Free-energy formalism for inhomogeneous nonlinear Fokker-Planck equations

Peter Rapčan, Gabriele Sicuro and Constantino Tsallis

Abstract We extend the free-energy formalism recently introduced for homogeneous Fokker–Planck equations to a wide class of inhomogeneous nonlinear Fokker–Planck equations, providing sufficient conditions for the equation coefficients to obtain a free-energy that does not increase with time. Some properties of the stationary solutions of these Fokker–Planck equations are discussed.

Consider a Fokker-Planck equation (FPE) in $(1+1)$ dimensions, i.e., a continuity equation for the probability density $\rho(x,t)$

$$\frac{\partial\rho(x,t)}{\partial t} = -\frac{\partial J[x,\rho(x,t)]}{\partial x}, \tag{1}$$

with a probability-current density given by

$$J[x,\rho(x,t)] := A(x)\Psi[\rho(x,t)] - D(x)\Omega[\rho(x,t)]\frac{\partial\rho(x,t)}{\partial x}. \tag{2}$$

We assume the following boundary conditions $\forall t \geq 0$:

$$\lim_{x\to\pm\infty}\rho(x,t) = \lim_{x\to\pm\infty}\frac{\partial\rho(x,t)}{\partial x} = \lim_{x\to\pm\infty}J[x,\rho] = 0. \tag{3}$$

Peter Rapčan
Centro Brasileiro de Pesquisas Físicas, Rua Dr. Xavier Sigaud, 150, 22290-180, Rio de Janeiro, Brazil; e-mail: rapcan@cbpf.br

Gabriele Sicuro
Centro Brasileiro de Pesquisas Físicas, Rua Dr. Xavier Sigaud, 150, 22290-180, Rio de Janeiro, Brazil; e-mail: sicuro@cbpf.br

Constantino Tsallis
Centro Brasileiro de Pesquisas Físicas and National Institute of Science and Technology of Complex Systems, Rua Dr. Xavier Sigaud, 150, 22290-180, Rio de Janeiro, Brazil, and Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, NM 87501, USA; e-mail: tsallis@cbpf.br

Moreover, we assume that, $\forall x\in\mathbb{R}$, $0<D(x)<\infty$ and that $\Omega[\rho]>0$ almost everywhere. We search therefore for a trace-form free-energy-like functional

$$F(t) := \int_{-\infty}^{\infty} f[x,\rho(x,t)]\mathrm{d}x \tag{4}$$

$$f[x,\rho(x,t)] := \varphi(x)\rho(x,t) - \Theta s[\rho(x,t)], \tag{5}$$

where f is a free-energy density, φ is an effective potential, s is an entropy density such that $s[0]=s[1]=0$, and $\Theta>0$ is a parameter that plays the role of a temperature. Evaluating the time derivative of F, and imposing Eq. (1), we obtain

$$\frac{\mathrm{d}F(t)}{\mathrm{d}t} = -\int_{-\infty}^{\infty} \Theta D(x)\Psi(x)\left[-\frac{A(x)}{D(x)}+\frac{\Omega[\rho]}{\Psi[\rho]}\frac{\partial\rho(x,t)}{\partial x}\right] \times\left[\frac{1}{\Theta}\frac{\partial\varphi(x)}{\partial x}-\left.\frac{\mathrm{d}^2 s[y]}{\mathrm{d}y^2}\right|_{y=\rho(x,t)}\frac{\partial\rho(x,t)}{\partial x}\right]\mathrm{d}x.$$

We assume, without loss of generality, that $\Psi[\rho]$ is positive. The integrand is non-negative, i.e., the free energy is non-increasing along the entire time evolution, if

$$\frac{1}{\Theta}\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x} = -\frac{A(x)}{D(x)}, \quad \frac{\mathrm{d}^2 s[\rho]}{\mathrm{d}\rho^2} = -\frac{\Omega[\rho]}{\Psi[\rho]}. \tag{6}$$

The relations above have been obtained for the first time in Refs. [1, 2] for the homogenous case $D(x)\equiv D = \mathit{constant}$.

One may wonder whether the structure of J presented in Eq. (2) and adopted in Eq. (1), might be substituted by a more general structure, like

$$J[x,\rho(x,t)] = \tilde{\Psi}[x,\rho(x,t)] - \tilde{\Omega}[x,\rho(x,t)]\frac{\partial\rho(x,t)}{\partial x}. \tag{7}$$

It turns out that the structure of our free-energy functional as defined in Eqs. (4) and (5) is not compatible with the structure of the above probability-current density unless $\tilde{\Psi}[x,\rho(x,t)] = A(x)\Psi[\rho(x,t)]$ and $\tilde{\Omega}[x,\rho(x,t)] = D(x)\Omega[\rho(x,t)]$. If we instead do not specify the structure of $f[x,\rho]$, we can still write down a set of equations such that $\frac{\mathrm{d}F(t)}{\mathrm{d}t}\leq 0$ which, in turn, constrain the pair $\tilde{\Psi},\tilde{\Omega}$ as follows

$$\left.\begin{array}{l}\frac{\partial^2 f[x,\rho]}{\partial x\partial\rho} = \tilde{\Psi}[x,\rho] \\ \frac{\partial^2 f[x,\rho]}{\partial\rho^2} = \tilde{\Omega}[x,\rho]\end{array}\right\} \Rightarrow \frac{\partial\tilde{\Psi}[x,\rho]}{\partial\rho} = \frac{\partial\tilde{\Omega}[x,\rho]}{\partial x}, \tag{8}$$

where the implied condition is not satisfied *a priori*.

Let us now come back to the factorized probability-current density in Eq. (2). It can be shown [3] that, if a stationary distribution of Eq. (1), $\rho_{st}(x)$, exists, then it is unique, coinciding with the limit distribution $\rho_{st}(x) = \lim_{t\to\infty}\rho(x,t)$, and it can be written in the form

$$\rho_{st}(x) = \exp_s[-\Theta^{-1}\varphi(x)+c], \tag{9}$$

where, given $g(\rho) := \frac{\mathrm{d}s(\rho)}{\mathrm{d}\rho}$, $\exp_s(x) := g^{-1}(-x)$ is a deformed exponential associated with the (generalized) entropy density s and c is a normalization constant. Hence, even for a fixed entropic form, one can obtain a wide class of stationary distributions by an appropriate choice of the argument of the deformed exponential, and in particular of $D(x)$.

Observe that (A, Ψ, D, Ω) and $(\gamma A, \gamma^{-1}\Psi, \delta D, \delta^{-1}\Omega)$, with $\gamma, \delta \neq 0$, lead to the same FPE. Therefore the quantities $\Theta^{-1}\partial_x\varphi$ and s are given up to a common multiplicative constant, unless additional information is available. In particular, the parameter Θ can be only fixed on the basis of the specific properties of the model under consideration. Supposing φ fixed in this way, and evaluating the second moment of the stationary distribution $\int_{-\infty}^{\infty} x^2 \rho_{st}(x)\mathrm{d}x$, the following identity can be written

$$\Theta = \frac{-\int_{-\infty}^{\infty} x^3 \frac{\mathrm{d}\varphi(x)}{\mathrm{d}x} \left(\frac{\mathrm{d}^2 s[z]}{\mathrm{d}z^2}\Big|_{z=\rho_{st}(x)} \right)^{-1} \mathrm{d}x}{3\int_{-\infty}^{\infty} x^2 \rho_{st}(x)\mathrm{d}x}. \tag{10}$$

Summarizing, we have extended the free-energy formalism introduced in [1, 2], to a wide class of inhomogeneous nonlinear Fokker–Planck equations. The connection with q-statistics (and its associated nonadditive entropy S_q) can be straightforwardly obtained as a particular case. A more complete analysis of the formalism, addressing properties of the free-energy functional, entropy production in the process of relaxation towards the equilibrium, derivation of the stationary solution, accompanied by a proof of the existence of a unique limit distribution, is being published elsewhere [3].

Acknowledgements We acknowledge financial support by CNPq and Faperj (Brazilian Agencies), and by the John Templeton Foundation (USA). P.R. also acknowledges financial support by the Institute of Physics, Slovak Academy of Sciences.

References

1. V. Schwämmle, M. E. Curado, and D. F. Nobre. A general nonlinear Fokker–Planck equation and its associated entropy. *The European Physical Journal B*, 58(2):159–165, 2007.
2. V. Schwämmle, F. D. Nobre, and E. M. F. Curado. Consequences of the *H* theorem from nonlinear Fokker–Planck equations. *Physical Review E*, 76:041123, 2007.
3. G. Sicuro, P. Rapčan, and C. Tsallis. Nonlinear inhomogeneous Fokker–Planck equations: entropy and free-energy time evolution. *https://arxiv.org/abs/1609.05980*, 2016.