Available online at www.sciencedirect.com
ScienceDirect
Physica A 374 (2007) 573–584
PHYSICA A
www.elsevier.com/locate/physa

Maximum entropy principle and classical evolution equations with source terms

J-H. Schönfeldt[a], N. Jimenez[b], A.R. Plastino[a,b,c], A. Plastino[b,*], M. Casas[c]

[a]Department of Physics, University of Pretoria, Pretoria 0002, South Africa
[b]Facultad de Ciencias Exactas y Observatorio, Universidad Nacional de La Plata, IFLP-CONICET, C.C. 727, 1900 La Plata, Argentina
[c]Departament de Fisica, Universitat de les Illes Balears, Mallorca, Spain

Received 27 March 2006
Available online 31 August 2006

Abstract

We devise a maximum entropy technique to construct (approximate) time-dependent solutions to evolution equations endowed with source terms and, consequently, not preserving normalization. In some special cases the method yields exact solutions. It is shown that the present implementation of the maximum entropy prescription always (even in the case of approximate solutions) preserves the exact functional relationship between the time derivative of the entropy and the time-dependent solutions of the evolution equation. Other properties of the maximum entropy solutions and some illustrative examples are also discussed.

Keywords: Maximum entropy; Jaynes relations; Diffusion-like equations with sources

1. Introduction

The application of information-entropic variational principles to the study of diverse systems and processes in physics, astronomy, biology, and other fields, has been the focus of considerable research activity in recent years. A (by no means exhaustive) list of important examples is given in Refs. [1–12]. The roots of this approach can be traced back (at least) to Gibbs [13] who pointed out that the canonical probability distribution is the one maximizing the entropy under the constraints imposed by normalization and the mean energy value. However, it was Jaynes who elevated the principle of maximum entropy to the status of a foundational starting point for the development of statistical mechanics, and the first to recognize its relevance as a general statistical inference principle [14–16].

A large amount of research has been devoted to the study of time-dependent maximum entropy solutions (either exact or approximate) of diverse evolution equations, such as the Liouville equation, the Vlasov equation, diffusion equations, and Fokker–Planck equations [17–27]. Most of these applications of the maximum entropy method to time-dependent scenarios involved evolution equations (linear or non-linear)

*Corresponding author. Fax: +54 2258238.
E-mail address: plastino@fisica.unlp.edu.ar (A. Plastino).

0378-4371/$ - see front matter © 2006 Published by Elsevier B.V.
doi:10.1016/j.physa.2006.07.046

exhibiting the form of a *continuity equation* and, consequently, preserving normalization in time. Our purpose here is to explore some aspects of the application of the maximum entropy approach to a special type of evolution equations: those endowed with source terms and, consequently, *not preserving normalization*.

It is a common assumption that entropic concepts, including the maximum entropy principle, can be applied only to *probability distributions*. A given function ρ, if it is to be interpreted as a probability distribution, has to be non-negative and normalized to unity. However, entropic concepts can be profitably applied also to the study of (positive) *densities*, which are non-negative quantities not necessarily normalized to 1. Indeed, a (positive) density can be normalized to any positive number $\mathcal{N}$. The application of the maximum entropy principle to the study of densities allows for the analysis of a variegated family of interesting problems. For example, densities may evolve according to non-linear evolution equations [25–27] (as contrasted to ensemble probabilities which, strictly speaking, must evolve linearly [28]). In this regard, it is worthwhile to remember that Boltzmann himself introduced his celebrated entropic functional in order to study the evolution of the density of particles in the $(\mathbf{x}, \mathbf{v})$ space which, by the way, obeys a non-linear transport equation. When applying the maximum entropy principle to the evolution of a density the normalization $\mathcal{N}$ may even change with time (i.e., $\mathcal{N} = \mathcal{N}(t)$). This is precisely the case with the (linear) evolution equations with source terms that we are going to consider in the present work. There are several possible scenarios where these equations with sources may arise. For instance, when considering the diffusion of a certain type of particles we may need to include explicitly, in the description of the diffusion process, the sources of those particles. This situation may arise in several problems in physics, astronomy, or biology. For example, when dealing with the transport equation of cosmic rays [17], if we want to include the sources of cosmic rays into our model, we have to incorporate the corresponding source-terms into the evolution equation. In spite of its possible practical applications, our principal interest in the present contribution will be to explore the structure of the dynamical equations connecting the (time-dependent) main characters of our maximum entropy scheme: the relevant mean values (constituting, at an initial time t_0, the available prior information), the associated Lagrange multipliers, the partition function, and the entropy. In particular, we are going to investigate the relationships between H-theorems verified by the exact solutions and the H-theorems verified by the maximum entropy approximate ones.

The paper is organized as follows. In Section 2 we explain, and provide some examples, of the type of evolution equations that we are going to consider in this work. Some properties of the exact time-dependent solutions to this equations are derived in Section 3. A maximum entropy formalism to treat these equations is implemented in Section 4, where some of its main features are investigated. In Section 5 some examples are considered, in order to illustrate the results obtained in the previous sections. Finally, some conclusions are drawn in Section 6.

2. Evolution equations with source terms

In Refs. [17–24] the maximum entropy principle has been used with reference to the study of *equations of evolution exhibiting the form of continuity equations*. We may mention, for instance, the Liouville equation, the Fokker–Planck equation, diffusion equations, the Von Neumann's equation in quantum mechanics, etc. The evolution equations that we are going to investigate here comprise a continuity-like equation *plus an extra term K describing a source or a sink*. Let us consider a classical system described by a time-dependent density distribution $F(\mathbf{z}, t)$ evolving according to the partial differential equation

$$\frac{\partial F}{\partial t} + \nabla \cdot \mathbf{J} = K, \tag{1}$$

where $\mathbf{z}$ denotes a point in the relevant N-dimensional phase space, $\mathbf{J}$ is the flux vector, and K represents a source-term ($\mathbf{J}$ and K may depend on the distribution F). As examples we have:

- The one-dimensional diffusion equation with a source term,

$$\frac{\partial F}{\partial t} - Q\frac{\partial^2 F}{\partial x^2} = K, \tag{2}$$

where Q denotes the diffusion coefficient, and the flux is given by

$$J = -Q\frac{\partial F}{\partial x}. \tag{3}$$

- The general Liouville equation with a source term K

$$\frac{\partial F}{\partial t} + \nabla \cdot (F\mathbf{w}) = K, \tag{4}$$

with flux

$$\mathbf{J} = F\mathbf{w}. \tag{5}$$

If $K = 0$ we recover the standard (general) Liouville equation [28,30,31]. The Liouville equation describes the evolution of an ensemble of classical, deterministic dynamical systems evolving according to the equations of motion

$$\frac{d\mathbf{z}}{dt} = \mathbf{w}(\mathbf{z}), \tag{6}$$

where $\mathbf{z}$ denotes a point in the concomitant N-dimensional phase space.
- Hamiltonian ensemble dynamics with sources, a particular instance of the Liouville equations (6). For Hamiltonian systems with n degrees of freedom we have
1. $N = 2n$;
2. $\mathbf{z} = (q_1, \ldots, q_n, p_1, \ldots, p_n)$;
3. $w_i = \partial H/\partial p_i, (i = 1, \ldots, n)$; and
4. $w_{i+n} = -\partial H/\partial q_i, (i = 1, \ldots, n)$;

where the q_i and the p_i stand for generalized coordinates and momenta, respectively.

With reference to the last item note that Hamiltonian dynamics exhibits the important feature of being divergenceless

$$\nabla \cdot \mathbf{w} = 0. \tag{7}$$

For it the Liouville equation simplifies to

$$\frac{\partial F}{\partial t} + \mathbf{w} \cdot \boldsymbol{\nabla} F = K, \tag{8}$$

which is equivalent to a relationship obeyed by the total time derivative

$$\frac{dF}{dt} = K, \tag{9}$$

that is computed along an individual phase-space's orbit.

As mentioned in the Introduction, there are several problems in physics, astronomy, and biology where the evolution equations with sources arise naturally. When studying diffusion problems we can include explicitly, in the description of the diffusion process, the sources of the diffusing particles. In that case, the most natural kind of source term $K(\mathbf{z}, t)$ is given by a positive function of $\mathbf{z}$ and t (if the source is time dependent) not depending on F itself. Another type of situation leading naturally to a source term is given by the diffusion of particles that undergo a certain decay process. In such a case, the changes in the evolving density $F(\mathbf{z}, t)$ have two different origins. On the one hand, the diffusion process itself. On the other one, the decay process. This last factor gives rise to a negative source-like term (that is, a sink-like term) proportional to $F(\mathbf{z}, t)$ itself,

$$K = -qF, \tag{10}$$

where the (negative) constant q is related to the mean life τ of the decaying particles.

3. Evolution of the entropy and the relevant mean values

In order to implement the maximum entropy method, we need to re-formulate our problem in terms of a density $f(\mathbf{z},t)$ that is normalized to unity and therefore can be regarded as a probability density. Consequently, it will prove convenient to re-cast the density distribution $F(\mathbf{z},t)$ under the guise,

$$F(\mathbf{z},t) = \mathcal{N}(t) f(\mathbf{z},t), \tag{11}$$

with

$$\int F(\mathbf{z},t)\,\mathrm{d}^N z = \mathcal{N}(t), \tag{12}$$

and

$$\int f(\mathbf{z},t)\,\mathrm{d}^N z = 1. \tag{13}$$

The evolution equations for $\mathcal{N}$ and f are, respectively,

$$\frac{\mathrm{d}\mathcal{N}}{\mathrm{d}t} = \int K\,\mathrm{d}^N z \tag{14}$$

and

$$\frac{\partial f}{\partial t} + \nabla\cdot\mathbf{j} = k - \frac{\dot{\mathcal{N}}}{\mathcal{N}} f, \tag{15}$$

where we have introduced the abbreviations

$$\mathbf{j} = \frac{\mathbf{J}}{\mathcal{N}} \tag{16}$$

and

$$k = \frac{K}{\mathcal{N}}. \tag{17}$$

3.1. Evolution of the entropy

Since the density f is properly normalized, we can consider its (time-dependent) Shannon entropy

$$S[f] = -\int f \ln f\,\mathrm{d}^N z, \tag{18}$$

whose time derivative is given by (cf. Eq. (15))

$$\begin{aligned}\frac{\mathrm{d}S}{\mathrm{d}t} &= \int \left[\frac{\dot{\mathcal{N}}}{\mathcal{N}} f + \nabla\cdot\mathbf{j} - k\right] \ln f\,\mathrm{d}^N z \\ &= -\frac{\dot{\mathcal{N}}}{\mathcal{N}} S + \int [\nabla\cdot\mathbf{j} - k] \ln f\,\mathrm{d}^N z.\end{aligned} \tag{19}$$

The following alternative (but equivalent) expression for the time derivative of the entropy is also useful:

$$\frac{\mathrm{d}S}{\mathrm{d}t} = -\frac{\dot{\mathcal{N}}}{\mathcal{N}} S - \int k \ln f\,\mathrm{d}^N z + \left\langle \nabla\cdot\left(\frac{\mathbf{j}}{f}\right)\right\rangle. \tag{20}$$

If the source $k(\mathbf{z})$ has a definite sign we can introduce the function

$$g(\mathbf{z},t) = \frac{\mathcal{N}}{\dot{\mathcal{N}}} k(\mathbf{z}), \tag{21}$$

which verifies,

$$g(\mathbf{z},t)\geqslant 0,$$

$$\int g(\mathbf{z},t)\,\mathrm{d}^N z = 1, \tag{22}$$

and can thus be interpreted as a probability density function associated with the source term. Now, adding and subtracting from (20) the integral,

$$\int k \ln\left(\frac{\mathcal{N} k}{\dot{\mathcal{N}}}\right) \mathrm{d}^N z, \tag{23}$$

one can re-cast (20) in the form

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{\dot{\mathcal{N}}}{\mathcal{N}}\{S[g] - S[f] - I[g,f]\} + \left\langle \nabla \cdot \left(\frac{\mathbf{j}}{f}\right)\right\rangle, \tag{24}$$

where

$$I[g,f] = \int g \ln(f/g)\,\mathrm{d}^N z \tag{25}$$

denotes the Kullback distance [29] between the probability densities g and f.

An interesting particular instance of Eq. (24) obtains when we have a source term proportional to F itself,

$$K = qF, \tag{26}$$

with q constant. If $q<0$ we can interpret this source term as describing the flow of particles that undergo a decay process. With a term like (26) we have $g=f$ and

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \left\langle \nabla \cdot \left(\frac{\mathbf{j}}{f}\right)\right\rangle. \tag{27}$$

In the particular case of Liouville equation with a source like (26) we get

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \langle \nabla \cdot \mathbf{w}\rangle, \tag{28}$$

which coincides with the expression for the time derivative of the entropy for the standard, norm preserving Liouville equation [31,32].

3.2. Evolution of the relevant mean values

Another important ingredient of the maximum entropy approach is given by the set of mean values

$$\langle A_i\rangle = \int A_i F\,\mathrm{d}^N z \tag{29}$$

of M relevant quantities A_i, $(i=1,\ldots,M)$. These M quantities are going to play the role of the prior information used to construct the maximum entropy ansatz. We are going to assume that these M mean values are known at an initial time t_0 (more on this later).

The time derivatives of the relevant mean values (29) are

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A_i\rangle = \int [-A_i \nabla \cdot \mathbf{J} + A_i K]\,\mathrm{d}^N z \quad (i=1,\ldots M). \tag{30}$$

Integrating by parts and making the usual assumption that $\mathbf{J}\to 0$ rapidly enough as $|z|\to\infty$, surface terms vanish (they do in 99.9% of physics problems!) and we finally obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A_i\rangle = \int [\mathbf{J}\cdot \boldsymbol{\nabla} A_i + A_i K]\,\mathrm{d}^N z \quad (i=1,\ldots,M). \tag{31}$$

We are also going to need, and thus introduce now, the "re-scaled" mean values,

$$a_i = \frac{1}{\mathcal{N}} \langle A_i \rangle. \tag{32}$$

4. MaxEnt ansatz for the evolution equation

4.1. Preliminaries

A central point for our present discussion is that of considering a specially important ansatz for solving the evolution equation (1), namely, the MaxEnt one,

$$F(\mathbf{z}, t) = \mathcal{N} f_{ME}(\mathbf{z}, t) = \frac{\mathcal{N}}{Z} \exp\left[-\sum_{i=1}^{M} \lambda_i A_i \right], \tag{33}$$

where the $A_i(\mathbf{z})$ are M appropriate quantities that are functions of the phase space location $\mathbf{z}$. The partition function Z is given by

$$Z = \int \exp\left[-\sum_{i=1}^{M} \lambda_i A_i \right] \mathrm{d}^N z. \tag{34}$$

The probability distribution f_{ME} appearing in (33) is the one that maximizes the entropy $S[f]$ under the constraints imposed by normalization and the relevant mean values $\langle A_i \rangle$ (or the $a_i = \langle A_i \rangle / \mathcal{N}$). The re-scaled relevant mean values a_i and the associated Lagrange multipliers λ_i are related by the celebrated Jaynes' relations [15]

$$\lambda_i = \frac{\partial S}{\partial a_i}, \tag{35}$$

$$a_i = \frac{\langle A_i \rangle}{\mathcal{N}} = -\frac{\partial}{\partial \lambda_i} (\ln Z), \tag{36}$$

$$S = \ln Z + \sum_i \lambda_i a_i, \tag{37}$$

and

$$\frac{\partial \lambda_i}{\partial a_j} = \frac{\partial^2 S}{\partial a_i \partial a_j} = \frac{\partial \lambda_j}{\partial a_i}. \tag{38}$$

It is not possible to exagerate the importance of Jaynes' relations (35)–(38). Within Jaynes' information-theoretical approach to statistical mechanics, the aforementioned relations constitute the basis of the connection between statistical mechanics and thermodynamics. All the basic equations of equilibrium thermodynamics are particular instances of (35)–(38), or can be derived from special instances of (35)–(38). *This fact alone provides already a strong motivation* for studying in detail the interplay between the various quantities appearing in Jaynes' relations, when applying the maximum entropy principle to diverse physical scenarios. Indeed, a special instance of this line of enquiry constitutes one of our main focuses of attention here.

All the time dependence of the maximum entropy distribution f_{ME} appearing in the ansatz (33) is contained in the Lagrange multipliers $\lambda_i(t)$, which are assumed to be time dependent. The Lagrange multipliers (and the normalization factor $\mathcal{N}$) change in time in order to accommodate to the evolving mean values $\langle A_i \rangle$ (and the evolving norm of $F(\mathbf{z}, t)$). We assume that the mean values of the M relevant quantities A_i at an initial time t_0,

$$\{\langle A_1 \rangle_{t_0}, \ldots, \langle A_M \rangle_{t_0}\}, \tag{39}$$

as well as the initial value $\mathcal{N}_{t_0}$, are known. They constitute our prior information. On the basis of these initial data we determine the initial values of the Lagrange multipliers λ_i and the partition function Z. Then, on the basis of an appropriate set of equations of motion for the relevant mean values (constructed using the evolving maximum entropy ansatz) we determine the (approximate) time evolution of the $\langle A_i \rangle$. Now, in general, the time derivatives of the aforementioned mean values are given by Eq. (31), that is re-written here for convenience,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A_i \rangle = \int [\mathbf{J} \cdot \nabla A_i + A_i K]\, \mathrm{d}^N z \quad (i = 1, \ldots, M). \tag{40}$$

The integrals appearing in the right-hand sides of these equations generally involve, unfortunately, new mean values not included in the original set $\langle A_i \rangle (i = 1, \ldots, M)$ (remember that the flux $\mathbf{J}$ depends on the distribution f). One way to implement the maximum entropy approach to solve the evolution equation (1) is to evaluate, at each instant of time, the right-hand sides of (40) using the maximum entropy ansatz (33). In this way, the system of equations (40) can be translated into a closed system of motion for the Lagrange multipliers λ_i. This (time-dependent self-consistent) approach will yield either exact solutions, or only approximate solutions, depending on the specific form of the evolution equation (1) (such is also the case, of course, in the case of continuity equations. See [19–23] and references therein).

4.2. Time evolution

We discuss now specific details of the temporal evolution, beginning with that of the Lagrange multipliers. Regarding the set of quantities $a_i, (i = 1, \ldots, M)$ as the set of independent parameters characterizing f_{ME}, we get

$$\begin{aligned}\frac{\mathrm{d}\lambda_i}{\mathrm{d}t} &= \sum_{j=1}^{M} \left(\frac{\partial \lambda_j}{\partial a_i}\right)\left(\frac{\mathrm{d}a_i}{\mathrm{d}t}\right) \\ &= \frac{\partial}{\partial a_i}\left(\sum_{j=1}^{M} \lambda_j \left(\frac{\mathrm{d}a_j}{\mathrm{d}t}\right)\right) - \sum_{j=1}^{M} \lambda_j \frac{\partial}{\partial a_i}\left(\frac{\mathrm{d}a_j}{\mathrm{d}t}\right).\end{aligned} \tag{41}$$

Now, since $\langle A_i \rangle = \mathcal{N} a_i$, we have

$$\begin{aligned}\frac{\mathrm{d}a_i}{\mathrm{d}t} &= \frac{1}{\mathcal{N}}\frac{\mathrm{d}\langle A_i \rangle}{\mathrm{d}t} - a_i \frac{\mathrm{d}\ln \mathcal{N}}{\mathrm{d}t} \\ &= \frac{1}{\mathcal{N}} \int [\mathbf{J} \cdot \nabla A_i + A_i K - \dot{\mathcal{N}} f A_i]\, \mathrm{d}^N z,\end{aligned} \tag{42}$$

and, as a consequence,

$$\sum_{i=1}^{M} \lambda_i \left(\frac{\mathrm{d}a_i}{\mathrm{d}t}\right) = \frac{1}{\mathcal{N}} \int \left(\mathbf{J} \cdot \nabla \sum_i \lambda_i A_i + K \sum_i \lambda_i A_i - \dot{\mathcal{N}} f \sum_i \lambda_i A_i\right) \mathrm{d}^N z. \tag{43}$$

Substituting now the MaxEnt ansatz (33) for f (remember that we have defined $\mathbf{j} = \mathbf{J}/\mathcal{N}$) one gets

$$\begin{aligned}\sum_{i=1}^{M} \lambda_i \left(\frac{\mathrm{d}a_i}{\mathrm{d}t}\right) &= \int f \nabla \cdot (\mathbf{j}/f)\, \mathrm{d}^N z + \frac{1}{\mathcal{N}} \int [\dot{\mathcal{N}} f - K][\ln(fZ)]\, \mathrm{d}^N z \\ &= \frac{1}{\mathcal{N}} \left[\langle \nabla \cdot (\mathbf{j}/f) \rangle + \int [\dot{\mathcal{N}} f - K][\ln(fZ)]\, \mathrm{d}^N z\right] \\ &= \frac{1}{\mathcal{N}} (\langle \nabla \cdot (\mathbf{j}/f) \rangle + \int [\dot{\mathcal{N}} f - K] \ln f\, \mathrm{d}^N z),\end{aligned} \tag{44}$$

where the fact has been used that (14) implies $\int [\dot{\mathcal{N}} f - K][\ln(Z)]\, \mathrm{d}^N z = 0$. Finally,

$$\begin{aligned}\frac{\mathrm{d}\lambda_i}{\mathrm{d}t} &= \frac{\partial}{\partial a_i} \int \left[f \nabla \cdot \left(\frac{\mathbf{j}}{f}\right) + \left(\frac{\dot{\mathcal{N}}}{\mathcal{N}} f - k\right) \ln f\right] \mathrm{d}^N z \\ &\quad - \sum_{j=1}^{M} \lambda_j \frac{\partial}{\partial a_i} \int \left[\mathbf{j} \cdot \nabla A_j + A_j k - \frac{\dot{\mathcal{N}}}{\mathcal{N}} f A_j\right] \mathrm{d}^N z.\end{aligned} \tag{45}$$

4.3. Evolution of the entropy

Now we are going to consider the time derivative of the entropy evaluated on the maximum entropy solution: $S[f_{ME}]$. From Eqs. (36) and (37) we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}S[f_{ME}] &= \frac{\mathrm{d}}{\mathrm{d}t}(\ln Z) + \frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{i=1}^{M}\lambda_i a_i\right)\\ &= \sum_i \frac{\mathrm{d}\lambda_i}{\mathrm{d}t}\frac{\partial}{\partial\lambda_i}(\ln Z) + \sum_i \frac{\mathrm{d}\lambda_i}{\mathrm{d}t}a_i + \sum_i \lambda_i \frac{\mathrm{d}a_i}{\mathrm{d}t}\\ &= \sum_i \lambda_i \frac{\mathrm{d}a_i}{\mathrm{d}t},\end{aligned} \tag{46}$$

and, using now (43), the important relation

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}S[f_{ME}] &= \frac{1}{\mathcal{N}}\int\left[\mathbf{J}\cdot\nabla\sum_i \lambda_i A_i + K\sum_i \lambda_i A_i - \dot{\mathcal{N}} f_{ME}\sum_i \lambda_i A_i\right]\mathrm{d}^N z\\ &= \int\left[-(\nabla\cdot\mathbf{j})\left(\sum_i \lambda_i A_i\right) + k\sum_i \lambda_i A_i - \frac{\dot{\mathcal{N}}}{\mathcal{N}} f_{ME}\sum_i \lambda_i A_i\right]\mathrm{d}^N z\\ &= \int\left[(\nabla\cdot\mathbf{j})(\ln Z + \ln f_{ME}) + \left(\frac{\dot{\mathcal{N}}}{\mathcal{N}} f_{ME} - k\right)(\ln Z + \ln f_{ME})\right]\mathrm{d}^N z\\ &= \int\left(\nabla\cdot\mathbf{j} + \frac{\dot{\mathcal{N}}}{\mathcal{N}} f_{ME} - k\right)\ln f_{ME}\,\mathrm{d}^N z\\ &= -\frac{\dot{\mathcal{N}}}{\mathcal{N}}S[f_{ME}] + \int(\nabla\cdot\mathbf{j} - k)\ln f_{ME}\,\mathrm{d}^N z.\end{aligned} \tag{47}$$

Summing up, we have,

$$\frac{\mathrm{d}}{\mathrm{d}t}S[f_{ME}] = -\frac{\dot{\mathcal{N}}}{\mathcal{N}}S[f_{ME}] + \int(\nabla\cdot\mathbf{j} - k)\ln f_{ME}\,\mathrm{d}^N z. \tag{48}$$

Comparing now the expression for the entropy's time derivative corresponding to the exact solutions (cf. Eq. (19)) with the expression just derived (48) for the maximum entropy ansatz, we can reach an important conclusion: our present maximum entropy scheme always (even in the case of approximate solutions) preserves the exact functional relationship between the time derivative of the entropy and the time-dependent solutions of the evolution equation. Consequently, any H-theorem verified when evaluating the entropy functional upon the exact solutions is also verified when evaluating the entropy upon the MaxEnt approximate treatments. This is of considerable relevance in connection with the consistency of the method as a maximum entropy approach.

5. Examples

5.1. Liouville equation with constant sources

According to Eq. (31), and remembering that, for the Liouville equation, the flux is given by $\mathbf{J} = F\mathbf{w}$, the temporal evolution of the mean values of the dynamical quantities A_i is

$$\begin{aligned}\frac{\mathrm{d}\langle A_i\rangle}{\mathrm{d}t} &= \int[F\mathbf{w}\cdot\nabla A_i + A_i K]\,\mathrm{d}^N z\\ &= \langle\mathbf{w}\cdot\nabla A_i\rangle + B_i \quad (i = 1,\ldots,M),\end{aligned} \tag{49}$$

where

$$B_i = \int A_i K \, d^N z \quad (i = 1, \ldots, M). \tag{50}$$

Here we are going to assume that f is given by the ansatz (33)–(34). We can then regard the quantities Z, f, and λ_i's as functions of the set $a_1, \ldots, a_M$. Alternatively, it is also possible to regard all relevant quantities as functions of the λ_i's instead.

Let us consider the important particular case where the following closure relationship holds:

$$\mathbf{w} \cdot \nabla A_i = \sum_j^M C_{ij} A_j \quad (i = 1, \ldots, M), \tag{51}$$

where the C_{ij} constitute a set of (structure) constants. This entails that

$$\frac{d\langle A_i \rangle}{dt} = \sum_j^M C_{ij} \langle A_j \rangle + B_i \quad (i = 1, \ldots, M). \tag{52}$$

It is useful also to introduce the quantity,

$$B_0 = \int K \, d^N z \quad (i = 1, \ldots, M). \tag{53}$$

The general solution of the equations of motion for the mean values is then seen to be of the form

$$\langle A_i \rangle(t) = \langle A_i \rangle_{\text{inhom.}} + \langle A_i \rangle_{\text{hom.}}, \tag{54}$$

where $\langle A_j \rangle_{\text{inhom.}}$ complies with

$$\sum_{j=1}^N C_{ij} \langle A_j \rangle_{\text{inhom.}} + B_i = 0, \tag{55}$$

and is a particular solution of the (inhomogeneous) set of linear differential equations, while $\langle A_i \rangle_{\text{hom.}}$ is the general solution of the homogeneous set of equations

$$\frac{d\langle A_i \rangle}{dt} = \sum_j^M C_{ij} \langle A_j \rangle \quad (i = 1, \ldots, M). \tag{56}$$

Now, if $\nabla \cdot \mathbf{w} = 0$ (that is, if the flux $\mathbf{w}$ is divergenceless) the temporal evolution of the Lagrange multiplier is given by

$$\begin{aligned}
\frac{d\lambda_i}{dt} &= \frac{\partial}{\partial a_i} \int \left[f \nabla \cdot \left(\frac{\mathbf{j}}{f} \right) + \left(\frac{\dot{\mathcal{N}}}{\mathcal{N}} f - k \right) \ln f \right] d^N z \\
&\quad - \sum_{j=1}^M \lambda_j \frac{\partial}{\partial a_i} \int \left[\mathbf{j} \cdot \nabla A_j + A_j k - \frac{\dot{\mathcal{N}}}{\mathcal{N}} f A_j \right] d^N z \\
&= \frac{\partial}{\partial a_i} \int \left[f \nabla \cdot \mathbf{w} + \frac{1}{\mathcal{N}} \left(\dot{\mathcal{N}} f - K \right) \ln f \right] d^N z \\
&\quad - \sum_{j=1}^M \lambda_j \frac{\partial}{\partial a_i} \int \left[f \mathbf{w} \cdot \nabla A_j + \frac{1}{\mathcal{N}} (A_j K - \dot{\mathcal{N}} f A_j) \right] d^N z
\end{aligned}$$

$$
\begin{aligned}
&= -\frac{\dot{\mathcal{N}}}{\mathcal{N}}\frac{\partial S}{\partial a_i} - \frac{1}{\mathcal{N}}\frac{\partial}{\partial a_i}\int K \ln f \, \mathrm{d}^N z \\
&\quad - \sum_{j=1}^{M} \lambda_j \frac{\partial}{\partial a_i}\int \left[f\left(\sum_k^M C_{jk} A_k\right) + \frac{1}{\mathcal{N}}(A_j K - \dot{\mathcal{N}} f A_j)\right] \mathrm{d}^N z \\
&= -\frac{\dot{\mathcal{N}}}{\mathcal{N}}\lambda_i - \frac{1}{\mathcal{N}}\frac{\partial}{\partial a_i}\int K \ln f \, \mathrm{d}^N z \\
&\quad - \sum_{j=1}^{M} \lambda_j \frac{\partial}{\partial a_i}\left[\left(\sum_k^M C_{jk} a_k\right) + \frac{1}{\mathcal{N}}\left(\int A_j K \, \mathrm{d}^N z\right) - \frac{\dot{\mathcal{N}}}{\mathcal{N}} a_j\right] \\
&= -\frac{\dot{\mathcal{N}}}{\mathcal{N}}\lambda_i - \frac{1}{\mathcal{N}}\frac{\partial}{\partial a_i}\int K \ln f \, \mathrm{d}^N z \\
&\quad - \sum_{j=1}^{M} \lambda_j \left[C_{ji} + \frac{1}{\mathcal{N}}\frac{\partial}{\partial a_i}\left(\int A_j K \, \mathrm{d}^N z\right) - \frac{\dot{\mathcal{N}}}{\mathcal{N}}\delta_{ij}\right],
\end{aligned} \tag{57}
$$

which ends up in

$$
\frac{\mathrm{d}\lambda_i}{\mathrm{d}t} = \left(\sum_{j=1}^{M} C_{ji}\lambda_j\right) - \frac{1}{\mathcal{N}}\frac{\partial}{\partial a_i}\int K \ln f \, \mathrm{d}^N z. \tag{58}
$$

5.2. A collisional Vlasov equation with sources

We are going to consider the following collisional Vlasov with sources:

$$
\frac{\partial F}{\partial t} + v\frac{\partial F}{\partial x} - \left[\frac{\partial \phi}{\partial x} + \gamma v\right]\frac{\partial F}{\partial v} - \gamma\alpha\frac{\partial^2 F}{\partial v^2} - \gamma F = [\beta_0 + \beta_1 x^2]F, \tag{59}
$$

where γ, α, β_0, and β_1 are constants (γ and α are positive) and the potential ϕ is of a quadratic form,

$$
\phi(x) = \tfrac{1}{2}\phi_2 x^2. \tag{60}
$$

Here we are also going to assume that $\phi_2 > 0$. Eq. (59) is a generalization of the source-free equation studied in Ref. [24]. Let us now consider a maximum entropy ansatz of the form

$$
\begin{aligned}
F(x, v, t) &= \exp[-\lambda_0 - \lambda_1 x - \lambda_2 v - \lambda_3 x^2 - \lambda_4 xv - \lambda_5 v^2], \\
&= \frac{\mathcal{N}}{Z}\exp[-\lambda_1 x - \lambda_2 v - \lambda_3 x^2 - \lambda_4 xv - \lambda_5 v^2] \\
&= \mathcal{N} f,
\end{aligned} \tag{61}
$$

where the $\lambda_i, i = 0, \ldots, 5$ are appropriate Lagrange multipliers and

$$
Z = \int \exp[-\lambda_1 x - \lambda_2 v - \lambda_3 x^2 - \lambda_4 xv - \lambda_5 v^2] \, \mathrm{d}x \, \mathrm{d}v. \tag{62}
$$

The (normalized) distribution f appearing in (61) maximizes the Boltzmann–Gibbs entropic functional,

$$
S[f] = -\int f(x, v, t) \ln f(x, v, t) \, \mathrm{d}x \, \mathrm{d}v, \tag{63}
$$

under the constraints imposed by normalization and the instantaneous mean values of the quantities $B_1 = x$, $B_2 = v$, $B_3 = x^2$, $B_4 = xv$, and $B_5 = v^2$. All the time dependence of the ansatz (61) is expressed through the Lagrange multipliers λ_i, which are time dependent. Inserting the ansatz (61) into the partial differential equation (59), and equating to zero, separately, terms proportional to $x^i v^j$ with different exponents i,j, it is possible to prove that the ansatz (61) constitutes an exact solution to (59), provided that the Lagrange multipliers comply with the set of coupled ordinary differential equations,

$$\frac{d\lambda_0}{dt} = -\gamma\alpha\lambda_2^2 + 2\gamma\alpha\lambda_5 - \gamma - \beta_0, \tag{64}$$

$$\frac{d\lambda_1}{dt} = \phi_2\lambda_2 - 2\gamma\alpha\lambda_4\lambda_2, \tag{65}$$

$$\frac{d\lambda_2}{dt} = -\lambda_1 + \gamma\lambda_2 - 4\gamma\alpha\lambda_2\lambda_5, \tag{66}$$

$$\frac{d\lambda_3}{dt} = \phi_2\lambda_4 - \gamma\alpha\lambda_4^2 - \beta_1, \tag{67}$$

$$\frac{d\lambda_4}{dt} = -2\lambda_3 + 2\phi_2\lambda_5 + \gamma\lambda_4 - 4\gamma\alpha\lambda_4\lambda_5, \tag{68}$$

and

$$\frac{d\lambda_5}{dt} = -\lambda_4 - 4\gamma\alpha\lambda_5^2 + 2\gamma\lambda_5. \tag{69}$$

Alternatively, we can focus our attention on the set of ordinary differential equations governing the evolution of the selected set of relevant mean values,

$$\frac{d}{dt}\langle x\rangle = \langle v\rangle + \beta_0\langle x\rangle + \beta_1\langle x^3\rangle, \tag{70}$$

$$\frac{d}{dt}\langle v\rangle = -\phi_2\langle x\rangle - \gamma\langle v\rangle + \beta_0\langle v\rangle + \beta_1\langle x^2 v\rangle, \tag{71}$$

$$\frac{d}{dt}\langle x^2\rangle = 2\langle xv\rangle + \beta_0\langle x^2\rangle + \beta_1\langle x^4\rangle, \tag{72}$$

$$\frac{d}{dt}\langle xv\rangle = -\phi_2\langle x^2\rangle - \gamma\langle xv\rangle + \langle v^2\rangle + \beta_0\langle xv\rangle + \beta_1\langle x^3 v\rangle, \tag{73}$$

and

$$\frac{d}{dt}\langle v^2\rangle = -2\phi_2\langle xv\rangle - 2\gamma\langle v^2\rangle + 2\alpha\gamma + \beta_0\langle v^2\rangle + \beta_1\langle x^2 v^2\rangle. \tag{74}$$

This example exhibits the peculiarity that, in spite of the fact that the maximum entropy ansatz (61) provides exact time-dependent solutions to Eq. (59), the equations of motion (70)–(74) for the five relevant mean values do not constitute a closed set of differential equations of motion for these quantities.

6. Conclusions

A maximum entropy approach to construct approximate, time-dependent solutions to evolution equations endowed with source terms was considered. We have shown that in some particular cases the method leads to exact time-dependent solutions. By construction our present implementation of the maximum entropy prescription complies with the exact equations of motion of the relevant mean values. Moreover, it always (even in the case of approximate solutions) preserves the exact functional relationship between the time derivative of the entropy and the time-dependent solutions of the evolution equation. This means that any H-theorem verified when evaluating the entropy functional upon the exact solutions is also verified when evaluating the entropy upon the MaxEnt approximate treatments. This is of considerable relevance in connection with the consistency of the method as a maximum entropy approach. Other features exhibited by the maximum entropy solutions and some illustrative examples were also discussed.

References

[1] E.T. Jaynes, Probability Theory: The Logic of Science, Cambridge University Press, Cambridge, 2005.
[2] B.R. Frieden, Physics from Fisher Information, Cambridge University Press, Cambridge, 1998.
[3] B.R. Frieden, Science from Fisher Information, Cambridge University Press, Cambridge, 2004.
[4] B.R. Frieden, B.H. Soffer, Phys. Rev. E 52 (1995) 2274.
[5] C. Beck, F. Schlogl, Thermodynamics of Chaotic Systems, Cambridge University Press, Cambridge, 1993.
[6] S. Sieniutycz, H. Farkas (Eds.), Variational and Extremum Principles in Macroscopic Systems, Elsevier, Amsterdam, 2005.
[7] M. Gell-Mann, C. Tsallis (Eds.), Nonextensive Entropy—Interdisciplinary Applications, Oxford University Press, Oxford, 2004.
[8] T.D. Franck, Nonlinear Fokker-Planck Equations, Springer, Berlin, 2005.
[9] T. Yamano, Eur. Phys. J. B 18 (2000) 103.
[10] B.M. Boghosian, Phys. Rev. E 53 (1996) 4754.
[11] E. Curado, A. Plastino, Phys. Rev. E 72 (2005) 047103.
[12] L. Borland, Physica D 99 (1996) 175.
[13] J.W. Gibbs, Elementary Principles in Statistical Mechanics, Yale University Press, New Haven, 1902.
[14] E.T. Jaynes, Papers on Probability, Statistics and Statistical Physics, in: R.D. Rosenkrantz (Ed.), Reidel, Dordrecht, 1987.
[15] A. Katz, Principles of Statistical Mechanics: The Information Theory Approach, Freeman, San Francisco, 1967.
[16] W.T. Grandy Jr., P.W. Milonni (Eds.), Physics and Probability. Essays in Honor of Edwin T. Jaynes, Cambridge University Press, New York, 1993.
[17] P. Hick, G. Stevens, Astron. Astrophys. 172 (1987) 350.
[18] J. Baker-Jarvis, M. Racine, J. Alameddine, J. Math. Phys. 30 (1989) 1459.
[19] A.R. Plastino, A. Plastino, Phys. Lett. A 226 (1997) 257.
[20] A.R. Plastino, H.G. Miller, A. Plastino, Phys. Rev. E 56 (1997) 3927.
[21] A.R. Plastino, H.G. Miller, A. Plastino, G.D. Yen, J. Math. Phys. 38 (1997) 6675.
[22] A. Plastino, A.R. Plastino, H.G. Miller, Phys. Lett. A 232 (1997) 349.
[23] E.D. Malaza, H.G. Miller, A.R. Plastino, F. Solms, Physica A 265 (1999) 224.
[24] S.A. El-Wakil, A. Elhanbaly, M.A. Abdou, Physica A 323 (2003) 213.
[25] C. Tsallis, D. Buckman, Phys. Rev. E 54 (1996) 2197.
[26] L. Borland, F. Pennini, A.R. Plastino, A. Plastino, Eur. Phys. J. B 12 (1999) 285.
[27] P.C. da Silva, L.R. da Silva, E.K. Lenzi, R.S. Mendes, L.C. Malacarne, Physica A 342 (2004) 16.
[28] N.G. van Kampen, Stochastic Processes in Physics and Chemistry, North-Holland, Amsterdam, 1992.
[29] S. Kullback, Information Theory and Statistics, Wiley, New York, 1959.
[30] J. Liouvile, J. Math. Pure Appl. 3 (1838) 342.
[31] L. Andrey, Phys. Lett. A 111 (1985) 45.
[32] D. Ruelle, Conversations on Nonequilibrium Physics with an Extraterrestrial, Phys. Today (2004) 48.