Generalized conformal Hamiltonian dynamics and the pattern formation equations

Partha Guha*
IHÉS, 35, Route de Chartres,
F-91440 Bures-sur-Yvette, France

S.N. Bose National Centre for Basic Sciences
JD Block, Sector III, Salt Lake
Kolkata - 700098, India

A.Ghose-Choudhury†
Department of Physics, Surendranath College,
24/2 Mahatma Gandhi Road, Calcutta-700009, India.

December 4, 2017

Abstract

We demonstrate the significance of the Jacobi last multiplier in Hamiltonian theory by explicitly constructing the Hamiltonians of certain well known first-order systems of differential equations arising in the activator-inhibitor (AI) systems. We investigate the generalized Hamiltonian dynamics of the AI systems of Turing pattern formation problems, and demonstrate that various subsystems of AI, depending on the choices of parameters, are described either by conformal or contact Hamiltonian dynamics or both. Both these dynamics are subclasses of another dynamics, known as Jacobi mechanics. Furthermore we show that for non Turing pattern formation, like the Gray-Scott model, may actually be described by generalized conformal Hamiltonian dynamics using two Hamiltonians. Finally, we construct a locally defined dissipative Hamiltonian generating function [13] of the original system. This generating function coincides with the "free energy" of the associated system if it is a pure conformal class. Examples of pattern formation equation are presented to illustrate the method.

MSC classification : 58A15, 70H15, 92B05.

*E-mail: partha@bose.res.in; guha@ihes.fr
†E-mail aghosechoudhury@gmail.com

PACS numbers : 45.20.-d, 05.45. -a, 45.50.Jf

Keywords and keyphrases Jacobi's last multiplier, singular Lagrangians, Autocatalysis system, morphogenesis, Turing pattern formation, Jacobi bracket.

Contents

1 Introduction

Many second-order ordinary differential equations (ODEs) of the form $\ddot{x} = F(t, x, \dot{x})$ admit a Lagrangian description because of the existence of a Jacobi Last Multiplier (JLM), μ, which can be shown to be equal to $\partial^2 L/\partial \dot{x}^2$. In a recent article Nucci *et al* [26] have shown how one can obtain the Lagrangians for certain well known biological models described by planar systems of ODEs using Jacobi's last multiplier. Although in some cases the corresponding Lagrangians are known, it may not always be possible to reduce a given planar system of ODEs

$$\dot{x} = f(x, y, t), \qquad \dot{y} = g(x, y, t), \tag{1.1}$$

to an equivalent second-order ODE. Therefore, the derivation of even a singular Lagrangian for such a system is interesting from the mathematical point of view. A singular Lagrangian is one for which the Hessian matrix

$$\mathcal{H} = \left(\frac{\partial^2 L}{\partial u_i \partial u_j} \right)$$

is singular. In such cases it is not possible to express the equation of motion in the form $\ddot{x} = F(x, \dot{x}, t)$. For such singular Lagrangians the usual definition of the conjugate momentum turns out to be velocity independent and consequently one cannot define a Hamiltonian by the usual Legendre transformation.

The JLM is a useful tool for deriving an additional first integral for a system of n first-order ODEs when $n-2$ first integrals of the system are known. Besides, the JLM allows us to determine the Lagrangian of a second-order ODE in many cases [14, 15, 34, 9]. In recent years a number of articles have dealt with this particular aspect [18, 25, 6]. However, when a planar system of ODEs cannot be reduced to a second-order differential equation the question of interest arises whether the JLM can provide a mechanism for finding the Lagrangian of the system.

In an interesting paper Nucci and Tamizhmani [26] showed that the method used by Trubatch and Franco in [32] and Paine [27] for finding Lagrangians of certain representative biological models actually relies on the existence of a JLM. Nucci *et al* have re-derived the linear Lagrangians of these first-order systems using JLM. They have also obtained the Lagrangians of the corresponding single second-order equations which the earlier authors had failed to do, for example in the case of the host-parasite model.

In this article we apply JLM to find the Lagrangian and the Hamiltonian of certain systems of differential equations which appear in spatio-temporal studies and in biology. It may be noted that a variational problem with a Lagrangian L and configuration space Q may fail to satisfy the Legendre condition, i.e., the fibre derivative map $FL : TQ \to T^*Q$ may fail to be a local diffeomorphism. Therefore direct Hamiltonization of a nonlinear system based on the JLM [3, 12] offers a distinct advantage over the usual process using Legendre transformations. In fact it also yields the canonical coordinates in terms of which one can express the underlying system in canonical form. A similar though more restricted result is given by Lucey and Newman [16], who have shown that for a given system of autonomous ODEs there exists, locally at least a symplectic structure and a Hamiltonian function such that the given system of equations can be expressed in Hamiltonian form.

In a seminal paper, Turing [33] proposed that the problem of pattern formation could be understood using a simple system of reaction-diffusion equations representing interactions of chemicals. In these models, a system of chemicals react with each other and diffuse across a space. These chemical reactions need an inhibitory agent, to suppress the reaction, and an existory agent to activate the reaction. The application of the pattern formation has been

linked to research in development biology. Morphogenesis [**?**] means the generation of tissue organization and shape in animal and plant embryos in the context of developmental biology. It is the evolution of shape of an organism together with the differentiation of its parts. The spatio-temporal distribution of gene expression patterns during morphogenesis together with its key regulators which are again given by gene expressions is one of the main recent achievements in developmental biology. Turing was the first to offer an explanation of morphogenesis through chemistry showing that differences in the diffusion constants of activator and inhibitor species can bring about destabilization of the uniform state and lead to spontaneous emergence of periodic spatial patterns.

Turing patterns emerge in various areas of biological systems, for example a very famous model is the Gierer-Meinhardt [8] system. Gierer and Meinhardt developed a model of two coupled reaction-diffusion equation for the production and diffusion of two different kinds of substances, called the activator and inhibitor (see for example, [28]). Let $u(t,x)$ and $v(t,x)$ stand for the concentration of the activator and inhibitor at (x,t) respectively, then the so called Gierer-Meinhardt model of morphogenesis is

$$\begin{aligned} u_t &= D_u u_{xx} + \rho\rho_0 + \lambda\rho\frac{u^2}{v} - bu \ , \\ v_t &= D_v v_{xx} + \lambda'\rho' u^2 - cv \ , \end{aligned} \tag{1.2}$$

where D_u and D_v are the diffusion constants of the activator and inhibitor, $\rho\rho_0$ stands for the source concentration for the activator and ρ' is the one for the inhibitor, b and c are respectively denote the degradation coefficients of the activator and inhibitor, λ and λ' are related to activator and inhibitor productions. In the absence of diffusion the model takes the form of a system of ODEs. The crucial idea of Turing was that it is possible to have such steady states which are stable in the absence of diffusion, but which turn unstable in the presence of diffusion and form spatially heterogeneous patterns, hence the name diffusion-driven instability or Turing pattern formation Normally diffusion tends to spread out concentrations as to create a homogeneous distribution and not a spatially heterogeneous mixture, so in this respect it is a counter intuitive.

Granero-Porati and Porati [10] considered the ODE version of the Gierer-Meinhardt model in the form

$$\begin{aligned} \dot{u} &= \rho\rho_0 + \lambda\rho\frac{u^2}{v} - bu \ , \\ \dot{v} &= \lambda'\rho' u^2 - cv \ . \end{aligned} \tag{1.3}$$

Not all reaction-diffusion systems generate patterns through Turing's prescription. In fact, small changes in parameters other than just spatial one can lead to very different patterns, one of the famous example is the Gray-Scott (GS) model [11, 4]. Unlike the Gierer-Meinhardt model which has one chemical acting as an activator and the other as an inhibitor, the GS model has two chemicals u and v, where v is transformed to an inert product and u and v react together to produce more v. Thus we find that the activator-inhibitor equations play a very

important role in the study of Turing pattern formation which provides a credible theoretical explanation of animal coat patterns (see for example [22]).

Result of this paper In this paper we study the generalized Hamiltonian mechanics, based on conformal or contact Hamiltonian geometry, of nonlinear ODEs appearing both in Turing and non-Turing pattern formations. We compute the Lagrangian and Hamiltonian of these equations using Jacobi's last multiplier.. It is well known that vector fields whose flows preserve a symplectic form, up to a constant, such as simple mechanical systems with friction, are called conformal. The Duffing oscillator being a typical example of this class. In fact, interestingly enough, the system also turns out to be a conformal Hamiltonian system [20, 23]. Tourigny [31] recently viewed two-component feedback loop equations as a deformed (q-deformation) Hamiltonian system using q-deformed symplectic form and standard separable Hamiltonian. Unfortunately in most physical cases Hamiltonians are non-separable or non-standard one, our approach is based on conformal or contact geometry and the Hamiltonians involved here are non-standard one. In particular, we map the pattern formation equation to generalized classical mechanics based on conformal and contact Hamiltonian method [1, 2, 23]. Both conformal and contact structures belong to a larger class, known as Jacobi structure. Jacobi manifolds were introduced independently by Kirillov [17] and Lichnerowicz [19], who used different but equivalent notions.

Following [13] we study the local equivalence problem between a given autonomous vector field associated to pattern formation equation and a pre-defined Hamiltonian dissipative realization, viewed as a reference system. Method uses a homotopy operator to decompose the (possibly) non-closed one-form into its exact and anti-exact parts on a star-shaped domain. It is known from Gardner [5] that exact part is used to derive a dissipative potential, while the anti- exact part associated with a nondissipative potential does not contribute to the dissipative potential on the star- shaped region.

Our goal is to study these generalized geometries so that non-conservative biological processes can be mapped to the classical formalism. We consider three different examples describing both Turing and non-Turing pattern formations. We illustrate how all these equations can be mapped to conformal and contact mechanics. The purpose of the paper is two fold: people from the field of biology may find it profitable to study pattern formation using the Hamiltonian formalism while for the mathematical physics community new examples of conformal/contact Hamiltonian dynamics are provided. We attempt to illustrate our results in such a way as to be intelligible to both these communities.

The paper is organized as follows. In Section 2 we describe the Jacobi Last Multiplier (JLM) formulation for singular Lagrangian equations illustrating our construction through examples. Section 3 is devoted to computation of the Hamiltonians of such singular activator-inhibitor type systems. Section 4 is devoted to conformal Hamiltonian description and descrition via contact Hamiltonian mecahnics is given section 5. We complete our paper with a modest conclusion in section 6.

2 Preliminaries: Illustrations of finding Lagrangians using JLM

Let us briefly recall the procedure described in [26] for finding Lagrangians for a planar system of ODEs from a knowledge of the last multiplier. We assume that the system (1.1) and (**??**) admits a Lagrangian and class of systems which we wish to deal in this paper are linear or affine in velocities, so that

$$L(t,x,y,\dot{x},\dot{y}) = F(t,x,y)\dot{x} + G(t,x,y)\dot{y} - V(t,x,y). \tag{2.1}$$

Then the Euler-Lagrange equations of motion

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{u}}\right) = \frac{\partial L}{\partial u}, \quad \text{with} \;\; u = x \text{ and } y$$

yield

$$\dot{y} = \left(\frac{F_t + V_x}{G_x - F_y}\right) = g(t,x,y), \tag{2.2}$$

and

$$\dot{x} = -\left(\frac{G_t + V_y}{G_x - F_y}\right) = f(t,x,y), \tag{2.3}$$

where the subscripts on F, G and V denote partial derivatives while the overdot represents derivative with respect to time. It is obvious that one must have $G_x \neq F_y$. In order to introduce the notion of Jacobi's last multiplier we assume that $G_x = -F_y$ and assign a common value,

$$\mu(t,x,y) := G_x = -F_y. \tag{2.4}$$

From (2.2) and (2.3) we have

$$2\mu f(t,x,y) = -(G_t + V_y) \tag{2.5}$$

$$2\mu g(t,x,y) = (F_t + V_x). \tag{2.6}$$

It is clear that the construction

$$\frac{\partial}{\partial x}(2\mu f) + \frac{\partial}{\partial y}(2\mu g)$$

leads to the following equation,

$$\frac{d}{dt}\log\mu + \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} = 0. \tag{2.7}$$

using the original system of ODEs $\dot{x} = f$ and $\dot{y} = g$. However, (2.7) is precisely the defining relation for JLM [34]. Thus we see that given the solution of this equation one can easily construct from (2.4) the coefficient functions F and G occurring in the expression for the Lagrangian since

$$F(t,x,y) = -\int \mu(t,x,y)dy \quad \text{and} \quad G(t,x,y) = \int \mu(t,x,y)dx. \tag{2.8}$$

Once these functions are determined one can obtain an expression for the partial derivatives of V from (2.2) and (2.3) as follows

$$\frac{\partial V}{\partial x} = 2\mu(t,x,y)g(t,x,y) + \frac{\partial}{\partial t}\left(\int \mu dy\right), \tag{2.9}$$

$$\frac{\partial V}{\partial y} = -2\mu(t,x,y)f(t,x,y) - \frac{\partial}{\partial t}\left(\int \mu dx\right). \tag{2.10}$$

In view of (2.7) it is easy to check the equality of the mixed derivatives,

$$\frac{\partial^2 V}{\partial x \partial y} = \frac{\partial^2 V}{\partial y \partial x}.$$

In the next sections we demonstrate the construction of the Lagrangians for spatio-temporal autocatalysis system and the celebrated Gierer-Meinhardt model, these are all auto-catalytic systems. We apply Jacobi's last multiplier method to compute there Lagrangians.

2.1 Lagrangians for Spatio-temporal autocatalysis system

The following is an example of an auto-catalysis and activator inhibitor system.

$$\dot{x} = \frac{a}{b+y} - cx := f(x,y) \tag{2.11}$$

$$\dot{y} = dx - hy := g(x,y). \tag{2.12}$$

From the defining relation (2.7) for the last multiplier, we have

$$\frac{d}{dt}\log\mu - (c+h) = 0,$$

which gives $\mu = e^{(c+h)t}$. It must be noted that μ is not necessarily a purely temporal function, *μ is defined up to a factor that is a constant of motion.* It follows that the functions $G(x,y)$ and $F(x,y)$ are given by

$$G(x,y) = xe^{(c+h)t}, \quad F(x,y) = -ye^{(c+h)t}. \tag{2.13}$$

From (2.9) and (2.10) we have therefore

$$\frac{\partial V}{\partial x} = 2e^{(c+h)t}(dx - hy)$$

$$\frac{\partial V}{\partial y} = -2e^{(c+h)t}(\frac{a}{b+y} - cx)$$

whence from the equality of the mixed derivatives we obtain the condition $c + h = 0$. Using this condition the expression for the potential term becomes

$$V(x,y) = 2cxy - 2a\log(b+y) + dx^2$$

and hence a Lagrangian for the reduced system

$$\dot{x} = \frac{a}{b+y} - cx, \quad \dot{y} = dx + cy$$

is given by

$$L = x\dot{y} - y\dot{x} + 2a\log(b+y) - dx^2 - 2cxy. \tag{2.14}$$

Notice that the condition $c + h = 0$ causes the last multiplier to reduce to unity.

2.2 Lagrangians for the Gierer-Meinhardt model

Our second example is provided by the following system

$$\dot{u} = a - bu + \frac{u^2}{v}, \quad \dot{v} = u^2 - v, \tag{2.15}$$

which is known as the *Gierer-Meinhardt* model. Here u is a short-range autocatalytic substance, i.e., activator, and v is its long-range antagonist, i.e., inhibitor. In other words, this scheme considers autocatalytic activation of chemical u and self inhibitation of v. The model was formulated by Alfred Gierer and Hans Meinhardt in 1972 [8].

From the defining relation (2.7) for the last multiplier, we find that when the parameter $a = 0$ the multiplier is given by

$$\mu = \frac{1}{u^2} e^{(1-b)t}.$$

In this case proceeding in the same manner as above one finds that a consistent expression for the potential term exists provided the parameter $b = 1$ and the final expression for a singular Lagrangian may be given by

$$L = \frac{v}{u^2}\dot{u} + \frac{1}{u}\dot{v} + 2(u + \frac{v}{u} - \log v), \tag{2.16}$$

under the condition $a = 0$ and $b = 1$. The reduced system therefore has the appearance

$$\dot{u} = -u + \frac{u^2}{v}, \quad \dot{v} = u^2 - v. \tag{2.17}$$

3 Time dependent Hamiltonian systems and the Jacobi Last Multiplier

Let $\mathcal{M}$ denote a real two dimensional manifold with local coordinates x and y. Consider the following non autonomous system of differential equations:

$$\dot{x} = f(x, y, t), \quad \dot{y} = g(x, y, t), \tag{3.1}$$

where f and g are smooth real valued functions. We can associate with the system (3.1) the following:
(a) a vector field

$$X := \frac{\partial}{\partial t} + f\frac{\partial}{\partial x} + g\frac{\partial}{\partial y}$$

defined on $\mathcal{M} \times \mathbb{R}$ whose integral curves are determined by the system (3.1), (b) alternatively we may consider the following set of one forms on $\mathcal{M} \times \mathbb{R}$

$$\alpha^{(1)} := dx - f(x, y, t)dt, \quad \alpha^{(2)} := dy - g(x, y, t)dt$$

and finally, (c) a two-form on $\mathcal{M} \times \mathbb{R}$ given by

$$\alpha^{(1)} \wedge \alpha^{(2)} = dx \wedge dy + (fdy - gdx) \wedge dt.$$

The classical Poincaré-Cartan form [29, 30] for a Hamiltonian H is given in the standard extended phase space coordinates $\{t, q^i, p^j \, 1 \geq i, j \geq n\}$, by

$$\Theta = p_i dq^i - Hdt. \tag{3.2}$$

The Poincaré-Cartan form consists of two terms - the standard "symplectic" 1-form $p_i dq^i$ and the Hamiltonian term. The duality between the Hamiltonian and Lagrangian formulations is well known by means of the Legendre transformation. Let $L : \mathbb{R} \times TQ \to \mathbb{R}$ be a non-autonomous Lagrangian. Let us recall that the Legendre transformation $FL : \mathbb{R} \times TQ \longrightarrow \mathbb{R} \times T^*Q$, is a fibre derivative. Given $f \in C^\infty(TQ, \mathbb{R})$ and a restriction $f_q := f|_{T_qQ}$ to the fibre over q, the fibre derivative of f is a mapping defined by

$$FL(f) : TQ \to T^*Q, \qquad FL\big(f(q, \dot{q})\big) := Df_q(\dot{q}).$$

The function f is said to be hyperregular if $FL(f)$ is a diffeomorphism. Therefore a Legendre transformation is locally given by

$$FL(t, q^i, \dot{q}^j) \equiv (t, q^i, FL(\dot{q}^j)) = (t, q^i, p_i = \partial L/\partial \dot{q}).$$

In terms of the jet coordinates $\{t, q^i, \dot{q}^j\}$ the one form Θ has a Lagrangian of the form

$$\Theta = Ldt + \frac{\partial L}{\partial \dot{q}^i}\big(dq^i - \dot{q}^i dt\big). \tag{3.3}$$

When L is hyperregular, i.e., FL is a diffeomorphism, then in such a situation both formulations are completely equivalent. Our focus here is on the Hamiltonian formulation. In Hamiltonian coordinates we have

$$d\Theta = \big(dp_i + \frac{\partial H}{\partial q^i}dt\big) \wedge \big(dq^i - \frac{\partial H}{\partial p_i}dt\big)$$

so the differential system takes the well-known Hamiltonian form

$$dp_i + \frac{\partial H}{\partial q^i}dt = 0, \qquad dq^i - \frac{\partial H}{\partial p_i}dt = 0.$$

In other words, if (3.1) admits a Hamiltonian description then

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}. \tag{3.4}$$

An alternative description is given in terms of the Euler vector field

$$X_E = \frac{\partial}{\partial t} + \frac{\partial H}{\partial p}\frac{\partial}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial}{\partial p}, \tag{3.5}$$

defined by

$$i_{X_E} d\Theta = 0 \qquad \text{and} \qquad i_{X_E} dt = 1. \tag{3.6}$$

Thus $X_E = \frac{\partial}{\partial t} + X_H$, where X_H is the standard Hamiltonian vector field defined by the canonical symplectic form $\omega = dp \wedge dq$. In fact the first equation yields the Hamiltonian equation in the following form

$$dH + i_{X_H}\omega = 0.$$

3.1 Jacobi's last multiplier and Hamiltonians

Our basic aim is to study the generalization of Hamiltonian mechanics and to construct an exact expression for dH using Jacobi's last multiplier. The algorithm to be employed for this purpose is based on an application of the exterior algebra and is described below. Let

$$\beta^{(1)} := dq - \frac{\partial H}{\partial p}dt, \quad \beta^{(2)} := dp + \frac{\partial H}{\partial q}dt. \tag{3.7}$$

Clearly the two-form

$$\Omega := \beta^{(1)} \wedge \beta^{(2)} = dq \wedge dp + (dH - \frac{\partial H}{\partial t}dt) \wedge dt = dq \wedge dp + dH \wedge dt, \tag{3.8}$$

and is *closed*. It is obvious that when (3.1) is expressible in the form of (3.4) then the two-form $\alpha^{(1)} \wedge \alpha^{(2)}$ must be proportional to the closed two-form $\beta^{(1)} \wedge \beta^{(2)}$, so that there exists a function $\sigma(x, y, t)$ such that

$$\sigma^{-1}[dx \wedge dy + (f dy - g dx) \wedge dt] = [dq \wedge dp + dH \wedge dt]. \tag{3.9}$$

Since the two-form on the rhs is necessarily closed it follows that we must have

$$\sigma^{-1}\left(\frac{\partial \sigma}{\partial t} + f\frac{\partial \sigma}{\partial x} + g\frac{\partial \sigma}{\partial y}\right) = \left(\frac{\partial f}{\partial x} + \frac{\partial g}{\partial y}\right). \tag{3.10}$$

The last equation may be written as

$$\frac{d \log \sigma}{dt} = \left(\frac{\partial f}{\partial x} + \frac{\partial g}{\partial y}\right),$$

and a comparison with (2.7), the determining equation for the JLM, shows that $\sigma^{-1} = \mu$. Hence from (3.9) we see that the existence of σ satisfying (3.10) implies that

$$\sigma^{-1}(fdy - gdx) = dH + \text{terms proportional to } \ dt, \tag{3.11}$$

provided $\frac{\partial \sigma}{\partial t} = 0$. The latter condition being true for autonomous differential equations.

For nonautonomous cases satisfying (3.9) form one must modify (3.11) by introducing two auxiliary functions ψ and ϕ [3] such that

$$\sigma^{-1}((f - \psi)dy - (g - \phi)dx) = dH + \text{terms proportional to } dt, \tag{3.12}$$

when $\frac{\partial \sigma}{\partial t} \neq 0$. This essentially removes the explicit time-dependent terms and allows for the construction of a Hamiltonian for the remaining autonomous part. However, the time dependence is not altogether lost; it being manifested in the the data of the new coordinates.

Note that (3.12) implies

$$\frac{\partial}{\partial x}\left(\sigma^{-1}(f - \psi)\right) + \frac{\partial}{\partial y}\left(\sigma^{-1}(g - \phi)\right) = 0. \tag{3.13}$$

It will now be observed that one may write (3.9) in the following manner

$$\sigma^{-1}[dx \wedge dy + (fdy - gdx) \wedge dt] = \sigma^{-1}[(dx - \psi dt) \wedge (dy - \phi dt) + (f - \psi)dy \wedge dt - (g - \phi)dx \wedge dt],$$

which in view of (3.12) becomes

$$\sigma^{-1}[dx \wedge dy + (fdy - gdx) \wedge dt] = \sigma^{-1}(dx - \psi dt) \wedge (dy - \phi dt) + dH \wedge dt. \tag{3.14}$$

But a comparison of (3.14) with (3.9) shows that

$$\sigma^{-1}(dx - \psi dt) \wedge (dy - \phi dt) = dq \wedge dp. \tag{3.15}$$

In view of (3.10) and (3.13) it is clear that the lhs of (3.15) is indeed closed. Thus the problem of recasting (3.1) into the form of Hamilton's equations reduces to a determination of the auxiliary functions ϕ and ψ such that H is identified from (3.12). As for the canonical variables q and p these are to be identified from (3.15) once ϕ and ψ are known and σ has been obtained by solving (3.10). We illustrate the application of the above procedure with a few examples.

4 Conformal Hamiltonians dynamics and activator-inhibitor system

Let (M, ω) be a symplectic manifold, where M is a differentiable manifold endowed with a symplectic form ω. Consider a diffeomorphism ϕ such that $(\phi^k)^*(\omega) = k\omega$, where $k \in \mathbb{R}$. The space of diffeomorphism $\{\phi^k\}$ form the pseudogroup $Diff^k_\omega$. Let $X_k \in Vect^k_\omega = T_{id}Diff^k_\omega$.

The vector field X_k is said to br conformal with parameter $k \in \mathbb{R}$ if the Lie derivative satisfies $L_{X_k}\omega = k\omega$.

We obtain $di_{X_k}\omega = k\omega$ using Cartan's magic formula, which imples ω must be exact, $\omega = -d\theta$. We assume $H^1(M) = 0$, then given X_k there exist a Hamiltonian function $H \in C^\infty(M)$ such that $X_k = X_H^k$ be a conformal vector field, which satisfies

$$i_{X_H^k}\omega = dH - k\theta.$$

Let Z be the Liouville vector field, given by $i_Z\omega = -\theta$ or $L_Z\omega = \omega$. We know for any $H \in C^\infty(M)$, we have $L_{X_H}\omega = 0$, hence it is clear $L_{X_H+Z}\omega = \omega$. Thus conformal vector field on M is given by $X_H^k = X_H + kZ$. Conversely, given X_H^k and $H^1(M) = 0$, using $i_{X_H^k}\omega = dH - k\theta$ and bundle morphism $\sharp : T^*M \to TM$, we abtain $(dH - k\theta)^\sharp = X_H + kZ$. Here we tacitly use the nondegeneracy of ω and $L_Z\omega = -d\theta = \omega$.
Putting all these arguments together we obtain the following result.

Theorem 4.1 *The conformal vector field X_H^k on the symplectic manifold $(T^*\mathbb{R}, \omega) \simeq (\mathbb{R}^2, \omega = dx \wedge dy)$ can be expressed $X_H + kZ$, where Z is the unique vector field defined by $i_Z\omega = -\theta$. Here $\theta = -ydx$ is the canonical one form of $T^*\mathbb{R}$. The equation described by the vector field X_H^k is given by*

$$\dot{x} = \frac{\partial H}{\partial y}, \qquad \dot{y} = -\frac{\partial H}{\partial x} - ky. \tag{4.1}$$

In this section we analyse Hamiltonian structure of both the activator-inhibitor systems. In the first case we map it to conformal Hamiltonian dynamics, but the Gierer-Meinhardt case yields almost conformal Hamiltonian structure.

4.1 Autocatalysis system and conformal Hamiltonian mechanics

Let us start our analysis with the autocatalysis system. One can check directly that Lie derivative of the dynamical vector field of the autocatalysis system satisfies $L_\Gamma\omega = (c + h)\omega$, hence Γ is said to be conformal vector field with parameter $c + h$. When we impose $c + h = 0$, Γ becomes symplectic or Hamiltonian vector field. When we restricted to the symplectic case, i.e., $c = -h$, the associated Hamiltonian is given by

$$H = a\log(b + y) - d\frac{x^2}{2} - cxy, \tag{4.2}$$

with standard Poisson Brackets $\{x, y\} = 1$ with the equations of motion given by

$$\dot{x} = \{x, H\} = \frac{\partial H}{\partial y} = \frac{a}{b + y} - cx$$

$$\dot{y} = \{y, H\} = -\frac{\partial H}{\partial x} = dx + cy.$$

When the manifold is $\mathbb{R}^2$ with coordinates (x, y) and $\omega = dx \wedge dy$, the conformal vector fieldsthose whose flow is conformalhave the form:

$$\dot{x} = \frac{\partial H}{\partial y}, \quad \dot{y} = -\frac{\partial H}{\partial x} + \kappa y$$

where $H : \mathbb{R}^2 \to \mathbb{R}$ is the Hamiltonian. Their flow has the property $\phi^*\omega = e^{\kappa t}\omega$, so the symplectic inner product of any two tangent vectors contracts exponentially if $\kappa < 0$. If ω is an locally symplectic structure (l.c.s.) then two l.c.s. ω and $\omega' = e^{\kappa t}\omega$ are conformally equivalent.

Thus general activator-inhibitor system can be expressed

$$\dot{x} = \frac{\partial H}{\partial y}, \quad \dot{y} = -\frac{\partial H}{\partial x} - (c + h)y.$$

Given $H \in C^\infty(M)$, the vector field Γ (or X^c_H- usual notation) satisfies

$$i_{X^c_H}\omega = dH - (c + h)\theta, \quad \theta = ydx$$

is conformal. The conformal vector field is given by $X_H + (c + h)Z$, where Z is defined by $i_Z\omega = -\theta$. Here it turns out $Z = y\partial_y$.

4.2 The Gierer-Meinhardt model and almost conformal Hamiltonian structure

At first we study $b = 1$ case, then the integrating factor becomes $\mu = u^{-2}$. Consider planar Hamiltonian system

$$\dot{u} = J(u, v)H_v, \qquad \dot{v} = -J(u, v)H_u,$$

where J is associated with the symplectic structure. Using last multiplier equation we obtain

$$\frac{d}{dt}\log\mu + \frac{\dot{J}}{J} = 0,$$

which yields $\mu = \frac{1}{J}$. Thus symplectic matrix is given by

$$\mathbb{J} = \begin{pmatrix} 0 & \mu^{-1} \\ -\mu^{-1} & 0 \end{pmatrix}.$$

Thus only multiplying with the inverse integrating factor $\mu^{-1} = u^2$ admits a Hamiltonian structure

$$H = \log v - u - \frac{v}{u}, \tag{4.3}$$

with fundamental Poisson Brackets given by

$$\{u, u\} = \{v, v\} = 0, \quad \{u, v\} = \mu^{-1} = u^2. \tag{4.4}$$

In general for any arbitrary nonsingular function $f(u)$ it is possible to change the nonstandard Poisson structure to standard Poisson structure by substituting $v \longmapsto f^{-1}(u)v$. Then the "new" Poisson bracket satisfies

$$\{u, v\}_f = f^{-1}(u)\{u, v\} = 1.$$

It is now easy to verify that the Hamiltonian (for nonstandard Poisson structure) equations

$$\dot{u} = \{u, H\} = u^2 \frac{\partial H}{\partial v} = -u + \frac{u^2}{v}, \tag{4.5}$$

$$\dot{v} = \{v, H\} = -u^2 \frac{\partial H}{\partial u} = u^2 - v, \tag{4.6}$$

reproduce the equations of the reduced system (2.17). Furthermore as $dH/dt = 0$ the Hamiltonian H is also a first integral of the reduced system (2.17). The Poisson structure associated with (4.4) is called nonstandard Poisson structure. It is clear that the equations (4.5) and (4.6) are not divergence free. The multiplication by the JLM μ yields volume preserving condition

$$\sum_{i=1}^{2} \frac{\partial}{\partial w_i} \mu \frac{dw_i}{dt} = 0, \qquad \text{where} \quad w_i = u, v,$$

so the phase space volume is preserved.

Let μ be the multiplier and the dynamical vector field associated to $b = 1$ Gierer-Meinhardt equation is given by

$$\Gamma = (-u + \frac{u^2}{v})\frac{\partial}{\partial u} + (u^2 - v)\frac{\partial}{\partial v}. \tag{4.7}$$

We consider transformation of vector field Γ corresponding to the transformation of Poisson bracket, $\Gamma \longmapsto \mu\Gamma$, which satisfies

$$i_{\mu\Gamma}\Omega = dH, \qquad \text{where} \qquad \Omega = du \wedge dv. \tag{4.8}$$

Here μ can be identified with the inverse integrating factor. The terminology "integrating factor" for the function V comes from the fact that $1/V$ is an integrating factor for the vector field Γ, i.e., that $V\Gamma$ is divergence-free. These allow the use of techniques from the theory of (local) Hamiltonian differential equations.

The vector field $\tilde{\Gamma}$ associated to the general equation satisfies

$$i_{\mu\tilde{\Gamma}}\Omega = dH - (b-1)\frac{dv}{u}. \tag{4.9}$$

Hence the conformal vector field can be decomposed into

$$\mu\tilde{\Gamma} = X_H - (b-1)u^{-1}\frac{\partial}{\partial u}, \tag{4.10}$$

where

$$X_H = (-\frac{1}{u} + \frac{1}{v})\frac{\partial}{\partial u} + (1 - \frac{v}{u^2})\frac{\partial}{\partial v}. \tag{4.11}$$

Thus we give a Hamiltonian description of the Gierer-Meinhardt model.

4.3 Application to non-Turing pattern formation: Gray-Scott model

Self-replicating patterns have recently been found in the reaction-diffusion of chemical species. Examples of such systems include the Gray Scott model, the Schnakenberg model etc. Numerical simulations show that the irreversible Gray-Scott model exhibits a broad array of new patterns, The irreversible Gray-Scott model governs the chemical reactions $U + 2V \to 3V$ and $V \to P$ in a gel reactor, where V catalyses its own reaction with U and P is an inert product. Letting $u = u(t)$ and $v = v(t)$ denote the concentrations of the two chemical species U and V, the pair of ordinary differential equations governing these reactions is :

$$\dot{u} = -uv^2 + \alpha(1-u) \tag{4.12}$$

$$\dot{v} = uv^2 - \beta v. \tag{4.13}$$

Here α denotes the rate at which u is fed from the reservoir into the reactor and β is the sum of α and the rate constant while k is the rate at which v is converted to an inert product.

We choose $\beta = -\alpha$, so the reduced Gray-Scott equation becomes

$$\dot{u} = vu^2 + \alpha u, \qquad \dot{v} = -vu^2 + \alpha(1-v), \tag{4.14}$$

This equation may be expressed in Hamiltonian form in the following manner:

$$\begin{pmatrix} \dot{u} \\ \dot{v} \end{pmatrix} = (J(u,v) \begin{pmatrix} \frac{\partial H_1}{\partial u} \\ \frac{\partial H_1}{\partial v} \end{pmatrix} - R(u,v) \begin{pmatrix} \frac{\partial H_2}{\partial u} \\ \frac{\partial H_2}{\partial v} \end{pmatrix}, \qquad H_1 = u + v, \qquad H_2 = \alpha(1-v)u. \tag{4.15}$$

where

$$J = \begin{pmatrix} 0 & vu^2 \\ -vu^2 & 0 \end{pmatrix} \qquad R = \begin{pmatrix} 0 & \alpha \\ -\alpha & 0 \end{pmatrix}.$$

Note that the (full) Gray-Scott model is given by

$$\begin{pmatrix} \dot{u} \\ \dot{v} \end{pmatrix} = (J(u,v) \begin{pmatrix} \frac{\partial H_1}{\partial u} \\ \frac{\partial H_1}{\partial v} \end{pmatrix} - R(u,v) \begin{pmatrix} \frac{\partial H_2}{\partial u} \\ \frac{\partial H_2}{\partial v} \end{pmatrix} - (\beta + \alpha) \begin{pmatrix} u \\ 0 \end{pmatrix}. \tag{4.16}$$

5 Contact geometry and Generalized Hamiltonian dynamics

The idea of using contact geometry in the context of classsical irreversible thermodynamics is an exciting area. This space permits us to encode thermodynamical constraints. We will see that all these activator-inhibitor equations can also be given Hamiltonian formalism using contact geometry.

Recall that a contact manifold is a pair (M, η) where η is a 1-form in the manifold M such that $\eta \wedge (d\eta)^{\wedge n}$ is a volume form in M. There is a uniquely defined vector field E (called Reeb or characteristic vector field) such that (see e.g. [19, 21])

$$i(E)\eta = 1, \qquad i(E)d\eta = 0. \tag{5.1}$$

For each function f in M there is a contact Hamiltonian vector field X_f such that

$$i(X_f)\eta = f, \qquad i(X_f)d\eta = df - E(f)\,\eta. \tag{5.2}$$

It is easy to check that if $c \in \mathbb{R}$, then $X_c = c\,E$ and in particular $X_1 = E$, and that $X_{f_1+f_2} = X_{f_1} + X_{f_2}$, while $X_{f_2\,f_1} = f_2\,X_{f_1} + f_1\,X_{f_2} - f_2\,f_1\,E$. Furthermore, $X_f(f) = f\,E(f)$ and more generally, $X_f(f^k) = k\,f^k\,E(f)$.

Consider the morphism $\sharp_\Lambda : \Omega^1(M) \to \mathcal{X}$ induced by Λ between C^∞-modules of one forms $\Omega(M)$ and vector fields $\mathcal{X}$ defined on M. This contact structure defines a Jacobi structure where the bivector field Λ is defined by $\Lambda(df_2, df_1) = d\eta(X_{f_2}, X_{f_1})$.

A Jacobi structure is the triplet (M, Λ, E) which satisfies the following integrability condition

$$[\Lambda, \Lambda] = 2E \wedge \Lambda, \qquad \mathcal{L}_E\Lambda = 0, \tag{5.3}$$

where $\mathcal{L}_E$ stands for Lie derivative with respect to E. If we drop the integrability conditions we obtain almost Jacobi structure. The bivector Λ defines a Jacobi bracket

$$\{f, g\} = \Lambda(df, dg) + fE(g) - gE(f), \qquad f, g \in C^\infty(M), \tag{5.4}$$

where the bracket is that of Schouten-Nijenhuis. This satisfies the weaker Leibnitz identity condition

$$\operatorname{supp}\{f, g\} \subseteq \operatorname{supp}\{f\} \cap \operatorname{supp}\{g\},$$

i.e., the support of $\{f, g\}$ is contained in the intersection of the supports of f and g. We recall that the support of a function is the closure of the set of points at which the function does not vanish. This condition imples that the Jacobi bracket is not a derivation in each argument, hence, the Leibniz derivation rule is weakened, but the Jacobi bracket satisfies Jacobi identity.

Vector fields associated with functions f on the algebra of smooth functions $C^\infty(M)$ are given by

$$X_f = \sharp_\Lambda(df) + fE.$$

This is known as Hamiltonian vector field with respect to Jacobi structure. The characteristic distribution $\mathcal{D}$ of TM is defined by Λ and E, given as

$$\mathcal{D}_x = \sharp_{\Lambda_x}(T_x^*M) + \Xi, \tag{5.5}$$

where Ξ denotes the subspace generated by the vector field E_p.

The analogous to Darboux theorem for symplectic manifolds establishes the existence of a set of coordinates (s, q^i, p^i), with $i = 1, \ldots, n$, such that

$$\eta = ds - \sum_{i=1}^{n} p_i\,dq^i \tag{5.6}$$

In such a coordinate set the expressions of E, Λ, $\{\cdot,\cdot\}$ and X_f are:

$$\begin{aligned} E &= \frac{\partial}{\partial s} \\ \Lambda &= \sum_{i=1}^{n}\left(\frac{\partial}{\partial q^i}\wedge\frac{\partial}{\partial p_i}+p_i\,\frac{\partial}{\partial s}\wedge\frac{\partial}{\partial p_i}\right) \\ \{f_1,f_2\} &= \left(f_1-\sum_{i=1}^{n}p_i\frac{\partial f_1}{\partial p_i}\right)\frac{\partial f_2}{\partial s}-\left(f_2-\sum_{i=1}^{n}p_i\frac{\partial f_2}{\partial p_i}\right)\frac{\partial f_1}{\partial s}+\sum_{i=1}^{n}\left(\frac{\partial f_1}{\partial q^i}\frac{\partial f_2}{\partial p_i}-\frac{\partial f_2}{\partial q^i}\frac{\partial f_1}{\partial p^i}\right) \\ X_f &= \left(\sum_{i=1}^{n}p_i\frac{\partial f}{\partial p_i}-f\right)\frac{\partial}{\partial s}+\sum_{i=1}^{n}\frac{\partial f}{\partial p_i}\,\frac{\partial}{\partial q^i}-\sum_{i=1}^{n}\left(\frac{\partial f}{\partial q^i}+p_i\frac{\partial f}{\partial s}\right)\frac{\partial}{\partial p_i} \end{aligned} \tag{5.7}$$

In the particular case of the damped harmonic oscillator the manifold M is $\mathbb{R}^3$ and η is then $\eta = ds - y\,dx$, and then the contact Hamiltonian vector field defined by the function f is:

$$X_f = \frac{\partial f}{\partial y}\frac{\partial}{\partial x}-\left(\frac{\partial f}{\partial x}+\frac{\partial f}{\partial s}\right)\frac{\partial}{\partial y}+\left(y\frac{\partial f}{\partial y}-f\right)\frac{\partial}{\partial s}.$$

Suppose (M,Λ,E) is a Jacobi manifold and $f\in C^\infty(M)$. Then it defines another Jacobi structure which is said to be f-conformal to the given one or almost Jacobi structure. The Reeb vector field E_f and the Poisson bivector Λ_f are modified by [21]

$$E_f = fE+\Lambda^\sharp(df),\qquad \Lambda = f\Lambda, \tag{5.8}$$

where $\Lambda^\sharp : T^*M\to TM$ stands for bundle morphism. This can be equivalently described in symplectic language when the Jacobi structure on M comes from a symplectic 2-form Ω, then almost Jacobi structure or f-conformal Jacobi structure is given by

$$\Lambda_f^\sharp = f(\Omega^\flat)^{-1},\qquad E_f = (\Omega^\flat)^{-1}(df)=\Lambda^\sharp(df). \tag{5.9}$$

One of our example, the Gierer-Meinhardt equation, belongs to this class.

5.1 Contact Hamiltonian description of conformal dynamics and reduced equations

We now reduce the original system (2.11) in a different way. We consider now $a=0$, i.e.

$$\dot{x} = \frac{a}{b+y},\qquad \dot{y} = d\,x - h\,y. \tag{5.10}$$

This equation can be well described by conformal Hamiltonian vector field $X_{H_t}+hZ$, where the "truncated Hamiltonian" is $H_t = a\log(b+y)-\frac{d}{2}x^2$. In this section we describe this equation in terms contact Hamiltonian formalism. The mixed term xy of the actual Hamiltonian acts like an entropy function. This can be viewed as the thermodynamical description of the equation (5.10).

The corresponding Hamiltonian $H_s = a\log(b+y) - \frac{d}{2}x^2 + hxy$ of the reduced system (5.10) can be expressed as $H_s = H + hS$. Here

$$H = a\log(b+y) - d\frac{x^2}{2}, \qquad \text{with} \qquad S = xy \equiv x\dot{x}.$$

Thus from the contact Hamiltonian equations of motion

$$\dot{x^i} = \frac{\partial H_s}{\partial y}, \qquad \dot{y} = -\frac{\partial H_s}{\partial x} - \frac{\partial H_s}{\partial S}y \qquad \dot{S} = y\frac{\partial H_s}{\partial y} - H_s,$$

we obtain the equations of the reduced activator-inhibitor model (2.11). Unlike the damped oscillator or Liénard system here the entropy function S flow satisfies

$$\dot{S} = \frac{ya}{b+y} - a\log(b+y) + \frac{d}{2}x^2.$$

A simple calculation shows

$$\frac{\partial \dot{S}}{\partial y} = -\frac{y^2 a}{(b+y)^2} \qquad \text{and} \ \frac{\partial \dot{S}}{\partial x} = dx.$$

Reduced GM equation Similarly, we can study the reduced form of the Gierer-Meinhardt equation $\dot{u} = \frac{u^2}{v}, \dot{v} = u^2 - kv$ using contact Hamiltonian framework. This equation can also be described via (almost) conformal Hamiltonian vector field $\tilde{J}X_{H_t} + kZ$, where $H_t = \log v - u$ is the truncated Hamiltonian and $\tilde{J} = u^2$ stands for multiplier.

We take away the mixed term v/u from the Hamiltonian $H = \log v - u - v/u$ just like the previous example. We identify the mixed term $s = -v/u$ as the entropy function. The contact Hamiltonian is defined as

$$H_s = \log v - u + S(s) = H_t + \tilde{S}(S), \qquad \text{where} \qquad S = ks.$$

Thus using

$$\dot{u} = u^2\frac{\partial h}{\partial v}, \qquad \dot{v} = -u^2\frac{\partial h}{\partial v} - v\frac{\partial S}{\partial s}$$

we obtain

$$\dot{u} = \frac{u^2}{v}, \qquad \dot{v} = u^2 - kv, \qquad \dot{s} = 1 - u + k\frac{v}{u}. \tag{5.11}$$

Hence we recast equation (5.11) in contact Hamiltonian form.

5.2 Full activator-inhibitor system and general Jacobi bracket

The full activator-inhibitor equation given in (2.11) can be described using the generalized Jacobi bracket formalism. We recall that on the compact set of $\mathbb{R}^{2n+1}$ we can define the contact one form as

$$\eta = ds + \sum_{j=1}^{n} \left(q^j dp_j - p_j dq^j\right).$$

This yields

$$\text{Ker } \eta = \left\{ (\frac{\partial}{\partial p_j} - q^j \frac{\partial}{\partial s}), (\frac{\partial}{\partial q^j} + p_j \frac{\partial}{\partial s}) \right\}.$$

In this setting the Jacobi vector field is defined as

$$\widehat{X}_f = \left(\sum_{i=1}^{n} p_i \frac{\partial f}{\partial p_i} - f \right) \frac{\partial}{\partial s} + \sum_{i=1}^{n} \left(\frac{\partial f}{\partial p_i} - q^i \frac{\partial f}{\partial s} \right) \frac{\partial}{\partial q^i} - \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q^i} + p_i \frac{\partial f}{\partial s} \right) \frac{\partial}{\partial p_i} \tag{5.12}$$

The vector field $\widehat{X}_f$ is the lifting of the Jacobi vector field to the generalized contact space $(\tilde{\Lambda}, E)$, where

$$\tilde{\Lambda} = \sum_{i=1}^{n} \left(\frac{\partial}{\partial q^i} \wedge \frac{\partial}{\partial p_i} + p_i \frac{\partial}{\partial s} \wedge \frac{\partial}{\partial q^i} - q^i \frac{\partial}{\partial s} \wedge \frac{\partial}{\partial p_i} \right). \tag{5.13}$$

In general, the flow $\hat{X}_f$ of (5.12) can be explicitly written in contact coordinates

$$\left\{ \begin{array}{rcl} \dot{q}^i & = & \frac{\partial f}{\partial p_i} - q^i \frac{\partial f}{\partial s}, \\ \dot{p}_i & = & -\frac{\partial f}{\partial q^i} - p_i \frac{\partial f}{\partial s}, \\ \dot{s} & = & p_i \frac{\partial f}{\partial p_i} - f \end{array} \right. \tag{5.14}$$

Now we choose contact Hamiltonian $H_s = H + S(s)$, and the two parameter generalized Jacobi vector field is defined as

$$\widehat{X}_s^{c,h} = \left(y \frac{\partial H_s}{\partial y} - H_s \right) \frac{\partial}{\partial s} + \left(\frac{\partial H_s}{\partial y} - cx \frac{\partial H_s}{\partial s} \right) \frac{\partial}{\partial x} - \left(\frac{\partial H_s}{\partial x} + hy \frac{\partial H_s}{\partial S} \right) \frac{\partial}{\partial y}, \tag{5.15}$$

This coincides with the usual one when $c = h = 1$. We obtain our equation using this two parameter deformed Jacobi vector field.

We can recast these equations as

$$\dot{x} = \frac{\partial h}{\partial y} - c \frac{\partial S}{\partial y}, \qquad \dot{y} = -\frac{\partial h}{\partial x} - h \frac{\partial S}{\partial x}, \tag{5.16}$$

where

$$h = a \log (b + y) - \frac{1}{2} d x^2, \qquad \text{and} \qquad S = xy.$$

This is a metriplectic way of writing the activator-inhibitor equation. If we include the "entropy" s equation, then the system contact lift of metriplectic systems. The idea of lifting a n-dimensional vector field to the contact phase space was introduced in the context of controlled irreversible systems by Eberard et al., where the contact lift was generated by the contact Hamiltonian function.

Illustration 2 : The (full) Gierer-Meinhardt equation

$$\dot{u} = a - bu + \frac{u^2}{v}, \qquad \dot{v} = u^2 - v,$$

where as usual u and v stand for activator and inhibitor respectively. The two parameter (almost) generalized Jacobi vector field is given by

$$\widehat{X}_s^{c,h} = \left(v\frac{\partial H_s}{\partial v} - H_s\right)\frac{\partial}{\partial s} + \left(J(u,v)\frac{\partial H_s}{\partial v} - (bu-a)\frac{\partial H_s}{\partial s}\right)\frac{\partial}{\partial u} - \left(J(u,v)\frac{\partial H_s}{\partial u} + v\frac{\partial H_s}{\partial S}\right)\frac{\partial}{\partial y},$$

where $J(u,v) = u^2$, $H_s = h + S(s) = \log v - u + s$. This equation can also be recasted to

$$\dot{u} = u^2\frac{\partial h}{\partial v} - (bu-a)\frac{\partial h}{\partial s}, \qquad \dot{v} = -u^2\frac{\partial h}{\partial u} - v\frac{\partial h}{\partial s}. \tag{5.17}$$

6 Equivalence problem and dissipative potentials for pattern formation equations

This section addresses the problem of deriving a generalized Hamiltonian potential for autonomous dynamical systems appearing in Turing pattern formation. Following [13], we know that for a given vector field one can construct a locally defined dissipative Hamiltonian generating function for autonomous dynamical systems. In their paper Hudon et al. proposed to study the local equivalence problem between a known autonomous vector field and a predefined Hamiltonian dissipative realization, viewed as a reference system. We explain their formalism in the next section.

6.1 Method and computation of a dissipative potential

It is useful to state the method from an algorithmic point of view. We consider here only planar systems and refer to [13] for further details.

1. Let $\Omega = dx \wedge dy$. Obtain a one-form (which is possibly non-closed) by taking the interior product of Ω with respect to the given vector field $\Gamma = f_1(x,y)\partial_x + f_2(x,y)\partial_y$ associated nonlinear dynamical system, i.e., $\omega = i_\Gamma \Omega$.

2. Let $\mathcal{X} = x\partial_x + y\partial_y$ be the Liouville vector field given in a star-shaped domain. An open subset S of $\mathbb{R}^n$ is said to be star-shaped with respect to a point $\tilde{\mathbf{p}} = (\tilde{x}_1, \cdots, \tilde{x}^n) \in S$ if the following conditions hold: (a) S is contained in a coordinate neighborhood U of $\tilde{\mathbf{p}}$; (b) The coordinate functions of U assign coordinates $(\tilde{x}_1, \cdots, \tilde{x}^n)$ to $\tilde{\mathbf{p}}$; (c) If $\tilde{\mathbf{p}}$ is any point in S with coordinates $(x_1, \cdots, x_n)$ assigned by functions of U , then the set of points $(\tilde{x} + \lambda(x - \tilde{x}))$ belongs to S, for all $\lambda \in [0,1]$.

3. A homotopy operator is constructed on a star-shaped domain, via

$$\big(\mathbb{H}\omega\big) = \int_0^1 i_{\mathcal{X}}\omega\big(\lambda x, \lambda y\big)d\lambda = \tilde{F}(x,y),$$

to decompose the non-closed one-form into its exact and non-exact parts. The homotopy operator $\mathbb{H}$ is a linear operator on elements of $\Lambda^k(\mathbb{R}^n)$ that satisfies the identity $\omega = d(\mathbb{H}\omega) + \mathbb{H}\omega$.

4. The exact part $\omega_e = \frac{\partial \tilde{F}}{\partial x}dx + \frac{\partial \tilde{F}}{\partial y}dy$ is used to derive a dissipative potential, while the non-exact part is associated with a non-dissipative potential that does not contribute to the dissipative potential on the star- shaped region.

5. (Equivalence of closed one-forms [5]) The goal is to compute a change of coordinates to express ω_e and the dissipative function. Suppose there exists a diffeomorphism $\Phi(\mathbf{x}) = \mathbf{z}$ preserving the exact form

$$\Phi^*(\tilde{\omega}_e) = \omega_e = \big(\frac{\partial F}{\partial x_i}dx_i\big), \qquad \text{where} \quad \tilde{\omega}_e = \sum_{i=1}^{2} -z_i dz_i.$$

Locally it is given by

$$dz_1 \wedge dz_2 = \big(\frac{\partial^2 F}{\partial x^2} + \frac{\partial^2 F}{\partial y^2}\big)dx \wedge dy.$$

6. z satisfy dissipative Hamiltonian equation

$$\dot{z} = \big(J(z) - R(z)\big)\nabla H(z), \qquad H(z) = \frac{1}{2}\big(z_1^2 + z_2^2\big),$$

where J is the standard symplectic matrix and $R = id_{2\times 2}$.

We must emphasize here that in order to compute the dissipative potential, we study the equivalence problem [5] between the closed one-form and a reference closed one-form derived from a known dissipative Hamiltonian realization. The locally defined dissipative potential for the original system is then expressed in these coordinates.

Now we state our result:

Claim 6.1 *a) The dissipative potential F computed from the homotopy operator $\mathbb{H}$ in the star shaped domain for the Gierer-Meinhardt equation*

$$\dot{u} = a - bu + \frac{u^2}{v}, \qquad \dot{v} = u^2 - v,$$

is given by

$$F = av - \frac{1}{2}(b-1)uv + \frac{u^2}{2} - \frac{u^3}{3},$$

and based on the equivalence of the closed one-forms we obtain new coordinates

$$z_1 = \big(-\frac{1}{2}(b-1)v + u(1-u)\big) \qquad z_2 = \big(a - \frac{1}{2}(b-1)u. \tag{6.1}$$

b) The dissipative potential and transformed coordinates of the activator inhibitor system.

$$\dot{x} = \frac{a}{b+y} - cx, \qquad \dot{y} = dx - hy$$

are given by

$$F = -\frac{1}{2}dx^2 + \frac{1}{2}(h-c)xy + a\log(y+b) - a\log b,$$

$$z_1 = -dx + \frac{1}{2}(h-c)y, \qquad z_2 = \frac{1}{2}(h-c)x + a\frac{dy}{b+y}.$$

The dissipative Hamilton generating function F derived for the activator-inhibitor pattern formation equation is the " free energy" of the associated system. Hence we can write $F = H + \lambda S$ up to some constant term, where H is the Hamiltonian and S stands for entropy function:

$$F_{AI} = H_{AI} - \frac{1}{2}S_{AI}, \qquad H_{AI} = -\frac{1}{2}dx^2 + a\log(y+b), \qquad S = (h-c)xy + 2a\log\, b, \quad (6.2)$$

where the last term of S is a constant one. But this observation is not valid for almost conformal Hamiltonian system like the Gierer-Meinhardt equation.

7 Conclusion

In this paper we have studied the Hamiltonization of systems of equations appearing in Turing as well as non-Turing pattern formations. The Hamiltonians described here are true in the sense that they allow us to reproduce the original equations through the standard Hamilton equations, although they are non-standard in nature. In fact, the method described here is specifically suited for systems which are intrinsically described by singular Lagrangians. We took three different types of systems, activator-inhibitor equation is described by conformal Hamiltonian mechanics, where as the Gierer-Meinhardt equation and the Gray-Scott equation are described by almost conformal and conformal with two potentials respectively. In particular, we have shown all these equations can be mapped to the framework of generalized classical mechanics using conformal, almost conformal or contact and f-conformal Jacobi geometry.

Using [13] we formulated the dissipative Hamilton generating potential F and study equivalence of closed one-forms for activator-inhibitor model and the the Gierer-Meinhardt equation. We have demonstrated that F is free energy function for the first model, which is a pure conformal class system. We now wish to find its connection to other systems. It would be interesting to study whether the formulation described here can be applied to other activator-inhibitor models; in particular to the Thomas model [22], proposed in 1975, which is an empirical model based on a specific reaction involving uric acid and oxygen. We propose to take up this issue in future.

Another interesting topic is to investigate the pattern formation equations of non-planar systems. Indeed in an interesting paper Wojkowski and Liverani [35] have studied the Lyapunov spectrum in locally conformal Hamiltonian systems and it has been demonstrated that Gaussian isokinetic dynamics, Nośe-Hoovers dynamics and other systems can also be studied through locally conformal Hamiltonian systems.

Acknowledgments

We would like to express our sincere appreciation to Professors Pepin Carinẽna, Ogul Esen, Christophe Soulé, Gerrado Torres del Castillo, Rui Diláo, Nadya Morozova, Bob Penner and Debshankar Roy for their interest and valuable comments in various stages of our work. This

work was done while PG was visiting IHES. He would like to express his gratitude to the members of IHES for their warm hospitality, especially to Christophe Soulé and Bob Penner for their constant encouragement.

References

[1] A. Bravetti, H. Cruz and D. Tapias, Contact Hamiltonian mechanics, *Ann. Phys.* **376** (2017) 17-39.

[2] J.F. Cariñena and P.Guha, *Non-standard Hamiltonian structures of Liénard equation and contact geometry*, Int.J. Geom. Modern Phys. (to appear).

[3] G. F. Torres del Castillo, *The Hamiltonian description of a second-order ODE*, J.Phys. A Math. Theor. **43** (2009) 265202 (9pp).

[4] A. Doelman, T. J. Kaper, and P. A. Zegeling, *Pattern formation in the 1-D Gray-Scott model*, Nonlinearity 10 (1997) 523-563.

[5] R. B. Gardner. *The Method of Equivalence and Its Applications*, SIAM, Philadelphia, PA, 1989.

[6] A. Ghose Choudhury, P. Guha and B. Khanra, *On the Jacobi last multiplier, integrating factors and the Lagrangian formulation of differential equations of the Painlevé-Gambier classification*, J. Math. Anal. Appl. 360 (2009), no. 2, 651–664.

[7] A. Ghose Choudhury and P. Guha, *Application of Jacobi's last multiplier for construction of Hamiltonians of certain biological systems*, Cent. J. Eur. Phys. 10(2) (2012) 398-404.

[8] A. Gierer and H. Meinhardt, *A theory of biological pattern formation.* Kybernetik 12 (1972) 30-39.

[9] A. Goriely, *Integrability and nonintegrability of dynamical systems.* Advanced Series in Nonlinear Dynamics, 19. World Scientific Publishing Co., Inc., River Edge, NJ, 2001. xviii+415 pp.

[10] M.I. Granero-Porati and A. Porati, *Temporal organization in a morphogenesis field*, J. Math. Biol 20 (1984) 153-157.

[11] P. Gray and S. K. Scott, *Chemical oscillations and instabilities*, Oxford University Press, Oxford, 1994, pp. 219-229.

[12] P. Guha and A. Ghose Choudhury, *Hamiltonization of Higher-Order Nonlinear Ordinary Differential Equations and the Jacobi Last Multiplier*, Acta Appl. Math (2011) 116:179-197.

[13] N. Hudon, K. Höffner and M. Guay, *Equivalence to dissipative Hamiltonian realization*, Proceedings of the 47th IEEE Conference on Decision and Control Cancun (Mexico, Dec. 9-11, 2008), pp 163 - 3168.

[14] C.G.J. Jacobi, *Sul principio dell'ultimo moltiplicatore, e suo uso come nuovo principio generale di meccanica,* Giornale Arcadico di Scienze, Lettere ed Arti **99** (1844), 129-146.

[15] C.G.J. Jacobi, *Theoria novi multiplicatoris systemati aequationum differentialium vulgarium applicandi,*J. Reine Angew. Math **27** (1844), 199-268, *Ibid* **29**(1845), 213-279 and 333-376. Astrophys. Journal, **342**, 635-638, (1989).

[16] C. A. Lucey, E. T. Newman, *On the construction of Hamiltonians*, J. Math. Phys. 29 (1998) 2430.

[17] A. Kirillov, *Local Lie algebras*, Russian Math. Surveys 31 (1976) 55-75.

[18] M.C.Nucci and P.G.L.Leach, *Jacobi's last multiplier and Lagrangians for multidimensional systems.arXiv:0709.3231v1.*

[19] A. Lichnerowicz, *Les varités de Jacobi et leurs algébres de Lie associées*, J. Math. pures et appl. 57 (1978) 453-488.

[20] C.-M. Marle, *A property of conformally Hamiltonian vector fields: Application to the Kepler problem*, arXiv:1011.5731v2 [math.SG] (2010).

[21] C.-M. Marle, *On Jacobi manifolds and Jacobi bundles*, in Symplectic Geometry, Groupoids, and Integrable Systems pp 227-246, edited by P. Dazord and A. Weinstein, Mathematical Sciences Research Institute Publications 20, Springer-Verlag (1991) New York Berlin Heidelberg.

[22] J. D. Murray, *Mathematical Biology I: An Introduction, volume I*, Springer-Verlag, 3rd edition, 2003. *Mathematical Biology II: Spatial Models and Biomedical Applications*, 3rd ed. Springer-Verlag, New York, 2003

[23] R.I. McLachlan and M. Perlmutter, *Conformal Hamiltonian systems*, J. Geom. Phys. 39 (2001) 276-300.

[24] A. Minarsky, N. Morozova, R. Penner and C. Soulé, *The theory of morphogenesis*IHES/M/17/13.

[25] M.C.Nucci, *Jacobi last multiplier and Lie symmetries: a novel application of an old relationship*, J. Nonlinear Math. Phys. 12 (2005) 284304.

[26] M.C.Nucci and K M Tamizhmani *Lagrangians for biological systems*, *arXiv:1108.2301v1.*

[27] G.H. Paine, *The development of Lagrangians for biological models*, Bull. Math. Biol. **44** (1982) 749-760.

[28] S. Ruan, *Diffusion-driven instability in the Gierer-Meinhardt model of morphogenesis*, Natural Resourse Modeling 11, no. 2, summer 1998.

[29] G. Sardanashvily, *Hamiltonian time-dependent mechanics*, J. Math. Phys. 39 (1998), no. 5, 2714–2729.

[30] J. Struckmeier, *Hamiltonian dynamics on the symplectic extended phase space for autonomous and non-autonomous systems*. J. Phys. A 38 (2005), no. 6, 1257–1278.

[31] D.S. Tourigny, *Two-component feedback loops and deformed mechanics*, Phys. Lett. A 379 (4) (2015) 342-347.

[32] S.L. Trubatch and A. Franco, *Canonical Procedures for Population Dynamics*, J. Theor. Biol. **48** (1974) 299-324.

[33] A.M. Turing, *The chemical basis of morphogenesis*. Phil. Trans. R. Soc. Lond. B237, 37-72 (1952).

[34] E.T. Whittaker, *A Treatise on the Analytical Dynamics of Particles and Rigid Bodies*. Cambridge University Press, Cambridge, 1988.

[35] M. P. Wojtkowski and C. Liverani, *Conformally symplectic dynamics and symmetry of the Lyapunov spectrum*, Comm. Math. Phys., 194 (1998) 4760.