ANALYTIC SOLUTIONS TO THE LOTKA-VOLTERRA
MODEL FOR SUSTAINED CHEMICAL OSCILLATIONS†

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ABSTRACT

The Lotka-Volterra (LV) model of oscillating chemical
reactions, characterized by the rate equations
\[
\begin{align*}
\dot{x}_1 &= ax_1 - bx_1x_2 \\
\dot{x}_2 &= -cx_2 + bx_1x_2 
\end{align*}
\]
has been an active area of research since it was originally
posed in the 1920s. In this Review, we present a simple
transformation which reduces the two-dimensional LV
system to a one-dimensional system modeled by a
second-order nonlinear autonomous ordinary differential
equation. The formal analytic solutions to the LV
problem are then derived for the first time. An
introductory analysis of these solutions is given which
leads to the development of an LV-related family of
dynamical systems. Analytic solutions to this family of
differential equations are presented, for certain cases, in
terms of known functions that exhibit oscillatory
behavior. The Hamiltonian nature of both the LV model
and the related family of differential equations is
developed, and future extensions of this treatment are
discussed.

1. INTRODUCTION

In this Review, we present analytic solutions to the
Lotka-Volterra (LV) model for sustained chemical
oscillations. During the analysis of these solutions, a
family of LV-related nonlinear autonomous ordinary
differential equations, all of which can be solved
analytically (some in terms of known functions) are
developed. The Hamiltonian forms of both the LV model
and its related family are explored in order to gain more
insight into the nature of dynamical systems which
possess invariants.

An oscillating chemical system is one in which some
macroscopic feature of the system undergoes periodic
temporal or spatial variations. (The LV system, for
example, exhibits sustained oscillations in time.) In
recent years, an increasing amount of attention has been
paid to oscillating chemical reactions because of the
discovery of oscillatory homogeneous biochemical and
inorganic systems [1,2].

Although much research has been done on the nature
of oscillating systems, such as the study by Prigogine and
co-workers on the thermodynamic and kinetic
requirements for the existence of oscillations [3,4], little
is known analytically about such systems. This lack of
knowledge is a result of the complexity of the differential
models used. Thus, the development of a systematic
technique for the solution of a set of n nonlinear first-
order differential equations could lead to new insights
into the nature of conservative systems which possess
sustained oscillations. Because of the highly nonlinear
nature of the differential equations used to model
chemical oscillators [5,6], much of the current research
has been aimed at analyzing the qualitative behavior of
the rate laws (e.g., [7]). The qualitative properties of
differential equations, including the requirements for a
system to be considered conservative, will be discussed in
more detail in Part 2, and applied throughout the
remainder of this work. In Part 3, reaction schemes used
to model some common chemical oscillators will be described, and the phenomenological rate laws will be developed.

In Part 4, we present a method which allows a two-dimensional nonlinear conservative system, namely the LV model, to be reduced to a one-dimensional system modeled by a second-order nonlinear ordinary differential equation. (The generalization of this method to systems with dimensionality greater than 2 is briefly discussed in Part 6.) The main reasons for the choice of the LV model for our study are that it is the simplest known model of a two-component system which exhibits sustained oscillations, and it has wide applicability in many fields. The analytic solution to the LV model, which is presented in Part 4, has a doubly periodic nature which implies that it represents a new type of elliptic function. An introductory analysis of this function is presented in Part 5 in terms of the analytic solutions to a LV-related family of differential equations. This family, which appears initially to be more complicated than the LV model, is capable in some cases of being solved analytically in terms of known functions, with the solutions representing approximations to the solution of the LV system.

The Hamiltonian form of the LV model is investigated in Part 4, leading to the definition of a new Hamiltonian in a four-dimensional phase space. A brief discussion of the further extension of this Hamiltonian to n-dimensional systems is presented in Part 6. The LV-related family of differential equations is also shown to possess a Hamiltonian, although the function constructed initially to be more complicated than the LV model, is

### 2. DYNAMICAL SYSTEMS

#### A. Qualitative Properties of Dynamical Systems

A dynamical system, by which any homogeneous chemical reaction is modeled [8-10], consists of a set of first-order ordinary differential equations. In this Section, we present a review of the qualitative properties of such systems. (A qualitative property, such as stability, of a dynamical system is one which may be determined without explicitly solving the system.) The mathematical results presented here will be used throughout the remainder of this work.

Consider a system of first-order ordinary differential equations (ODEs) represented by

\[ \dot{x}_i = f_i(t, x_1, ..., x_n), \quad \forall \ i = 1, ..., n, \]  

(2.1)

where \( \dot{x}_i = dx_i/dt \). By allowing \( x_1, ..., x_n \) to be components of a n-dimensional vector \( x \), eq. (2.1) can be written as

\[ \dot{x} = f(t, x), \]  

(2.2)

where \( f(t, x) \) is a vector-valued function. In order to be well defined, eq. (2.2) requires that the function \( f \) be continuous in both the one-dimensional real Euclidean space of the scalar \( t \in \mathbb{R} \) and the n-dimensional real Euclidean space of the vector \( x \in \mathbb{R}^n \). The function \( f \) maps an open subset \( G \) of \( \mathbb{R}^{n+1} \) to \( \mathbb{R}^n \), which can be written symbolically as \( f: G \rightarrow \mathbb{R}^n \) where \( G \subset \mathbb{R}^{n+1} \) [11,12].

A solution to eq. (2.2) is a function \( \Phi(t) \) which is defined on an interval \( I \) of the t-axis \( (I \subset \mathbb{R}) \), such that \( \Phi: I \rightarrow \mathbb{R}^n \) is continuously differentiable and \( \Phi(t) \) satisfies eq. (2.2) [12]. The solution of eq. (2.2) is the curve \( \Gamma \) lying in region \( G \), where each point of the curve has the coordinates \( (t, \Phi(t)) \), and where the tangent to \( \Gamma \) at each point is represented by \( f(t, \Phi(t)) \) [11].

One of the most important conditions that \( f(t, x) \) must satisfy is the Lipschitz condition for continuous differentiability. The condition for a function to be Lipschitz continuous in the neighborhood of a certain point \( p_0 \) is that

\[ \| f(t, x) - f(t, x') \| \leq L \| x - x' \|, \]  

(2.3)

where \( L \) is a constant and \( \| r \| \) is the Euclidean length (norm) of the vector given by

\[ |r| = \left[ \sum_{i=1}^{n} r_i^2 \right]^{1/2}, \]  

(2.4)

and where \( x, x' \) belong to a bounded domain \( D \subset \mathbb{R}^n \) [13,14]. The neighborhood of a point \( p_0 \) defined by the coordinates \( (t_0, x^0) \) in \( \mathbb{R}^{n+1} \) \( \{ p := (t, x) \in \mathbb{R}^{n+1} \} \) is the set of points \( N(t_0, x^0) \) satisfying the conditions that for every \( (t, x), \| t - t_0 \| < \tau \) and \( \| x - x^0 \| < \rho \), where \( \tau \) and \( \rho \) are positive constants. A boundary point of \( G \) is defined as the point \( (t_0, x^0) \) in \( \mathbb{R}^{n+1} \) such that every neighborhood of \( (t_0, x^0) \) contains both points in \( G \) and points outside of \( G \). The set \( G \subset \mathbb{R}^{n+1} \) is open if and only if it contains none of its boundary points, and is closed if it contains all of its boundary points [11].

The requirement of Lipschitz continuity in the neighborhood of the point \( p_0 \) implies that there exists a unique solution to the initial value problem, namely, the problem of finding a solution to eq. (2.2) which satisfies the condition \( \Phi(t_0) = x^0 \) [12-14]. This existence-uniqueness theorem may also be stated as follows: there exists one and only one solution \( x = \Phi(t, p_0) \) of eq. (2.2) which satisfies the initial condition \( \Phi(t_0, p_0) = x^0 \) if \( f(t, x) \) and its first partial derivatives \( \partial f / \partial x \) are continuous in \( G \subset \mathbb{R}^{n+1} \). Thus, each solution \( \Phi(t, p_0) \) exists and is
continuous on some interval $I \subset \mathbb{R}$ containing $t_0$, and every solution is continuous with respect to variations in the values of the initial condition $p_0$ [11,15].

If eq. (2.2) is autonomous, $f$ is not an explicit function of time:

$$\dot{x} = f(x) .$$

(2.5)

This is a special case of eq. (2.2), where the domain of $f$ is some real $n$-dimensional region $(G \subset \mathbb{R}^n)$ instead of an $(n+1)$-dimensional region. Throughout the remainder of this discussion, $f(x)$ and its first partial derivatives will be assumed to be continuous so that the existence-uniqueness theorem discussed above applies. If, for aid of visualization, we assume that eq. (2.5) governs the motion of a physical system, then the components of $x$ may be viewed as the generalized coordinates for the system. This set of coordinates, $\{x_i \mid i = 1, \ldots, n\}$, constitutes the configuration space for the system. The solution curves for this system, referred to as trajectories or orbits, represent the history of the positional variations of the system, since the position $x$ of the system at any given time will lie on one of these trajectories [13]. The trajectory that the position $x$ moves along as time advances is determined by the initial conditions chosen for the system.

The velocity of the point $x$ at any given time along the trajectory is the tangent vector to the point $x$ [i.e., eq. (2.5)]. Thus the solution to eq. (2.5) can be viewed as a point moving along a curve in an $n$-dimensional space with a position dependent velocity given by eq. (2.5). (By convention, the orientation of trajectories is in the direction of increasing time.) A trajectory which passes through the initial point $x^0 \in \mathbb{R}^n$, represents an infinite set of solutions $\{\phi(t+c,x^0) \mid c \in \mathbb{R}\}$ which differ from each other in phase. The invariance of the solutions of autonomous systems to translations of the independent variable $t$ can be shown as follows.

If $\alpha(t) = \phi(t,x^0)$ is a solution to eq. (2.5) on the interval $(a,b)$, then $\beta(t) = \phi(t-c,x^0)$ is a solution on the interval $(a-c,b-c)$, where $c$ is any real constant. Since for every $\tau \in (a,b)$, $\dot{x}(\tau) = \beta(\tau-c)$, $\alpha(\tau)$ and $\beta(\tau)$ define identical trajectories in configuration space [11]. Thus, the solutions of eq. (2.5) are invariant to translations in time.

The solution $\alpha(t) = \phi(t,x^0)$ of eq. (2.5) is periodic with period $T$ if there exists some real finite positive number $T$ such that $\alpha(t+T) = \alpha(t) \forall t \in \mathbb{R}$ (excluding the trivial case of $\alpha(t) =$ constant). A system has periodic solutions if and only if it possesses trajectories which are closed curves [16]. (Let $\gamma$ be a closed curve that solves eq. (2.5) and is defined by $\alpha \forall t \in \mathbb{R}$. Since $\gamma$ is closed, there exists a time $t_1$ and a number $T > 0$ such that $\alpha(t_1) = \alpha(t_1 + T)$.)

A stronger condition for stability is that there exist some $\delta > 0$ such that

$$\|x^0 - x^c\| < \delta \rightarrow \lim_{t \rightarrow \infty} \|\phi(t,x^0) - x^c\| = 0 .$$

A critical point which satisfies this condition for stability is said to be asymptotically stable [13]. A critical point which does not meet any of the criteria for stability is said to be unstable.

To develop a better understanding of stability, let us consider the two-dimensional autonomous system where

$$\dot{x} = f(x) ,$$

$x := (x_1,x_2)$ and $f(x) := (f_1(x), f_2(x))$, and investigate the geometric implications of stability for this system. In a two-dimensional system, the neighborhood of a point is a circle centered about that point with some radius $r > 0$, which will be referred to as the $r$-neighborhood of the point. For a critical point to be stable, there must exist a sufficiently small $\delta$-neighborhood $N(\delta)$ of $x^c$ contained in any $\epsilon$-neighborhood $N(\epsilon)$ of $x^c$ such that every trajectory which passes through $N(\delta)$ at some time $t = t_0$, remains in

![Fig. 1. Example of a trajectory which shows Lyapunov stability.](image)
N(ɛ) for all future times [12,17] (see Fig. 1). The critical point is asymptotically stable if there exists a sufficiently small N(δ) of x such that every trajectory which passes through N(δ) at some time t = t₀ approaches the critical point as t approaches infinity (see Fig. 2). All critical points which are asymptotically stable are also Lyapunov stable; however, the converse is not true. For a critical point to be unstable, a trajectory must exist which passes through N(δ) but does not remain in N(ɛ) (see Fig. 3).

The stability of critical points is important in the analysis of physical systems since, for example, an equilibrium state of a chemical system corresponds to an asymptotically stable critical point. Thus, if a system is perturbed from its equilibrium point by a small amount, the system will return to the equilibrium point in a sufficiently long period of time. This is an example of Le Châtelier’s Principle.

B. Conservative Systems

A conservative system is defined as a system given by eq. (2.5) which possesses at least one first integral on a region R ⊂ G. A first integral is a differentiable function F(x) on R such that for any solution x = φ(t,x₀) ∈ R of eq. (2.5),

\[ F(φ(t,x₀)) = C \equiv \text{constant} , \quad ∀ \ t ∈ I , \quad (2.6) \]

such that x = φ(t,x₀) ∈ R. (The trivial case of F identically constant is excluded.) The integral represented in eq. (2.6) defines a family of (n-1)-dimensional surfaces, referred to as level surfaces, on which each trajectory lies [11]. A trajectory lies on a level surface Lᵢ if that trajectory touches the surface at at least one point. This can be seen by allowing F to be an integral on R ⊂ G and defining the level surface Lᵢ = \{x ∣ F(x) = C\} where C is some constant. Let φ(t,x₀) ∈ R be a solution of eq. (2.5) on the interval I, ∀ t ∈ I. Then for some t₁ ∈ I, φ(t₁,x₀) = x₁ ∈ Lᵢ implies that φ will define a trajectory γ which touches Lᵢ at the point x₁ ∈ R. The condition that x₁ ∈ Lᵢ implies that but since F is an integral of R by hypothesis, the above relationship must hold for all t ∈ I. This allows eq. (2.7) to be written as

\[ F(φ(t₁,x₀)) = F(x₁) = C , \quad (2.7) \]

which implies that F is equal to a constant on every point of the trajectory γ. Thus, every point of γ is an element of Lᵢ, implying that the trajectory must lie completely on the level surface Lᵢ. An integral, therefore, represents a special constraint on the system of equations which reduces the dimensionality of the system by one. (In classical mechanics, general constraints are referred to as holonomic when the variable x represents spatial coordinates [18].) Since for a two-dimensional system (n=2) the level surfaces reduce to trajectories [16], the trajectories of a conservative two-dimensional autonomous system are completely defined by a single integral.

In order to illustrate this, let us consider the two dimensional system

\[ \dot{x}_1 = f₁(x₁, x₂) , \quad \dot{x}_2 = f₂(x₁, x₂) , \quad (2.9) \]

where f₁ and ∂f₁/∂x₂, (i,j = 1,2) are continuous in some region D ⊂ R². Eq. (2.9) implies that

\[ f₂(x₁, x₂) \dot{x}_1 - f₁(x₁, x₂) \dot{x}_2 = 0 , \quad (2.10) \]

which is an exact differential if there exists a function F such that

\[ F(φ(t,x₀)) = C \equiv \text{constant} , \quad ∀ \ t ∈ I , \quad (2.6) \]
\[ \frac{\partial F}{\partial x_1} = \lambda f_2(x_1, x_2), \quad \frac{\partial F}{\partial x_2} = -\lambda f_1(x_1, x_2) \] (2.11)

where \( \lambda \) is a function of \( x_1 \) and \( x_2 \) which insures that

\[ \frac{\partial^2 F}{\partial x_2 \partial x_1} = \frac{\partial^2 F}{\partial x_1 \partial x_2}. \] (2.12)

If an integrating factor \( \lambda \) can be found such that the solution to eq. (2.12) holds for every point \((x_1, x_2) \in \mathbb{D}\), then

\[ F(x_1, x_2) = C, \] (2.13)

where \( C \) is a constant, thus defining a conservative system.

Eq. (2.13) defines a family of curves, with each curve corresponding to a different value of \( C \) as determined by the initial conditions, which fills the \((x_1, x_2)\) plane. Since these curves are the trajectories of eq. (2.9), and since the existence-uniqueness theorem implies that one and only one trajectory passes through every point in the plane, the existence of a first integral for a two-dimensional system enables one to find all of the trajectories which solve the system. In other words, the existence of a first integral, or invariant, reduces the dimensionality of the system by one.

In general, an \( n \)-dimensional system is completely integrable if a set of \( n-1 \) independent integrals for eq. (2.5) can be found [19]. Because of this, the implicit solution of eq. (2.5) is often written as

\[ C_i = F_i(x), \quad \forall \ i = 1, \ldots, n-1. \]

A set of integrals is independent if no integral of the set is derivable from the other integrals of the set or, in other words, if there does not exist a function having the form \( \phi(F_1, \ldots, F_{n-1}) = 0 \), where \( F_i \) are the integrals. The independence of a set of integrals is determined by the existence of a nonzero functional determinant or Jacobian [20],

\[ \frac{\partial (F_1, \ldots, F_{n-1})}{\partial (x_2, \ldots, x_n)} = \begin{vmatrix} \frac{\partial F_1}{\partial x_2} & \cdots & \frac{\partial F_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_{n-1}}{\partial x_2} & \cdots & \frac{\partial F_{n-1}}{\partial x_n} \end{vmatrix} \neq 0. \]

If this condition is satisfied, the variables \( x_i, \forall \ i = 2, \ldots, n \), can be expressed as unique, continuous, differentiable functions of the one independent variable \( x_1 \) [19]:

\[ x_i = \psi_i(x_1), \quad \forall \ i = 2, \ldots, n. \] (2.14)

As a final note, conservative systems cannot possess asymptotically stable singular points [13]. This can be illustrated by defining an invariant \( F \) for eq. (2.9) and letting \( F(x_1', x_2') = C_0 \), where \( C_0 \) is a known constant. The condition for \((x_1', x_2')\) to be an asymptotically stable point is that every trajectory in a sufficiently small neighborhood of the critical point approaches this point as \( t \to -\infty \). But, by hypothesis, \( F \) is an invariant, implying that \( F \) is a constant on every trajectory in the \((x_1, x_2)\) plane. If \( \gamma \) is a trajectory which approaches the point \((x_1', x_2')\) as \( t \to -\infty \), and \( F(x_1, x_2) = C_1 \) along every point of \( \gamma \), then

\[ \lim_{t \to -\infty} F(x_1(x_2)) = F(x_1'(x_2')) = C_1 = C_0. \] (2.15)

Since every trajectory in a sufficiently small neighborhood approaches the point \((x_1', x_2')\) as \( t \to -\infty \), \( F \) attains the value of \( C_0 \) for every trajectory in some small region \( R \) about the point \((x_1', x_2')\). This contradicts the hypothesis that \( F \) is invariant, since the value of \( F \) should change for each trajectory. Although the previous argument is for a two-dimensional system, similar arguments can be applied to systems with higher dimensionality.

The fact that no conservative system can possess an asymptotically stable critical or equilibrium point has many implications for oscillating chemical reactions. The major implication is that oscillating chemical systems occur far from equilibrium. On the other hand, some systems which possess asymptotically stable points in configuration space may possess invariants in the reaction coordinate space, which is a space defined not only by the position but also by the velocity [11]. These systems may be completely specified by a reaction Hamiltonian, which is a conservative integral of the motion. The next Section will discuss the nature of conservative integrals which possess Hamiltonian structure, and how these integrals can be used to determine the phase-space trajectories of a system.

C. The Hamiltonian

Although the Hamiltonian approach to dynamical systems adds nothing new to the physical nature of the problem, it does allow for the development of new and more powerful approaches to working with physical properties of the system which have already been established. The Hamiltonian can be developed either from the properties of work done on a conservative physical system, or from a variational calculus approach applied to Hamilton’s principle [22]. The latter approach will be presented in this Section.

For a \( 2n \)-dimensional dynamical system which can be written in the form
\[ \dot{x} = ay, \quad \dot{y} = g(x,y) \]  

(2.16)

where \( a \) is a proportionality constant, the components of the vector \( x \in \mathbb{R}^n \) are the coordinates of the system, and the components of the vector \( y \in \mathbb{R}^n \) are the momenta of the system. The 2n-dimensional real Euclidean space in which the solution curves to eq. (2.16) lie will be referred to as the phase space of the system, with the n-dimensional spaces in which the solution curves of \( \dot{x} = ay \) and \( \dot{y} = g(x,y) \) lie being referred to as configuration space and momentum space, respectively. For convenience, the proportionality constant \( a \), which in a mechanical system would be related inversely to mass, will be assumed to be one. The velocity of the system represented by eq. (2.16) is \( \ddot{x} \) and the acceleration is \( \dddot{x} \).

 Kinetic energy is the energy that the system possesses as a result of the motion of the system, and is classically defined as

\[ T = \frac{1}{2} \sum_{i=1}^{n} \dot{x}_i^2. \]  

(2.17)

The potential energy \( V \) is the energy that a system possesses as a result of the configuration of the system. (A system which is subject to dissipative forces can have a potential linearly dependent on the velocity; in general, forces in a conservative system are derivable from the negative gradient of the potential energy.)

One immediate result of eq. (2.16) is

\[ \ddot{x} = \ddot{y} = g(x,y) \]  

(2.18)

implying that any 2n-dimensional system having the form of eq. (2.16) can be written as a n-dimensional system of second-order autonomous differential equations. The converse of this argument is also true. In general, a set of \( n \) th order differential equations can be expressed as a set of \( mn \) first-order differential equations [13]. Thus, any second-order differential equation can be viewed as a system which models a fictitious particle with a position and momentum defined by eq. (2.16).

Hamilton’s principle [21] states that out of all possible paths along which a dynamical system may travel from one point to another in a specific amount of time, the actual path followed is the one which minimizes the time integral of the difference between the kinetic and potential energies. Hamilton’s principle can be summarized by stating that the action integral,

\[ I = \int_{t_1}^{t_2} L(x, \dot{x}) \, dt, \]  

(2.19)

where \( L = T - V \), is constant for the actual path of motion. Thus, the variation [22] of eq. (2.19) is

\[ \delta I = \int_{t_1}^{t_2} \delta L(x, \dot{x}) \, dt = 0, \]  

(2.20)

which is a sufficient condition for deriving the equations of motion for a dynamical system having the form of eq. (2.16) [18]. The function \( L(x, \dot{x}) \) is termed the Lagrangian of the system.

The variation of \( I \) is obtained by considering \( I \) as a function of some parameter \( \alpha \) which labels a set of curves \( x_i(t, \alpha) \) such that

\[ x_i(t, \alpha) = x_i(t, 0) + \alpha \eta_i(t), \quad \forall i = 1, \ldots, n, \]  

(2.21)

where \( x_i(t, 0) \) are the solutions to the extremum problem (to be obtained), and \( \eta_i \) are independent functions of \( t \) which vanish at the end points and are continuous up through second derivatives (C2) [18,22]. With the use of eq. (2.21), eq. (2.20) becomes

\[ \frac{\partial I}{\partial \alpha} \, d\alpha = \int_{t_1}^{t_2} \sum_{i=1}^{n} \left( \frac{\partial L}{\partial x_i} \frac{\partial \dot{x}_i}{\partial \alpha} + \frac{\partial L}{\partial \dot{x}_i} \frac{\partial \ddot{x}_i}{\partial \alpha} \right) \, d\alpha \, dt = 0, \]

(2.22)

which can be integrated by parts to give

\[ \frac{\partial I}{\partial \alpha} \, d\alpha = \int_{t_1}^{t_2} \sum_{i=1}^{n} \left( \frac{\partial L}{\partial x_i} \frac{\partial \dot{x}_i}{\partial \alpha} - \frac{\partial x_i}{\partial \alpha} \frac{d \partial L}{\partial \dot{x}_i} \right) \, d\alpha \, dt + \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{x}_i} \frac{\partial \ddot{x}_i}{\partial \alpha} \bigg|_{t_1}^{t_2} = 0. \]

Since all curves pass through the fixed end points, implying

\[ \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{x}_i} \frac{\partial \ddot{x}_i}{\partial \alpha} \bigg|_{t_1}^{t_2} = 0, \]

(2.23)

eq (2.22) reduces to

\[ \frac{\delta I}{\delta \alpha} \, d\alpha = \int_{t_1}^{t_2} \sum_{i=1}^{n} \left( \frac{\partial L}{\partial x_i} - \frac{d \partial L}{\partial \dot{x}_i} \right) \delta x_i \, dt = 0, \]

where
The fundamental lemma from variational calculus [22] states that if
\[ \int_{x^0}^{x^1} M(x) \eta(x) \, dx = 0 \]
for any arbitrary function \( \eta(x) \in C^2 \), then \( M(x) \) must vanish identically in the interval \((x^1), x^2)\). Applying this lemma to eq. (2.23) gives
\[ \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_i} - \frac{\partial L}{\partial x_i} = 0, \quad \forall \ i = 1, \ldots, n. \quad (2.24) \]
This system of equations [eq. (2.24)] is referred to as Lagrange’s equations and is equivalent to the original equations of motion [eq. (2.16)]. Thus, the dynamical system is now defined by a Lagrangian,
\[ L = \frac{1}{2} \sum_{i=1}^{n} \dot{x}_i^2 + V(x) \dot{x}_i, \quad (2.25) \]
which satisfies Lagrange’s equations [eq. (2.24)]. The conjugate momentum is now given by
\[ p_i = \frac{\partial L}{\partial \dot{x}_i} = \dot{x}_i + \frac{\partial V}{\partial \dot{x}_i}, \quad (2.26) \]
which reduces to the form of eq. (2.16) if the system does not have a velocity-dependent potential. The transition from a Lagrangian formulation to a Hamiltonian formulation is mathematically equivalent to a coordinate transformation from \((x, \dot{x})\) to \((x, p)\). This switch in coordinates is accomplished by performing a Legendre transformation on the Lagrangian.

A Legendre transformation, in general, concerns a function \( f \) of two variables \((x, y)\) which has a total differential given by
\[ df = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy = u \, dx + v \, dy. \]
In order to change the coordinates from \((x, y)\) to \((u, v)\), with the differential quantities expressed in terms of \( du \) and \( dv \), a new function \( g \) is defined such that
\[ g = f - u \, x. \]
Direct differentiation of \( g \) gives
\[ dg = df - u \, dx - x \, du, \]
which, upon substituting in the relationship for \( df \), reduces to
\[ dg = v \, dy - x \, du. \]
By direct comparison of the last equation to the total differential of \( g \), the functional form of \( x \) and \( v \) must satisfy the relationships
\[ v = \frac{\partial g}{\partial y} \quad \text{and} \quad x = - \frac{\partial g}{\partial x}. \]
Applying this transformation to eq. (2.25) gives the Hamiltonian as
\[ H(x, y) = \sum_{i=1}^{n} p_i y_i - L(x, \dot{x}) \]
which, if the potential is linear in the velocity, reduces to
\[ H(x, y) = \frac{1}{2} \sum_{i=1}^{n} \left( y_i - \frac{\partial V}{\partial y_i} \right)^2 + V(x, y) \quad (2.27) \]
where
\[ \frac{\partial H}{\partial y_i} = \dot{x}_i \quad \text{and} \quad \frac{\partial H}{\partial x_i} = - \dot{y}_i, \quad \forall \ i = 1, \ldots, n. \quad (2.28) \]
The Hamiltonian, which is the sum of the potential and kinetic energy of a system, represents the total energy. Eq. (2.28) are Hamilton’s equations, which completely define the motion of the system. It is important to note that not all systems of first-order autonomous differential equations can be placed into Hamiltonian form, although all conservative systems should possess a transformation which allows the equations to be placed into a form which solve Hamilton’s equations. If a system can be placed into a form which solves Hamilton’s equations, and if
\[ \frac{\partial^2 H}{\partial x_i \partial y_j} = \frac{\partial^2 H}{\partial y_i \partial x_j}, \quad \forall \ i, j = 1, \ldots, n, \]
where \( i \neq j \), the system possesses a Hamiltonian.

The invariance of the Hamiltonian is easily shown for a system with a velocity-independent potential by a direct time differentiation of eq. (2.27). When the potential is velocity independent, eq. (2.27) reduces to
\[ H(x, y) = \frac{1}{2} \sum_{i=1}^{n} y_i^2 + V(x) = T + V, \quad (2.29) \]
which has the time derivative
\[ \frac{dH}{dt} = y \dot{y} + \frac{dV}{dt} \dot{x}. \quad (3.30) \]
Using eq. (2.26) and Hamilton’s equations [eq. (2.28)], reduces eq. (3.30) to
Since $H$ represents an invariant, similar to the invariants discussed in the previous Section, it defines a family of curves in the phase plane which are the possible trajectories of the particle. The particular trajectory of the particle is determined as soon as the initial position and momentum of the particle are specified.

Although the form of the potential $V(x)$ has not been given, several qualitative properties of the trajectories can be determined from eq. (2.29). Since $H$ is quadratic in $y$ and $y_0 \leq n$, $H(x, y) = H(x, -y)$, which implies that the trajectories will be symmetric with respect to reflection across the $x$-axis. Furthermore, since $T > 0$, the potential must be less than or equal to the total energy of the system, thus confining the trajectories to that region of phase space.

The equilibrium points for a Hamiltonian system [i.e., a system solving eq. (2.28)] are $y = 0$ and $dV/dx = -g(x) = 0$. This implies that the singular points of eq. (2.16), or equivalently eq. (2.28), lie on the $x$-axis and must be at a point where the potential energy is an extremum. If the potential energy attains a maximum at the singular point, the singular point is unstable; if the potential is at a minimum, the singular point will be stable [13,17].

The existence of a Hamiltonian for a given dynamical system can be used to discover the other constants of the motion, since the Poisson bracket of the Hamiltonian with a function $N(x, y)$ is the time derivative of $N$. The Poisson bracket of $H$ with $\Phi$ is defined by

$$\{H, \Phi\} = \sum_{i=1}^{n} \left( \frac{\partial H}{\partial y_i} \frac{\partial \Phi}{\partial x_i} - \frac{\partial H}{\partial x_i} \frac{\partial \Phi}{\partial y_i} \right) \frac{d\Phi}{dt} . \quad (2.31)$$

Later in this Review, a new approach to obtaining Hamiltonians for the Lotka-Volterra model will be presented. Also, the existence of a Hamiltonian structure for a family of nonlinear differential equations related to the Lotka-Volterra model will be shown. The ability to write a Hamiltonian for a dynamical system allows the application of new techniques, such as Hamilton-Jacobi theory [18], in an attempt to develop analytic solutions.

3. THE DYNAMICS OF CHEMICAL SYSTEMS

A. Introduction

The dynamics of chemical systems (i.e., chemical kinetics) is the study of the mechanism and rate of transformation of one set of compounds (the reactants) into another set (the products). As mentioned in Part 2, the rate of reaction of a system is modeled by a set of first-order autonomous differential equations [10], which are referred to as the rate laws. Recall from the previous Section that the variables $x_i \in \mathbb{R}^n, \forall i = 1, \ldots, n$, were taken to be the generalized coordinates of a system modeled by a set of $n$ first-order differential equations, and that the vector $x$ in configuration space completely specified the state of the system at a given time. The generalized coordinates $x_i$ of the dynamical system [eq. (2.5)] can be interpreted as composite variables of the amount of the chemical components in a system and are then referred to as reaction coordinates.

The reaction coordinates for a system are defined chemically as follows. The total mass of a system of $r$ components at any given time can be written

$$m(t) = \sum_{a=1}^{r} m_a(t),$$

where $m_a(t)$ is the mass of the $a$th component at time $t$. The change of the $a$th component can be expressed as

$$dm_a = d_{i}m_a + d_{E}m_a, \quad \forall a = 1, \ldots, r, \quad (3.1)$$

where $d_{i}m_a$ and $d_{E}m_a$ are the (differential) mass changes of the $a$th component resulting from reactions within the system, and from mass transfer with the exterior, respectively. The conservation of mass during a reaction implies that

$$d_{i}m = \sum_{a=1}^{r} d_{i}m_a = 0, \quad (3.2)$$

and, therefore, that

$$dm = d_{E}m = \sum_{a=1}^{r} d_{E}m_a. \quad (3.3)$$

The differential reaction coordinate for a chemical system is defined by

$$dx_i = \frac{1}{v_{ia}} dn_{ia}, \quad (3.4)$$

where $dn_{ia}$ is the change in the number of moles of the $a$th component due to the $i$th reaction, and $v_{ia}$ is the stoichiometric coefficient of the $a$th component in the $i$th reaction [11]. (By convention, the sign of $v_{ia}$ is positive if the component is a product and negative if it is a reactant.) Converting to moles and substituting eqs. (3.2) and (3.4) into eq. (3.1) gives

$$dn_a = \sum_{i=1}^{r} v_{ia} dx_i + d_{E}n_a, \quad \forall a = 1, \ldots, r. \quad (3.5)$$
If \( d_{\beta n_a} = 0 \) for some component \( \beta \), then eq. (3.5) can be integrated to give
\[
n_\beta(t) - n_\beta(0) = \sum_{j=1}^{n} v_{j\beta} \left[ x_j(t) - x_j(0) \right],
\]
which, if the component \( x_j \) only appears in the \( i \)th reaction, reduces to
\[
x_i(t) = \frac{1}{v_{i\beta}} \left[ n_\beta(t) - n_\beta(0) \right] + x_i(0). \tag{3.6}
\]

When the change in volume during the course of the reaction is negligible, this reaction coordinate [eq. (3.6)] can be expressed in terms of the molar concentrations of the components.

Chemical reactions are classified by how eqs. (3.2) and (3.3) are related, the type of mechanism followed, and the order of the system. An open chemical reaction is a reaction where some of the components gain or lose mass by interaction with sources external to the system \( (d_\beta m \neq 0) \). If the mass of some of the components in the reaction is maintained constant via interactions with an external reservoir, while the remaining components undergo mass changes due only to reactions within the system, the reaction is said to be simply open. In this case,
\[
\begin{align*}
dm_a &= d_j m_a, \quad \forall \alpha = 1, \ldots, s < r, \\
d_j m_a &= -d_k m_a, \quad \forall \alpha = s + 1, \ldots, r.
\end{align*}
\]

A system is closed if the total change in mass is zero, implying that the mass of the system is conserved during the course of the reaction. In most kinetic studies, only simply open or closed systems are considered.

The general mechanisms which are used to construct a model for a chemical system are either reversible or irreversible simple chemical reactions, or autocatalytic chemical reactions. A simple chemical reaction is a closed single step reaction having the form
\[
\sum_{\alpha=1}^{r} A_\alpha \frac{k_\alpha}{k_\alpha'} \sum_{\alpha=r+1}^{n} A_\alpha
\]
where \( k_\alpha \) and \( k_\alpha' \) are rate constants, which are independent of the concentrations of the components but dependent on temperature [23]. If \( k_\alpha' = 0 \), the reaction is irreversible; otherwise it is classified as a reversible reaction. The order of a system refers to the highest power to which the concentrations of the components are raised (e.g., a second-order reaction will have at least one quadratic term) in the rate law. When a single-step reaction creates, as a product, one of the reactants, such that the total concentration of that reactant is constant for the reaction, the reaction is said to be autocatalytic. An oscillating chemical system is a complicated system modeled by a combination of simple and autocatalytic reactions with at least one autocatalytic step, since an autocatalytic step is a necessary condition for chemical oscillations to exist [3,4].

The solutions to the rate laws, usually referred to as integrated rate laws, give the concentrations of the chemical components of a system as functions of time, thus allowing for predictions of the amount of a specific compound in the reaction vessel at any given time. Two approaches for obtaining these solutions are the phenomenological approach [10,23] and the Hamiltonian approach [11,24-26], with the latter being a simple mathematical extension of the former. The phenomenological approach to chemical kinetics involves writing the rate law for each reaction in terms of one component for that reaction and solving the resulting system of differential equations. This approach can become complicated even for systems containing a small number of chemical reactions. The Hamiltonian approach develops a set of reaction coordinates and their conjugate momenta, and uses these to write a reaction Hamiltonian for the system. Once a reaction Hamiltonian is defined, powerful solution techniques, such as Hamilton-Jacobi theory, can be applied in order to obtain analytic solutions.

The reaction Hamiltonian for a system can in principle be derived as follows. Let a system of \( n \) chemical reactions possess the set of \( n \) corresponding rate equations
\[
\dot{x} = f(x), \tag{3.8}
\]
where \( x = (x_1, \ldots, x_n) \) and \( f(x) = (f_1(x), \ldots, f_n(x)) \). The second time derivative of eq. (3.8) is
\[
\ddot{z} = \sum_{j=1}^{n} \frac{\partial f}{\partial x_j} \dot{x}_j = \sum_{j=1}^{n} \frac{\partial f}{\partial x_j} f_j(x) = g(x), \tag{3.9}
\]
which, using the same line of reasoning as that presented in Part 2, can be expressed as a set of \( 2n \) first-order differential equations
\[
\dot{z} = f(x), \quad \dot{y} = g(x),
\]
thus defining the reaction coordinates \( x \) and the reaction momenta \( y \) of the system. If the system possesses a potential \( V(x) \) such that
\[
g_i(x) = -\frac{\partial V}{\partial x_i}, \quad \forall i = 1, \ldots, n, \tag{3.10}
\]
then a reaction Hamiltonian, defined by
\[
H(x, y) = \frac{1}{2} \sum_{i=1}^{n} y_i^2 + V(x), \tag{3.11}
\]
exists. The existence of a Hamiltonian guarantees that...
the dynamical behavior of the system will be described by eq. (2.28), and that the solutions to the system will define closed curves in the reaction phase space. The particular phase space trajectory of the system is fixed by the specification of a set of 2n initial conditions. Both the phenomenological and the Hamiltonian approaches to the solution of the rate laws of simple and autocatalytic reactions will be presented in the following sections. The formalism developed will then be used to set up the dynamical equations for the complex systems of some common chemical oscillators.

B. Simple Chemical Reactions

As mentioned in the previous section, a simple chemical reaction is a closed or simply open single-step reaction having the form [eq. (3.7)]

$$\sum_{a=1}^{r} A_{a} \frac{k_{a}}{k_{1}^{'}} \sum_{a=r+1}^{s} A_{a},$$

where the forward reaction is of order r and the reverse reaction is of order s-r. Processes which are modeled by simple chemical reactions include radioactive decay, absorption and emission of electromagnetic radiation, and some formation and degradation reactions.

For an irreversible reaction \(k_{1}^{' = 0}\), the phenomenological rate law is

$$\dot{x} = k_{1} \prod_{a=1}^{r} [n_{a}(0) - x],$$

where \(n_{a}(0)\) is the number of moles of the \(a\)th component at \(t = 0\), and \(x\) is the reaction coordinate as given in eq. (3.6) with \(x(0) = 0\). The integrated rate law is

$$t = \int_{0}^{x} \left[ \prod_{a=1}^{r} [n_{a}(0) - x'] \right]^{-1} dx',$$

(3.13)

the solution of which depends upon the initial concentrations of the components \(n_{a}(0)\) for \(r > 1\). When \(r = 1\), the solution to eq. (3.13) is

$$x(t) = n_{1}(0) \left[ 1 - e^{-k_{1}t} \right],$$

or, equivalently,

$$n_{1}(t) = n_{1}(0) e^{-k_{1}t},$$

which is the familiar equation for first-order exponential decay. If the initial concentrations of all the components in the reaction are equal [i.e., \(n_{a}(0) = n_{a+1}(0) \equiv n(0), \forall a\)]

$$= 1, \ldots, r - 1\), eq. (3.13) can be integrated and solved for \(x\) to give

$$x = n(0) - \left[ n(0)^{1-r} + (1-r) k_{1} t \right]^{1/(1-r)},$$

(3.14)

for all \(r > 1\).

When the reaction is a reversible reaction, the phenomenological rate law is

$$\dot{x} = k_{1} \prod_{a=1}^{r} [n_{a}(0) - x] - k_{1}^{' \prod_{\beta=r+1}^{s} [n_{\beta}(0) + x],}$$

which when written in integral form becomes

$$t = \int_{0}^{x} \left[ k_{1} \prod_{a=1}^{r} [n_{a}(0) - x'] - k_{1}^{' \prod_{\beta=r+1}^{s} [n_{\beta}(0) + x'] \right]^{-1} dx'.$$

(3.15)

Eq. (3.15) can be integrated only in very limited cases, such as the second-order \((r = 2, s = 4)\) case, where the values of \(n_{a} (a = 1,2)\) are equal, and the initial concentrations of \(n_{a} (\beta = 3,4)\) are zero.

The Hamiltonian approach [11,24,25] to the solution of an irreversible reaction modeled by eq. (3.7) when \(k_{1}^{'} = 0\) begins with the reaction rate defined by eq. (3.12) where the reaction coordinate \(x\) is defined by eq. (3.6) without the assumption of \(x(0) = 0\). Eq. (3.10) implies that the second time derivative of eq. (3.12) is equal to the negative gradient of the potential for the system. Thus, the reaction potential is given by [11,24,25]

$$V(x) = -\frac{1}{2} k_{1}^{2} \prod_{a=1}^{r} [x - x(0) - n_{a}(0)]^{2},$$

which implies that the reaction Hamiltonian is

$$H(x,p) = \frac{1}{2} p^{2} - \frac{1}{2} k_{1}^{2} \prod_{a=1}^{r} [x - x(0) - n_{a}(0)]^{2}.$$

(3.17)

The dynamical equations for the chemical reaction are now given by the solution to Hamilton’s equations [eq. 2.28]. The analytic solutions to these equations can be obtained by solving eq. (3.17) using Hamilton-Jacobi theory [18] and, in every instance, agree with those solutions obtained using the phenomenological approach [24,25]. For a reversible reaction [eq. (3.7) with \(k_{1}^{'} \neq 0\), the reaction Hamiltonian has the form of eq. (3.11) with a potential given by [11,24,25]
Although the Hamiltonian formulation of chemical kinetics initially appears more complicated, as the complexity of a chemical system increases, the ability to write a reaction Hamiltonian and to use the solution techniques developed for solving Hamiltonian systems \[18,22\] improves the chance of obtaining analytic solutions to the rate equations.

C. Autocatalytic Reactions \[11,26\]

Consider a chemical system having a fixed number of reactions \( n \) which are coupled via a single intermediate \( X \):

\[
a_{i\alpha}A_{\alpha} + c_i^{(1)}X \rightleftharpoons d_{i\alpha}'A'_{\alpha} + c_i^{(2)}X, \tag{3.18}
\]

for all \( i = 1, \ldots, n \), where the components \( A_\alpha \) and \( A'_{\alpha}, \alpha = 1, \ldots, r \), are maintained constant, and the coefficients \( a_{i\alpha}, d_{i\alpha}' \), and \( c_i^{(j)} (j = 1, 2) \) for the \( i \)th reaction are non-negative integers \[11,26\]. An autocatalytic reaction is a reaction which produces as a product a larger quantity of one of the reactants than is used in the reaction. An autocatalytic scheme is a special case of eq. (3.18), where for at least one of the reactions \( c_i^{(2)} > c_i^{(1)} \).

The phenomenological rate law for the above reaction scheme, if \( k_i' = 0 \), is

\[
\frac{d[X]}{dt} = \sum_{i=1}^{n} \frac{d[X]^{(i)}}{dt}, \tag{3.19}
\]

where

\[
\frac{d[X]^{(i)}}{dt} = \pm k_i [A_{\alpha_0}]^{n_{\alpha_0}} [X]^{c_i^{(0)}}
\]

is the rate of change of the concentration of component \( X \) (denoted by \([X]\)) in the \( i \)th reaction. The sign of eq. (3.20) is positive if \( c_i^{(2)} > c_i^{(1)} \) and negative if \( c_i^{(1)} > c_i^{(2)} \). If the reaction scheme is reversible, eq. (3.20) becomes

\[
\frac{d[X]}{dt} = \pm k_i [A_{\alpha_0}]^{n_{\alpha_0}} [X]^{c_i^{(0)}}
\]

In general eq. (3.19) can only be solved for small \( n \) in terms of known functions.

The development of a reaction Hamiltonian for the chemical system of eq. (3.18) with \( k_i' = 0 \) \[11,26\] begins by defining the reaction coordinate for the system,

\[
x = n_0 + \sum_{i=1}^{n} v_i x_i
\]

where \( n_0 \) is the initial number of moles of component \( X \), \( x_i \) is the reaction coordinate of the \( i \)th reaction [as defined by eq.(3.6)], and \( v_i \) is the stoichiometric coefficient of \( X \) in the \( i \)th reaction \[11,26\]. The reaction Hamiltonian for the chemical system represented by eq. (3.18) when \( k_i' = 0 \) is \[11,26\]

\[
H(x,y) = \frac{1}{2} y^2 + \sum_{i=1}^{n} V'(x) + \sum_{j=1}^{n} V''(x), \tag{3.22}
\]

where the potential \( V'(x) \), given by

\[
V'(x) = -k_i [A_{\alpha}]^{-2} x^{2} x^{c_i^{(0)}},
\]

constitutes the contribution from the \( i \)th reaction, and the potential \( V''(x) \), given by

\[
V''(x) = \pm \left[ 4 V'(x) V'(x) \right]^{1/2},
\]

represents the coupling between the \( i \)th and \( j \)th reactions, with the sign being determined by the particular set of reactions under consideration. Since every possible combination of binary coupling appears in the Hamiltonian, the total number of coupling terms for a set of \( n \) reactions is \[11,26\] \( C^n = n! [2! (n - 2)!] \). Eq. (3.22) can also be used for reversible reactions by realizing that a set of \( n \) reversible reactions can be written as a set of \( 2n \) irreversible reactions \[11,26\]. Once a reaction Hamiltonian is known, the solution techniques employed in Hamiltonian dynamics can be used to analytically solve the dynamical system \[18,21,22\].

D. Oscillating Chemical Reactions

In this Section, a brief introduction to chemical systems which exhibit sustained oscillations is presented.
This introduction will be expanded in Part 4 to a more thorough investigation of one of the models presented below, namely the Lotka-Volterra model. Oscillating chemical reactions are multi-component, multi-step systems which must possess at least one autocatalytic step and have a component which exhibits sustained oscillations in space or time. The autocatalytic step creates a feed-back loop which, in a sequence of chemical reactions, is defined as the inhibition or activation of one step in the reaction by a product of a later step in the reaction.

The simplest reaction scheme which exhibits sustained oscillations in time is the Lotka-Volterra system. This system, originally introduced in 1920 by A. Lotka [27], and later modified by V. Volterra [28] for use in ecology, is modeled by the following set of reactions:

\[
\begin{align*}
A_1 + X_1 &\rightarrow 2X_1 \\
X_1 + X_2 &\rightarrow 2X_2 \\
A_2 + X_2 &\rightarrow A_2 + A_3
\end{align*}
\]

(LV)

We assume here that the concentration of \(A_1\) is held constant by contact with an external reservoir, the concentration of \(A_2\) is constant during the course of the reaction, and \(A_3\) is unreactive. Under these conditions, the dynamics of the system are completely defined by the changes in the concentrations of the two autocatalytic intermediates \(X_1\) and \(X_2\).

The phenomenological rate laws for the LV reaction scheme are

\[
\begin{align*}
\dot{x}_1 &= a x_1 - b x_1 x_2 \\
\dot{x}_2 &= -c x_2 + b x_1 x_2 
\end{align*}
\]  

(3.23)

where, if the volume of the reaction remains constant during the course of the reaction, \(x_i = [X_i] \ (i=1,2), a = k_1, b = k_2, \) and \(c = k_3, [A_{20}]\), with \([A_{i0}]\) symbolizing the initial concentration of the component \(A_i\). Numerical integration of eq. (3.23), which will be considered further in Part 4, shows that the LV model has closed trajectories (see Fig. 4), indicating the existence of periodic solutions. Until recently [29], however, the analytic form of these solutions was unknown. In Part 4, we present the technique used to obtain the analytic solutions to eq. (3.23).

Continued interest in the LV problem is a result of the ease with which it can be modified to model a variety of systems in many different fields. Today, one of the main applications of the Lotka-Volterra system is in modeling the interaction of biological species [30,31], not chemical reactions. However, G. Rabal and co-workers [1] have used the LV scheme, and a modification of this scheme, to model pH regulated oscillating systems which were designed for a continuously stirred tank reactor. The modified reaction scheme which they [1] used is

\[
\begin{align*}
A_1 + A_2 &\rightarrow X_2 \\
A_1 + A_2 + X_1 &\rightarrow A_3 \\
A_1 + X_1 + X_2 &\rightarrow 2X_1 + A_4
\end{align*}
\]

(MLV)

The dynamical equations for this system are

\[
\begin{align*}
\dot{x}_1 &= -a x_1 + b x_1 x_2 \\
\dot{x}_2 &= c - b x_1 x_2 
\end{align*}
\]  

(3.24)

where \(a = k_2 [A_{10}] [A_{20}], b = k_3 [A_{10}]\), and \(c = k_1 [A_{10}] [A_{20}]\). This system, which is similar to Lotka’s 1910 reaction scheme [32], has an unstable critical point at \((c/a, a/b)\) [see Fig. 5], indicating that the intermediates exhibit forced oscillations (i.e., oscillations that increase in amplitude over time).

The next major advance in the study of chemical

![Fig. 4. Solution curves to eq. (3.23) of text showing the closed trajectories indicative of periodic solutions.](image)

![Fig. 5. Solution curves to eq. (3.24) of text indicating growing oscillations.](image)
oscillators was in 1952, when A. M. Turing [33] showed that a chemical reaction coupled with diffusion could exhibit stable spatial patterns. Later, Prigogine and co-workers [34,35] illustrated this phenomenon with the reaction mechanism

$$
A_1 \rightarrow X_1
$$

$$
A_2 + X_1 \rightarrow X_2 + A_3 \quad \text{(BR)}
$$

$$
2X_1 + X_2 \rightarrow 3X_1
$$

$$
X_1 \rightarrow A_4.
$$

This mechanism, and any modifications to this mechanism which possess a 3rd order autocatalytic step, are referred to as the Brusselator [36] (since Prigogine and his associates were working in Brussels at the time). The intermediates $X_1$ and $X_2$ show sustained oscillations in time without including diffusion. If diffusion terms are included, however, spatial patterns also develop. The phenomenological rate laws, if diffusion is not considered and if the concentrations of $A_i$ (i=1,...,4) are constant throughout the course of the reaction, are

$$
\frac{dx_1}{dt} = a - bx_1 + cx_1^2x_2 - dx_1
$$

$$
\frac{dx_2}{dt} = bx_1 - cx_1^2x_2,
$$

where $a = k_1 [A_{10}]$, $b = k_2 [A_{20}]$, $c = k_3$, and $d = k_4$. The solution curves of eq. (3.25) exhibit a stable limit cycle (see Fig. 6). A limit cycle is a closed trajectory in configuration space which has the property that every trajectory sufficiently near the limit cycle approaches this cycle either as $t \to \infty$ (a stable limit cycle) or as $t \to -\infty$ (an unstable limit cycle) [13]. When a stable limit cycle exists, the structure of the oscillation will be stable for small perturbations of the initial values of $x_1$ and $x_2$ [13], implying that the qualitative behavior of the oscillations is less dependent on the initial concentrations of the system.

Until recently [37], the LV reaction scheme and the Brusselator were the only two-component reaction mechanisms known which had intermediates exhibiting sustained oscillations. N. Samardzija and co-workers [37] have developed a method which allows them to transform the Van der Pol [12,13] rate equations,

$$
\frac{dx_1}{dt} = x_2
$$

$$
\frac{dx_2}{dt} = -x_1 + \mu (1 - x_2^2)x_2
$$

where $\mu$ is a positive constant, into phenomenological rate laws which can be modeled by a complex (10 step) reaction scheme with intermediates that show sustained oscillations.

The first reaction known to exhibit both spatial and temporal oscillations is the three-component reaction of the cerium-ion catalyzed oxidation of malonic acid by bromate in a sulfuric acid medium [38,39]. The reaction mechanism proposed by Field, Körös, and Noyes (FKN) for this so-called Belousov-Zhabotinskii reaction [2] consists of two processes, as summarized in Table 1. The first process, process A, is the reduction of bromate ions by bromide ions through a series of oxygen transfers. When the concentration of the bromide level goes below a certain critical concentration, the reaction switches to the second process, process B, which is the oxidation of Ce(III) by the radical BrO$_2^\cdot$ species. This reaction autocatalytically produces bromous acid, which is a component in the first process. The Ce(IV) produced by the oxidation of Ce(III) reacts with one of the products of process A to produce the bromide ion. As the concentration of the bromide ion increases past the critical concentration, the reaction switches back to process A. Thus, the bromide ion can be viewed as a delayed negative feedback component [2,5].

A generalization of the FKN mechanism, generally referred to as the Oregonator, leads to the following reaction scheme [2,5]:

$$
A_1 + X_2 \xrightleftharpoons[k_1']{k_1} X_1
$$

$$
X_1 + X_2 \xrightleftharpoons[k_2']{k_2} X_2 + A_2
$$

$$
A_2 + X_1 \xrightleftharpoons[k_3']{k_3} 2X_1 + X_3
$$

continued on next page
Table 1. FKN [2,5] mechanism for the Belousov-Zhabotinskii reaction.

<table>
<thead>
<tr>
<th>Process A</th>
<th>Process B</th>
<th>Net Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2 \text{H}^+ \rightleftharpoons \text{Br}^- + \text{Br}_2\text{O}_2 + \text{HOBr})</td>
<td>(\text{Br}^- + \text{HBrO}_2 + \text{H}^+ \rightleftharpoons 2 \text{HOBr})</td>
<td>(\text{Br}^- + \text{HOBr} + \text{H}^+ \rightleftharpoons \text{Br}_2 + \text{H}_2\text{O}) \times 3</td>
</tr>
<tr>
<td>(\text{Br}_2 + \text{CH}_2(\text{COOH})_2 \rightleftharpoons \text{BrCH(CHOH)}_2 + \text{Br}^- + \text{H}^+) \times 3</td>
<td>(2 \text{Br}^- + \text{Br}_2\text{O}_2 + 3 \text{CH}_2(\text{COOH})_2 \rightleftharpoons 3 \text{BrCH(CHOH)}_2 + 3 \text{H}_2\text{O})</td>
<td></td>
</tr>
</tbody>
</table>

where \(f\) is a stoichiometric factor [5]. If the rate constants for the reverse reactions are close to zero, and the concentrations of \(A_i, \forall i = 1, \ldots, 4\), are held constant, then the rate laws for the Oregonator can be written

\[
\begin{align*}
\dot{x}_1 &= a x_2 - k_2 x_1 x_2 + b x_1 - 2 k_4 x_1^2 \\
\dot{x}_2 &= -a x_2 - k_2 x_1 x_2 + f k_3 x_3 \\
\dot{x}_3 &= k_3 x_1 - k_3 x_3 ,
\end{align*}
\]

(3.26)

where \(a = k_1 [A_{10}]\) and \(b = k_3 [A_{20}]\). The solutions of eq. (3.26) exhibit stable limit cycle behavior.

Using the law of mass action, N. Samardzija and co-workers [36] have transformed numerous well known multi-dimensional dynamical systems, such as the Rössler rate equations [40], the Lorenz attractor rate equations [41], and the rate equations for the forced Duffing system [42], into phenomenological rate laws which can be used to model large multi-step chemical reaction schemes. The intermediates in these schemes not only show oscillatory behavior but also show chaotic behavior like period-doubling (when the period of the limit cycle successively doubles, causing the system to circulate twice around the cycle before the initial concentrations are restored).

Since the first introduction of chemical reaction schemes which possess rate equations exhibiting sustained oscillations [27], and the discovery of an actual oscillating chemical system [38,39], the theory of oscillating chemical reactions has been an extremely active area of research. Nevertheless, oscillatory phenomena are still not well understood, mainly due to the lack of a sufficiently developed mathematical treatment of the highly nonlinear first-order differential equations which model these systems. In the next Section, a method for obtaining analytic solutions to conservative dynamical systems possessing two degrees of freedom will be developed and applied to the Lotka-Volterra (LV) model.

4. THE LOTKA-VOLterra MODEL

A. Introduction

Since the Lotka-Volterra problem was originally posed in 1920 by Lotka [27], it has been one of the most studied models for a two-dimensional dynamical system exhibiting sustained oscillations. Among the reasons for the popularity of this model are the relative simplicity of the differential equations which characterize the system, and the wide applicability of this system to a variety of different physical, chemical and biological problems.

The chemical reaction scheme originally developed by Lotka [27] is

\[
\begin{align*}
\text{A}_1 + \text{X}_1 &\rightarrow 2 \text{X}_1 \\
\text{X}_1 + \text{X}_2 &\rightarrow 2 \text{X}_2 \\
\text{A}_2 + \text{X}_2 &\rightarrow \text{A}_2 + \text{A}_3 ,
\end{align*}
\]

(LV)

which, when the concentrations of \(A_1, A_2,\) and \(A_3\) are assumed to be constant, leads to the rate equations given by eq. (3.23), namely

\[
\begin{align*}
\dot{x}_1 &= a x_1 - b x_1 x_2 \\
\dot{x}_2 &= -c x_2 + b x_1 x_2 ,
\end{align*}
\]

where \(a, b,\) and \(c\) are as defined in Chapter 3. V. Volterra
[28] later recast this model in terms of the populations of two interacting biological species, where one species preys upon the other. Both Lotka [27] and Volterra [28] generalized the two species model [eq. (3.23)] to an n-dimensional system (GLV) modeled by the rate equations

$$\dot{x}_i = \varepsilon_i x_i + \frac{1}{\beta_i} \sum_{j=1}^{n} \alpha_{ij} x_i x_j ,$$  

(4.1)

for all $i = 1, ..., n$, where $\varepsilon_i$ is the coefficient of increase or decrease of the $i$th species, $\beta$, measures the strength of coupling of the $i$th species to predator-prey interactions, and $\alpha_{ij}$ gauges the interaction between the $i$th and the $j$th species.

The LV and GLV models have been adapted and applied to neural networks [43], epidemiology [44], and mode-specific coupling in lasers [45], as well as being used in population biology [30, 46] and chemical kinetics [1, 47]. Recently, V. Fairen and B. Hernández-Bermejo [48] showed that any set of kinetic equations can be associated to an equivalent GLV representation by the introduction of suitable collective variables. These results have later been expanded for application to general nonlinear systems [49].

Despite the increasing number of LV applications, the analytic solutions to this problem have never been explicitly determined until the present work. Since the original publications [27, 28], the system was known to be conservative, thus implying that the solutions are periodic, but the analytic form of the solutions was unknown. Many different techniques have been applied and developed in the attempt to derive analytic solutions to the LV model. One of the first methods applied when trying to determine the nature of the solutions to an ordinary differential equation is numerical integration, since the numerical integration of an equation generates data which can then be plotted allowing for the visualization of solution curves. The technique of numerical integration will be discussed and applied to the LV model later in this Chapter. Another traditional approach is linearization of the rate equations in order to simplify the system [50]. The linearization of the LV model [51] leads to the rate equations

$$\dot{x}_1 = -c x_2 + \frac{a c}{b}$$
$$\dot{x}_2 = a x_1 - \frac{a c}{b} ,$$

which are the familiar differential equations for the harmonic oscillator, and which have the general solutions [51]

$$x_1(t) = A + B \cos \omega t + C \sin \omega t$$
$$x_2(t) = D + E \cos \omega t + F \sin \omega t ,$$

where $A, B, C, D, E, F$ (not all independent) are determined by the initial conditions, and $\omega$ is determined by $a, b,$ and $c$. Other methods used in order to attempt to determine directly analytic solutions to eq. (3.23) have included decomposition methods [52], iterative solution techniques [53], and perturbation techniques [54, 55]. None of these methods leads directly to analytic solutions to the LV model. Later in this Part, we present a direct method involving a transformation which uses the invariant of the LV system to derive the form of the analytic solutions to eq. (3.23).

Another approach to obtaining analytic solutions to the LV problem is to analyze the invariant, or first integral, of the system, since the existence of a first integral reduces the system to a one-dimensional problem. Since Lotka’s 1920 paper [27], the form of the first integral of eq. (3.23), namely

$$A = b x_1 + b x_2 - c \ln x_1 - a \ln x_2 ,$$  

(4.2)

has been known. Normally when the invariant for a two-dimensional system is known, the invariant can be used to eliminate one of the variables. However, eq. (4.2) cannot be easily solved for either $x_1$ or $x_2$ once given a fixed $A$. The inability to solve eq. (4.2) in a straightforward manner has led to the development of Hamiltonian forms for the LV model. In the 1960s, E. H. Kerner [56] showed that a simple logarithmic transformation of eq. (3.23) allows the LV model to be written in Hamiltonian form with the transformed eq. (4.2) being the Hamiltonian. Kerner then expanded this logarithmic transformation to make it applicable to the GLV system [eq. (4.1)]. Recent interest in the Hamiltonian nature of the LV problem has led to the rediscovery of this transformation for both the two-dimensional and multi-dimensional cases [57-60]. The ability to write a Hamiltonian for the LV model led R. Dutt [61] in the 1970s to apply Hamilton-Jacobi theory to Kerner’s Hamiltonian, but because of the nontraditional form of the Hamiltonian, only approximate solutions to the rate equations could be obtained. In an attempt to develop a traditional Hamiltonian for the LV model, T. Georgian and G. L. Findley [11] transformed the two-dimensional LV system into a four dimensional system involving both the rate equations and the acceleration equations. Later in this Chapter the Hamiltonian nature of the two-dimensional LV model will be discussed in greater detail.

The form of the invariants for the GLV model [eq. (4.1)] has been an important area of research in the past few years. L. Cairó and M. R. Feix [62] used a Carleman embedding method [63] to develop the linear polynomial family of invariants for the GLV model, whereas B. Grammaticos and co-workers [64] used a method based...
on the Frobenius integrability theorem [65] to develop the same invariants for the three-dimensional case. The study done by Grammaticos and co-workers was later clarified by S. Labrunie [66], who derived the conditions which must be satisfied by polynomial first-integrals for the three-dimensional LV system. Another technique used by M. A. Almeida and co-workers [67] to determine the invariants for the GLV model is a Lie symmetry method permitted by M. A. Almeida and co-workers [68]. The Lie symmetry method has been used by M. A. Almeida and co-workers to determine the three-dimensional LV system. Another technique which must be satisfied by polynomial first-integrals for the existence of invariants for the GLV system has been clarified by S. Labrunie [66], who derived the conditions on the Frobenius integrability theorem to develop the analytic solutions for the GLV model.

Although a large amount of research has been done on the conservative nature and Hamiltonian forms of the LV and GLV systems, none of this research has led to analytic solutions for either model until now. In this Part, we present (for background purposes) a simple technique for numerically integrating eq. (3.23). Then, with the use of eq. (4.2), a coordinate transformation is introduced to reduce the LV system to a one-dimensional problem, which can be modeled by a second-order nonlinear ordinary differential equation. This characteristic differential equation is then formally integrated to give the quadrature which represents the analytic solution to the LV problem. Finally, the Hamiltonian nature of the LV model is explored from a novel perspective.

B. Numerical Integration

In the study of nonlinear differential equations, analytic solutions are usually unknown; therefore, one of the first steps in analyzing a nonlinear system is the numerical integration of the differential equations for different initial conditions. Numerical integration generates a set of data which can be plotted, thus allowing visualization of the solution curves which can help to determine the stability of the system (as well as other qualitative properties). Because of the frequency with which this technique is used, many different methods for numerical integration have been developed; all of these techniques can be placed into one of three sub-divisions, however: extrapolation/interpolation, single-step methods, or multi-step methods [71]. In this Section, a brief introduction to these methods will be given, and then a detailed explanation of one type of single-step method, namely the Runge-Kutta method, will be presented and applied to the LV model.

Extrapolation/interpolation methods involve the approximation of an integral of the function $f(t)$ over some interval $(a, b)$ by a summation. In other words [72],

$$\int_{a}^{b} f(t) \, dt = \sum_{i=0}^{n} c_i f(t_i) \, ,$$

where the form of $c_i$ and $t_i$ are determined by the method used, and where $n$ determines the level of approximation. (For example, in the Newton-Cotes (NC) methods $t_i = t_0 + i \, h$, $\forall i = 0, \ldots, n$, with $h = (b-a)/n$, $t_0 = a$ and $t_n = b$ for a closed NC method, and $h = (b-a)/(n+2)$, $t_0 = a+h$, and $t_n = b-h$ for an open NC method.) This method can only be used if the differential equation can be written as a first-order, separable differential equation. (A separable differential equation in this context is a differential equation which can be written in the form $\dot{x} = f(t) \, g(x)$.)

Single-step and multi-step methods use weighted average values of $f(x,t)$ taken at different points in the interval $t_n \leq t \leq t_{n+1}$. This weighted average is defined by [71]

$$x_{n+k} = \sum_{i=1}^{k} \alpha_i x_{n+k-i} + h \sum_{i=1}^{k} \beta_i \dot{x}_{n+k-i} \, ,$$

where $h$ is the step size, or distance between the points along an interval, and $\alpha_i$ and $\beta_i$ are constants $\forall i = 1, \ldots, k$. If $k = 1$, implying that the value of $x$ is dependent on the previous step only, the method is a single-step method. If $k > 1$, the value of $x$ is dependent on several previous steps, and the method is known as multi-step. The technique used for determining the constants $\alpha_i$ and $\beta_i$ separate the different single-step or multi-step methods [71]. Common single-step methods include the Euler, or tangent-line method, and the Runge-Kutta method. Common multi-step methods are the Milne Predictor-Corrector method and the Adams-Moulton methods. The most popular method for numerical integration, because of the accuracy and ease of programming, is the single-step Runge-Kutta method which will now be discussed in more detail.

The single-step Runge-Kutta method involves the general equation [71]

$$x_{n+1} = x_n + \sum_{i=1}^{r} w_i k_i \, ,$$

where $w_i$ is a weighting coefficient to be determined, $r$ is the number of $f(t,x)$ substitutions, and

$$k_i = h \left( t_n + c_i h \, , x_n + \sum_{j=1}^{r} a_{ij} k_j \right) \, , \quad c_1 = 0 \, ,$$

for all $i = 1, \ldots, r$. The determination of the parameters
w, c, and a are done by Taylor series expansion of w in powers of h, such that this expansion agrees with the solution of the differential equations to a specified number of terms in the Taylor series [71]. The number r of terms in the Taylor series defines the order of the Runge-Kutta method. The local truncation error for a general Runge-Kutta method is proportional to h^{r+1}, and the global truncation error for a finite interval is proportional to h^r [51]. Since both the error and the stability of the numerical integration using a Runge-Kutta method are related to the step-size h chosen for the integration [71], J. B. Rosser [73] has developed techniques which allow the step-size to be adjusted during the numerical integration. This modification allows the Runge-Kutta methods to be used for stiff differential equations. (A stiff differential equation is one which has at least one rapidly decaying solution [50,71].)

The most common Runge-Kutta method used for numerical integration is the classic fourth-order Runge-Kutta. This method can be applied to both first-order and second-order differential equations with only slight modifications to the general Runge-Kutta formula. The general fourth-order Runge-Kutta formula for numerical integration of a first order differential equation \( \dot{x} = f(t,x) \) is [74]

\[
x(t+\Delta t) = x(t) + \frac{\Delta t}{6} \left( k_1 + 2k_2 + 2k_3 + k_4 \right),
\]

(4.3)

where

\[
k_1 = h f(t, x) \]
\[
k_2 = h f \left( t + \frac{\Delta t}{2}, x + \frac{\Delta t}{2} k_1 \right) \]
\[
k_3 = h f \left( t + \frac{\Delta t}{2}, x + \frac{\Delta t}{2} k_2 \right) \]
\[
k_4 = h f \left( t + \Delta t, x + \Delta t k_3 \right)
\]

When the differential equation is a second-order differential equation \( \ddot{x} = f(t,x,\dot{x}) \), the numerical integration formula becomes

\[
x(t+\Delta t) = x(t) + \Delta t \left( \dot{x}(t) + \frac{\Delta t}{6} \left( k_1 + 2k_2 + 2k_3 + k_4 \right) \right)
\]

(4.4)

\[
\dot{x}(t+\Delta t) = \dot{x}(t) + \frac{\Delta t}{6} \left( k_1 + 2k_2 + 2k_3 + k_4 \right)
\]

where

\[
k_1 = h f(t, x, \dot{x}) \]
\[
k_2 = h f \left( t + \frac{\Delta t}{2}, x + \frac{\Delta t}{2} \dot{x} + \frac{\Delta t}{8} k_1 \ddot{x} \right) \]
\[
k_3 = h f \left( t + \frac{\Delta t}{2}, x + \frac{\Delta t}{2} \dot{x} + \frac{\Delta t}{8} k_2 \ddot{x} \right) \]
\[
k_4 = h f \left( t + \Delta t, x + \Delta t \dot{x} + \frac{\Delta t}{2} k_3 \ddot{x} \right)
\]

All of the solution curves which are used as figure illustrations in the present work were obtained by numerically integrating the relevant differential equations using one of the two Runge-Kutta methods presented above.

The numerical integration of the LV system can be accomplished in three different ways using a fourth-order Runge-Kutta technique. Each of these methods produces the same numerical results, although the stability of the integration for different initial conditions differs for each method. The first method is the direct numerical integration of eq. (3.23) using eq. (4.3). This method is easily coded as an executable program, or even as a macro in a spreadsheet, making the data easily accessible for analysis. This integration of the rate equations is stable over a wide range of initial conditions. The second method involves the numerical integration of the second time derivatives of eq. (3.23), namely

\[
\ddot{x}_1 = a^2 x_1 - b^2 x_1^2 x_2 + b^2 x_1 x_2^2 + b(c - 2a) x_1 x_2 \\
\ddot{x}_2 = c^2 x_2 + b^2 x_1^2 x_2 - b^2 x_1 x_2^2 + b(a - 2c) x_1 x_2,
\]

(4.5)

using a modification of eq. (4.4). Although this method produces the same numerical results, it is not as stable as the first method, which means that this method cannot be used for extreme initial conditions. The final method numerically integrates the four-dimensional system derived by expressing eq. (4.5) as a system of first-order differential equations. This method proved to be the least stable of the three methods used for numerical integration.

The numerical integration of the LV system [eq. (3.23)] allows for the shape of the solution curves to be visualized. The solution curves for \( x_1 \) and \( x_2 \) are doubly periodic functions, with the solution of \( x_2 \) being slightly out of phase with respect to \( x_1 \) (see Fig. 7). This double periodicity suggests that the solutions to eq. (3.23) are related to the family of elliptic functions [74]. Later in this work, the relationship between the analytic solutions
to the LV problem, which will be derived in the next section, and the elliptic functions will be shown.

C. Analytic Solutions [29]

The numerical integration of the LV problem allows the solution curves to be visualized, but does not give the form of the analytic solution. In this section, a simple coordinate transformation will be presented which reduces the LV system to a one-dimensional problem characterized by a second-order nonlinear autonomous ordinary differential equation. The integral quadrature which represents the solution to this differential equation is then derived.

The development of the analytic solution to eq. (3.23) begins by using the invariant $\Lambda$ [eq. (4.2)] to define new coordinates $z_1(t)$ and $z_2(t)$ such that

$$z_1^2 + z_2^2 = 1.$$  \hspace{1cm} (4.6)

Several different ways of partitioning eq. (4.2) into two new coordinates consistent with eq. (4.6) are possible. We choose to define the new coordinates by placing the linear terms of the invariant into one coordinate, and the nonlinear terms of the invariant into another, to give

$$z_1 = \left(\frac{b}{\Lambda} (x_1 + x_2)\right)^{1/2},$$

$$z_2 = \left(-\frac{1}{\Lambda} (c \ln x_1 + a \ln x_2)\right)^{1/2}.$$  \hspace{1cm} (4.7)

This choice allows for the original coordinates $x_1$ and $x_2$ to be expressed in terms of the new coordinates as

$$x_1 = \frac{\Lambda}{b (a + c)} (c z_1^2 - 2 z_2 \dot{z}_2),$$

$$x_2 = \frac{\Lambda}{b (a + c)} (a z_1^2 + 2 z_2 \dot{z}_2).$$ \hspace{1cm} (4.8)

Because of eq. (4.6), the new coordinates can be written as a single angle $\Phi$ defined by

$$\tan \Phi = z_1/z_2.$$  \hspace{1cm} (4.9)

With $z_1$ and $z_2$ now being defined as

$$z_1 = \sin \Phi, \quad z_2 = \cos \Phi,$$

both eq. (3.23) and the time derivative of eq. (4.2) reduce to the same second-order nonlinear autonomous ordinary differential equation, namely

$$\ddot{\Phi} + \left(\sec \Phi - \tan \Phi - \frac{2 \Lambda}{a + c} \cos \Phi \sin \Phi\right)\dot{\Phi}^2$$

$$+ (c - a) \left(1 - \frac{\Lambda}{a + c} \sin^2 \Phi\right) \dot{\Phi}$$

$$- \frac{1}{2} a c \left(1 - \frac{\Lambda}{a + c}\right) \tan \Phi$$

$$- \frac{1}{2} a c \Lambda \sin \Phi \cos \Phi = 0.$$  \hspace{1cm} (4.10)

Since solving eq. (4.10) is equivalent to solving the rate equations for the LV model [i.e., eq. (3.23)], simplification of eq. (4.10) is in order. By defining a new angle $\Phi = 2 \Phi$, and by using the half-angle formulas [72], eq. (4.10) reduces to

$$\ddot{\Phi} + \left(\cot \Phi - \frac{1}{2} \frac{\Lambda}{a + c} \sin \Phi\right)\dot{\Phi}^2$$

$$+ \frac{1}{2} (c - a) \left[2 - \frac{\Lambda}{a + c} (1 - \cos \Phi)\right] \dot{\Phi}$$

$$+ \frac{1}{2} a c \left[2 - \frac{\Lambda}{a + c} (1 - \cos \Phi)\right]$$

$$\times (\cot \Phi - \csc \Phi) = 0.$$  \hspace{1cm} (4.11)

Eq. (4.11) still cannot be solved formally as yet, but it can be further simplified by defining a new variable $w$ as

$$w = \frac{1}{2} \frac{\Lambda}{a + c} (1 - \cos \Phi),$$  \hspace{1cm} (4.12)

which reduces eq. (4.11) to

$$\ddot{w} - \dot{w}^2 - (c - a) (w - 1) \dot{w}$$

$$+ a c w (w - 1) = 0.$$  \hspace{1cm} (4.13)

Transforming eq. (4.8) to the new variable gives the values of the original coordinates $x_1$ and $x_2$ as

$$x_1 = \frac{1}{b} (c w + \dot{w}), \quad x_2 = \frac{1}{b} (a w - \dot{w}).$$  \hspace{1cm} (4.14)

Eq. (4.13) can be formally integrated using a symbolic
Fig. 8. Numerical solution of eq. (4.13) of text showing the doubly periodic nature of the formal solution, namely eq. (4.15) of text.

processor [75] for the special case of $a = c$ to give the analytic solution (via quadrature)

$$t - t_0 = \pm \int_0^w \left[ \frac{dw'}{a^2 w'^2 + w_0 e^{2w'}} \right]^{1/2} , \quad (4.15)$$

where $t_0$ and $w_0$ are dependent on initial data. Eq. (4.15) represents a new function. Numerical analysis of eq. (4.13) using eq. (4.3) shows that the implicit function $w$ is doubly periodic (see Fig. 8), indicating a relationship to the Jacobian elliptic functions [74]. This relationship will be explored further in the next Part.

When $c \neq a$, the solution of eq. (4.13) is more problematic, but straightforward. The first step in solving eq. (4.13) is the rearrangement of the invariant [eq. (4.2)] to yield

$$b x_1 x_2 = - \frac{k^2}{b} x_1^{1-a} e^{b(x_1 x_2)/a}, \quad (4.16)$$

where $\alpha = c/a$ and $k^2 = - b^2 e^{2\alpha \alpha}$. Substituting eq. (4.16) into the rate equations [eq. (3.23)] gives

$$\dot{x}_1 = a x_1 + \frac{k^2}{b} x_1^{1-a} e^{b(x_1 x_2)/a} \quad (4.17)$$

$$\dot{x}_2 = - a x_2 - \frac{k^2}{b} x_1^{1-a} e^{b(x_1 x_2)/a},$$

which, upon using the transformation given by eq. (4.14), allows eq. (4.13) to be written as

$$\begin{align*}
0 &= \alpha a \left[ \frac{b}{a} (a + 1) w - b \alpha a \phi \right] \\
&\quad + \frac{k^2}{b} \left( \frac{\alpha a}{b} \right)^{-a} e^{(a + 1) \nu} e^{-b \phi} = 0 . \quad (4.20)
\end{align*}$$

When $\alpha = 1$ ($a = c$), eq. (4.19) reduces to eq. (4.15), with $w_0 = k^2$.

Even though eq. (4.18) cannot be integrated in terms of known elementary functions, it does represent the analytic solution to the LV problem, since substitution of the values of $w$ and $\dot{w}$ obtained from a numerical integration of eq. (4.18) into eq. (4.14) generates the same solutions as a direct numerical integration of eq. (3.23). An introductory analysis of eq. (4.18) using a power series expansion will be presented in the next Part in the context of generating analytical solutions to a LV-related family of differential equations.

D. Hamiltonians

As mentioned in Section 4.A, a great deal of interest has been expressed in the Hamiltonian form of the LV model, mainly because of the powerful solution techniques which can be applied if a Hamiltonian exists. Although the analytic solution to the LV model was derived in the last Section without using a Hamiltonian technique, in this Section we will review different approaches to developing Hamiltonians for the LV problem, since Hamiltonian methods are important when considering the symmetry of the system.

In the 1960s, while studying the dynamical aspects of chemical kinetics, E. H. Kerner [56] showed that the LV model could be placed into Hamiltonian form using a simple logarithmic transformation. This transformation defined the position $q$ and the momentum $p$ as [56]

$$q = \ln x_2 , \quad p = \ln x_1 ,$$

which allowed the rate equations to be written as

$$\dot{q} = - \left( b e^p - a \right) , \quad \dot{p} = b e^p - c .$$

The invariant for the transformed system is the Hamiltonian and is defined by [56]

$$H = b e^q + b e^p - c p - a q , \quad (4.21)$$

which by direct differentiation with respect to $q$ and $p$ yields Hamilton’s equations. This Hamiltonian, however, because of its nontraditional nature, cannot be solved using Hamilton-Jacobi theory or any of the other advanced solution techniques that Hamiltonian dynamics allows. (A traditional Hamiltonian is defined by an invariant having the form of eq. (2.27).)

In an attempt to develop a more traditional
Hamiltonian, T. Georgian and G. L. Findley defined a possible reaction Hamiltonian as [11]
\[ H = \frac{1}{2} (y_1^2 + y_2^2) - \frac{1}{2} (a^2 x_1^2 + c^2 x_2^2 + b^2 x_1^2 x_2^2) - b \xi x_1 x_2, \]  
(4.22)
where \( y_i = \dot{x}_i \) and
\[ \xi = -b x_1^2 + (c - 2a) x_1 \]
\[ = -b x_2^2 + (a - 2c) x_2, \]
(4.23)
which comes from assuming that \( M_i = M_i/\xi \) for \( i = 1, 2 \). Eq. (4.23) was proposed initially as a holonomic constraint [11]. However, the Hamiltonian represented by eq. (4.22) is not constant because the condition implied by eq. (4.23) does not hold for any arbitrary trajectory (although it does hold for the critical point). This approach does allow, however, for modifications in terms of a coordinate transformation and an integrating factor.

We begin the modification of eq. (4.22) by defining new coordinates \( q_1 \) and \( q_2 \) such that
\[ q_1 = \ln x_1, \quad q_2 = \ln x_2, \]
(4.24)
which transform the rate equations [eq. (3.23)] to
\[ \dot{q}_1 = -(b e^{\xi_1} - a), \quad \dot{q}_2 = b e^{\xi_1} - c. \]
(4.25)
This transformation is similar to the transformation which Kerner applied [56], except that both of the original coordinates are kept as position coordinates. The Hamiltonian for the system can now be defined by
\[ H = \frac{\mu}{2} (p_1^2 + p_2^2) + V(q_1, q_2), \]
(4.26)
where the form of the conjugate momenta \( p_i \) will be discussed below, \( \mu = \mu(p_1, p_2) \) is an integrating factor which will also be discussed below, and \( V \) is a potential which solves
\[ dV = V_{q_1} dq_1 + V_{q_2} dq_2 = -\xi (\dot{q}_1 dq_1 + \dot{q}_2 dq_2) = 0 \]
(4.27)
with \( \dot{q}_i \) being the accelerations and \( \xi = \xi(q_1, q_2) \). The acceleration equations, derived by taking the second time derivative of eq. (4.25), are
\[ \ddot{q}_1 = -b e^{\xi_1} (b e^{\xi_1} - c), \dot{q}_2 = -b e^{\xi_1} (b e^{\xi_2} - a). \]
(4.28)
In order for eq. (4.27) to be satisfied and for \( dV \) to be an exact differential, the second derivatives of the potential must commute. In other words,
\[ \partial_2 (\xi \dot{q}_1) = \partial_1 (\xi \dot{q}_2), \]
(4.29)
which gives the characteristic partial differential equation in terms of \( \xi \) as
\[ \xi_{12} \ddot{q}_1 - \xi_{11} \ddot{q}_2 = \xi \left[ b e^{\xi_1} (b e^{\xi_1} - c) - b e^{\xi_2} (b e^{\xi_2} - a) \right]. \]
(4.30)
The solution of eq. (4.30) for \( \xi \), which defines the potential since
\[ V = b e^{\xi_1} \int \xi (b e^{\xi_1} - c) dq_1 + b e^{\xi_1} \int \xi (b e^{\xi_2} - a) dq_2 \]
\[ - \int \partial_1 \left[ \xi b e^{\xi_2} (b e^{\xi_2} - a) \right] dq_1 dq_2, \]
(4.31)
begins by defining a new function \( \beta(q_1, q_2) \) such that
\[ \frac{V_{q_1}}{V_{q_2}} = \left( \frac{b e^{\xi_1} - c}{e^{\xi_1}} \right) \left( \frac{e^{\xi_2}}{b e^{\xi_2} - a} \right) = \frac{\beta_{q_1}}{\beta_{q_2}}, \]
(4.32)
which is solved by
\[ \beta = b q_1 + b q_2 + \frac{a}{e^{\xi_1}} + \frac{c}{e^{\xi_2}}. \]
(4.33)
If the potential is defined as \( V = -\beta \), then the accelerations [eq. (4.28)] can be written as
\[ \ddot{q}_1 = -\frac{\beta_{q_1}}{\xi}, \quad \ddot{q}_2 = -\frac{\beta_{q_2}}{\xi}, \]
(4.34)
with \( \xi \) being defined as
\[ \xi = -\frac{1}{b e^{\xi_1} e^{\xi_2}}. \]
(4.35)
Thus, the Hamiltonian is now
\[ H = \frac{\mu}{2} (p_1^2 + p_2^2) - b q_1 - b q_2 - \frac{a}{e^{\xi_1}} - \frac{c}{e^{\xi_2}}. \]
(4.36)
Hamilton’s equations [eq. (2.28)] imply that
\[ \dot{q}_1 = \frac{1}{2} (p_1^2 + p_2^2) \frac{\partial \mu}{\partial p_1} + \mu p_1 \]
\[ \dot{q}_2 = \frac{1}{2} (p_1^2 + p_2^2) \frac{\partial \mu}{\partial p_2} + \mu p_2 \]
(4.37)
which can be used to develop relationships for \( p_i \) which define the form of the function \( \mu \). At this time, we have not investigated the functional form for either \( p_i \) or \( \mu \) other than the relationships given in eq. (4.37).
Another method which can be used to develop a Hamiltonian for the LV system also uses the coordinate transformation represented by eq. (4.24). G. D. Birkhoff [76] showed that any dynamical system with two degrees of freedom can be transformed into a system possessing a Lagrangian

$$L = \frac{1}{2} \left( \dot{q}_1^2 + \dot{q}_2^2 \right) + \alpha_1 \dot{q}_1 + \alpha_2 \dot{q}_2 + \gamma , \quad (4.38)$$

where $\alpha_i$ ($i = 1,2$) and $\gamma$ are functions of $q_1$ and $q_2$ only, and satisfy the following conditions:

\begin{align*}
(\text{I}) & \quad \ddot{q}_1 + \lambda \dot{q}_2 = \frac{\partial \gamma}{\partial q_1} \\
(\text{II}) & \quad \ddot{q}_2 - \lambda \dot{q}_1 = \frac{\partial \gamma}{\partial q_2} \\
(\text{III}) & \quad \lambda = \frac{\partial \alpha_1}{\partial q_2} - \frac{\partial \alpha_2}{\partial q_1} .
\end{align*} \quad (4.39)

A Legendre transformation of eq. (4.38) defines the Hamiltonian as

$$H = \frac{1}{2} \left( \left( p_1 - \alpha_1 \right)^2 + \left( p_2 - \alpha_2 \right)^2 \right) - \gamma , \quad (4.40)$$

where the conjugate momenta $p_i$ are defined by

$$p_1 = \frac{\partial L}{\partial \dot{q}_1} = \dot{q}_1 + \alpha_1 , \quad p_2 = \frac{\partial L}{\partial \dot{q}_2} = \dot{q}_2 + \alpha_2 , \quad (4.41)$$

and where the potential $\gamma$ is determined by eq. (4.39). If we want the system to satisfy the condition that the time derivative of the momenta equal the accelerations, then $\alpha_1$ and $\alpha_2$ must be constants for any set of initial conditions. Therefore, we define $\alpha_1$ and $\alpha_2$ as

$$\alpha_1 = \Lambda , \quad \alpha_2 = - \Lambda , \quad (4.42)$$

since $\Lambda$ is invariant for any set of initial conditions. Substitution of eq. (4.42) into eq. (4.39) gives the partial differential equations which the potential must solve. Since the second derivatives of $\gamma$ commute, eq. (4.39) can be integrated to define the potential as

$$\gamma = \frac{1}{2} b^2 \left( e^{2q_1} + e^{2q_2} \right) - b \left( c e^{q_1} + a e^{q_2} \right) - (a + c) \Lambda . \quad (4.43)$$

With this definition of the potential, the Hamiltonian becomes

$$H = \frac{1}{2} \left[ \left( p_1 - \Lambda \right)^2 + \left( p_2 + \Lambda \right)^2 \right] - \frac{1}{2} b^2 \left( e^{2q_1} + e^{2q_2} \right) \quad + b \left( c e^{q_1} + a e^{q_2} \right) + (a + c) \Lambda , \quad (4.44)$$

with the derivatives being given as follows:

$$\frac{\partial H}{\partial p_1} = p_1 - \Lambda = \dot{q}_1$$

$$\frac{\partial H}{\partial p_2} = p_2 + \Lambda = \dot{q}_2$$

$$\frac{\partial H}{\partial q_1} = \left( p_2 + \Lambda \right) - \left( p_1 - \Lambda \right) \left( b e^{q_1} - c \right)$$

$$- \frac{\partial \gamma}{\partial q_1} = - \dot{p}_1$$

$$\frac{\partial H}{\partial q_2} = \left( p_2 + \Lambda \right) - \left( p_1 - \Lambda \right) \left( b e^{q_2} - a \right)$$

$$- \frac{\partial \gamma}{\partial q_2} = - \dot{p}_2 . \quad (4.45)$$

The partial derivatives of the potential $\gamma$ are:

$$\frac{\partial \gamma}{\partial q_1} = \left( b e^{q_1} - c \right) \times \left[ \left( b e^{q_1} - c \right) + \left( b e^{q_2} - a \right) - b e^{q_1} \right]$$

$$\frac{\partial \gamma}{\partial q_2} = \left( b e^{q_2} - a \right) \times \left[ \left( b e^{q_1} - c \right) + \left( b e^{q_2} - a \right) - b e^{q_1} \right] .$$

The Hamiltonian represented by eq. (4.44) is in the traditional form, but with a velocity dependent potential.

Since the system being characterized by eq. (4.44) is a four-dimensional system, three constants of the motion should exist. Two of the constants, namely the original invariant [eq. (4.2)] and the Hamiltonian [eq. (4.44)], have now been developed. As discussed in Part 2, the Hamiltonian for a dynamical system can be used to find the other constants of the motion by construction of a Poisson bracket. If $f(q,p)$ is an invariant for the dynamical system, then the Poisson bracket of $f(q,p)$ with $H$ [eq. (4.44)] can be reduced using eq. (4.45) to the condition

$$\left( \frac{\partial f}{\partial q_1} + b e^{q_1} \frac{\partial f}{\partial p_1} \right) \dot{q}_1$$

$$+ \left( \frac{\partial f}{\partial q_2} - b e^{q_2} \frac{\partial f}{\partial p_1} \right) \dot{q}_2 = 0 . \quad (4.46)$$
One approach to solving eq. (4.46) is to define a function $\psi$ such that

\[
\frac{\partial \psi}{\partial q_1} + b e^{q_1} \frac{\partial \psi}{\partial p_2} = b e^{q_1} - c, \\
\frac{\partial \psi}{\partial q_2} - b e^{q_2} \frac{\partial \psi}{\partial p_1} = b e^{q_2} - a,
\]

which is solved by

\[
\psi = p_2 - p_1 - c q_1 - a q_2. \tag{4.47}
\]

The existence of three independent invariants (represented by $\Lambda$ [eq. (4.2)], $H$ [eq. (4.44)] and $\psi$ [eq. (4.47)]) implies that the system is completely integrable. (The linear independence of the three invariants was checked by computing the Jacobian of the system, which is non-zero.) Complete integrability implies that the LV system can be represented by one independent variable, which was shown explicitly in the last section.

5. LOTKA-VOLterra RELATED FAMILY OF DIFFERENTIAL EQUATIONS

A. Development [77]

As mentioned in Part 4, the technique used to solve the LV model leads to a family of LV-related differential equations. In this Part, this family will be derived, and the analytic solutions (which represent approximate solutions to the LV model) will be presented. The family of invariants for this system will be developed, and a simple transformation will be shown which allows these systems to be written in Hamiltonian form.

In Section 4.C, the rate equations for the LV model were rewritten as [eq. (4.17)]

\[
\dot{x}_1 = ax_1 + \frac{k^2}{b} x_1^{1-\alpha} e^{b(x_1 + x_2)/a}, \\
\dot{x}_2 = -ax_2 - \frac{k^2}{b} x_1^{1-\alpha} e^{b(x_1 + x_2)/a},
\]

where $k^2 = -b^2 e^{\Lambda_0}$. Introducing a power series expansion for the exponential term yields

\[
\dot{x}_1 = ax_1 + \frac{k^2}{b} x_1^{1-\alpha} \sum_{m=0}^{\infty} \frac{1}{m!} \left( \frac{b}{a} \right)^m (x_1 + x_2)^m, \\
\dot{x}_2 = -ax_2 - \frac{k^2}{b} x_1^{1-\alpha} \sum_{m=0}^{\infty} \frac{1}{m!} \left( \frac{b}{a} \right)^m (x_1 + x_2)^m. \tag{5.1}
\]

A family of differential equations related to the LV model can be derived by truncating the power series in eq. (5.1) to give

\[
\dot{x}_1 = ax_1 + \frac{k^2}{b} x_1^{1-\alpha} \sum_{m=0}^{n} \frac{1}{m!} \left( \frac{b}{a} \right)^m (x_1 + x_2)^m, \\
\dot{x}_2 = -ax_2 - \frac{k^2}{b} x_1^{1-\alpha} \sum_{m=0}^{n} \frac{1}{m!} \left( \frac{b}{a} \right)^m (x_1 + x_2)^m, \tag{5.2}
\]

for $n = 0, \ldots, \infty$, with $n = \infty$ corresponding to the LV model. (Although the value of $k^2$ can be any negative number, for the system to become the LV model as $n \to \infty$, $k$ must be defined by $k^2 = -b^2 e^{\Lambda_0}$, where $\Lambda$ is the value of eq. (4.2) at $t = 0$.) The family of differential equations represented by eq. (5.2), even though it appears to be more complicated than the original LV problem, will be shown in the next Section to possess analytic solutions in terms of known functions for the cases when $\alpha = 1$ and $n \leq 3$. The integral quadrature for the cases of $n = 2$ and $n = 3$ will also be presented. Numerical integration of eq. (5.2) shows that for $n \geq 2$, the solution curves are closed, which implies the existence of periodic solutions (see Fig. 9). Thus, eq. (5.2) represents a family of two-dimensional dynamical systems which show sustained oscillations.

Eq. (5.2) may have applications in a variety of areas. In the 1970s, J. J. Tyson and J. C. Light [6] developed a technique for deriving two-component reaction schemes modeled by equations similar to this family. (Due to the complexity of the rate laws, however, no attempt was made to obtain analytic solutions.) Another area in which this family may have applications is population biology, since eq. (5.2), when $n = 2$ and $\alpha = 1$, has the quadratic coupling term which appears in the LV predator-prey system.

Fig. 9. The configuration space trajectories of eq. (5.2) of text for different values of $n$. The initial conditions for the numerical integration where $x_1(0) = 0.70000, x_2(0) = 0.55560$ and the structural constants were $a = 1.0, \alpha = 1.0$, and $k = 0.35845 i$ (where $i = \sqrt{-1}$).
model [eq. (3.23)], as well as the quadratic terms dependent only upon $x_i$ and $x_j$ (which is reminiscent of the LV competition model [78]).

B. Analytic Solution [77]

In this Section, eq. (5.2) will be reduced to a one-dimensional system modeled by a second-order nonlinear differential equation. The analytic solutions to this equation in terms of known functions will be derived for the special cases $\alpha = 1$ and $n \leq 3$, and the integral quadratures will be derived which represent the analytic solutions for the special cases $\alpha = 2$ and $\alpha = 3$. The relationship between these analytic solutions and the analytic solution to the LV model [eqs. (4.15) and (4.19)] will be discussed.

Since the family of differential equations represented by eq. (5.2) is directly related to the LV model, the same transformation, namely eq. (4.14), can be used to reduce the present system to a one-dimensional problem modeled by the variable $w(t)$. This one-dimensional system is characterized by the second-order differential equation

$$\ddot{w} - a(1 - \alpha) \dot{w} - a^2 \alpha w$$

$$- k^2 \left[ \frac{1}{b} (a \alpha w + \dot{w}) \right]^{1-\alpha}$$

$$+ \sum_{m=0}^{n} \frac{1}{m!} (\alpha + 1)^m w^m = 0,$$

for $n = 0, \ldots, \infty$. Eq. (5.3), which as $n \to \infty$ becomes the characteristic differential equation for the LV model [eq. (4.18)], can be integrated using a symbolic processor [75] to give the quadrature

$$t - t_0 = \int_0^w [a a (\rho - w')]^{-1} dw', \quad (5.4)$$

where $\rho$ is given by the solution to the polynomial

$$(n+1)! a a \left[ - b a \rho^{n+1} + b a (a + 1) w' \rho^n \right. \left. + k^2 \left( \frac{b}{a a} \right) \sum_{m=0}^{n+1} \frac{1}{m!} (\alpha + 1)^m w'^m \right] = 0,$$

for all $n = 0, \ldots, \infty$. Eq. (5.5) can be solved in terms of radicals for $\alpha \leq 3$ with the aid of a symbolic processor [75]. Numerical integration of eq. (5.3) for a specified value of $\alpha > 0$ and $n > 1$ shows that the solution curves are doubly periodic functions with the same general shape as that for the LV model (see Fig. 10). As the value of $n$ increases, the solution curves of eq. (5.4) become better approximations to the LV model.

When $\alpha = 1$, eq. (5.5) is a second order polynomial which can be solved using the quadratic formula to give

$$\rho = w' \pm \frac{1}{a} \left[ a^2 w'^2 + k^2 \sum_{m=0}^{n+1} \frac{2^m}{m!} w'^m \right]^{1/2},$$

which when substituted into eq. (5.4) yields the integral quadrature

$$t - t_0 = \pm \int_0^w \left[ a^2 w'^2 + k^2 \sum_{m=0}^{n+1} \frac{2^m}{m!} w'^m \right]^{-1/2} dw'. \quad (5.6)$$

Eq. (5.6), which reduces to eq. (4.15) when $n = \infty$, can be solved in terms of known functions for $n \leq 3$ (with the use of a symbolic processor [75,79]); these solutions are presented in Table 2. From these solutions it becomes obvious that the doubly periodic nature of the LV problem appears as a result of the higher-order terms in the power series expansion, since the solutions for the $n = 0$ and $n = 1$ case are exponential (although the solution for the $n = 1$ case can become periodic when $a^2 < 2 k^2$). Elliptic functions, like the solutions to the $n = 2$ and $n = 3$ case, are known for their doubly periodic nature [74].

For the case of $\alpha = 2$, the solution of eq. (5.5) has three branches which, when substituted back into eq. (5.4), give

$$t - t_0 = \int_0^w \left[ \frac{1}{2} p_2^{1/3} + 2 a^2 w'^2 p_2^{-1/3} - a w' \right]^{-1} dw'. \quad (5.7)$$
Table 2. Analytic solutions to eq. (5.6) of text for \( n \leq 3 \).

<table>
<thead>
<tr>
<th>( n )</th>
<th>Solution</th>
<th>( n )</th>
<th>Solution</th>
</tr>
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<tbody>
<tr>
<td>0</td>
<td>[ w(t) = \frac{1}{2a} e^{ax(t-x)} + \frac{k^2}{2a^2} (k^2 - a) e^{x(t-x)} - \frac{k^2}{a^2} ]</td>
<td>3</td>
<td>[ \frac{\sqrt{2}}{2} k \left[ (\beta_2 - \beta_4)(\beta_1 - \beta_3) \right]^{1/2} (t - t_b) ]</td>
</tr>
<tr>
<td></td>
<td>[ w(t) = \frac{1}{2a} e^{ax(t-x)} + \frac{k^2}{2a^2} (k^2 - \lambda) e^{x(t-x)} - \frac{k^2}{\lambda^2} ]</td>
<td></td>
<td>[ F \left( \sin^{-1} \left( \frac{w - \beta_3}{\beta_2 - \beta_3} \right), \frac{\beta_2 - \beta_3}{\beta_1 - \beta_3} \right) ]</td>
</tr>
<tr>
<td></td>
<td>where ( \lambda = \sqrt{a^2 + 2k^2} )</td>
<td>where</td>
<td>[ F \left( \sin^{-1} \left( \frac{w - \beta_3}{\beta_2 - \beta_3} \right), \frac{\beta_2 - \beta_3}{\beta_1 - \beta_3} \right) ]</td>
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<tr>
<td>2</td>
<td>[ \frac{\sqrt{2}}{3} k \sqrt{\beta_1 - \beta_3} (t - t_b) = F \left( \sin^{-1} \left( \frac{w - \beta_3}{\beta_2 - \beta_3} \right), \frac{\beta_2 - \beta_3}{\beta_1 - \beta_3} \right) ]</td>
<td>[ \beta_1 = -\frac{1}{2} + \frac{\sqrt{2}}{4} k^{-1} \left[ p_3^{1/2} + (a^2 + 2k^2)^2 p_3^{-1/2} - 2(a^2 + k^2) \right]^{-1/2} ]</td>
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<tr>
<td></td>
<td>where ( F ) is an elliptic function of the first kind and</td>
<td>[ \beta_2 = -\frac{1}{2} + \frac{\sqrt{2}}{4} k^{-1} \left[ p_3^{1/2} + (a^2 + 2k^2)^2 p_3^{-1/2} + 4(a^2 + k^2) \right]^{-1/2} ]</td>
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<td></td>
<td>[ \beta_1 = -\frac{1}{4} \frac{a^2 + 2k^2}{k^2} - \frac{1}{8} (1 + i\sqrt{3}) k^{-2} p_2^{1/2} ]</td>
<td>[ \beta_2 = -\frac{1}{4} \frac{a^2 + 2k^2}{k^2} - \frac{1}{8} (1 - i\sqrt{3}) k^{-2} p_2^{1/2} ]</td>
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<td></td>
<td>[ -\frac{1}{8} (1 - i\sqrt{3}) k^{-2} (a^4 + 4a^2 k^2 - 4k^4) p_2^{-1/2} ]</td>
<td>[ \beta_3 = -\frac{1}{4} \frac{a^2 + 2k^2}{k^2} - \frac{1}{4} k^{-2} (a^4 + 4a^2 k^2 - 4k^4) p_2^{-1/2} ]</td>
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<td></td>
<td>[ \beta_3 = -\frac{1}{4} \frac{a^2 + 2k^2}{k^2} - \frac{1}{4} k^{-2} (a^4 + 4a^2 k^2 - 4k^4) p_2^{-1/2} ]</td>
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<td>with ( p_2 ) defined as</td>
<td>[ \beta_3 = -\frac{1}{4} \frac{a^2 + 2k^2}{k^2} - \frac{1}{4} k^{-2} (a^4 + 4a^2 k^2 - 4k^4) p_2^{-1/2} ]</td>
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<tr>
<td></td>
<td>[ p_2 = -a^6 - 6a^4 k^2 - 8k^4 ]</td>
<td>[ \beta_3 = -\frac{1}{2} - \frac{\sqrt{2}}{4} k^{-1} \left[ p_3^{1/2} + (a^2 + 2k^2)^2 p_3^{-1/2} - 2(a^2 + k^2) \right]^{1/2} ]</td>
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<td></td>
<td>[ + 4\sqrt{3} a^2 k^2 (a^2 - 4k^2) + k^4 (3a^4 + 8k^4) ]</td>
<td></td>
<td>[ -\frac{1}{4} \frac{a^2 + 2k^2}{k^2} - \frac{1}{4} k^{-2} (a^4 + 4a^2 k^2 - 4k^4) p_2^{-1/2} ]</td>
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<td></td>
<td>[ \beta_4 = -\frac{1}{4} \frac{a^2 + 2k^2}{k^2} - \frac{1}{4} k^{-2} (a^4 + 4a^2 k^2 - 4k^4) p_2^{-1/2} ]</td>
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<td>[ + 4\sqrt{2} k (2k^2 - 3a^2) \left[ p_3^{1/2} + (a^2 + 2k^2)^2 p_3^{-1/2} \right]^{-1/2} ]</td>
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<tr>
<td></td>
<td>[ -\frac{1}{4} \frac{a^2 + 2k^2}{k^2} - \frac{1}{4} k^{-2} (a^4 + 4a^2 k^2 - 4k^4) p_2^{-1/2} ]</td>
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<td>[ + 2\sqrt{2} k (2k^2 - 3a^2) \left[ p_3^{1/2} + (a^2 + 2k^2)^2 p_3^{-1/2} \right]^{-1/2} ]</td>
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<tr>
<td></td>
<td>[ -\frac{1}{4} \frac{a^2 + 2k^2}{k^2} - \frac{1}{4} k^{-2} (a^4 + 4a^2 k^2 - 4k^4) p_2^{-1/2} ]</td>
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<tr>
<td></td>
<td>[ + 2\sqrt{2} k (2k^2 - 3a^2) \left[ p_3^{1/2} + (a^2 + 2k^2)^2 p_3^{-1/2} \right]^{-1/2} ]</td>
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<tr>
<td></td>
<td>[ -\frac{1}{4} \frac{a^2 + 2k^2}{k^2} - \frac{1}{4} k^{-2} (a^4 + 4a^2 k^2 - 4k^4) p_2^{-1/2} ]</td>
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<tr>
<td></td>
<td>[ -\frac{1}{4} \frac{a^2 + 2k^2}{k^2} - \frac{1}{4} k^{-2} (a^4 + 4a^2 k^2 - 4k^4) p_2^{-1/2} ]</td>
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</table>

and

\[
\begin{align*}
    t - t_0 &= \int_0^w \left[ -2 \frac{1}{4} (1 \pm i \sqrt{3}) p_2 \right]^{1/3} \\
    &\quad - a^2 (1 \mp i \sqrt{3}) w^2 p_2^{1/3} - aw' \, dw',
\end{align*}
\]

(5.8)

where \( p_2 \) is defined as

\[
p_2 = 8 a^3 w^3 + 4 k^2 b \sum_{m=0}^{n+1} \frac{3^m}{m!} w^m
\]

\[
+ 4 \left[ \frac{k^2 b}{m!} \sum_{m=0}^{n+1} \frac{\beta^m}{m!} \right]^{1/2}
\]

(5.9)

When the summation in eq. (5.9) is allowed to go to infinity, eqs. (5.7) and (5.8) represent the integral quadratures for the LV model when \( a = 2 \).

When \( a = 3 \), the four solutions to eq. (5.5), upon substitution into eq. (5.4), lead to the integral quadratures presented below:

\[
t - t_0 = \int_0^w \left[ -2 a w' + 12 a^3 w^3 (3 b k^2 S p_3)^{1/3} \right]
\]

\[
- p_3^{1/3} - 6 a^2 w'^{-1/2} + \frac{\beta}{6} \left( (3 b^2 k^2 S p_3)^{1/3} \right)
\]

\[
- p_3^{1/3} - 6 a^2 w'^{1/2} \left( (3 b^2 k^2 S p_3)^{1/3} - p_3^{1/3} \right)
\]

\[
- 12 a^2 w'^2 \right]^{-1} dw'
\]

and

\[
t - t_0 = \int_0^w \left[ -2 a w' + 12 a^3 w^3 (3 b^2 k^2 S p_3)^{1/3} \right]
\]

\[
- p_3^{1/3} - 6 a^2 w'^{-1/2} - \frac{\sqrt{6}}{} \left( (3 b^2 k^2 S p_3)^{1/3} \right)
\]

\[
- p_3^{1/3} - 6 a^2 w'^{1/2} \left( (3 b^2 k^2 S p_3)^{1/3} - p_3^{1/3} \right)
\]

\[
- 12 a^2 w'^2 \right]^{-1} dw'
\]

where

\[
p_3 = \frac{3 k^2 b^2 S}{6} \left[ 9 a^2 w'^2 + (3 k^2 b^2 S + 81 a^4 w'^4)^{1/2} \right]
\]

and

\[
S = \sum_{m=0}^{n+1} \frac{4^m}{m!} w^m.
\]

These analytic solutions to eq. (5.3) also represent the solutions to the LV model when \( a = 3 \), if the summation is allowed to go to infinity.

The integral quadratures presented above, although not reducible to known functions, do represent analytic solutions to eq. (5.3) for finite \( n \), and to eq. (4.18) for infinite \( n \). The numerical integration of these quadratures leads to periodic solutions which are indicative of a conservative system. In the next Section, the invariants for eq. (5.2) will be derived, and a simple transformation which allows this system to be written in Hamiltonian form will be presented.

C. Invariants and Hamiltonians [77]

The fact that eq. (5.2) possesses closed curves as solutions (see Fig. 5.1) is indicative of the existence of an invariant for the system. The derivation of the invariant for any two-dimensional system modeled by a set of first-order differential equations begins by taking the ratio of the rate equations. For the system represented by eq. (5.2), this ratio is

\[
\frac{dx_1}{dx_2} = \frac{ax_1 + \frac{k^2}{b} x_1^{1-a} \sum_{m=0}^{n} \frac{1}{m!} \left( \frac{b}{a} \right)^m (x_1 + x_2)^m}{-a a x_2 - \frac{k^2}{b} x_1^{1-a} \sum_{m=0}^{n} \frac{1}{m!} \left( \frac{b}{a} \right)^m (x_1 + x_2)^m},
\]

which can be rewritten as

\[
\left[ -a a x_2 - \frac{k^2}{b} x_1^{1-a} \sum_{m=0}^{n} \frac{1}{m!} \left( \frac{b}{a} \right)^m (x_1 + x_2)^m \right] \, dx_1 = 0
\]

(5.10)

Eq. (5.10) can be integrated to give
\[ I_n = a x_1^n x_2 \]
\[ + k^2 \sum_{m=1}^{n+1} \frac{1}{m!} a^{1-m} b^{m-2} (x_1 + x_2)^m , \]  
(5.11)

which can be shown by induction to be the first integral of the system as follows.

The condition for eq. (5.11) to be invariant is
\[
\frac{dI_n}{dt} = \partial_I I_n \dot{x}_1^{(0)} + \partial_J I_n \dot{x}_2^{(0)} = 0 ,
\]  
(5.12)

where \( \partial_I f_n = \frac{\partial f}{\partial x_i} \), and \( \dot{x}_j^{(0)} = \dot{x}_j \) for some specific value of \( n \). When \( n = 0 \), eq. (5.12) can be written as
\[
\frac{dI_0}{dt} = a a x_1^{1-a} x_2 + k^2 b \left( a x_1 + \frac{k^2}{b} x_1^{1-a} \right) + \left( a x_2^{1-a} \right) \left( -a a x_2 - \frac{k^2}{b} x_1^{1-a} \right) ,
\]
which simplifies to zero. Now, eq. (5.2) can be written recursively as
\[
\dot{x}_1^{(j+1)} = \dot{x}_1^{(0)} + \left( (j + 1)! \right)^{-1} k^2 b^j a^{-j-1} x_1^{1-a} (x_1 + x_2)^{j+1}
\]
\[
\times \left( a x_1 + \frac{k^2}{b} x_1^{1-a} \right) \left( -a a x_2 - \frac{k^2}{b} x_1^{1-a} \right),
\]  
(5.13)

and \( I_{j+1} [\text{eq. (5.11)}] \) can be rewritten as
\[
I_{j+1} = I_j + \left( (j + 2)! \right)^{-1} k^2 b^j a^{-j-1} (x_1 + x_2)^{j+2} . \]
(5.14)

Substitution of eq. (5.13) and the derivatives of eq. (5.14) into eq. (5.12) gives, upon rearrangement,
\[
\frac{dI_{j+1}}{dt} = \left( \partial_I I_j \dot{x}_1^{(j)} + \partial_J I_j \dot{x}_2^{(j)} \right)
\]
\[
+ \left( (j + 1)! \right)^{-1} k^2 b^j a^{-j-1} x_1^{1-a} (x_1 + x_2)^{j+1}
\]
\[
\times \left( \partial_I I_j - \partial_J I_j \right) + \left[ \dot{x}_1^{(j)} + \dot{x}_2^{(j)} \right] ,
\]
which (since \( \partial_I I_j \dot{x}_1^{(j)} + \partial_J I_j \dot{x}_2^{(j)} = 0 \) by assumption) reduces to
\[
\frac{dI_{j+1}}{dt} = \left( (j + 1)! \right)^{-1} k^2 b^{j} a^{-j-1} (x_1 + x_2)^{j+1}
\]
\[
\times \left[ a x_1^{1-a} (x_1 + x_2)^{j+1} - a x_1^{1-a} (x_1 + x_2)^{j+1} \right] .
\]  
(5.15)

Expansion and rearrangement simplifies eq. (5.15) to zero, thus completing the proof that eq. (5.11) is invariant.

Another method leading to the characteristic differential equation [eq. (5.3)] for eq. (5.2) begins by defining new coordinates \( z_1 \) and \( z_2 \) in the same manner as developed in Part 4 for the solution to the LV problem. The coordinate \( z_1 \) is defined such that it contains only the terms linear in \( x_1 \) and \( x_2 \) in the invariant, while the coordinate \( z_2 \) contains the remaining terms of the invariant. Applying the remaining coordinate transformations of Part 4 reduces eq. (5.2) to eq. (5.3).

The transformation of eq. (5.2) into Hamiltonian form begins by introducing new variables \( q \) and \( p \) such that
\[
q = x_1 , \quad p = x_1^{1-a} x_2 .
\]  
(5.16)

This transformation allows the rate equations [eq. (5.2)] for the system to be written as
\[
\dot{q} = a q + k^2 q^{1-a}
\]
\[
\times \sum_{m=0}^{n} \frac{1}{m!} a^{-m} b^{m-1} (q + p q^{1-a})^m \]
\[
\dot{p} = -a p - k^2 [1 + (1-a) p q^{-a}]
\]
\[
\times \sum_{m=0}^{n} \frac{1}{m!} a^{-m} b^{m-1} (q + p q^{1-a})^m ,
\]  
(5.17)

and the invariant [eq. (5.11)] to be rewritten as
\[
H_n = a q p + k^2
\]
\[
\times \sum_{m=0}^{n} \frac{1}{m!} a^{1-m} b^{m-2} (q + p q^{1-a})^m .
\]  
(5.18)

The derivation of Hamilton’s equations from eq. (5.18) may be shown simply as follows. The derivatives of eq. (5.18) with respect to \( q \) and \( p \) are
where by direct comparison with eq. (5.17) leads to Hamilton’s equations, namely
\[
\frac{\partial H_n}{\partial p} = \dot{q} \quad \text{and} \quad \frac{\partial H_n}{\partial q} = -\dot{p}.
\]

The Hamiltonian of eq. (5.18), like Kerner’s Hamiltonian for the original LV problem, does not treat both coordinates equally. An extension of this system to a full four-dimensional space in order to develop a more traditional Hamiltonian has not been attempted. If a more traditional Hamiltonian can be developed for this general family of functions, the nature of the third invariant for the general system could be compared to the third invariant of the LV model [eq. (4.47)] to perhaps give more insight into the symmetry of both the LV problem and its related family.

6. CONCLUSIONS

In this Review, we have presented the analytic solutions to the Lotka-Volterra problem. Our presentation began with a brief discussion of the qualitative properties of dynamical systems in Part 2. This treatment was then used in Part 3 for the development and solution of the rate laws pertaining to various chemical reaction schemes. Part 3 also provided a brief introduction to the study of systems which exhibit sustained chemical oscillations. Our study of chemical oscillations was then expanded in Part 4 to a more thorough investigation of the LV model, which led ultimately to the development of a new coordinate transformation for the LV system. This transformation [eq. (4.7)] reduced the dimensionality of the LV problem by one and allowed for the development of an equivalent second-order differential equation [eq. (4.13)], which was then solved analytically via quadratures. These quadratures [eqs. (4.15) and (4.19)], although not capable of being integrated in terms of known elementary functions, define new functions which represent the analytic solutions to the Lotka-Volterra problem. In Part 5, an introductory analysis of these analytic solutions was provided, one which led to the development of a new family of LV-related dynamical systems [eq. (5.2)]. This family of dynamical systems, although appearing more complex than the LV system, could in some instances be solved in terms of known functions (Table 2). The Hamiltonian forms for both the LV problem (Section 4.D) and the LV-related family [eq. (5.18)] were also explored. The analytic solutions to the LV problem represent, if fully analyzed, the definition of new elliptic-type functions. The full analysis of any quadrature begins by comparing the form of its solutions to the solutions of known functions. This comparison leads to the development of approximations to the quadrature in terms of known functions, as well as to insight into the nature of the function. For the analytic solutions to the LV problem [eq. (4.19)], we began this comparison by performing a power series expansion on the exponential term in the quadrature. When \( a = c \), truncation of this expansion led to a relationship (given in Table 2) between this function and the family of elliptic functions [74]. A future full analysis of eq. (4.19) will involve showing that eq. (4.19) is convergent, determining the exact nature of the two periods of the solution, and defining the singularities of the function (see, for example, E. T. Whittaker and G. N. Watson’s book on modern analysis [80]).

The coordinate transformation employed to solve the LV model [eq. (4.7)], which involved the first integral of the system [eq. (4.2)], may have the capability of being generalized to an n-dimensional system such as GLV (cf. Part 4). For example, an integrable four-dimensional system will possess three invariants. If two of these invariants were known, four new coordinates \( z_i (i = 1, \ldots, 4) \) could be defined such that the system could be represented by two angles \( \Psi \) and \( \Omega \), with these angles being given by
\[
\tan \Psi = \frac{z_1}{z_2} \quad \text{and} \quad \tan \Omega = \frac{z_3}{z_4}.
\]

With eq. (6.1), the old system could be represented by the solution to two second-order characteristic differential equations in terms of \( \Psi \) and \( \Omega \), which may or may not be coupled. (The coupling would depend upon the nature of the original invariants, and on how the coordinates \( z_i \) are defined.) If the differential equations are coupled, it might be possible to use the same technique to reduce the system to one dimension if an invariant in terms of \( \Psi \) and \( \Omega \) can be found.

The determination of the invariants of any n-
dimensional system, however, is a problem in its own right. This problem can be solved in part if the system can be written in Hamiltonian form, since once a Hamiltonian is known, the construction of the Poisson bracket with a general function can lead to insight into the form of other invariants. The Lagrangian that Birkhoff [76] developed for a two-dimensional system [cf. eq. (4.38)] can be generalized to an n-dimensional Lagrangian given by

$$ L = \sum_{i=1}^{n} \left[ \frac{1}{2} \ddot{q}_{i}^{2} + \alpha_{i} \dot{q}_{i} \right] + \gamma , \quad (6.2) $$

where $\alpha_{i}, \forall i = 1,\ldots,n$, and $\gamma$ are functions dependent only upon the coordinates $q_{i}$. These functions can be determined as follows. For eq. (6.2) to truly define a Lagrangian, Lagrange’s equations [i.e., eq. (2.24)] must be satisfied. This condition leads to the function $\gamma$ being defined by a system of $n$ partial differential equations, namely

$$ \frac{\partial \gamma}{\partial q_{i}} = \ddot{q}_{i} + \sum_{j=1}^{n} \left( \frac{\partial \alpha_{i}}{\partial q_{j}} - \frac{\partial \alpha_{j}}{\partial q_{i}} \right) \dot{q}_{j} , \quad (6.3) $$

for all $i = 1,\ldots,n$. If there exists a set of functions $\alpha_{i} (i = 1,\ldots,n)$ such that $\gamma$ possesses a complete differential (in other words, if all of the mixed partial derivatives of $\gamma$ commute), the system will be able to be written in Lagrangian form. Once the Lagrangian is defined, a Legendre transformation (defined in Section 2.C, above) of eq. (6.2) leads to a Hamiltonian having the form

$$ H = \frac{1}{2} \sum_{i=1}^{n} (p_{i} - \alpha_{i})^{2} - \gamma , \quad (6.4) $$

where the momenta of the system $p_{i}$ are defined by

$$ p_{i} = \frac{\partial L}{\partial \dot{q}_{i}} = \dot{q}_{i} + \alpha_{i} . \quad (6.5) $$

Once eq. (6.4) is determined for the system, the Poisson bracket [i.e., eq. (2.31)] can be constructed and analyzed in order to develop the other invariants for the system. The existence of eq. (6.4) can also be used to determine the analytic solutions to the system by applying Hamilton-Jacobi theory [22].

The family of LV-related differential equations developed in Part 5 [eq. (5.2)] represents a set of two-dimensional systems which show sustained oscillations (see Fig. 5.2). The applications for which these systems may provide models have not yet been explored. It may be possible (using the techniques of J. J. Tyson and J. C. Light [6], or the approach of N. Samardzija and co-workers [37]) to develop oscillating chemical reaction schemes, modeled by eq. (5.2), in which the analytic solutions to the rate laws are known in terms of well-defined functions. Eq. (5.2) should also be able to be recast in terms of complex interactions between populations of biological species. This family of dynamical systems clearly provides a rich analytical ground for a plethora of future model studies.

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