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INVARIANTS OF KINETIC DIFFERENTIAL EQUATIONS*

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Abstract

Polynomial differential equations showing chaotic behavior are investigated using polynomial invariants of the equations. This tool is more effective than the direct method for proving statements like the one: the Lorenz equation cannot be transformed into an equation which would be a mass action type kinetic model of a chemical reaction.

Keywords: algebraic invariants, polynomial differential equations, chaotic behavior, chemical kinetics, negative cross-effects
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1 Introduction

There is a considerable interest in whether or not real chemical systems can exhibit chaos [2, 18, 19], be it understood in any sense usually used.

As the overwhelming majority of chaotic polynomial differential equations cannot be considered as chemical kinetic models, the question is still open: are realistic models of chemical reactions able to exhibit chaotic behavior? As a contribution to the answer to this question Tóth and Hárs [27] investigated orthogonal transforms of the Lorenz equation and of a model by Rössler. Here we present a more effective method to obtain similar results which is based on the use of algebraic invariants.

Let us suppose we have a complex chemical reaction with a finite number (M) of chemical species $X_1, X_2, ...X_M$ and suppose there are a finite number (R) of reaction steps. The reaction can be displayed as:

$$\sum_{m=1}^{M} \mu(m,r)X_m \xrightarrow{k_r} \sum_{m=1}^{M} \nu(m,r)X_m \qquad (r = 1, 2, \ldots, R) \tag{1}$$

*This paper is in final form and no version of it will be submitted for publication elsewhere.—Dedicated to the memory of K. S. Sibirsky.

The positive real numbers k_r are *the reaction rate coefficients*, and the nonnegative integers $\mu(m,r)$ and $\nu(m,r)$ are *the stoichiometric coefficients.* The usual *mass action type* deterministic model of the reaction above is a polynomial differential equation:

$$\dot{y}_m = \sum_{r=1}^{R} (\nu(m,r) - \mu(m,r)) k_r \prod_{p=1}^{M} y_p^{\mu(p,r)} \qquad (m = 1, 2, \ldots, M), \tag{2}$$

where the dependent variables are the concentrations of species ($y_m := [X_m]$) and the independent variable is the time.

Equation (2) is the *induced kinetic differential equation* of reaction (1). Kinetic differential equations are polynomial differential equations. But not every polynomial differential equation can be considered as being induced by a reaction. Let us consider the Lorenz equation [8]:

$$\begin{aligned} \dot{x} &= -\sigma(x - y) \\ \dot{y} &= rx - y \boxed{-xz} \qquad (\sigma, b, r \in \mathbb{R}^+) \\ \dot{z} &= xy - bz \end{aligned}$$

This equation is not a kinetic one as it contains the term $\boxed{-xz}$. Such a term is said to express *negative cross-effect* as it expresses that y decreases in a process in which it does not take part. (A mathematical definition will be presented in the next section.) This characteristic property of kinetic differential equations has been used to study kinetic gradient systems [24], to design oscillatory reactions [26], to obtain necessary conditions for oscillation [17], or for the Turing instability [22, 23] etc.

Another quite well-known nonkinetic, polynomial differential equation is the Rössler equation [12]:

$$\begin{aligned} \dot{x} &= x - xy - y \\ \dot{y} &= x^2 - ay \qquad (a, b, c, d \in \mathbb{R}^+) \\ \dot{z} &= bx - cz + d \end{aligned}$$

Tóth and Hárs [27] investigated the question whether there exist orthogonal transformations to specific nonkinetic models (e.g. the Lorenz and the Rössler equation) which transform these models into kinetic ones. They had shown by lengthy calculations with the coefficients that no transformation of the form $\mathbf{MA}$ (where $\mathbf{M}$ is an orthogonal and $\mathbf{A}$ is a positive definite diagonal transformation) transforms the Lorenz equation into a kinetic one, and there exists no universal transformation to a similar model by Rössler transforming it to a kinetic equation at all the values of the parameters. This result can be achieved much easier by using algebraic invariants.

Many interesting polynomial differential equations showing other types of exotic behavior, like oscillation (the harmonic oscillator, the Van der Pol oscillator) or pattern formation (Turing's example, [28, p. 42–43]) are also nonkinetic in the sense defined above, and methods have been proposed to eliminate negative cross-effects.

Why would it be useful to transform chaotic equations into kinetic ones and which are the methods to achieve this goal? The answers to the first question are obvious: Having kinetic equations one can construct (at least, formal) chemical reactions with a given type of exotic behavior. Another advantage would be a small contribution to the structural characterization of polynomial differential equations with chaotic behavior. The characterization would reflect behavior under certain transformations: under linear, nonsingular, orthogonal ones.

As an answer to the second question we mention two methods. Samardzija et al. [16] proposed the following transformation. First, the stationary point would be transformed into the first orthant of the state space, and then the jth right hand side would be multiplied by the jth variable. The equation obtained in this way will really become a kinetic equation as it will be a polynomial equation of the Kolmogorov type: $\dot{y}_j = y_j f_j \circ y_j \quad (j = 1, 2, \ldots, M)$. Scott [18, p. 125–126] accepts the transformation proposed by Samardzija et al. as a chemical model for the harmonic oscillator and for the Lorenz equation. Although the qualitative resemblance of the solutions of the two models to each other is quite good in this case, the method in general gives a model which has different eigenvalues of the Jacobian at the equilibrium point. (Contrary to the expectation of Peng et al. [9] who say that 'the transform does not alter the qualitative features of a particular model, thus allowing known dynamical features to be applied to a corresponding chemical system.') To exclude this, an additional condition should be met, which has, by the chance, happened in the special cases investigated in [16]. A criticism from the chemical side has been expressed by Györgyi and Field [4, p. 48], who say that the resulting models contain more autocatalytic steps than found in any known chemical system.

Another method has originally been proposed by Korzukhin, improved by Farkas and Noszticzius [3], and reinvented by Poland [10]. The method relies heavily upon chemical intuition, although the results can be supported by mathematical proofs based upon singular perturbation [29]. The essence is to construct a chemical reaction whose quasi steady state approximation is the given original (nonkinetic) differential equation.

In this paper we apply the theory of algebraic invariants of differential equations [20] to study the effect of transformations. We are looking for polynomial invariants which take on values different from that taken on by any kinetic differential equation. If such an invariant has been found the transformations corresponding to this invariant cannot transform the given equation into a kinetic one. Application of algebraic invariants is an especially powerful method because as *large equations* can be treated by this method as we wish. We will show an example of coupled models with a negative value of such an invariant which can only be nonnegative for coupled kinetic differential equations.

The structure of our paper is as follows. Sec. 2 presents the fundamental definitions and statements connected with algebraic invariants of polynomial differential equations. Sec. 3 applies algebraic invariants to obtain negative results similar to the ones obtained before. In cases where it is not impossible we try to find linear transformations to transform nonkinetic equations into kinetic ones in Example 7. Finally, we discuss the possible directions of further investigations.

2 Algebraic Invariants

Let us consider the following differential equation (we use the upper index to denote the coordinates):

$$\dot{y}^i = a^i + \sum_{j=1}^{n} a^i_j y^j + \sum_{j_1=1}^{n}\sum_{j_2=1}^{n} a^i_{j_1 j_2} y^{j_1} y^{j_2} + \ldots + \sum_{j_1, j_2, \ldots, j_D} a^i_{j_1 j_2 \ldots j_D} y^{j_1} y^{j_2} \ldots y^{j_D}, \quad (3)$$

or to use Einstein's summation convention:

$$\dot{y}^i = \sum_{\omega\in\Omega} a^i_{j_1 j_2 \ldots j_\omega} y^{j_1} y^{j_2} \ldots y^{j_\omega} \ (i, j_1, \ldots, j_\omega = 1, 2, \ldots, n;\ a^i_{j_1 j_2, \ldots, j_\omega} \in \mathbb{R}). \quad (4)$$

where $\Omega := \{0, 1, \ldots, D\}$ with some nonnegative integer D, is the *degree* of the right hand side.

Definition 1 (Negative cross-effect) *Let us rewrite equation (4) in such a way that all the summands are different monomials of the variables, and let us denote the new coefficients by $\bar{a}^i_{j_1 \ldots j_\omega}$. Then, equation (4) is said to contain a* negative cross-effect *if there exists $\bar{a}^i_{\mathbf{j}} < 0$ such that $\neg\exists j_k : j_k = i$.*

Theorem 1 ([5]) *A polynomial differential equation can be considered as the mass action type deterministic model of a chemical reaction if and only if it does not contain terms expressing negative cross-effect.*

Remark 1 *This definition and theorem have been generalized for nonpolynomial equations in [23].*

If $y = (y^1, y^2, \ldots, y^n)$ is the vector of unknown variables of (4) then $\hat{y} := qy$ with $q \in GL(n, \mathbb{R})$ obeys the equation

$$\dot{\hat{y}}^r = \sum_{\omega\in\Omega} b^r_{r_1, \ldots, r_\omega} \hat{y}^{r_1} \ldots \hat{y}^{r_\omega} \ (r, r_1, \ldots, r_\omega = 1, \ldots, n;\ b^r_{r_1, \ldots, r_\omega} \in \mathbb{R}). \quad (5)$$

The relation between the coefficient tensors of equation (4) and (5) can be expressed as

$$b = B(a, q) \quad (6)$$

where B denotes the polynomial function to express b using a and q.

Let $GL(n, \mathbb{R}) := \{q \in \mathbb{R}^{n\times n}; \det(q) \neq 0\}$ be the *general linear group* of linear, invertible transformations, and let $Q \subset GL(n, \mathbb{R})$ be a subgroup with respect to multiplication of transformations.

Definition 2 (Polynomial invariant) *Let us denote the set of all possible coefficients by* $A := \mathbb{R}^n \times \mathbb{R}^{n\times n} \times \cdots \times \mathbb{R}^{n\times\cdots\times n}$ *(where the last product consists of* $D+1$ *factor). The polynomial* $I : A \to \mathbb{R}$ *is said to be a* polynomial invariant *of equation (4) under the group* Q*, if there exists a functional (called* multiplier*)* $\lambda : Q \to \mathbb{R}$ *for which* $I(B(a,q)) = \lambda(q)I(a) \quad (q \in Q,\ a \in A)$ *holds.*

Definition 3 (Absolute/relative invariant) *If* $\lambda(q) = 1$ *for all* $q \in Q$ *then* I *is an* absolute invariant*, otherwise* I *is a* relative invariant.

Definition 4 *We will also use the following groups:*

$$\begin{aligned} \textit{Orthogonal group} \qquad & O(n,\mathbb{R}) = \{q \in \mathbb{R}^{n\times n},\ qq^T = I\} \\ \textit{Special orthogonal group} \qquad & SO(n,\mathbb{R}) = \{q \in \mathbb{R}^{n\times n},\ qq^T = I,\ \det(q) = 1\}. \end{aligned}$$

Remark 2 *In reference to* GL, O *and* SO *we can state the following relationship* $SO \subset O \subset GL$.

Definition 5 (Reducible polynomial invariant) *A polynomial invariant is said to be* reducible *if it is a polynomial of polynomial invariants of lower degree.*

Definition 6 (Generating system) *The set of polynomial invariants* $\mathcal{B}$ *is said to be a* generating system *if all the polynomial invariants of equation (4) under* Q *can be obtained as a polynomial of the elements of the set* $\mathcal{B}$.

Example 1 *Let us consider the following (linear) system*

$$\dot{y}^i = a^i_j y^j \qquad (\Omega = \{1\};\ i,j = 1,2;\ a^i_j \in \mathbb{R}).$$

A generating system of invariants of the system above under $Q = GL$ *is*

$$\begin{aligned} & I_1(a) = a^1_1 + a^2_2 = \mathrm{tr}(a) \\ & I_2(a) = \mathrm{tr}(a^2) \\ & I_3(a) = \mathrm{tr}(a^3) \\ & (I_3 \textit{ is reducible as } \mathrm{tr}(a^3) = \mathrm{tr}(a^2)\mathrm{tr}(a) - \frac{1}{2}\mathrm{tr}(a)(\mathrm{tr}^2(a) - \mathrm{tr}(a^2))) \\ & \textit{and thus } I_3 = I_2 I_1 - \frac{1}{2} I_1(I_1^2 - I_2) \\ & I_4(a) = \ldots \quad (\textit{reducible}) \\ & \vdots \end{aligned}$$

Consequently $\{I_1, I_2\}$ *is a generating system. [20, Thm. 2.6]*
A possibly more familiar generating system is formed from $\{\mathrm{tr}(a), \det(a)\}$ *used to determine the qualitative behavior of the origin.*

Definition 7 (Minimal generating system) *The generating system* $\mathcal{B}$ *is said to be* minimal*, if no elements of it can be discarded without destroying the generating property.*

As no elements of the set $\{I_1, I_2\}$ can be discarded without destroying the generating property, it is a minimal generating system.

Definition 8 (Signature) *The components of the* signature tensor ε *is defined in the following way:*

$$\varepsilon^{p_1 p_2 \dots p_n} = \begin{cases} 1 & \text{if } (p_1, p_2, \dots p_n) \text{ is an even permutation of } (1, 2, \dots n); \\ -1 & \text{if } (p_1, p_2, \dots p_n) \text{ is an odd permutation of } (1, 2, \dots n); \\ 0 & \text{if there are } i, j \in (1, 2, \dots n) \text{ such that } i \neq j \text{ but } p_i = p_j. \end{cases} \tag{7}$$

$\varepsilon^{p_1 p_2 \dots p_n}$ *is not defined if* $p_1, p_2, \dots p_n$ *are not from the first* n *positive integers.*

Definition 9 (Alternation, generalized alternation) *Let us start from the tensor* $(a^{i_1 i_2 \dots i_k}_{j_1 j_2 \dots j_l})$ *and let us multiply it with a signature tensor* $(\varepsilon^{j_2 j_3 \dots j_{n+1}})$ $(n + 1 \leq l)$ *and let us apply Einstein's convention of summing for identical indices to obtain the tensor* $(b^{i_1 i_2 \dots i_l}_{j_1 j_{n+1} j_{n+3} j_l})$ *in the following way:*

$$b^{i_1 i_2 \dots i_l}_{j_1 j_{n+1} j_{n+3} j_l} := a^{i_1 i_2 \dots i_k}_{j_1 j_2 \dots j_l} \varepsilon^{j_2 j_3 \dots j_{n+1}}.$$

Then, tensor b *is obtained by* alternation *from the tensor* a *with respect to the lower indices. One can do the same with upper indices. If lower and upper indices are taken as well, then* b *is obtained by* generalized alternation *from the tensor* a.

Example 2 *By* alternation *we get* $a^i_j \varepsilon^j = a^1_1$ *(here* $n = 1$*), whereas* generalized alternation *gives us* $a^i_j \varepsilon^{ij} = a^1_2 - a^2_1$ *(here* $n = 2$*).*

Definition 10 ((Generalized) complete contraction) *If a tensor has the same number of upper and lower indices, then one can form pairs from upper and lower indices and making them equal, afterwards one can apply Einstein's summation convention for identical indices. This process is said to be a* complete contraction. *If pairs are formed from indices no matter where the indices are, the process is said to be a* generalized complete contraction.

Example 3 *The trace is obtained by complete contraction, as* $\mathrm{tr}(a^i_j) = a^i_i$.

Theorem 2 ([20]) *A base of polynomial invariants of equation (4) under the group* $GL(n, \mathbb{R})$ *(under* $O(n, \mathbb{R})$*) can be obtained by alternation followed by complete contraction (by generalized alternation followed by generalized complete contraction) of the indices of the products of the coefficient tensors.*

Let us consider the equation

$$\dot{y}^j = a^j_\alpha y^\alpha + a^j_{\alpha\beta} y^\alpha y^\beta \qquad (j, \alpha, \beta = 1, 2, \dots, n). \tag{8}$$

This equation is a special case of (4) with the conditions:

$$\Omega = \{1, 2\}, \; (i, j_1, j_2, \dots, j_\omega = 1, 2, \dots, n).$$

A minimal generating system of polynomial invariants *of not more than the second degree* of this equation is:

$I_1^* = a_\alpha^\alpha$	GL	≥ 1
$I_2^* = a_q^p \varepsilon^{pq}$	SO	$= 2$
$I_3^* = a_{\alpha p}^\alpha \varepsilon^p$	GL	$= 1$
$I_4^* = a_\beta^\alpha a_\alpha^\beta$	GL	≥ 2
$I_5^* = a_\beta^\alpha a_\beta^\alpha$	O	≥ 3
$I_6^* = a_q^p a_s^r \varepsilon^{pqrs}$	SO	$= 4$
$I_7^* = a_q^p a_{\alpha r}^\alpha \varepsilon^{pqr}$	SO	$= 3$
$I_8^* = a_q^\alpha a_{\alpha r}^p \varepsilon^{pqr}$	SO	$= 3$
$I_9^* = a_r^p a_{\alpha\alpha}^q \varepsilon^{pqr}$	SO	$= 3$
$I_{10}^* = a_{\alpha\beta}^\alpha a_{\gamma\gamma}^\beta$	O	≥ 3
$I_{11}^* = a_{\alpha\gamma}^\alpha a_{\beta\gamma}^\beta$	O	≥ 2
$I_{12}^* = a_{\beta\beta}^\alpha a_{\gamma\gamma}^\alpha$	O	≥ 2
$I_{13}^* = a_{\beta\gamma}^\alpha a_{\beta\gamma}^\alpha$	O	≥ 2
$I_{14}^* = a_{\beta\gamma}^\alpha a_{\alpha\gamma}^\beta$	O	≥ 2
$I_{15}^* = a_{\alpha p}^\alpha a_{\beta\beta}^q \varepsilon^{pq}$	SO	$= 2$
$I_{16}^* = a_{\alpha q}^p a_{\alpha s}^r \varepsilon^{pqrs}$	SO	$= 4$

The *first column* contains the sign of the invariant and the invariant itself, where ε is the signature tensor defined above. The *second column* shows the sign of the group under which the given invariant is really invariant. The *third column* contains the dimension of the equation which the invariant is related to.

Example 4 *If the dimension of the equation is* not suitable, *I_n^* is not invariant. We will examine part of a concrete model (Boissonade, De Kepper [1]) and I_5^*. The original model is:*

$$\begin{aligned}\dot{x} &= \mu x \boxed{-ky} - \lambda - x^3\\ \dot{y} &= \tau x - \tau y\end{aligned}$$

As I_5^* only depends on the coefficients of first degree we examine only the following modified equation:

$$\begin{aligned}\dot{x} &= \mu x \boxed{-ky}\\ \dot{y} &= \tau x - \tau y\end{aligned} \tag{9}$$

Let us choose a linear orthogonal transformation $q \in O$. If $q = \begin{pmatrix} 1 & -1 \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$, q^{-1} is its inverse matrix and A is the coefficient matrix of the equation (9), then *the new transformed equation is:*

$$\begin{pmatrix}\hat{x}\\ \hat{y}\end{pmatrix}^{\cdot} = q \cdot A \cdot q^{-1} \cdot \begin{pmatrix}\hat{x}\\ \hat{y}\end{pmatrix}.$$

As $I^*_{5orig} = \mu^2 + k^2 + 2\tau^2$ *and* $I^*_{5tr} = 1.5625k^2 - 1.875k\mu + 1.5625\mu^2 - 0.75k\tau - 0.75\mu\tau + 1.25\tau^2$ *and* $\neg\exists\lambda \in \mathbb{R}$ *constant such that* $I^*_{5tr} = \lambda \cdot I^*_{5orig}$, I^*_5 *is* not invariant. *(*I^*_{5orig} *and* I^*_{5tr} *are respectively* I^*_5 *in case of the equation (9) and of the transformed equation.)*

3 Application of Algebraic Invariants

In this section we test in the case of several concrete nonkinetic models with at least two variables whether the negative cross-effect can be transformed out of them. First of all we offer some remarks.

1. Let us start with model (8), and its (orthogonal or nonsingular) transform

$$\dot{\hat{y}}^j = b^j_\alpha \hat{y}^\alpha + b^j_{\alpha\beta}\hat{y}^\alpha\hat{y}^\beta \ (j, \alpha, \beta = 1, 2, \dots, n). \tag{10}$$

2. Orthogonal or regular invariants are looked for which take on different values when calculated from the coefficients of (8) and from those of (10). One can only know the sign of the invariants as we know only the general form of the transformation hence the exact numerical value of the invariants are unknown. Therefore, those invariants are looked for which take on *values of different sign* when calculated from the coefficients of (8) and from those of (10). In this case we can tell that there are no (orthogonal or nonsingular) transformations which transform the negative cross-effect out of the nonkinetic differential equation.

3. In this paper we examine second degree, *at most* 4 variable equations and investigate the polynomial invariants of not more than second degree. (Should the model contain terms of the degree higher than two, it causes no problem as the coefficients of the ith degree terms in the transformed equation only depend on the ith degree terms in the original one. Therefore, these invariants are invariants of equations containing higher degree terms too.)

4. The invariants $I^*_2, I^*_3, I^*_6, I^*_{15}$ and I^*_{16} are *not related to 3 variable* equations, so they cannot be used for equations in 3 variables. If we are interested in 4 variable equations, we might try to use I^*_6 or I^*_{16}. I^*_6 only contains nonnegative coefficients in the case of kinetic differential equations, its sign, however, can be negative or positive as well. I^*_{16} can also be positive or negative.

5. I^*_1 and I^*_{11} are polynomials of coefficients *irrelevant* from the point of view of negative cross-effect (see **Definition 1**), they cannot be used either.

6. The invariants $I_5^*, I_{12}^*, I_{13}^*$ are sums of squares, therefore they are nonnegative for all possible coefficients.

7. The sign of the invariants $I_7^*, I_8^*, I_9^*, I_{10}^*, I_{14}^*$ is not unambiguously defined (even it is known that they are calculated from the coefficients of a kinetic differential equation), that is why they generally cannot be used either.

8. The sign of the absolute invariant I_4^* is *always nonnegative* when calculated from the coefficients of a kinetic differential equation as

$$I_4^* = \sum_{i=1}^{n}(a_i^i)^2 + \sum_{j,k=1 j\neq k}^{n} a_j^k a_k^j,$$

thus I_4^* might be appropriate. But only such equations should be considered in which negative cross-effects are manifested in first degree terms, as I_4^* is a polynomial of linear terms. (Therefore e.g. *the Lorenz equation cannot be investigated by this invariant.*) Nonnegativity of I_4^* however does not imply the absence of negative cross-effect, see e.g. Example 6 and Example 7 below.

Let us consider the following four variable model.

Example 5 ([14])

$$\begin{aligned}
\dot{x} &= \boxed{-y-z} \\
\dot{y} &= x + \frac{1}{4}y + w \\
\dot{z} &= 3 + xz \\
\dot{w} &= \boxed{-\frac{1}{2}z} + \frac{1}{20}w
\end{aligned} \tag{11}$$

$$I_4^* = -\frac{387}{200}$$

I_4^* being negative, the equation cannot be transformed into a kinetic differential equation.

The table below contains the value of I_4^* for a series of models. As it can be seen for some values of the parameters, it can have a negative sign, therefore for these values of the parameters (which form an open set in the parameter space) the models cannot be transformed into kinetic differential equations. (The boxed term(s) here and below show(s) the negative cross-effect.) Nothing can be said about other parts of the parameters space.

No.	Equations	I_4^*	Reference
1	$\begin{aligned} \dot{x} &= \boxed{-y-z} \\ \dot{y} &= x+ay \\ \dot{z} &= b-cz+xz \end{aligned}$	a^2+c^2-2	[18, p. 94],[11, 13]
2	$\begin{aligned} \dot{x} &= x\boxed{-z}-xy \\ \dot{y} &= x^2-ay \\ \dot{z} &= bx-cz+d \end{aligned}$	$1+a^2+c^2-2b$	[6]
3	$\begin{aligned} \dot{x} &= ax\boxed{-y-bz} \\ \dot{y} &= x+1.1 \\ \dot{z} &= c(1-z^2)(x+y)-z \end{aligned}$	$a^2+(c-1)^2-2-2bc$	[6]
4	$\begin{aligned} \dot{x} &= \boxed{-y-z} \\ \dot{y} &= x+ay \\ \dot{z} &= b-cz+xz \end{aligned}$	a^2+c^2-2-2b	[6]
5	$\begin{aligned} \dot{x} &= -ax\boxed{-z}-xy \\ \dot{y} &= \boxed{-x}+by+cz \\ \dot{z} &= b+exz+fx \end{aligned}$	a^2+b^2-2f	[6]
6	$\begin{aligned} \dot{x} &= \boxed{-y-z} \\ \dot{y} &= x \\ \dot{z} &= a(y\boxed{-y^2})-bz \end{aligned}$	b^2-2	[6]
7	$\begin{aligned} \dot{x} &= (z-\beta)x\boxed{-\omega y} \\ \dot{y} &= \omega x+(z-\beta)y \\ \dot{z} &= \lambda+\alpha z+\varepsilon z x^3 \\ & -\tfrac{z^3}{3}\boxed{-(x^2+y^2)(1}+\varrho z) \end{aligned}$	$2\beta^2+\alpha^2-2\omega^2$	[7],[18, p. 244]
8	$\begin{aligned} \dot{x} &= \mu x\boxed{-ky-\lambda}-x^3 \\ \dot{y} &= \tau x-\tau y \end{aligned}$	$\mu^2+\tau^2-2k\tau$	[1]

Let us remark, that models **6** and **7** contain negative cross-effects in second degree terms, too, but the negative cross-effect manifested in the first degree terms are used only.
Finally, let us consider a model obtained by (linear) diffusional coupling from two smaller models.

Example 6 *Adding $\dot{w}=0$ to the model **6** from the table above and then coupling* *this equation and the four variable model of Example 5 gives*

$$\begin{aligned}
\dot{x}_1 &= -y_1 - z_1 + D_{12}^1(x_2 - x_1) \\
\dot{y}_1 &= x_1 + D_{12}^2(y_2 - y_1) \\
\dot{z}_1 &= a(y_1 - y_1^2) - bz_1 + D_{12}^3(z_2 - z_1) \\
\dot{w}_1 &= 0 + D_{12}^4(w_2 - w_1) \\
\dot{x}_2 &= -y_2 - z_2 + D_{21}^1(x_1 - x_2) \\
\dot{y}_2 &= x_2 + \frac{1}{4}y_2 + w_2 + D_{21}^2(y_1 - y_2) \\
\dot{z}_2 &= 3 + x_2 z_2 + D_{21}^3(z_1 - z_2) \\
\dot{w}_2 &= -\frac{1}{2}z_2 + \frac{1}{20}w_2 + D_{21}^4(w_1 - w_2).
\end{aligned}$$

As $I_4^* = -4 + 2\sum_{i=1}^4 D_{12}^i D_{21}^i + \sum_{i=1}^4 (D_{12}^i)^2 + \sum_{i=1}^4 (D_{21}^i)^2 + 2bD_{12}^3 + b^2 + \frac{1}{2}D_{21}^2 + \frac{1}{16} + D_{21}^4 + \frac{1}{4}$, *therefore depending on the value of the diffusion coefficients this expression can be made nonnegative, without affecting terms which express negative cross-effects.*

Remark 3 *Obviously models with a nonnegative value of* I_4^* *coupled with linear diffusion result in a model with a nonnegative value of* I_4^*. *As* I_4^* *only depends on the coefficients of linear terms, nonlinear diffusion could also be allowed.*

Let us consider the following hypothetical model.

Example 7 (2 variable predator-prey system.)

$$\begin{aligned}
\dot{x} &= -ax \boxed{-by} + cxy \\
\dot{y} &= dy \boxed{-ex} - fxy
\end{aligned} \tag{12}$$

Here we find that $I_4^* = a^2 + d^2 + 2be$ which is always nonnegative. *This means that the value of* I_4^* *does not exclude the possibility that (12) can be transformed into a kinetic differential equation. Calculating the eigenvalues of the coefficient matrix of the linear part it turns out that they are both real (one negative, one positive). Therefore, turning to the* Jordan-form *of the linear part we receive a linear part without negative cross-effects. This argument holds for all such linear parts whose eigenvalues are real. (This is not the case if we treat e.g. the model of the harmonic oscillator.) But in each single case we should study the effect of this transformation on the nonlinear terms. In the present case let us introduce the new variables by the definition:* $\begin{pmatrix} \xi \\ \eta \end{pmatrix} := U^{-1} \begin{pmatrix} x \\ y \end{pmatrix}$, *where* U *is the matrix of the eigenvectors of* $\begin{pmatrix} -a & -b \\ -e & d \end{pmatrix}$. *A straightforward calculation shows that negative cross-effects do appear in the second degree terms.*

4 Discussion and perspectives

As a part of a possible structural approach to chaotic and kinetic differential equations we investigated if it was possible to transform out negative cross-effects from chaotic nonkinetic equations. It turned out that the investigations can greatly be simplified by the use of some algebraic invariants. By this more powerful method we have found a new series of nonkinetic models which cannot be transformed into kinetic ones, at least not for an open set in the parameter space. We also think that the use of other invariants may provide similar results for other models, and for other qualitative properties [17], as well.

Another approach to extend the results and methods of [27] would be to automatize the calculations, i.e. to carry out the transformations and the proof of insolvability of the emerging inequalities by a mathematical program package.

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5 Notation

$a, b, c, d, e, f, k, \alpha, \beta, \varepsilon, \mu, \omega, \varrho, \tau$	coefficients in differential equations
$D_{12}^1, D_{12}^2, D_{12}^3, D_{12}^4$	diffusion coefficients in the first coupled system
$D_{21}^1, D_{21}^2, D_{21}^3, D_{21}^4$	diffusion coefficients in the second coupled system
σ, r	coefficients of the Lorenz-equation
$\mu(m, r)$	the stoichiometric coefficient of the m-th chemical species of the reactants in the r-th reaction
$\nu(m, r)$	the stoichiometric coefficient of the m-th chemical species of the products in the r-th reaction
X_m	the m-th chemical species
y_m	the concentration of the m-th chemical species
y^i	the i-th variable of a differential equation
$a^i_{j_1, j_2, \ldots, j_\omega}$	the coefficient of $y^{j_1} y^{j_2} \ldots y^{j_\omega}$ in the i-th equation in a model
GL, O, SO	the general linear, orthogonal, special orthogonal group
Q	a subgroup of GL, O or SO
q	a linear transformation
a, b	coefficient tensors
$a^{i_1 i_2 \ldots i_k}_{j_1 j_2 \ldots j_l}, b^{i_1 i_2 \ldots i_l}_{j_1 j_{n+1} j_{n+3} j_l}$	element of coefficient tensors
$tr(a)$	trace of the tensor a
$\varepsilon^{p_1 p_2 \cdots p_n}$	signature tensor
$\mathcal{B}$	generating system
$I_1, I_2, \ldots$	invariants of an equation
$I_1^*, I_2^*, \ldots$	invariants of the equation $\dot{y}^j = a^j_\alpha y^\alpha + a^j_{\alpha\beta} y^\alpha y^\beta$ $(j, \alpha, \beta = 1, 2, \ldots, n)$

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