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ORIGINAL PAPER

A study for the microwave heating of some chemical reactions through Lie symmetries and conservation laws

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Abstract In this paper, we consider an equation describing microwave heating and we find the subclasses of equations which are nonlinearly self-adjoint. From a general theorem on conservation laws proved by Ibragimov we obtain conservation laws for this equation.

Keywords Classical symmetries · Partial differential equation · Conservation laws

1 Introduction

Lie's infinitesimal transformation method is an effective and systematic technique in handling partial differential equations (PDEs). Many phenomena in chemistry, biology, classical mechanics, fluid dynamics, elasticity, and many other applied areas as in the engineering are described by PDEs and the symmetry group techniques provide one method for obtaining solutions of this equations. In [12] is determined an infinite three-dimensional symmetry group of point transformations allowing a similarity reduction from which are obtained solutions of the equation from the electromagnetics from a quasi static perspective:

$$u_{xx} + \tau\, u_{xxt} - \mu^2\, u_t\, e^{-\eta u} = 0, \qquad u = u(x,t), \qquad -\infty < x < \infty$$

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where $u = u(x, t)$ is an unknown time-depending potential function.

The classical method for finding symmetry reductions of partial differential equations is the Lie group method [13,16,17]. The fundamental basis of this method is that, when a differential equation is invariant under a Lie group of transformations, a reduction transformation exists. For PDEs with two independent variables a single group reduction transforms the PDE into an ordinary differential equation (ODE), which in general are easier to solve. Symmetry groups can also be used to obtain, for example, exact solutions and conservation laws of PDEs: [1–4].

The application of Lie groups methods to concrete physical systems involves tedious, mechanical computations. Programmable computer algebra systems such as MATHEMATICA, MACSYMA, MAXIMA, MAPLE and REDUCE, among other, are very powerful in such computations. An excellent survey of the different packages presently available and a discussion of their strengths and applications is given by Hereman [8].

The use of microwave radiation for heating is common in many industrial situations such as cooking, sterilising, melting, smelting, sintering and drying. Microwaves are widely used in chemical industry to accelerate chemical reactions. Some research results have shown that microwave heating can significantly accelerate the reaction. In general, a mathematical analysis of microwave heating requires solving both the heat equation and Maxwell's equations of electromagnetism, which all thermal, electrical and magnetic properties depend on the temperature. In [11] Huang, Lin and Yang presented a numerical model to study the microwave heating on saponification reaction in test tube, where the reactant was considered as a mixture of dilute solution. In [9] Hill and Pincombe considered the one-dimensional microwave heating of the half-space $x \geq 0$ which involves solving a system consisting of the nonlinear heat equation and Maxwell's equations for a linear conducting medium of density ρ being

$$\begin{aligned}
&\rho c(T)\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(K(T)\frac{\partial T}{\partial x}\right) + q(T)|E|^2,\\
&\frac{\partial H}{\partial x} + \frac{\partial}{\partial t}\left[\epsilon(T)E\right] + \sigma(T)E = 0,\\
&\frac{\partial E}{\partial x} + \frac{\partial}{\partial t}\left[\mu(T)H\right] = 0,
\end{aligned}$$

where $T = T(x, y)$ is the temperature, $E = E(x, t)$ the electricity, $H = H(x, t)$ the magnetic fields, $c(T)$, $k(T)$ and $q(T)$ denote the temperature-dependent specific heat, thermal conductivity and body heating coefficient respectively, while $\mu(T)$, $\epsilon(T)$ and $\sigma(T)$ denote the temperature-dependent magnetic permeability, electric permittivity and electrical conductivity of the medium and $|E|^2$ denotes the square of the modulus of the complex electric intensity. The authors attempted to improve the simple model utilised in both Hill and Smyth [10] and Coleman [7] by incorporating a spatial dependence on the heat source. They proved that the model is consistent with that proposed by Coleman [6] in examining the Stefan problem for microwave heating.

The aim of this paper is to make an analysis of the heat equation

$$u_t = [A(u)u_x]_x + E(x,t)C(u) \tag{1}$$

where $u = u(x,t)$ is an unknown function, $A(u) \neq 0$, $E(x,t)$ and $C(u)$ are arbitrary differentiable functions, by using Lie classical symmetries. We determine, for the Eq. (1) the subclasses of equations which are nonlinearly self-adjoint. For these classes of nonlinearly self-adjoint equations we obtain conservation laws.

2 Methodology

To apply the classical method to Eq. (1) we consider the one-parameter Lie group of infinitesimal transformations in (x,t,u) given by

$$\begin{aligned} x^* &= x + \epsilon\xi(x,t,u) + O(\epsilon^2),\\ t^* &= t + \epsilon\tau(x,t,u) + O(\epsilon^2),\\ u^* &= u + \epsilon\eta(x,t,u) + O(\epsilon^2), \end{aligned}$$

where ϵ is the group parameter. We require that this transformation leaves invariant the set of solutions of (1). This yields to an overdetermined, linear system of partial differential equations for the infinitesimals $\xi(x,t,u)$, $\tau(x,t,u)$ and $\eta(x,t,u)$. The associated Lie algebra of infinitesimal symmetries is the set of vector fields of the form

$$\mathbf{v} = \xi(x,t,u)\partial_x + \tau(x,t,u)\partial_t + \eta(x,t,u)\partial_u. \tag{2}$$

Invariance of Eq. (1) under a Lie group of point transformations with infinitesimal generator (2) leads to a set of nine determining equations. Solving this system we obtain $\xi = \xi(x,t)$, $\tau = \tau(t)$ and $\eta = \eta(x,t,u)$ where ξ, τ and η are related by the following conditions:

$$\begin{aligned} &\eta A_u + \tau_t A - 2\xi_x A = 0,\\ &2\eta_x A_u + 2\eta_{ux} A - \xi_{xx} A + \xi_t = 0,\\ &\eta A A_{uu} - \eta\,(A_u)^2 + \eta_u A A_u + \eta_{uu} A^2 = 0,\\ &-\xi ACE_x - \tau ACE_t - \eta AC_u E + \eta A_u CE + \eta_u ACE\\ &\quad -2\xi_x ACE - \eta_{xx} A^2 + \eta_t A = 0. \end{aligned}$$

The solutions of this system depend on the functions A, C and E of Eq. (1). We proceed to give non-trivial Lie symmetries of Eq. (1) for certain values of A and C and the equation must satisfy the function E. We assume the following, k_1, k_2, k_3, k_4, $k \neq 0$, $n \neq 0$ are arbitrary constants, and:

$$\begin{aligned} \mathbf{v}_1 &= \partial_x,\\ \mathbf{v}_2 &= \partial_t,\\ \mathbf{v}_3 &= x\partial_x + 2t\partial_t, \end{aligned}$$

Table 1 Infinitesimal generators of Eq. (1) depending on A and C functions

N	$A(u)$	$C(u)$	Infinitesimal generators
1.	Arbitrary	Arbitrary	$\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$
2.	e^{ku}	$e^{nu}, (n \neq k)$	$\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \mathbf{v}_4$
3.	e^{ku}	e^{ku}	$\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_5, \mathbf{v}_6$
4.	u^k	$u^n, (n \neq k+1)$	$\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \mathbf{v}_7$
5.	u^k	$u^{k+1}, (k \neq -1, -\frac{4}{3})$	$\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_8, \mathbf{v}_9$

Table 2 Equation for function E

N	$E(x,t)$
1.	$(k_1x + k_3)\, E_x + (2k_1t + k_2)\, E_t + 2k_1 E = 0$
2.	$(k_1x + k_3)\, E_x + (2k_1t - kk_4t + k_2)\, E_t + (k_4n + 2k_1 - kk_4)\, E = 0$
3.	$(2kk_1x + 2k_2x + k_3)\, E_x + (3k_2t + k_4)\, E_t + (4k_2 + 4kk_1)\, E = 0$
4.	$(k_1x + k_3)\, E_x + (2k_1t - kk_4t + k_2)\, E_t + (k_4n + 2k_1E - kk_4 - k_4)\, E = 0$
5.	$(2kk_1x + 2(k+1)k_3x + k_4)\, E_x + ((3k+4)k_3t + k_2)\, E_t + (4kk_1 + 4(k+1)k_3)\, E = 0$

$$\begin{aligned}
\mathbf{v}_4 &= t\partial_t - \frac{1}{k}\partial_u,\\
\mathbf{v}_5 &= x\partial_x + \frac{2}{k}\partial_u,\\
\mathbf{v}_6 &= 2x\partial_x + 3t\partial_t + \frac{1}{k}\partial_u,\\
\mathbf{v}_7 &= t\partial_t - \frac{1}{k}u\partial_u,\\
\mathbf{v}_8 &= x\partial_x + \frac{2}{k}u\partial_u,\\
\mathbf{v}_9 &= 2(k+1)x\partial_x + (3k+4)t\partial_t + u\partial_u,
\end{aligned} \tag{3}$$

are infinitesimal generators of Eq. (1) (Tables 1, 2).

3 Symbolic manipulation program

In this section we show how the free software MAXIMA program symmgrp2009.max derived by W. Heremann can be used to calculate the determining equations for Eq. (1). To use symmgrp2009.max, we have to convert (1) into the appropriate MAXIMA syntax: x[1] and x[2] represent the independent variables x and t, respectively, u[1] represents the dependent variable u, u[1, [1, 0]] represents u_x, u[1, [0,1]] represents u_t and u[1, [2, 0]] represents u_{xx}. Hence (1) is rewritten as

$$u[1,[0,1]] - diff(C, u[1]) * u[1,[1,0]]^2 - A * u[1,[2,0]] - E * C = 0$$

The infinitesimals ξ, τ and η are represented by eta1, eta2 and phi1, respectively. The program symmgrp2009.max automatically computes the determining equations for the infinitesimals. The batch file containing the MAXIMA commands to implement the program symmgrp2009.max, which we have called clasico.mac is

```
kill(all);
batchload(``C:\\CLA\\symmgrp2009.max'');
/*classical symmetries Maxwell equation*/
batch(``C:\\clasico.dat'');
symmetry(1,0,0);
printeqn(lode);
save(``lodegnlh.lsp'',lode);
for j thru q do (x[j]:=concat(x,j));
for j thru q do (u[j]:=concat(u,j));
ev(lode)$
gnlhode:ev(%,x1=x,x2=t,u1=u);
grind:true$
stringout(``gnlhode'',gnlhode);
derivabbrev:true;
```

The first lines of this file are standard to symmgrp.max and are explained in [5]. The last lines are provided in order to create a suitable output for solving the determining equations. This changes x[1], x[2] and u[1] to x, t and u, respectively. The file clasica.mac in turn batches the file clasica.dat which contains the required data about (1).

```
p:2$
q:1$
m:1$
parameters:[a,b,c,n,k,s]$
warnings:true$
sublisteqs:[all]$
subst_deriv_of_vi:true$
info_given:true$
highest_derivatives:all$
depends([eta1,eta2,phi1],
depends([A,C],u[1],E,[x[1],x[2]]);
[x[1],x[2],u[1]]);

e1:u[1,[0,1]]-diff(A,u[1])*u[1,[1,0]]^2-A*u[1,[2,0]]-E*C;
v1:u[1,[2,0]];
```

The program symmgrp2009.max automatically computes the determining equations for the infinitesimals.

4 Determination of self-adjointness, nonlinear self-adjointness equations

Definition 1 Consider an sth-order PDE

$$F(x, u, u_{(1)}, \dots, u_{(s)}) = 0 \tag{4}$$

with independent variables $x = (x^1, \dots, x^n)$ and a dependent variable u, where $u_{(1)} = \{u_i\}$, $u_{(2)} = \{u_{ij}\}, \dots$ denote the sets of the partial derivatives of the first, second, etc. orders, $u_i = \partial u/\partial x^i$, $u_{ij} = \partial^2 u/\partial x^i \partial x^j$. The formal Lagrangian is defined as

$$\mathcal{L} = v\,F\left(x, u, u_{(1)}, \ldots, u_{(s)}\right), \tag{5}$$

where $v = v(x, t)$ is a new dependent variable. The adjoint equation to (4) is

$$F^*(x, u, v, u_{(1)}, v_{(1)}, \ldots, u_{(s)}, v_{(s)}) = 0, \tag{6}$$

with

$$F^*(x, u, v, u_{(1)}, v_{(1)}, \ldots, u_{(s)}, v_{(s)}) = \frac{\delta(v\,F)}{\delta u},$$

where

$$\frac{\delta}{\delta u} = \frac{\partial}{\partial u} + \sum_{s=1}^{\infty}(-1)^s D_{i_1} \cdots D_{i_s} \frac{\partial}{\partial u_{i_1 \cdots i_s}}$$

denotes the variational derivatives (the Euler-Lagrange operator). Here

$$D_i = \frac{\partial}{\partial x^i} + u_i \frac{\partial}{\partial u} + u_{ij} \frac{\partial}{\partial u_j} + \ldots$$

are the total derivatives.

Definition 2 Equation (4) is said to be nonlinear self-adjoint if the equation obtained from the adjoint Eq. (6) by the substitution

$$v = h(x, u), \tag{7}$$

such that $h(x, u) \neq 0$,

$$F^*(x, u, u, u_{(1)}, u_{(1)}, \ldots, u_{(s)}, u_{(s)}) = 0$$

is identical with the original Eq. (4), i.e.

$$F^* \left|_{v=h}\right. = \lambda F. \tag{8}$$

If $h = u$ or $h = h(u)$ and $h'(u) \neq 0$, Eq. (4) is said self-adjoint or quasi-self-adjoint, respectively, [15].

In [14] Ibragimov introduced a general theorem on conservation laws. The new theorem does not require existence of a Lagrangian and is based on the concept of an adjoint equation for nonlinear equations.

Given

$$F = u_t - [A(u)u_x]_x - E(x, t)C(u),$$

we obtain

$$F^* \equiv -v\, C_u\, E - v_{x\,x}\, A - v_t. \tag{9}$$

Setting $v = u$,

$$F^* \equiv -u\, C_u\, E - u_{x\,x}\, A - u_t.$$

Comparing F^* with F we obtain the following result:

Proposition 1 *Equation $F \equiv u_t - [A(u)u_x]_x - E(x,t)C(u) = 0$ is not self-adjoint.*

Many equations having remarkable symmetry properties and physical significance are not self-adjoint. Therefore one cannot eliminate the nonlocal variables from conservation laws of these equations by setting $v = u$. Using the concept of nonlinear self-adjoint we get the following result:

Proposition 2 *Equation $F \equiv u_t - [A(u)u_x]_x - E(x,t)C(u) = 0$ is nonlinearly self-adjoint in the following cases:*

- *If $C = c$ and $v = k$, with c and k arbitrary constants.*
- *If $C = a_1 u + a_2$, where $a_1 \neq 0$, a_2 are arbitrary constants, and $v = v(t)$ verifies*

$$v_t + a_1 E v = 0. \tag{10}$$

- *If $A = C_u$ and $v = v(x)$ verifies*

$$v_{xx} + E v = 0. \tag{11}$$

5 Conservation laws

Given a PDE a conservation law is of the form

$$D_t\, \rho + D_x\, J = 0,$$

where ρ is the conserved density, J is the associated flux, $D_x J = \dfrac{\partial J}{\partial x} + \sum_{k=0}^{N} \dfrac{\partial J}{\partial u_{kx}} u_{(k+1)x}$, N is the order of J, and $D_t \rho = \dfrac{\partial \rho}{\partial t} + \sum_{k=0}^{M} \dfrac{\partial \rho}{\partial u_{kx}}\, D_x^k u_t$, with M the order of ρ.

In order to construct conservation laws we use the following theorem on conservation laws proved in [14].

Theorem 1 *Any Lie point, Lie-Bäcklund or non-local symmetry*

$$X = \xi^i(x, u, u_{(1)}, \ldots)\frac{\partial}{\partial x^i} + \eta(x, u, u_{(1)}, \ldots)\frac{\partial}{\partial u} \tag{12}$$

of Eq. (4) provides a conservation law $D_i(C^i) = 0$ for the simultaneous system (4), (6). The conserved vector is given by

$$\begin{aligned} C^i &= \xi^i \mathcal{L} + W\left[\frac{\partial \mathcal{L}}{\partial u_i} - D_j\left(\frac{\partial \mathcal{L}}{\partial u_{ij}}\right) + D_j D_k\left(\frac{\partial \mathcal{L}}{\partial u_{ijk}}\right) - \ldots\right] \\ &\quad + D_j(W)\left[\frac{\partial \mathcal{L}}{\partial u_{ij}} - D_k\left(\frac{\partial \mathcal{L}}{\partial u_{ijk}}\right) + \ldots\right] \\ &\quad + D_j D_k(W)\left[\frac{\partial \mathcal{L}}{\partial u_{ijk}} - \ldots\right] + \ldots, \end{aligned} \tag{13}$$

where W and $\mathcal{L}$ are defined as follows:

$$W = \eta - \xi^j u_j, \quad \mathcal{L} = v\, F\left(x, u, u_{(1)}, \ldots, u_{(s)}\right). \tag{14}$$

Let us apply Theorem 1 to the quasi self-adjoint Eq. (10). We will write generators of point transformation group admitted by Eq. (10) in the form

$$X = \xi^1 \frac{\partial}{\partial t} + \xi^2 \frac{\partial}{\partial x} + \eta \frac{\partial}{\partial u}$$

by setting $t = x^1,\ x = x^2$. The conservation law will be written

$$D_t(C^1) + D_x(C^2) = 0. \tag{15}$$

For C constant function, Eq. (1) is nonlinearly self-adjoint when $v = k$. This equation admits the generator $\mathbf{v}_3 = x\partial_x + 2t\partial_t$.
From generator $\mathbf{v}_3 = x\partial_x + 2t\partial_t$, the normal form for this group is

$$W = -u_x\, x - 2\, t\, u_t.$$

The vector components are

$$\begin{aligned} C^1 &= -2\, t\, v\, C\, E - 2\, t\, (u_x)^2\, v\, A_u - 2\, t\, u_{xx}\, v\, A - u_x\, v\, x, \\ C^2 &= -v\, x\, C\, E + 2\, t\, u_t\, u_x\, v\, A_u - u_x\, v_x\, x\, A - 2\, t\, u_t\, v_x\, A \\ &\quad + u_x\, v\, A + 2\, t\, u_{tx}\, v\, A + u_t\, v\, x. \end{aligned} \tag{16}$$

Setting $v = k$ in (16)

$$\begin{aligned} C^1 &= -2\, k\, t\, C\, E - 2\, k\, t\, (u_x)^2\, A_u - 2\, k\, t\, u_{xx}\, A - k\, u_x\, x, \\ C^2 &= -k\, x\, C\, E + 2\, k\, t\, u_t\, u_x\, A_u + k\, u_x\, A + 2\, k\, t\, u_{tx}\, A + k\, u_t\, x. \end{aligned} \tag{17}$$

Transfering the terms $D_x(\ldots)$ from C^1 to C^2 and simplifying, we obtain the conserved vector $\mathbf{C} = (C^1, C^2)$ with components given by

$$\begin{aligned} C^1 &= k\, u - 2\, k\, t\, C\, E, \\ C^2 &= -k\, x\, C\, E - k\, u_x\, A. \end{aligned}$$

For generators $\mathbf{v_1}$ and $\mathbf{v_2}$ we obtain trivial conservation laws.

6 Conclusions

In this work we have considered an equation describing microwave heating. By using free software Maxima, we have derived the Lie classical symmetries. We have determined the subclasses of this equation which are self-adjoint and nonlinearly self-adjoint. We found a class of nonlinearly self-adjoint of this equation which are not self-adjoint. By using a general theorem on conservation laws proved by Nail Ibragimov we derived conservation laws for some of these PDEs without classical Lagrangians.

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