

Thermodynamic geometry and critical aspects of bifurcations

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This work presents an exploratory study of the critical aspects of some well-known bifurcations in the context of thermodynamic geometry. For each bifurcation its *normal form* is regarded as a geodesic equation of some model analogous to a thermodynamic system. From this hypothesis it is possible to calculate the corresponding metric and curvature and analyze the critical behavior of the bifurcation.

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I. INTRODUCTION

The mean-field approximation is widely used in the study of complex systems. In such an approach the time evolution of the variable(s) $\vec{x} \in \mathbb{R}^D$ is described by a system of coupled differential equations [1]. For $D = 1$

$$\dot{x} \equiv \frac{d}{d\tau}x = \phi(x, \mu), \quad (1)$$

where μ is a control parameter.

Systems described by Eq. (1) may have bifurcations when μ reaches a critical value μ_c . Bifurcation is a qualitative change that occurs in the behavior of a dynamic system when the value of a control parameter (μ) undergoes a small and smooth change. In complex systems bifurcations are in general associated with critical transitions in many different contexts: from ecosystems to models of information traffic on the Internet, and from epidemic to social models [1].

But if a complex system undergoes a transition when $\mu \sim \mu_c$, it could be interesting to further investigate the critical aspects of such a transition. Inspired by thermodynamic geometry (TG), we develop in this paper an exploratory study of critical aspects of bifurcations.

TG is an approach based on Riemannian geometry for the study of thermodynamical and statistical mechanical systems in equilibrium. The main idea is that the space (manifold) of equilibrium states of a system is described by a metric, which in turn is proportional to the Hessian matrix of entropy (or other thermodynamic potential) of the system with respect to the thermodynamic parameters. In this context, the notion of “distance” between two states is associated with probability of fluctuation between them: the less likely the fluctuation between the states, the more distant they are.

From the metric one can obtain the curvature scalar R , which is proportional to the correlation volume ξ^d and therefore closely related to phase transitions.

Our main objective here is to study the critical aspects of bifurcations using, with some adaptations, the tools provided by thermodynamic geometry. For this purpose we consider the normal form of a bifurcation as a geodesic equation of some hypothetical model. Eventually the curvature scalar of the bifurcation can be obtained by an analysis of the inferred metric tensor. For illustrating the approach proposed, we analyze three well-known bifurcations: transcritical, saddle node, and pitchfork. For each case it was observed that the corresponding curvature diverges, according to a power law, for $\mu \rightarrow \mu_c$. From the point of view of TG, that is a typical

behavior of continuous phase transition, and it is possible to obtain a critical exponent from the curvature.

The paper is organized as follows. A brief summary of the formalism of TG and how it is applied to the study of phase transitions are presented in next section. In Sec. III a strategy is proposed of how to apply TG for the study of bifurcations. In Sec. IV the strategy is applied for three bifurcations; the corresponding curvatures are computed and analyzed. Conclusions are presented in Sec. V.

II. THERMODYNAMIC GEOMETRY AND PHASE TRANSITIONS

Thermodynamic geometry (TG) is an approach based on Riemannian geometry for studying equilibrium thermodynamics, with a relevant role in the study of phase transitions. The main idea is that all physical properties of the system under consideration are encoded in the metric that describes its thermodynamic state space.

The line element between two equilibrium states is given by (following the Einstein summation notation¹)

$$d\ell^2 = g_{ij}(X)dX^i dX^j \equiv \sum_{i,j} g_{ij}(X)dX^i dX^j, \quad (2)$$

where X^i are the “coordinates” of the thermodynamic state space (which can be the parameters such as temperature, density, chemical potential, etc.) and the metric tensor g_{ij} is proportional to the Hessian of entropy or of free energy [2]. For a single-component fluid system, the metric tensor is given by

$$g_{ij} = -\frac{1}{k_B} \frac{\partial^2 s(u, \rho)}{\partial X^i \partial X^j}, \quad i, j = 1, 2 \quad (3)$$

where k_B is the Boltzmann constant, s is entropy density, and the “coordinates” $X^1 = u, X^2 = \rho$ are internal energy and particle number per unit volume, respectively.

By appropriate changes of coordinates and using the Maxwell relations one can obtain other forms for the metric [2]. For example, the following line element (again for a single-component fluid system) has a diagonal metric:

$$d\ell^2 = \frac{1}{k_B T} \left[\frac{\partial^2 f}{\partial \rho^2} d\rho^2 - \frac{\partial^2 f}{\partial T^2} dT^2 \right], \quad (4)$$

¹Einstein summation notation: when an index variable appears twice in a single term (and not otherwise defined), it implies summation of that term over all the values of the index.

where $f(\rho, T) = u - T \cdot s$ is the Helmholtz free energy per unit volume. By a formal analogy between magnetic and fluid systems, Eqs. (3) and (4) above can also be used for magnetic systems by replacing ρ with m , the magnetization per spin [2].

The main purpose in TG is to obtain the curvature scalar (or thermodynamic curvature) R from the metric that describes the thermodynamic state space. Several studies suggest the physical interpretation of thermodynamic curvature R : in models with phase transitions [3,4] one can observe that R is proportional to the correlation volume ξ^d (where ξ is the correlation length and d the spatial dimensionality), mainly in the critical region. The sign of R appears to be related with the character of interparticle interactions: $R > 0$ if repulsive interactions dominate and $R < 0$ if attractive interactions dominate. See [5] and references therein. And for a single-component classical ideal gas the curvature is zero, indicating the absence of interactions and phase transitions.

With the thermodynamic curvature one can study all the phase diagrams of a system. Several examples of application for fluid and magnetic systems can be found, for instance, in [4,6,7].

In summary, given a thermodynamic potential of the system under consideration, one can compute the metric of the corresponding state space, by taking the second derivatives of the potential with respect to the coordinates (thermodynamic parameters). Eventually from the metric one can obtain the thermodynamic curvature R . On the other hand, once the metric is given, in general it is not a trivial task to obtain R . The usual steps in Riemannian geometry are as follows: (i) calculate the Christoffel symbols

$$\Gamma_{ij}^n = \frac{1}{2} g^{nk} (g_{ki,j} + g_{kj,i} - g_{ij,k}), \quad (5)$$

where g^{ij} (with upper indices) is the inverse of the metric, $g^{ij} g_{jk} = \delta^i_k$, and with the following notation: $g_{ki,j} = \partial_j g_{ki} = \partial g_{ki} / \partial X^j$; (ii) compute the fourth-rank (Riemann) curvature tensor

$$R_{ijk}^\ell = \partial_j \Gamma_{ik}^\ell - \partial_k \Gamma_{ij}^\ell + \Gamma_{jn}^\ell \Gamma_{ik}^n - \Gamma_{kn}^\ell \Gamma_{ij}^n; \quad (6)$$

and finally (iii) the curvature scalar R is given by²

$$R = g^{ij} g^{\ell m} R_{i\ell j m}, \quad (7)$$

For more details, see [2] and references therein.

One can also study the phases of a system with geodesics [8,9], curves between two points (in this case two thermodynamic states) that extremize the line element. In curved spaces geodesics play the same role of straight lines in flat spaces. The geodesic curves are solutions of a set of coupled nonlinear differential equations

$$\ddot{X}^\ell + \Gamma_{jk}^\ell \dot{X}^j \dot{X}^k = 0, \quad (8)$$

where each dot over X denotes a derivative with respect to τ , a variable that parametrizes the curve joining the two points and can be thought of as ‘‘time.’’ If one considers the diagonal metric of Eq. (4) it is not difficult to note that in the inverse metric (g^{ij}) will appear the inverse of second derivatives

of the free energy, and as a consequence the corresponding geodesic equations and (Riemannian) curvature scalar will be singular in the spinodal curve. Nearby the critical point the thermodynamic curvature follows a power law [2]

$$R \sim t^{\alpha-2}, \quad t = (T - T_c)/T_c, \quad (9)$$

where α is the critical exponent related to heat capacity. In a classical thermodynamical model (e.g., van der Waals) R is singular in the spinodal line and nearby the critical point it behaves as $R \sim t^{-2}$, indicating that $\alpha = 0$, as one would expect for mean-field theories.

In Refs. [8,9] the geodesic equations of the van der Waals model are studied. A natural question one could ask is whether given an arbitrary set of initial conditions [in this case, $X_0 \equiv (T_0, \rho_0)$ and $\dot{X}_0 \equiv (\dot{T}_0, \dot{\rho}_0)$] in the liquid phase, for instance, the geodesic reaches the other phase or terminates at the coexistence curve. After numerical analysis they conclude that (i) a geodesic beginning in a gas or liquid phase (with temperature below the critical temperature) does not reach the other phase; it either terminates at the spinodal curve or continues in the (thermodynamical) supercritical region; (ii) the geodesics do not show any special behavior at the coexistence (or binodal) curve, which is not so surprising since metric and curvature are both regular in that curve. A similar behavior for the geodesics is observed for the Curie-Weiss ferromagnetic model in Ref. [9].

III. TG AND BIFURCATIONS

For the study of critical aspects of bifurcations, the normal form of a bifurcation was regarded as a geodesic equation of a hypothetical model (M) analogous to some thermodynamical system. In Ref. [10] a mathematical model for phase transitions is discussed in the framework of bifurcation theory. There the time evolution of the order parameter x is described by a nonlinear first-order differential equation [see Eq. (1) of Ref. [10]]

$$\dot{x} \equiv \frac{dx}{d\tau} = f(x; \alpha_1, \dots, \alpha_n), \quad (10)$$

where $\alpha_1, \dots, \alpha_n$ are the control parameters. We follow a similar approach here: Eq. (10) is the normal form of a bifurcation, with only one control parameter ($\alpha_1 = \mu$), equivalent to Eq. (1), with x and μ playing, respectively, the analogous role of the magnetization and the (reduced) temperature in a model of magnetic system, for example. But it is necessary to transform the above equation in order to make it similar to Eq. (8); such a transformation will be shown later.

The bifurcations analyzed here are described by one-dimensional (1D) differential equations such as Eq. (1). In general, one considers that μ is constant. However, in the framework of TG it is interesting to consider x and μ as variables, in order to establish an analogy with thermodynamics. Moreover, the system

$$\dot{x} = \phi(x, \mu), \quad \dot{\mu} \approx 0 \quad (11)$$

is equivalent to Eq. (1). It is considered here a state space described by the pair of coordinates (x, μ) .

²By contraction with the metric it is possible to lower indices, e.g., $g_{ln} R_{ijk}^n = R_{lij k}$.

With $X^1 = x$ and $X^2 = \mu$, we considered that the metric is diagonal [analogous to Eq. (4) above] with the ansatz

$$g_{11} = \mathcal{F}(x, \mu), \quad g_{22} = \mathcal{G}(x, \mu), \quad g_{12} = 0 = g_{21}. \quad (12)$$

For such a metric the Christoffel symbols are given by partial derivatives of \mathcal{F} and \mathcal{G} , and the geodesic equations are

$$\ddot{x} = -\left(\frac{1}{\mathcal{F}} \frac{\partial \mathcal{F}}{\partial \mu}\right) \dot{x} \dot{\mu} - \frac{1}{2} \left(\frac{1}{\mathcal{F}} \frac{\partial \mathcal{F}}{\partial x}\right) \dot{x}^2 + \frac{1}{2} \left(\frac{1}{\mathcal{F}} \frac{\partial \mathcal{G}}{\partial x}\right) \dot{\mu}^2, \quad (13)$$

$$\ddot{\mu} = -\left(\frac{1}{\mathcal{G}} \frac{\partial \mathcal{G}}{\partial \mu}\right) \dot{x} \dot{\mu} + \frac{1}{2} \left(\frac{1}{\mathcal{G}} \frac{\partial \mathcal{F}}{\partial \mu}\right) \dot{x}^2 - \frac{1}{2} \left(\frac{1}{\mathcal{G}} \frac{\partial \mathcal{G}}{\partial \mu}\right) \dot{\mu}^2. \quad (14)$$

One should notice that μ also depends on “time” and the curvature scalar depends on the partial derivatives of \mathcal{F} and \mathcal{G} . The idea here is to obtain the metric, i.e., write \mathcal{F} and \mathcal{G} in terms of ϕ , by comparing the (transformed) normal form of some bifurcation with Eq. (13) and thus compute the corresponding curvature scalar. Now Eq. (1) must be transformed into a form similar to Eq. (13) above. We use here the same procedure used in Ref. [11] to rewrite Eq. (1) as a second order differential equation: (i) derive Eq. (1) with respect to time, but also considering μ as a function of time and (ii) divide the resulting equation by Eq. (1). Therefore, Eq. (1) becomes

$$\ddot{x} = \frac{1}{\phi} \frac{\partial \phi}{\partial x} \dot{x}^2 + \frac{1}{\phi} \frac{\partial \phi}{\partial \mu} \dot{x} \dot{\mu}, \quad (15)$$

and by comparing it with Eq. (13) one can observe that

$$\begin{aligned} \left(\frac{1}{\mathcal{F}} \frac{\partial \mathcal{F}}{\partial x}\right) &= (-2) \left(\frac{1}{\phi} \frac{\partial \phi}{\partial x}\right), \\ \left(\frac{1}{\mathcal{F}} \frac{\partial \mathcal{F}}{\partial \mu}\right) &= -\left(\frac{1}{\phi} \frac{\partial \phi}{\partial \mu}\right), \end{aligned} \quad (16)$$

and \mathcal{G} is not a function of x . On the other hand, in the study of dynamical systems one usually considers μ as a constant, and there is no equation describing the time evolution of μ . In order to simplify the calculations it is considered here that $\mathcal{G} = C = \text{const}$.

Solutions of Eqs. (16) can be obtained for (multiplicatively) separable functions: $\mathcal{F}(x, \mu) = F_1(x)F_2(\mu)$ and $\phi(x, \mu) = \xi(x)\eta(\mu)$. One can easily observe that

$$\mathcal{F}(x, \mu) = \frac{A}{[\xi(x)]^2 \eta(\mu)}, \quad (17)$$

with $A = \text{const}$, satisfies Eqs. (16).

Our approach presented above is not a new idea. In Ref. [11] ordinary differential equations are considered as geodesic equations in order to obtain their invariants. However, one should note that we do not use the Riemann extension of Ref. [11] for computing invariants of a system of equations.

Brief summary of the approach

It is assumed here that there is some hypothetical model M , whose dynamical behavior is described by $\dot{x} = \phi(x, \mu)$. The space of states of M has a line element $d\ell^2 = \mathcal{F}(x, \mu)dx^2 + C d\mu^2$, with \mathcal{F} given by Eq. (17), and C is a constant. M is analogous to some thermodynamic model in such a way that x and μ are analogous to the order parameter and to (reduced) temperature, respectively.

Following the usual steps of Riemannian geometry, one can compute the geodesic equations

$$\ddot{x} = \left(\frac{1}{\xi} \frac{d\xi}{dx}\right) \dot{x}^2 + \left(\frac{1}{\eta} \frac{d\eta}{d\mu}\right) \dot{x} \dot{\mu}, \quad (18)$$

$$\ddot{\mu} = -\frac{A}{2C} \frac{d\eta}{d\mu} \frac{1}{[\xi(x)\eta(\mu)]^2} \dot{x}^2. \quad (19)$$

It is not difficult to see that Eq. (18) is exactly Eq. (15) with the condition $\phi(x, \mu) \equiv \xi(x)\eta(\mu)$. Equation (19) in turn has actually a simple form:

$$\ddot{\mu} = -\frac{A}{2C} \frac{d\eta}{d\mu}. \quad (20)$$

And the curvature scalar is given by

$$R = \left[\frac{1}{C\eta} \frac{d^2\eta}{d\mu^2} - \frac{3}{2C} \left(\frac{1}{\eta} \frac{d\eta}{d\mu}\right)^2 \right]. \quad (21)$$

Usually in complex (or dynamical) systems one does not take into account the time dependence of the control parameter, just by assuming it is a constant. On the other hand, A and C are arbitrary constants, so one can consider $A \ll C$ in such a way that $\ddot{\mu} \approx 0$ and μ is nearly constant.

Some illustrative examples of the proposed approach are provided in the next section. However, in general the right-hand side of normal forms [Eq. (1)] are not separable functions of x and μ , i.e., $\phi(x, \mu) \neq \xi(x)\eta(\mu)$. But it is possible to change variables in such a way to obtain a separable function of x and μ .

IV. ANALYZING THE BIFURCATIONS

For the examples below, the normal forms of bifurcations are written in terms of the variables $y = y(\tau)$ and σ (= control parameter), with the dynamics governed by a differential equation of the form $\dot{y} = f(y, \sigma)$. In general $f(y, \sigma)$ is not a separable function, so a change of variables shall be performed: $(y(\tau), \sigma) \rightarrow (x(\tau), \mu)$ obtaining $\dot{x} = \phi(x, \mu)$ but with $\phi(x, \mu) = \xi(x)\eta(\mu)$. The curvature scalar $R(x, \mu)$ shall be performed using Eq. (21). Finally the variables (x, μ) are changed to the original ones in order to obtain $R(y, \sigma)$.

A. Transcritical bifurcation

The normal form for a transcritical bifurcation is given by the equation

$$\dot{y} \equiv \frac{dy}{d\tau} = \sigma y - y^2, \quad (22)$$

with the fixed points $\bar{y}_0 = 0$ and $\bar{y}_1 = \sigma$. The stability of the fixed points [12] depends on the value of σ : (i) for $\sigma < 0$, \bar{y}_0 is stable and \bar{y}_1 is unstable; (ii) for $\sigma = 0$ the origin is a half-stable fixed point; and (iii) for $\sigma > 0$, \bar{y}_1 is stable and \bar{y}_0 is unstable. The fixed points are presented in the first diagram of Fig. 1.

As mentioned above the right-hand side (RHS) of Eq. (22) is not a separable function of y and σ . Thus the following change of variable is performed: $y \rightarrow \mu(x + 1/2)$, with $\mu = \text{const}$. Equation (22) becomes

$$\dot{x} = (\sigma - \mu)x - \mu x^2 + (\sigma/2 - \mu/4). \quad (23)$$

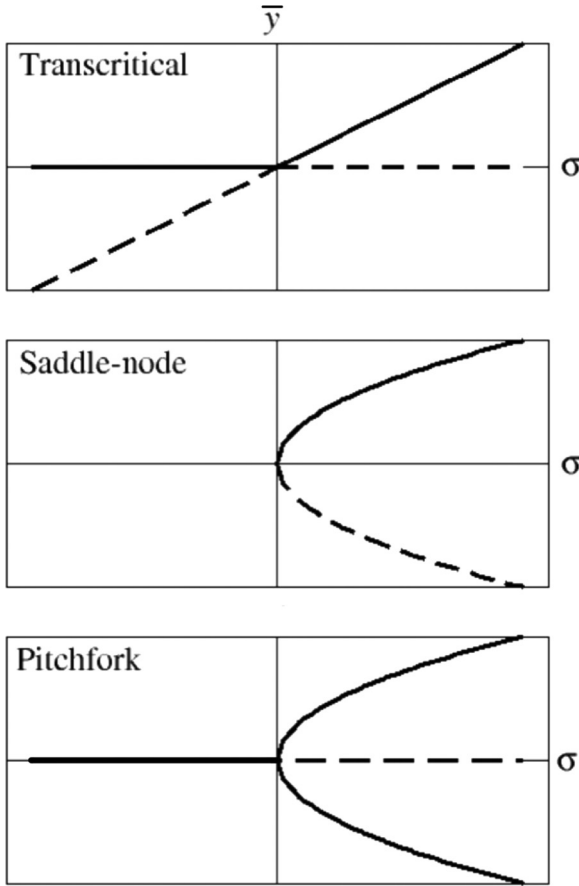


FIG. 1. Bifurcation diagrams: dependence of the fixed points \bar{y} with the control parameter σ . The stable points are represented by thick solid lines and the unstable points by dashed lines.

The purpose of this change of variable is to obtain a separable function of x and μ in RHS of the equation above; then the last term can vanish, so that $\sigma = \mu/2$. Now Eq. (22) is written as

$$\dot{x} = -\mu x(x + 1/2), \quad (24)$$

with the following relations among the variables: $y = \mu(x + 1/2)$ and $\sigma = \mu/2$.

Equation (24) has the same dynamical properties of Eq. (22). It has also two fixed points: $\bar{x}_0 = 0$ (corresponding to \bar{y}_1) and $\bar{x}_1 = -1/2$ (corresponding to \bar{y}_0). But now the RHS of Eq. (24) is a separable function of x and μ . One can easily observe that $\eta(\mu) = -\mu$ and $\xi(x) = x(x + 1/2)$; then the curvature is

$$R(x, \mu) = -\frac{3}{2C} \frac{1}{\mu^2}, \quad (25)$$

and in terms of the original variables:

$$R(y, \sigma) = -\frac{3}{8C} \frac{1}{\sigma^2}. \quad (26)$$

Following the analogy with a thermodynamical model (now with y playing the same role of an order parameter and σ playing the role of reduced temperature), one can observe that the curvature and thus the correlation length diverge for $\sigma \rightarrow \sigma_c = 0$, a typical behavior of second-order phase transition. By comparing the equation above with Eq. (9) one

could conclude (naively) that the transcritical bifurcation has the critical exponent $\alpha = 0$.

On the other hand, Eq. (22) is not difficult to be integrated in order to obtain $y(\tau)$ and one can observe that $y \rightarrow \sigma = \sigma^1$ asymptotically. Continuing the analogy with thermodynamics, this behavior corresponds to a critical exponent $\beta = 1$.

B. Saddle-node bifurcation

For the saddle-node bifurcation, the following equation is considered:

$$\dot{y} \equiv \frac{dy}{d\tau} = \sigma - y^2, \quad (27)$$

which has two fixed points: $\bar{y}_0 = -\sqrt{\sigma}$ (unstable) and $\bar{y}_1 = +\sqrt{\sigma}$ (stable), for $\sigma \geq 0$. See the second diagram of Fig. 1.

This time the change of variables $(y(\tau), \sigma) \rightarrow (x(\tau), \mu)$ is given by $y \rightarrow \mu(x - 1/2)$ and Eq. (27) takes the form of the logistic equation

$$\dot{x} = \mu x(1 - x), \quad \text{with } \mu = 2\sqrt{\sigma} \geq 0. \quad (28)$$

By proceeding with the same analysis of the previous subsection, one can compute the curvature of the saddle-node bifurcation

$$R(x, \mu) = -\frac{3}{2C} \frac{1}{\mu^2} \Rightarrow R(y, \sigma) = -\frac{3}{8C} \frac{1}{\sigma}, \quad (29)$$

with critical exponent $\alpha = 1$. On the other hand, from the asymptotic behavior of the solution of Eq. (27) one can infer that $\beta = 1/2$.

C. Pitchfork bifurcation

The normal form is given by

$$\dot{y} = (\sigma - y^2)y. \quad (30)$$

For $\sigma < 0$, $\bar{y} = 0$ is the only fixed point, and it is stable. For $\sigma > 0$ the system has three fixed points: $\bar{y}_0 = 0$ (unstable) and $\bar{y}_1 = \pm\sqrt{\sigma}$ (stable). See the third diagram of Fig. 1.

By using the change of variables $y \rightarrow \mu \cdot x$, Eq. (30) becomes

$$\dot{x} = \mu^2(x - x^3), \quad \text{with } \mu^2 = \sigma. \quad (31)$$

The curvature is

$$R(x, \mu) = -\frac{4}{C} \frac{1}{\mu^2} \Rightarrow R(y, \sigma) = -\frac{4}{C} \frac{1}{\sigma}, \quad (32)$$

and one can observe for this bifurcation the same critical exponents of the previous case: $\alpha = 1$ and $\beta = 1/2$.

V. FINAL REMARKS

In this work we presented an exploratory study of the critical aspects (in the sense of phase transitions) of some bifurcations from the perspective of thermodynamic geometry (TG). The normal forms of some well-known bifurcations were considered as geodesic equations of some hypothetical models analogous to thermodynamical models. From the geodesic equation it is possible to obtain an estimate of the corresponding metric and eventually the (thermodynamic) curvature R .

In all cases studied here it was observed that the curvature diverges (according to a power law) when the control parameter approaches its critical value (in which the system bifurcates). In the context of TG this is a clear indication of continuous phase transition. Following the analogy with thermodynamics it is possible to obtain naively the critical exponent α .

The thermodynamic curvature has dimensions of (length)^{*d*}, where *d* is the spatial dimensionality of the system. In lattice models, curvature and correlation length appear as dimensionless quantities, but it is understood that these quantities are given in units of the lattice spacing. In complex systems (e.g., epidemic models, population dynamics) one can, in general, nondimensionalize the first-order differential equation, in such a way that *x*, μ , and τ are dimensionless variables. Therefore, the curvature of each bifurcation shown in the manuscript is dimensionless. On the other hand, if applicable one could consider that *R* (and correlation length) is given in units of *L*^{*d*}

(and *L*, respectively), where *L* is a typical distance between “particles” of the system.

In TG the sign of *R* is related to the character of the interactions among the particles of the thermodynamic system. For complex systems, and specifically for the bifurcations studied in this paper, it is reasonable to expect that the curvature (and its sign) is also determined by the details of interactions among the particles of the complex system. It could be interesting to analyze the character of the interactions; however, depending on the model, it may not make any sense to say if the dominant interaction is attractive or repulsive.

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