Journal of Nonlinear Mathematical Physics Volume 15, Supplement 1 (2008), 69–76 Article

# Alternate Derivation of the Critical Value of the Frank-Kamenetskii Parameter in Cylindrical Geometry

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**Abstract**

Noether's theorem is used to determine first integrals admitted by a generalised Lane-Emden equation of the second kind modelling a thermal explosion. These first integrals exist for rectangular and cylindrical geometry. For rectangular geometry the first integrals show the symmetry of the temperature gradients at the rectangular walls. For a cylindrical geometry the first integrals show the dependence of the critical parameter on the temperature gradient at the cylinder wall. The well known critical value for the Frank-Kamenetskii parameter, $\delta = 2$, is obtained in a very natural way.

## 1 Introduction

The steady-state heat balance equation,

$$k_c \nabla^2 T + \sigma Q A \exp\left(-\frac{E}{RT}\right) = 0, \tag{1.1}$$

is used to model a thermal explosion in a vessel. The constant $k_c$ is the thermal conductivity, $\sigma$ the density, $Q$ is the heat of reaction, $A$ the frequency factor, $E$ the energy of activation of the chemical reaction, $R$ the universal gas constant and $T$ the gas temperature. The heat balance equation (1.1) is non-dimensionalised by the substitution

$$\theta = \frac{E}{RT_0^2}\left(T - T_0\right), \tag{1.2}$$

where $T_0$ is the ambient temperature. The heat balance equation (1.1) reduces to

$$\nabla^2\theta + \delta \exp\left(\frac{\theta}{1+\epsilon\theta}\right) = 0, \tag{1.3}$$

where

$$\delta = \left[ \frac{\sigma Q A}{k_c} \frac{E}{R T_0^2} \exp\left( -\frac{E}{R T_0} \right) \right] \tag{1.4}$$

and

$$\epsilon = \frac{R T_0}{E} << 1. \tag{1.5}$$

The Laplacian operator $\nabla^2$ is given by

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{N-1}{r} \frac{\partial}{\partial r}. \tag{1.6}$$

The constant $\delta$ is known as the Frank-Kamenetskii [10] parameter. By ignoring coefficients of $\epsilon$ and letting $\theta = y$ and $N = k + 1$ equation (1.3) reduces to

$$y'' + \frac{k}{x} y' + \delta \exp(y) = 0. \tag{1.7}$$

For well defined geometries we have $k = 0$ for a rectangular slab, $k = 1$ for an infinite circular cylinder and $k = 2$ for a sphere. Boundary conditions for the thermal explosion problem in a rectangular geometry are given by [10]

$$y(\pm 1) = 0. \tag{1.8}$$

The boundary conditions (1.8) fix the temperature at the walls. Boundary conditions for the thermal explosion problem in a cylindrical geometry are given by [10]

$$y'(0) = 0, \quad (a) \qquad y(1) = 0. \quad (b) \tag{1.9}$$

Boundary condition (1.9a) ensures continuity at the centre of the vessel. Boundary condition (1.9b) fixes the non-dimensional temperature at the wall.

The existence and uniqueness of solutions of (1.7) solved subject to (1.9) has been proved by Russell and Shampine [18]. They develop three numerical approaches to solving singular boundary value problems of the form (1.7) solved subject to (1.9). Balakrishnan et al. [4] have solved (1.7) numerically for non-integer values of $k$. Harley and Momoniat [12] use Lie point symmetries to investigate the stability of the boundary conditions (1.9) for non integer values of $k$. Frank-Kamenetskii [10] (see also Chambré [8] and Chandrasekhar [9]) has determined closed form solutions to (1.7) for the cases $k = 0$ and $k = 1$. Closed form solutions for the case $k = 2$ have not been determined. Nonlocal symmetries admitted by (1.7) have been investigated by Harley and Momoniat [11]. These nonlocal symmetries lead to new solutions which are valid after blow-up. Wazwaz [19] has used the Adomian decomposition method to obtain a power series solution to (1.7) for constant $\delta$. Momoniat and Harley [15] improved the radius of convergence of the power series solution based on a symmetry reduction approach.

The rest of the paper is divided up as follows: in Section 2 we discuss the theory of first integrals. In Section 3 we obtain and analyze first integrals admitted by (1.7) for $k = 0$ and $k = 1$. Concluding remarks are made in Section 4.

## 2 First integrals

In this section we discuss some of the theory of first integrals and symmetries. We write a second-order ordinary differential equation as

$$F(x, y, y', y'') = 0, \tag{2.1}$$

where $' = d/dx$. A first integral or conservation law admitted by (2.1) satisfies

$$D_x I(x, y, y')\big|_{(2.1)} = 0, \tag{2.2}$$

where $D_x$ is the operator of total differentiation given by

$$D_x = \frac{\partial}{\partial x} + y'\frac{\partial}{\partial y} + y''\frac{\partial}{\partial y'} + \dots . \tag{2.3}$$

A first integral $I(x, y, y')$ can be calculated by solving (2.2) directly where a suitable ansatz for $I(x, y, y')$ is chosen.

The Lie group method applied to differential equations [5, 13, 17] is a useful tool for determining the solutions admitted by differential equations. The Lie group approach considers an infinitesimal local transformation of the dependent and independent variables of the differential equation under consideration. A Taylor expansion of these local transformations is given by

$$\overline{x} \approx x + a\xi(x, y) + O(a^2), \qquad \overline{y} \approx y + a\eta(x, y) + O(a^2), \tag{2.4}$$

to first order in $a$. The transformations (2.4) leave the equation under consideration form invariant, i.e. (2.1) is transformed into

$$F\left(\overline{x}, \overline{y}, \frac{d\overline{y}}{d\overline{x}}, \frac{d^2\overline{y}}{d\overline{x}^2}\right) = 0. \tag{2.5}$$

The transformations (2.4) form a group. The constant $a$ is the group parameter. The generator of the group is given by

$$X = \xi\partial_x + \eta\partial_y, \tag{2.6}$$

where $\partial_x = \partial/\partial x$ and $\partial_y = \partial/\partial y$. The coefficients $\xi$ and $\eta$ of the symmetry generator (2.6) are calculated by solving a determining equation

$$X^{[2]}F(x, y, y', y'')\Big|_{(2.1)} = 0. \tag{2.7}$$

The generator $X^{[2]}$ is a second prolongation of $X$ given by

$$X^{[2]} = X + \zeta^{(1)}\partial_{y'} + \zeta^{(2)}\partial_{y''}, \tag{2.8}$$

where

$$\zeta^{(1)} = \eta_x + (\eta_y - \xi_x)y' - \xi_y y'^2, \tag{2.9}$$

$$\zeta^{(2)} = \eta_{xx} + (2\eta_{xy} - \xi_{xx})y' + (\eta_{yy} - 2\xi_{xy})y'^2 - \xi_{yy}y'^3 + (\eta_y - 2\xi_x)y'' - 3\xi_y y' y'', \quad (2.10)$$

and where subscripts denote differentiation (see e.g. Bluman and Kumei [5]). The symmetry generator (2.6) can be used to determine a group invariant solution admitted by (2.1) or reduce the order of (2.1).

In this paper we are interested in constructing first integrals of the equation under consideration. Noether's theorem [16] gives a relationship between symmetries and Lagrangians admitted by the equation under consideration. Noether's theorem [16] states that if we can find an operator $X$ given by

$$X = \xi\partial_x + \eta\partial_y, \quad (2.11)$$

where

$$X(L) + LD_x\xi = D_x B, \quad (2.12)$$

where $D_x$ is the operator of total differentiation given by (2.3) and $L$ is a solution of the Euler-Lagrange equation

$$\frac{d}{dx}\frac{\partial L}{\partial y'} - \frac{\partial L}{\partial y} = 0, \quad (2.13)$$

where $B$ is a gauge term, then

$$I = L\xi + \left(\eta - \xi y'\right)\frac{\partial L}{\partial y'} - B, \quad (2.14)$$

is a first-integral of the equation under consideration, i.e. solving

$$I = \text{constant} \quad (2.15)$$

gives a solution of the equation under consideration. The operator $X$ is known as a Noether or variational symmetry of the Lagrangian.

If the equation (2.1) admits a Lagrangian formulation, then Noether's theorem [16] can be used to determine first integrals admitted by (2.1). Bluman [6] and Anco and Bluman [1, 2, 3] introduced the Direct Construction Method to determine conservations laws or first integrals of systems of equations that do not possess a Lagrangian formulation. Kara and Mahomed [14] have investigated the relationship between symmetries and conservation laws. They have determined a formula from which symmetries of conservation laws can be constructed without recourse to a Lagrangian.

Bozkhov and Martins [7] have shown that for $k = 0$ (1.7) admits the generator of Lie point symmetries

$$Z = \partial_x, \qquad X = x\partial_x - 2\partial_y, \quad (2.16)$$

where $\partial_x = \partial/\partial x$, $\partial_y = \partial/\partial y$. For the case $k = 1$ (1.7) admits the generator of Lie point symmetries $X$ and

$$Y = x(\log x - 1)\partial_x - 2\log x\partial_y. \quad (2.17)$$

For values of $k \neq 0, 1$ (1.7) only admits $X$ as a Lie point symmetry. Bozkhov and Martins [7] show that $X$ is in fact a Noether symmetry of (1.7) for $k = 1$. This implies that for $k = 1$ in (1.7) we can use $X$ coupled with Noether's theorem [16] to determine a first integral admitted by (1.7).

# 3 First integrals of a Lane-Emden equation

## 3.1 k=0

We first consider the case $k = 0$. Equation (1.7) reduces to the autonomous

$$y'' + \delta \exp(y) = 0. \tag{3.1}$$

The second-order autonomous ordinary differential equation (3.1) admits the Lagrangian

$$L = y'^2 - 2\delta \exp(y) + f(x), \tag{3.2}$$

where $f(x)$ is a gauge term. A straightforward application of (2.12) shows that $Z$ is a Noether symmetry of (3.2), where

$$B(x, y) = f(x). \tag{3.3}$$

From (2.14) we find that

$$I = y'^2 + 2\delta \exp(y). \tag{3.4}$$

It is easy to check that $D_x I = 0$ on (3.1).

Equation (3.1) admits another Lagrangian

$$L = y'^2 + y' \left(2\delta x \exp(y) + g(y)\right), \tag{3.5}$$

with $Z$ as the corresponding Noether symmetry,

$$B(x, y) = 2\delta \exp(y) \tag{3.6}$$

and (3.4) as the corresponding first-integral.

A solution to (1.7) for $k = 0$ can be obtained by solving

$$I = \text{constant} = c_0, \tag{3.7}$$

for $c_0$ a constant. Substituting (3.4) into (3.7) we obtain

$$y'^2 = c_0 - 2\delta \exp(y). \tag{3.8}$$

Imposing (1.8) we find that

$$y'^2(-1) = y'^2(1). \tag{3.9}$$

This result confirms the symmetry of the boundary conditions at the boundary walls. We can use (3.10) instead of (1.8) to solve (1.7) for $k = 0$ and we will get the same solution. This result allows us to then only consider half of the rectangular geometry. We can thus impose boundary conditions (1.9). Imposing $y'(0) = 0$ we find that (3.8) can be written as

$$y'^2 = 2\delta \left[\exp(y(0)) - \exp(y)\right]. \tag{3.10}$$

Imposing the boundary condition $y(1) = 0$ we find that

$$y'^2(1) = 2\delta \left[\exp(y(0)) - 1\right]. \tag{3.11}$$

In Figure 1 we plot the implicit function (3.11) for $y(0)$ by specifying values of $y'(1)$. From Figure 1 we note that by increasing the magnitude of the temperature gradient at the wall of the rectangular vessel, the temperature at the centre of the vessel increases in an exponential way.

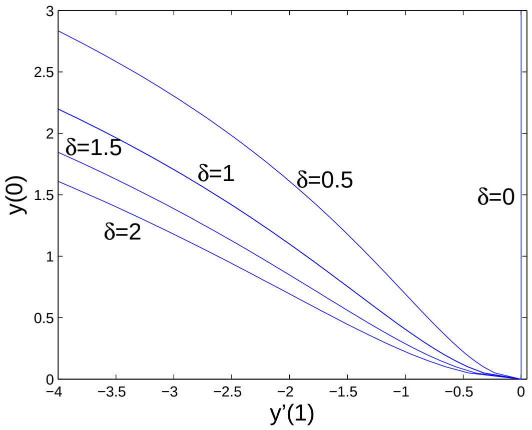


Figure 1: Plot of (3.11) for different values of $\delta$.

### 3.2 k=1

For $k = 1$ Bozkhov and Martins [7] show that $X$ from (2.16) is a Noether (variatonal) symmetry of (1.7). Equation (1.7) admits the Lagrangian

$$L = ax\left(\frac{1}{2}y'^2 - \delta e^y\right) + f(x) \tag{3.12}$$

where $a$ is a constant. Using (2.14) we find the corresponding first integral

$$I = \frac{1}{2}x^2y'^2 + 2xy' + \delta x^2 e^y. \tag{3.13}$$

The approach taken by Chambré [8] is to solve the equation

$$I = c_1, \tag{3.14}$$

where $c_1$ is a constant. Substituting (3.13) into (3.14) and imposing $y'(0) = 0$ we obtain $c_1 = 0$. Imposing $y(1) = 0$ we find that

$$\delta = -\frac{1}{2}y'^2(1) - 2y'(1). \tag{3.15}$$

We plot the expression (3.15) in Figure 2. From (3.15) we find the maximal value of $\delta$ is 2. Hence $y'(1) = -2$. The critical value of $\delta$ was obtained by Frank-Kamenetskii [10] and Chambré [8] after solving (1.7) for $k = 1$. Here we have shown that we can determine this critical value without having to first obtain a solution to the ordinary differential equation .

## 4 Concluding remarks

In this paper we have used Noether's theorem [16] to determine first integrals of the generalised Lane-Emden equation of the second-kind (1.7). For the case $k = 0$, a rectangular

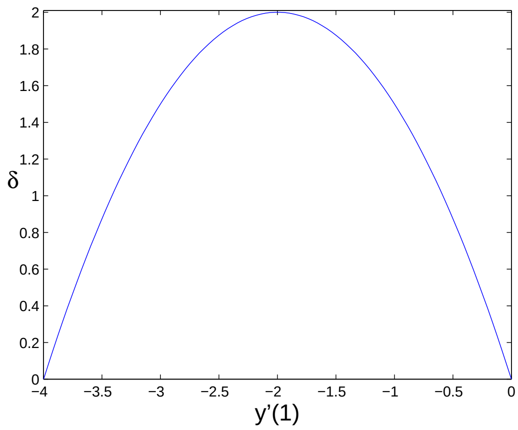


Figure 2: Plot of (3.15).

geometry, we have shown the symmetry of the temperature gradient at the boundary walls. We have also obtained two new boundary conditions that can be use to solve (1.7) for $k = 0$. By using this physical symmetry and imposing the boundary conditions that correspond to the cylindrical geometry case we have shown how the temperature at the centre of the rectangular vessel can be controlled by modifying the temperature gradient at the walls of the rectangular vessel. For the case $k = 1$, a cylindrical geometry, we have shown how the critical value of $\delta = 2$ can easily be obtained without recourse to a solution of the problem. These results have given us both mathematical and physical insights into the problem. Future work involves applying the approach presented here to other boundary value problems.

**Acknowledgments.** *The authors thank Prof A. Qadir for the comments made during the presentation of this work as well as for discussions after the seminar. EM acknowledges support from the National Research Foundation, South Africa, under grant number 2053745.*

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