Chapter

Differential Geometry and Macroscopic Descriptions in Nonequilibrium Process

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Abstract

The method of Riemannian geometry is fruitful in equilibrium thermodynamics. From the theory of fluctuations it has been possible to construct a metric for the space of thermodynamic equilibrium states. Inspired by these geometric elements, we will discuss the geometric-differential approach of nonequilibrium systems. In particular we will study the geometric aspects from the knowledge of the macroscopic potential associated with the Uhlenbeck-Ornstein (UO) nonequilibrium process. Assuming the geodesic curve as an optimal path and using the affine connection, known as α-connection, we will study the conditions under which a diffusive process can be considered optimal. We will also analyze the impact of this behavior on the entropy of the system, relating these results with studies of instabilities in diffusive processes.

Keywords: nonequilibrium processes, Uhlenbeck-Ornstein process, statistical manifold, α-connections, macroscopic potential

1. Introduction

The use of Riemannian geometry associated with the space of thermodynamic equilibrium states has been successful. In this framework the geometric elements are constructed from the knowledge of the thermodynamic potential. In this sense, one of the most interesting ideas is associated with the study of the phase transitions visualized by means of the singularities of the scalar curvature [1, 2]. As a geometric-differential approach of nonequilibrium systems, we consider in our study the geometric properties of a statistical manifold associated with trajectory-dependent entropy [3]. In statistics mechanics it is known that any statistical system has an associated metric-affine manifold having a special affine connection whether it is in equilibrium or not. The affine connection, called the α-connection [4], is a generalization of the Levi-Civita connection in Riemannian geometry, and in the case $\alpha = 0$ the metric-affine manifold reduces to the so-called Riemannian manifold. A first element that appears for nonequilibrium systems is the visualization of the phase transitions through the curvature tensor [5]. A second issue is the study of temporal evolution of a statistical system in order to study the optimal evolution.

In other words, it is the analysis of the dynamic behavior of the system and the study of the conditions that are optimal.

In the previous context, this chapter will focus on the analysis of the optimal evolution. In particular we consider the Uhlenbeck-Ornstein (UO) nonequilibrium process described by the probability density function (PDF) solution of the Fokker-Planck Equation [6]. From this probability density function, we build a two-dimensional metric-affine manifold in the coordinates (μ, σ), where μ is the mean and σ the standard deviation. In this coordinates and for the connections $\alpha = 0$ and $\alpha = -1$, the system evolves on a geodesic curve [7].

However, due to simplicity in geometric construction, we are interested in studying the behavior of the system in coordinates (θ_1, θ_2), where $\theta_1 = 1/(2\sigma^2)$ and $\theta_2 = -\mu/\sigma^2$. In these coordinates the probability density function belongs to the exponential family, and using this formal expression and analogously with the equilibrium probability density function, we build a macroscopic potential $\psi(\theta_1, \theta_2)$ for the UO process. From the geometry constructed using the $\psi(\theta_1, \theta_2)$ potential, we show that for $\alpha = 3$ and $\alpha = 2$, the system evolves on a geodesic curve. In particular for $\alpha = 3$, we show that the manifold is flat and for the steady state the macroscopic potential and entropy have the same functional dependence. Thinking the geodesic curve as an optimal trajectory, our results allow us to conjecture that the entropy describes the steady state of an optimal evolution.

In the second section of this chapter, we summarize the most relevant aspects of the theory of the statistical manifold. The geometric development associated with the fundamental solution of the Fokker-Planck equation of UO process is found in the third section. The fourth section is devoted to the construction of the potential. In the fifth section, we analyze the geometric relationship between macroscopic potential and entropy. In the sixth section, we present our conclusions and perspectives.

2. Elements of statistical manifold

In this section we briefly review the information of geometrical theory [4] that is used to analyze geometrically a family of probability density functions (PDF) and its application to thermodynamics. Let $p(x, \theta)$ be a PDF described by a random variable x and parameters $\theta = (\theta_1, \theta_2, \dots, \theta_m)$ that characterize a system. The set of PDFs

$$M = \{ p(x, \theta) : \theta \in \Omega \subset \mathbb{R}^m \} \tag{1}$$

becomes an m-dimensional statistical manifold having θ_i coordinates. According to the information geometrical theory, we can make a metric tensor g_{ij}

$$g_{ij}(\theta) = E\left[\partial_i l(x, \theta) \partial_j l(x, \theta)\right] = -E\left[\partial_i \partial_j l(x, \theta)\right], \tag{2}$$

where $l(x, \theta) = \ln [p(x, \theta)]$ and $E[.]$ means the expectation operation with respect to $p(x, \theta)$. The last expression is obtained by the use of the normalization condition $E[\partial_i l(x, \theta)] = 0$. This metric tensor is the Fisher information matrix in information theory.

In the statistical manifold M, we can introduce a natural derivative of the vector field B toward the tangent vector A, denoted by $\nabla_A^\alpha B$. It is obtained through the covariant coefficients [7]:

$$\Gamma_{ijk}^{(\alpha)}(\theta) = E\left[\left(\partial_i \partial_j l(x, \theta) + \frac{1-\alpha}{2} \partial_i l(x, \theta) \partial_j l(x, \theta)\right) \partial_k l(x, \theta)\right]. \tag{3}$$

We now restrict our attention to a special family of probability density function, called an exponential family, which is described by [8].

$$p(x,\theta) = \exp\left(C(x) + \sum_i^m \theta_i F_i(x) - \psi(\theta)\right), \tag{4}$$

where $C(x)$ and $F_i(x)$ are arbitrary functions of x and $\psi(\theta)$ is a function of θ_i coordinates.

Particularly for a probability density function belonging to the exponential family, from Eqs. (2) and (3) the covariant coefficients and metric tensor are written as [9, 10].

$$\Gamma_{ijk}^{(\alpha)}(\theta) = -\frac{(1-\alpha)}{2}\partial_i\partial_j\partial_k\psi(\theta), \tag{5}$$

$$g_{ij}(\theta) = \frac{\partial^2\psi(\theta)}{\partial\theta_i\partial\theta_j}. \tag{6}$$

These coefficients, for $\alpha \in \mathbb{R}$, determine a one-parameter family of affine connections, and each element of this family is called an α-connection. An affine connection allows one to compare vectors in nearby tangent spaces [9]. Moreover, the covariant coefficients satisfy the following relation:

$$\Gamma_{ij}^{k(\alpha)} = g^{km}\Gamma_{ijm}^{(\alpha)}, \tag{7}$$

where $\left(g^{km}\right)$ is the inverse matrix of the metric and $\left(g_{ij}\right)$ and $\Gamma_{ij}^{k(\alpha)}$ are the contravariant coefficients.

In the case $\alpha = 0$, the coefficients reduce to the Levi-Civita's connection:

$$\Gamma_{ijk}^{(0)} = \frac{1}{2}\left(\partial_i g_{jk} + \partial_j g_{ik} - \partial_k g_{ij}\right). \tag{8}$$

From Eq. (3) the curvature tensor for an α-connection is written as

$$R_{ijkm}^{(\alpha)} = \left(\partial_i\Gamma_{jk}^{s(\alpha)} - \partial_j\Gamma_{ik}^{s(\alpha)}\right)g_{sm} + \left(\Gamma_{irm}^{(\alpha)}\Gamma_{jk}^{r(\alpha)} - \Gamma_{jrm}^{(\alpha)}\Gamma_{ik}^{r(\alpha)}\right). \tag{9}$$

Since $\Gamma_{ijk}^{(\alpha)}(\theta)$ vanishes identically for $\alpha = 1$, any exponential family of PDF constitutes an uncurved space when the $\alpha = 1$ connection is used. The one connection is therefore called the exponential connection as we mentioned above [11]. The relationships (Eqs. (5) and (6)) lead to the simplification of the geometric construction associated with the probability density function (Eq. (4)).

For systems in thermodynamic equilibrium, the parameters θ_i may include inverse temperature, chemical potential, pressure, magnetic field, and so on. Also, $\psi(\theta)$ represents the thermodynamic potential of the system [8]. It is worth noting that, if we consider the equilibrium density functions and $\alpha = 0$, this formalism reproduces the geometric structure found by Ruppeiner for the space of equilibrium states. In the Ruppeiner formalism, the metric is constructed using the theory of fluctuations, and the geometric elements are obtained as the second derivatives of the corresponding thermodynamic potential [2]. In this paper we have chosen the approach of statistical manifold because it allows us to address nonequilibrium problems.

3. Fokker-Planck equation and macroscopic potential

A diffusion process can be thought of as a process of Uhlenbeck-Ornstein. The Uhlenbeck-Ornstein process is a stochastic process that, roughly speaking, describes the velocity of a massive Brownian particle under the influence of friction. The probability density function $P(x,t)$ of the Uhlenbeck-Ornstein process satisfies the Fokker-Planck equation [6]:

$$\frac{\partial P}{\partial t} = \frac{1}{\tau}\frac{\partial}{\partial x}[(x-x_0)P] + D\frac{\partial^2 P}{\partial x^2}. \tag{10}$$

The fundamental solution of this linear parabolic partial differential equation, and the initial condition consisting of a unit point mass at location y, is:

$$P(x,t) = \sqrt{\frac{1}{2\pi D\tau(1-e^{-2t/\tau})}}\exp\left\{-\frac{1}{2D\tau}\left[\frac{\left(x-x_0-(y-x_0)e^{-t/\tau}\right)^2}{1-e^{-2t/\tau}}\right]\right\} \tag{11}$$

which is the Gaussian density function with mean

$$\mu = x_0 + (y-x_0)e^{-t/\tau} \tag{12}$$

and variance

$$\sigma^2 = D\tau\left(1-e^{-2t/\tau}\right) \tag{13}$$

where x_0 represents the average length of the displacement, D is the diffusion coefficient, and τ is a characteristic time. Without loss of generality, in the rest of the work, we consider $y = 0$.

Considering Eqs. (12) and (13), we think the function (Eq. (11)) as a probability density function dependent on two parameters μ and σ, formally:

$$p(x,\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-(x-\mu)^2/2\sigma^2}. \tag{14}$$

Considering these parameters as the coordinates (μ,σ) of the manifold M and taking into account Eqs. (2) and (4), it can be seen that for $\alpha = 0$ and $\alpha = -1$, the system evolves on a geodesic curve [7].

Inspired by the simplicity of relations (Eqs. (5) and (6)), we use an alternative description of the UO process through the coordinates:

$$(\theta_1,\theta_2) = \left(\frac{1}{2\sigma^2}, -\frac{\mu}{\sigma^2}\right). \tag{15}$$

In these coordinates the probability density function (Eq. (14)) belongs to the exponential family and is written as

$$p(x,\theta_1,\theta_2) = \exp\left[-\theta_1 x^2 - \theta_2 x - \psi(\theta_1,\theta_2)\right] \tag{16}$$

where

$$\psi(\theta_1,\theta_2) = \frac{\theta_2^2}{4\theta_1} - \ln\left[\sqrt{\frac{\theta_1}{\pi}}\right]. \tag{17}$$

By analogy with the probability density functions for systems in equilibrium, we will call the relationship (Eq. (17)) “nonequilibrium potential” [8].

Using the potential (Eq. (17)) we calculate the coefficients (Eq. (5))

$$\begin{aligned} \Gamma^{(\alpha)}_{111} &= -\frac{(\alpha-1)}{2}\left(\frac{1}{\theta_1^3}+\frac{3\theta_2^2}{2\theta_1^4}\right), \ \Gamma^{(\alpha)}_{222}=0 \\ \Gamma^{(\alpha)}_{112} &= \Gamma^{(\alpha)}_{121}=\Gamma^{(\alpha)}_{211}=\frac{(\alpha-1)}{2}\frac{\theta_2}{2\theta_1^3} \\ \Gamma^{(\alpha)}_{122} &= \Gamma^{(\alpha)}_{221}=\Gamma^{(\alpha)}_{212}=-\frac{(\alpha-1)}{4\theta_1^2} \end{aligned} \tag{18}$$

Using Eqs. (18) and (19), we calculate the curvature tensor component in the coordinates (θ_1, θ_2)

$$R^{(\alpha)}_{1212}(\theta_1,\theta_2) = -\frac{(\alpha-3)(\alpha-1)}{8\theta_1^3}. \tag{19}$$

From Eq. (19) we observe that there are two α values for which the manifold is flat, $\alpha = 3$ and $\alpha = 1$. The case $\alpha = 1$ is a direct consequence of Eq. (5).

In a manifold with a connection, we can generalize the straight line of Euclidean geometry. The generalized straight line is called geodesic, and it is defined by the characteristic that its tangent vector does not change its direction. It satisfies the Eq. (11)

$$\frac{d^2\theta_i}{du^2}+\Gamma^i_{jk}\frac{d\theta_k}{du}\frac{d\theta_j}{du} = -\frac{d^2u/ds^2}{(du/ds)^2}\frac{d\theta_i}{du} \tag{20}$$

with an arbitrary parameter u. The special parameter s is called the affine parameter. We note that if u is a linear transformation of s, the right-hand side vanishes. Let us now prove that the curve defined by Eq. (15) of the UO process is a geodesic. We choose the Newtonian time t for the arbitrary parameter u. From Eq. (20) for the study of geodetic curves, we consider that the temporal dependence of the coordinates (θ_1, θ_2) is given by

$$\begin{cases} \theta_1(t) = \dfrac{1}{2D\tau\left(1-e^{-2t/\tau}\right)}, \\ \theta_2(t) = -\dfrac{x_0\left(1-e^{-t/\tau}\right)}{D\tau\left(1-e^{-2t/\tau}\right)}. \end{cases} \tag{21}$$

The tangent vector coordinate $d\theta_i/dt$ and the acceleration coordinate $d^2\theta_i/dt^2$ are

$$\frac{d\theta_1}{dt} = -\frac{\cosh^2(t/\tau)}{4D\tau^2}, \quad \frac{d^2\theta_1}{dt^2} = \frac{\coth(t/\tau)\mathrm{csch}^2(t/\tau)}{2D\tau^2} \tag{22}$$

and

$$\frac{d\theta_2}{dt} = -\frac{x_0\mathrm{sech}^2(t/(2\tau))}{4D\tau^2}, \quad \frac{d^2\theta_2}{dt^2} = \frac{2x_0\sinh^4(t/(2\tau))\mathrm{csch}^3(t/\tau)}{D\tau^3}. \tag{23}$$

Substituting Eqs. (22) and (23) in Eq. (20) for the coordinate θ_1, we have

$$\frac{1}{2D\tau^2}\left\{2D\tau[(\alpha-1)-(\alpha-3)\coth(t/\tau)]-(\alpha-1)x_0^2\right\}=\frac{d^2t/ds^2}{(dt/ds)^2}, \tag{24}$$

and for the coordinate θ_2

$$\begin{aligned}&\frac{\operatorname{csch}(t/\tau)}{2D\tau^2}\{2D\tau[-1-(\alpha-2)\cosh(t/\tau)+(\alpha-1)\sinh(t/\tau)]\}+\\&\frac{\operatorname{csch}(t/\tau)}{2D\tau^2}\left[\left(1+e^{-t/\tau}\right)(\alpha-1)x_0^2\right]=\frac{d^2t/ds^2}{(dt/ds)^2}.\end{aligned} \tag{25}$$

The results (Eqs. (24) and (25)) are compatible if we choose α as

$$\alpha=1+2\frac{D\tau}{x_0^2}. \tag{26}$$

Taking as reference the geometric study in the coordinates (μ,σ) [7], we consider two possible relationships between the characteristic time τ and the other two parameters, $\tau=x_0^2/D$ or $\tau=x_0^2/(2D)$. The first case leads to a flat geometry, that is, if $\tau=x_0^2/D$, we have that $\alpha=3$ and for Eq. (19) $R^{(3)}_{1212}(\theta_1,\theta_2)=0$. This case is equivalent to the connection $\alpha=-1$ in the coordinates (μ,σ), where the manifold is also flat and the affine time s and Newtonian time t are related by the differential equation

$$\frac{1}{\tau}=\frac{d^2t/ds^2}{(dt/ds)^2} \tag{27}$$

whose solution has the form

$$t=-\tau\ln(s+a\tau)+b. \tag{28}$$

On the other hand if $\tau=x_0^2/(2D)$, we have that $\alpha=2$ and the affine and Newtonian time are now related by

$$\frac{\coth(t/\tau)}{\tau}=\frac{d^2t/ds^2}{(dt/ds)^2}. \tag{29}$$

Due to its nature, the equation (Eq. (29)) has been solved numerically. For each τ we find solutions that make sense in the context of our problem. In **Figure 1** we show two examples of these solutions.

In the coordinates (μ,σ), Eqs. (27) and (29) correspond to the choices $\alpha=-1$ and $\alpha=0$, respectively [7]. On the other hand in the context of geometric construction from the potential (Eq. (17)), the main interpretation of the equation (Eq. (26)) is that the temporal evolution described by Eq. (21) coincides with a geodesic curve of space (θ_1,θ_2). In this sense we find two relationships $\tau=x_0^2/D$ and $\tau=x_0^2/(2D)$ between the parameters x_0, D, and τ for which the evolution is optimized.

It is interesting to note that if we assume that $v=x_0/\tau$, the relationship $\tau=x_0^2/D$ leads us to $D=v^2\tau$. This is a well-known and a widely used relationship, for example, in the understanding of bacterial mobility through a diffusive model.

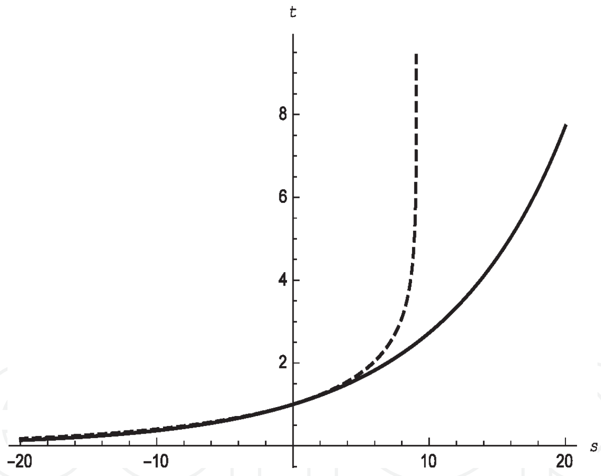

Figure 1.
t as a function of s for two values of τ. $\tau = 10$ in the solid line and $\tau = 1$ in the dashed line.

In this case the characteristic time τ represents the tumbling time, and ν represents the average speed of bacteria [12].

4. Optimal trajectory and entropy

Thinking the geodesic curve as an optimal trajectory, from Eq. (21) we will analyze the optimal evolution of the system in terms of the behavior of the macroscopic potential (Eq. (17)) and the entropy function. To begin with this discussion, we first notice that the common definition of a nonequilibrium Gibbs entropy

$$H(\theta) = -\int_{-\infty}^{\infty} p(x,\theta) \ln [p(x,\theta)] dx = \langle h(x,\theta) \rangle \tag{30}$$

suggests to define a trajectory-dependent entropy for the particle (or "system") $h(x,\theta) = -\ln [p(x,\theta)]$ [3]. The trajectory-dependent entropy is related to the function $l(x,\theta)$ used in the construction of the metric of the statistical manifold M by means of the relation $h(x,\theta) = -l(x,\theta)$. In our analysis we are interested in the entropy averaged over trajectories $H(\theta)$.

Moreover, given that the probability density function (Eq. (16)) belongs to the exponential family, we can calculate the entropy by means of the relation [13].

$$H(\theta) = \psi - \theta_1 \frac{\partial \psi}{\partial \theta_1} - \theta_2 \frac{\partial \psi}{\partial \theta_2}. \tag{31}$$

In any case, using Eqs. (30) or (31), we obtain

$$H(\theta) = \frac{1}{2} - \ln \left[\sqrt{\frac{\theta_1}{\pi}} \right]. \tag{32}$$

In order to study the temporal evolution of potential ψ and entropy H, we use the relations Eqs. (12) and (13) in Eq. (21). In particular, we focus on investigating the asymptotic behavior, that is, the behavior for $t \to \infty$. In this limit and using Eq. (21), we have that $\theta_1 = 1/(2D\tau)$ and $\theta_2 = -x_0/(D\tau)$. Therefore, the asymptotic behavior of the potential and entropy is written as

$$\psi = \frac{x_0^2}{2D\tau} + \frac{1}{2}\ln\left[2\pi D\tau\right] \tag{33}$$

and

$$H = \frac{1}{2} + \frac{1}{2}\ln\left[2\pi D\tau\right]. \tag{34}$$

If we think that in the coordinates (θ_1, θ_2), with $\alpha = 3$, the system evolves on a geodesic of a flat manifold ($R^{(3)}_{1212}(\theta_1, \theta_2) = 0$), we have $\tau = x_0^2/D$, and both the potential ψ and the entropy H tend to the same asymptotic value. In other words the entropy describes the asymptotic behavior of an optimal evolution:

$$\psi = H = \frac{1}{2} + \ln\sqrt{2\pi D\tau}. \tag{35}$$

In this last result, it can be seen that the asymptotic behavior depends fundamentally on the transport coefficient D. In this sense, the relevant variable in the description of the process is the diffusion coefficient D. It is interesting to note that the relations (Eq. (21)) are not invariant when we change t by $-t$. In this context, the evolution of the system is irreversible.

While in the coordinates (θ_1, θ_2) are two α-connections which leads to the system on a geodesic curve ($\alpha = 3$ and $\alpha = 2$), only $\alpha = 3$ makes that the macroscopic potential and entropy have the same functional dependence. It is interesting to note that for this choice of α, the manifold in the coordinates (θ_1, θ_2) is flat.

In the study of processes, the speed at which they occur is important. In this sense we will study the rate of change of potential:

$$\begin{aligned}\dot{\psi} &= \frac{x_0^2}{4D\tau^2}\operatorname{sech}\left(\frac{t}{2\tau}\right) + \frac{1}{2\tau}\left[\coth\left(\frac{t}{\tau}\right) - 1\right] = \\ &= \frac{1}{2\tau}\operatorname{sech}\left(\frac{t}{2\tau}\right) + \frac{1}{2\tau}\left[\coth\left(\frac{t}{\tau}\right) - 1\right] \geq 0,\end{aligned} \tag{36}$$

and the entropy

$$\dot{H} = \frac{1}{2\tau}\left[\coth\left(\frac{t}{\tau}\right) - 1\right] \geq 0. \tag{37}$$

The equal sign in Eqs. (36) and (37) corresponds to the steady state [14]. In this regard, we associate the asymptotic behavior with the steady state, and we can indicate that the entropy describes the steady state of an optimal evolution.

From the perspective of the probability density function (PDF), when the diffusion coefficient takes small values, the distribution (Eq. (14)) diffuses from a uniform state to a sharp concentrated state, that is, from a stable state to an unstable state [15]. Although in this chapter we have not studied the behavior of the curvature tensor in the (μ, σ) coordinates, these instabilities observed from the perspective of the PDF can be expressed in the singularity of the curvature tensor $R^{(0)}_{1212}(\mu, \sigma)$. An example of this behavior is the formation of density patterns in the populations of self-propelled bacteria whose mobility can be investigated in terms of the diffusion coefficient D [5]. We also observe from Eq. (35) that for $D \to 0$, the entropy and the macroscopic potential have a singular behavior. The behavior that we observe both the tensor $R^{(0)}_{1212}(\mu, \sigma)$ and the potential ψ allows us to conjecture that the instabilities of the system can also be observed in the singularities or discontinuities of the macroscopic potential.

5. Discussion and perspectives

In this chapter we have studied the PDF (Eq. (14)) that is the fundamental solution of the Fokker-Planck equation associated with the UO process. Our main interest was relating the geometric aspects of the process with the steady-state behavior. In our analysis we used the theoretical framework of the statistical manifold M with α-connections for two different coordinates (μ, σ) and (θ_1, θ_2) [4, 7]. In the first case, there exist two interesting values of α, namely, $\alpha = -1$ and $\alpha = 0$, for which the process evolves on a geodesic of space (μ, σ) with different values of τ. However, in the search for a simpler geometric construction, we find that for the coordinates (θ_1, θ_2), we can define a macroscopic potential $\psi(\theta_1, \theta_2)$, and the values of α that lead to the system evolving on a geodesic curve are $\alpha = 3$ and $\alpha = 2$. In our study we show that the connection $\alpha = -1$ for the coordinates (μ, σ) corresponds to the connection $\alpha = 3$ for the coordinates (θ_1, θ_2) in the sense that both connections lead to a flat curvature and the same relationship between the parameters of the system. An important consequence of this behavior is that when the system evolves over geodesics, the macroscopic potential ψ and entropy H have the same functional dependence in the steady state. If we think of the geodesic curve as an optimal trajectory, our results allow us to conjecture that the entropy describes the steady state of an optimal evolution in a flat manifold.

Additionally and poorly developed in this chapter is the use of geometric aspects in the study of instabilities in nonequilibrium system. In equilibrium thermodynamics this information is contained in the scalar curvature of the manifold of equilibrium states [2]. For nonequilibrium problems, the instabilities are associated with the singularities or discontinuities of the curvature tensor [5, 15]. In the case of diffusive problems, the instabilities can be found by studying the singularities of $R^{(0)}_{1212}(\mu, \sigma)$. In terms of diffusivity, we see that as it decreases, the system has different macroscopic behavior. An example of this behavior is the formation of density patterns in the populations of self-propelled bacteria whose mobility can be investigated in terms of the diffusion coefficient D [12]. From the perspective of the macroscopic potential ψ, the instabilities can be associated to singularities or discontinuities of ψ. In this sense, from a wider point of view, we consider that the potential ψ represents an alternative way to study the phase transitions in nonequilibrium systems.

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