



Entropy generation and the Fokker–Planck equation



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HIGHLIGHTS

- The Fokker–Planck equation is fundamental in transport processes.
- Entropy generation is fundamental in irreversibility analysis.
- The link between the two approaches is obtained.

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ABSTRACT

Stochastic differential equations are important to model many complex systems. The Fokker–Planck equation is fundamental in statistical thermodynamic analysis and in the study of fluctuations in complex systems. Entropy generation is a fundamental quantity in the analysis of irreversibility. This paper develops a link between the Fokker–Planck equation and entropy generation. The result suggests linking the entropy generation approach also to statistical processes.

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1. Introduction

Stochastic differential equations are used to model many complex systems in physics, chemistry, biology, finance and economics, and engineering, including population dynamics, protein kinetics, turbulence, etc. In this context, the Fokker–Planck equation represents the probability density for the position or the velocity of a particle of which the motion is described by a corresponding Langevin equation. Consequently it results as being fundamental in statistical thermodynamic analysis and in the study of fluctuations in complex systems [1–3]. The Fokker–Planck equation is an excellent approximation near the free energy minimum, just as Boltzmann's definition of entropy follows from finding the maximum entropy state.

The study of the solution of the stochastic differential equations leads to the analysis of the trajectories of the system considered in the phase space used to describe its behavior. The result is to obtain information on the probability transition function of the stochastic processes, on the stationary distribution and on the evolution of the system considered [4].

A link between the Fokker–Planck dynamics and the free energy functional was pointed out, and it is minimized over an appropriate class of probability densities [1]. These results allow us to describe metastability and hysteresis in physical systems [1,5]; indeed, the Fokker–Planck equation describes, in a statistical way, how a collection of initial physical data evolves with time.

Moreover, these results underline also the fundamental role of dissipation analysis in metastable systems. An important link appears between the Fokker–Planck equation and the global thermodynamic quantities which is useful in the analysis

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of dissipation in irreversible systems [6]. In the literature, usually, entropy production is used and there exist many links between entropy production and the Fokker–Planck equation [7,8].

As underlined in many papers on the entropy generation approach [6], there exist fundamental differences between entropy production and entropy generation approaches; indeed, the entropy generation approach [9–19]:

1. does not need the local equilibrium hypothesis;
2. introduces the lifetime of the process, the time of occurrence of a process;
3. analyzes the systems over a time greater than or equal to the lifetime of the entire process occurring in the system,

while the entropy production needs the local equilibrium hypothesis and does not consider the times. They are two different approach which allow us to analyze systems in a complementary way. The two approaches are complementary, so it is interesting to link also entropy generation to the Fokker–Planck equation.

In this paper the link will be developed to introduce the Fokker–Planck equation in terms related to dissipation, with particular regard to entropy generation. The result is fundamental in also providing irreversible phenomena with a statistical description.

2. The non-equilibrium Fokker–Planck equation

In order to introduce the Fokker–Planck equation, a set of n interacting particles is considered. The particles evolve in time following the Langevin equations:

$$\frac{dx_i}{dt} = f_i(\mathbf{x}) + r_i(t) \tag{1}$$

where x_i is the position of the i th particle, $\mathbf{x} = \{x_i\}$, f_i is the force acting on the i th particle, r_i is the noise mathematically considered as a stochastic variable such that:

$$\begin{aligned} \langle r_i(t) \rangle &= 0 \\ \langle r_i(t) r_j(t') \rangle &= 2D_i \delta_{ij} \delta(t - t') \end{aligned} \tag{2}$$

with $D_i \geq 0$, different constants for each particle. The associated Fokker–Planck equation describes the time evolution of the probability distribution $P(\mathbf{x}, t)$; it can be written as [7]:

$$\begin{aligned} \frac{\partial P(\mathbf{x}, t)}{\partial t} &= - \sum_i \frac{\partial J_i(\mathbf{x}, t)}{\partial x_i} \\ J_i(\mathbf{x}, t) &= \left[f_i(\mathbf{x}) + D_i \frac{\partial}{\partial x_i} \right] P(\mathbf{x}, t). \end{aligned} \tag{3}$$

This equation can be solved inside a space spanned by the set variable \mathbf{x} under boundary conditions related to the behavior of $P(\mathbf{x}, t)$ and $J_i(\mathbf{x}, t)$ at the boundary surface of the integration space itself. The condition of irreversibility can be expressed as follows:

$$\begin{aligned} D_i \neq D_j \quad i \neq j \text{ or} \\ D_i = D_j = D \quad i \neq j \quad \text{but} \quad \frac{\partial f_i}{\partial x_j} \neq \frac{\partial f_j}{\partial x_i}. \end{aligned} \tag{4}$$

The first of the relations (4) can represent a system in contact with two or more heat reservoirs at different temperatures, while the second relation can describe the contact of an irreversible system with a heat reservoir, but in the case of non-conservative forces.

3. Different extrema for internal and external dissipations

A thermodynamic system is a physical system whose interactions with the environment are reflected by different transfers of heat and work. For such a system, it is possible to write the kinetic energy theorem as [20,21]:

$$W_{es} + W_{fe} + W_i = \Delta E_k \tag{5}$$

where W_{es} is the work done by the environment (external to the system) on the system, the work done from external forces on the border of the system, W_{fe} is the work lost due to external irreversibility, E_k is the kinetic energy of the system, and W_i is the internal work, such that [20,21]:

$$W_i = W_i^{rev} - W_{fi} \tag{6}$$

with W_i^{rev} the reversible internal work and W_{fi} the work lost due to internal irreversibility. Moreover, the following relation must be taken in account [20,21]:

$$W_{se} = -W_{es} - W_{fe} \tag{7}$$

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