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New special solutions of the 'Brusselator' reaction model

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Abstract. Using the invariant formalism of the Painlevé analysis, we get the confluent hypergeometric equation from which we derive new special solutions of the 'Brusselator' reaction model. The previously known results are particular cases of the new ones. Other types of solutions are also obtained within the higher-order truncation of this invariant Painlevé analysis.

1. Introduction

The 'Brusselator' model was proposed by Prigogine and Lefever (1968). This biochemical model aimed to describe qualitative behaviour of a reaction scheme, compatible with the laws of thermodynamics and chemical kinetics.

Lefever *et al* (1977) studied the 'Brusselator' model adding spatial diffusion and altering slightly the reaction mechanism. Assuming equal diffusion coefficients for both chemical components, the set of equations they treated is

$$\frac{\partial u}{\partial t} = u^2 w - Bu + K \frac{\partial^2 u}{\partial x^2} \tag{1a}$$

$$\frac{\partial w}{\partial t} = -u^2 w + Bu + K \frac{\partial^2 w}{\partial x^2} \tag{1b}$$

where B is a constant parameter and K is the diffusion coefficient; the quantities $u(x, t)$ and $w(x, t)$ describe the (positive) concentrations. Lefever *et al* (1977) have analysed the steady-state solutions under the boundary condition $u+w =$ constant. The latter assumption has also been made by Vani *et al* (1993) to reduce system (1) to an equation in one dynamical variable only.

Seeking a wave solution, Vani *et al* (1993) have then performed the usual Painlevé analysis for the resulting ordinary differential equation (ODE) and have found a one-parameter family of particular solutions.

Many investigations of system (1) have been carried out by different authors. Recently Larsen (1993) performed the Weiss–Tabor–Carnevale (WTC) Painlevé analysis (Weiss *et al* 1983) and showed that system (1) possesses only the conditional Painlevé property. Using the standard truncation procedure, he has derived one- and two-parameter families of special solutions which can be reduced, after some algebraic manipulations to tanh-like solutions (Ndayirinde 1996a). Note also that the reduction $u + w =$ constant of system (1) is the Kolmogorov–Petrovsky–Piskunov (KPP) equation for which exact solutions have been derived by Cariello and Tabor (1991).

In this paper, we investigate system (1) within the invariant Painlevé formalism introduced by Conte (1989) and derive new special solutions from which Larsen's results

(Larsen 1993) appear as particular cases. An advantage of this invariant analysis is that the expressions for the coefficients of expansion (see equation (10) in the next section) are greatly shortened if compared with the WTC approach (see Larsen 1993). Furthermore, the expansion variable satisfies a Riccati system which allows the possibility of truncating the Laurent series at positive power (Pickering 1993). Hence the class of exact solutions is extended in comparison with the solutions originating from the standard truncated Painlevé expansion.

The present work is organized as follows. In section 2, we use the standard truncation procedure in the invariant formalism to derive new special solutions of (1). In section 3 we perform a higher-order truncation to look for special solutions one is not able to obtain with the standard truncation. Finally, some concluding remarks will be given in section 4.

2. Standard truncation procedure and special solutions

Before proceeding, let us first recall the main ideas of the invariant Painlevé analysis (Conte 1989).

Given a partial differential equation (PDE), algebraic in u and its derivatives

$$E(u, x, t) = 0 \tag{2}$$

around a movable singular manifold

$$\phi - \phi_0 = 0 \tag{3}$$

one looks for a solution as an expansion of the form

$$u = \chi^{-\alpha} \sum_{j=0}^{\infty} u_j \chi^j \tag{4}$$

where the coefficients u_j are invariant under a group of homographic transformations on ϕ. The expansion variable χ, which must vanish as $\phi - \phi_0$ is chosen to be

$$\chi = \frac{\psi}{\psi_x} = \left(\frac{\phi_x}{\phi - \phi_0} - \frac{\phi_{xx}}{2\phi_x} \right)^{-1} \qquad \psi = (\phi - \phi_0)\phi_x^{\frac{1}{2}}. \tag{5}$$

The variable χ satisfies the Riccati equations

$$\chi_x = 1 + \tfrac{1}{2} S \chi^2 \tag{6a}$$

$$\chi_t = -C + C_s \chi - \tfrac{1}{2}(CS + C_{xx})\chi^2 \tag{6b}$$

and the variable ψ satisfies the linear equations

$$\psi_{xx} = -\tfrac{1}{2} S \psi \tag{7a}$$

$$\psi_t = \tfrac{1}{2} C_x \psi - C \psi_x. \tag{7b}$$

The Schwarzian derivative S and the function C, given by

$$S = \{\phi; x\} = \frac{\phi_{xxx}}{\phi_x} - \frac{3}{2} \left(\frac{\phi_{xx}}{\phi_x} \right)^2 \qquad C = -\frac{\phi_t}{\phi_x} \tag{8}$$

respectively, are linked by the cross-derivative condition

$$S_t + C_{xxx} + 2C_x S + C S_x = 0. \tag{9}$$

The truncation procedure in the Painlevé analysis has been shown to be very powerful and systematic in deriving special solutions for nonlinear differential equations (see for instance Cariello and Tabor 1989, Estévez and Gordoa 1990, Pickering 1993, Larsen 1993).

Before applying this procedure to system (1), we may take without loss of generality $K = 1$ through a scaling procedure. Next, looking for solutions of type (4), i.e.

$$u = \chi^{-\alpha} \sum_{j=0}^{\infty} u_j \chi^j \qquad w = \chi^{-\beta} \sum_{j=0}^{\infty} w_j \chi^j \tag{10}$$

the leading-order analysis applied to (1) gives

$$\alpha = \beta = 1 \qquad \text{and} \qquad u_0 = \pm\sqrt{2} \equiv m \qquad w_0 = -u_0. \tag{11}$$

The standard truncation procedure suggests then to look for special solutions of (1) in the form

$$u_T = m\chi^{-1} + u_1 \tag{12a}$$

$$w_T = -m\chi^{-1} + w_1. \tag{12b}$$

Substituting (12) into (1), we get

$$j = 1 \qquad C - mw_1 + 2mu_1 = 0 \tag{13}$$

$$j = 2 \qquad C_x + 2u_1 w_1 - u_1^2 - B + S = 0 \tag{14}$$

$$j = 3 \qquad \tfrac{1}{2}mCS + \tfrac{1}{2}mC_{xx} + u_{1,t} - u_1^2 w_1 + Bu_1 + \tfrac{1}{2}mS_x - u_{1,xx} = 0 \tag{15a}$$

$$-\tfrac{1}{2}mCS - \tfrac{1}{2}mC_{xx} + w_{1,t} + u_1^2 w_1 - Bu_1 - \tfrac{1}{2}mS_x - w_{1,xx} = 0. \tag{15b}$$

The problem is now to solve the system (13)–(15) together with the compatibility condition (9) for u_1, w_1, C, χ and S.

From (13), we immediately get

$$w_1 = \frac{C}{m} + 2u_1 \tag{16}$$

while from (14), using (16), we get

$$-mC_x - 2Cu_1 - 3mu_1^2 + mB - mS = 0. \tag{17}$$

Adding (15a) and (15b), we get, with the aid of (16),

$$3(u_{1,t} - u_{1,xx}) + \frac{1}{m}(C_t - C_{xx}) = 0. \tag{18}$$

Since a derivation of the general solution of the truncation equations (13)–(15) or (16)–(18) together with (9), is a very hard task to do (if not impossible), such systems are usually solved, in literature, by assuming that the invariants S and C are constants (see for instance Cariello and Tabor 1989, Larsen 1993, Pickering 1993). Indeed, when the invariants S and C are constants and given by

$$S = -\tfrac{1}{2}k^2 \qquad C = c \tag{19}$$

(c and k being arbitrary constants), the general solution of the Riccati system (6) is (Hille 1976)

$$\chi^{-1} = \frac{k}{2} \tanh\left(\frac{k}{2}(x - ct + \delta)\right) \tag{20}$$

where δ is an arbitrary constant. The truncated solutions of solitary wave type are thus polynomials in tanh, which relates this approach directly with the tanh method (Malfliet 1992, Malfliet and Hereman 1996). Therefore, special solutions (12) are written in the form

$$u(x,t) \equiv u_T = \pm\sqrt{2}\frac{k}{2} \tanh\left(\frac{k}{2}(x - ct + \delta)\right) + u_1 \tag{21a}$$

$$w(x,t) \equiv w_T = \mp\sqrt{2}\frac{k}{2} \tanh\left(\frac{k}{2}(x - ct + \delta)\right) + w_1 \tag{21b}$$

where u_1, w_1, k, c are determined from (16)–(19).

On the other hand, as one of us has shown recently (Ndayirinde 1996b), the relaxation of such assumptions may lead to other types of solutions of physical interest. We thus proceed to find these solutions and therefore solve system (13)–(15) or equivalently (16)–(18) together with (9) in a more general way.

Guided by the fact that the function C has the dimension of a velocity (indeed C plays the role of the travelling wave speed in solitary wave solutions, see (19) and (20) for instance), we assume it here as a constant but let the invariant S be free. Therefore, the compatibility condition (9) becomes

$$S_t + CS_x = 0. \tag{22}$$

Extracting S from (17), keeping in mind that C is a constant, the relation (22) becomes

$$(u_{1,t} + Cu_{1,x})\left(-\frac{2C}{m} - 6u_1\right) = 0. \tag{23}$$

Two cases are now possible from (23):

(a) First,

$$u_1 = -\frac{C}{3m}. \tag{24}$$

This case implies (see (17)) that both S and C are constant, and consequently the sum $u_1 + w_1$ (see (16)). Therefore, the analysis reduces again to the customary assumption made in the literature as stated above. We recover explicit form (21) where k and c are related, provided system (13)–(15) is compatible, through (17) and (19), by

$$S = B + \frac{C^2}{3m^2} = B + \frac{C^2}{6}. \tag{25}$$

As previously stated (Vani *et al* 1993, Larsen 1993), the sum of the two components $u(x,t)$ and $w(x,t)$ is a constant. Note also that the same results have been derived with the tanh method (Ndayirinde 1996a).

(b) Secondly,

$$u_{1,t} + Cu_{1,x} = 0. \tag{26}$$

The coefficient u_1 is easily determined if one takes into consideration relations (26) and (18) as:

$$u_1 = \alpha + \beta \exp(-Cx + C^2 t) \equiv \alpha + \beta e^{\theta} \tag{27}$$

where α and β are arbitrary constants. Using form (27), we can write the explicit form of S from (17) as:

$$S = B - \frac{2\alpha C}{m} - 3\alpha^2 - \beta\left(\frac{2C}{m} + \alpha B\right) e^{\theta} - 3\beta^2 e^{2\theta}. \tag{28}$$

To know special solutions (12), one needs to determine the explicit form of χ. This is done by solving the linear ODE (7*a*) with S given by (28) and where t acts as a parameter; i.e.

$$\psi_{xx} + \frac{1}{2}\left[B - \frac{2\alpha C}{m} - 3\alpha^2 - \beta\left(\frac{2C}{m} + \alpha B\right) e^{\theta} - 3\beta^2 e^{2\theta}\right]\psi = 0. \tag{29}$$

Performing a change of the independent variable

$$z = e^{\theta} \tag{30}$$

we are able to rewrite equation (29) in the form

$$\psi_{zz}+\left[\frac{1}{C^2}\left(\frac{B}{2}-\frac{\alpha C}{m}-\frac{3\alpha^2}{2}\right)\frac{1}{z^2}-\frac{\beta}{C^2}\left(3\alpha+\frac{C}{m}\right)\frac{1}{z}-\frac{3\beta^2}{2C^2}\right]\psi=0. \tag{31}$$

It may be emphasized here that equation (31) is the confluent hypergeometric equation (Abramowitz and Stegen 1964). As a result, various confluent hypergeometric functions may be obtained by playing with the parameters entering in (31). For instance, if $\alpha\beta\neq 0$, a closer look at the Coulomb wave equation (Abramowitz and Stegun 1964) and equation (31) suggests that if

$$\frac{\beta^2}{C^2}=-\frac{2}{3}\qquad \frac{\beta}{C^2}\left(3\alpha+\frac{C}{m}\right)=2\eta\qquad \frac{1}{C^2}\left(\frac{B}{2}-\frac{\alpha C}{m}-\frac{3\alpha^2}{2}\right)=L(L+1) \tag{32}$$

with $m=\pm\sqrt{2}$ (see (11)), we can write down the general solution of (31) as

$$\psi=AF_L(\eta,z)+DG_L(\eta,z) \tag{33}$$

where A and D are arbitrary constants. The functions F_L and G_L are, respectively, the regular and irregular Coulomb wavefunctions.

Taking into consideration the definition of χ (see (5)), we write down special solutions (12) as

$$u(x,t)=m\frac{AF_L'+DG_L'}{AF_L+DG_L}+\alpha+\beta\mathrm{e}^{\theta} \tag{34a}$$

$$w(x,t)=-m\frac{AF_L'+DG_L'}{AF_L+DG_L}+\frac{C}{m}+2\alpha+2\beta\mathrm{e}^{\theta} \tag{34b}$$

where the functions F_L' and G_L' are respectively the derivatives (with respect to z) of the regular and irregular Coulomb wavefunctions. Note that the Coulomb wavefunctions play an important role in quantum mechanics, precisely in describing the behaviour of a charged particle in a Coulomb potential (Landau and Lifchitz 1967).

3. Higher-order truncation and special solutions

Due to the fact that the expansion variable in the invariant analysis satisfies a system of Riccati equations (see the introduction), one can proceed to higher-order truncation in series (10) to extend the class of exact solutions. In this case, with S and C constant, simple trigonometric identities allow the identification of negative and positive powers of χ (Pickering 1993).

Given any pair of expansion families characterized by (α,u_0) and $(\bar{\alpha},\bar{u}_0)$, (β,w_0) and $(\bar{\beta},\bar{w}_0)$, we may seek, following Pickering's idea (Pickering 1993), a solution of (1) as

$$u_T=\chi^{-\alpha}\sum_{j=0}^{\alpha+\bar{\alpha}}u_j\chi^j \tag{35a}$$

$$w_T=\chi^{-\beta}\sum_{j=0}^{\beta+\bar{\beta}}w_j\chi^j \tag{35b}$$

with the last coefficients given by

$$u_{\alpha+\bar{\alpha}}=(-\tfrac{1}{2}S)^{\bar{\alpha}}\bar{u}_0\qquad w_{\beta+\bar{\beta}}=(-\tfrac{1}{2}S)^{\bar{\beta}}\bar{w}_0. \tag{36}$$

Note that in this higher-order truncation, one must require that $S\neq 0$.

Considering the following identities (Pickering 1993)

$$\pm(\chi^{-1} + \tfrac{1}{2}S\chi) = \mp \mathrm{i}k\,\mathrm{sech}(k(x - ct + F)) \tag{37a}$$

$$\pm(\chi^{-1} - \tfrac{1}{2}S\chi) = \pm k\tanh(k(x - ct + F)) \tag{37b}$$

one may realize that the choice $u_0 = \bar{u}_0$, $w_0 = \bar{w}_0$ leads to the standard truncation results.

Taking into consideration the leading-order analysis (11), different choices of $(u_0, \bar{u}_0)$, and $(w_0, \bar{w}_0)$ are possible. However, the only choice leading to a solution different from the tanh one previously obtained is $(u_0, \bar{u}_0) = (\sqrt{2}, -\sqrt{2})$ and $(w_0, \bar{w}_0) = (-\sqrt{2}, \sqrt{2})$. Indeed, substituting

$$u_T = \sqrt{2}\chi^{-1} + u_1 + \frac{\sqrt{2}}{2}S\chi = \sqrt{2}\left(\chi^{-1} + \frac{1}{2}S\chi\right) + u_1 \tag{38a}$$

$$w_T = -\sqrt{2}\chi^{-1} + w_1 - \frac{\sqrt{2}}{2}S\chi = -\sqrt{2}\left(\chi^{-1} + \frac{1}{2}S\chi\right) + w_1 \tag{38b}$$

into (1) gives

$$j = 1 \qquad \frac{\sqrt{2}}{2}C - w_1 + 2u_1 = 0 \tag{39}$$

$$j = 2 \qquad 2u_1 w_1 - u_1^2 - B - 2S = 0 \tag{40}$$

$$j = 3 \qquad 4u_1 S + Bu_1 - u_1^2 w_1 - 2Sw_1 = 0 \tag{41}$$

$$j = 4 \qquad 2S^2 + u_1^2 S - 2Su_1 w_1 + BS = 0 \tag{42}$$

$$j = 5 \qquad 2u_1 - w_1 - \frac{\sqrt{2}}{2}C = 0. \tag{43}$$

Solving system (39)–(43), we get

$$u_1 = \pm\sqrt{\frac{B}{2}} \qquad C = 0 \qquad w_1 = \pm 2\sqrt{\frac{B}{2}} \qquad S = \frac{B}{4}. \tag{44}$$

Therefore, the solutions to (38) are explicitly written down as

$$u_T = \mp\sqrt{B}\,\mathrm{sech}\left(\pm\sqrt{\frac{B}{2}}x + \delta\right) \pm \sqrt{\frac{B}{2}} \tag{45a}$$

$$w_T = \pm\sqrt{B}\,\mathrm{sech}\left(\pm\sqrt{\frac{B}{2}}x + \delta\right) \pm 2\sqrt{\frac{B}{2}}. \tag{45b}$$

These static solutions could not be obtained neither by Larsen (1993) nor by Vani *et al* (1993) since they used the standard truncation procedure.

4. Concluding remarks

In comparison with the known results from the standard truncation procedure, it is easy to realize that the relaxation of the usual assumption made on the invariants S and C may lead to more general results of physical interest.

Besides the importance of Coulomb wavefunctions in quantum mechanics (Landau and Lifchitz 1967), the connection of the special functions derived from (31) with Bessel functions, whose physical interest has been established recently (Ndayirinde 1996b) testifies their wide application.

It is worth noticing that Vani *et al* (1993) and Larsen's (1993) results are particular cases of those obtained here. Indeed, one can easily show, using additional formulae for circular functions together with the definition of hyperbolic functions, that their results are tanh-like solutions as we have shown here for the S and C constants. We should also emphasize here that the results derived in section 3 could not be obtained with the standard truncation procedure.

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