About an H-theorem for systems with non-conservative interactions

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Received 29 May 2013
Accepted 10 July 2013
Published 9 August 2013

Abstract. We present some arguments in favor of an H-theorem for a generalization of the Boltzmann equation including non-conservative interactions and a linear Fokker–Planck-like thermostatting term. Such a non-linear equation describing the evolution of the single particle probability \( P_i(t) \) of being in state \( i \) at time \( t \) is a suitable model for granular gases and is referred to here as the Boltzmann–Fokker–Planck (BFP) equation. The conjectured H-functional, which appears to be non-increasing, is \( H_C(t) = \sum_i P_i(t) \ln \frac{P_i(t)}{\Pi_i} \) with \( \Pi_i = \lim_{t \to \infty} P_i(t) \), in analogy with the H-functional of Markov processes. The extension to continuous states is straightforward. A simple proof can be given for the elastic BFP equation. A semi-analytical proof is also offered for the BFP equation for so-called inelastic Maxwell molecules. Other evidence is obtained by solving particular BFP cases through numerical integration or through ‘particle schemes’ such as the direct simulation Monte Carlo.

Keywords: granular matter, kinetic theory of gases and liquids, Boltzmann equation
1. Introduction

The H-theorem is a consequence of the Boltzmann equation (whose validity, at least for
diluted gases, is now well understood) and has a great relevance in statistical mechanics
because it leads to two basic results [1]. First it provides a dynamical proof of the stationary
Maxwell–Boltzmann distribution for the particle velocity

\[ p_{MB}(v) = \left[ \frac{2\pi}{\beta m} \right]^{-3/2} e^{-\beta mv^2/2} \]

and second it states that the approach of the probability distribution \( p(v, t) \) toward \( p_{MB}(v) \)
is monotonic. The latter result can be interpreted as an instance of the second law of the
thermodynamics.

The literature about this subject is enormous and it is impossible to enter into
details. A discussion about the deep and intriguing issues concerning the reversibility
and recurrence paradoxes, as well the rigorous derivation of the Boltzmann equation in
the Grad–Boltzmann limit, can be found in [2]–[5].

doi:10.1088/1742-5468/2013/08/P08003
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After the seminal results by Boltzmann obtained employing his transport equation describing the behavior of diluted gases, similar H-theorems had been obtained for systems described by Markov processes, that is systems ruled by master equations or Fokker–Planck equations [6]. There is however an important difference with respect to the original Boltzmann H-theorem, where the functional $H_G[p]$ depends only on $p(v, t)$ and the knowledge of the asymptotic stationary probability $p_{MB}(v)$ is not required: for Markov processes the functional $H_C[p, \Pi]$ depends both on $p(v, t)$ and the asymptotic stationary probability $\Pi(v)$ which must be determined, see section 2 for details.

One of the basic features of the Boltzmann equation is the presence of bilinear terms, describing the binary collisions. Although the Boltzmann equation had been originally derived for systems with conservative dynamics, it is not difficult, at least at the formal level, to write down a similar evolution equation for the one-particle probability distribution for some dissipative systems (e.g. diluted granular gases). Due to the dissipative nature of granular gases, it is necessary to introduce an external mechanism pumping energy into the system, in order to have a statistical stationary state (mathematically a non-trivial stationary probability distribution). As a result the evolution equation for $p(v, t)$ includes a linear term representing the coupling to the ‘external bath’ and a bilinear term accounting for binary collisions [7].

In the classical derivation of Boltzmann a key feature used to prove the H-theorem is the presence of time reversal symmetry. The absence of such a property in dissipative systems is one of the technical difficulties in deriving a more general H-theorem. In view of its physical and mathematical relevance, the study of relaxation toward invariant probability, in terms of entropic functions, has attracted the interest of many scientists [8]–[11].

Previous studies have shown that both the stationary and dynamical statistical features are the combined results of bath and collisions [12]. We will see that in granular systems H-theorems, if any, must be the outcomes of both the linear and bilinear part of the evolution equation. The control of such contributions is not easy: we are able to show an H-theorem in the particular limit of ‘elastic granular’ gases in an external bath. Such a system, although quite artificial, presents non-trivial dynamical features. In addition we give some semi-analytical treatment of a Maxwell model of granular gas, and detailed numerical computations supporting our idea.

The paper is organized as follows. Section 2 is a quick summary of known different H-theorems for the Boltzmann equation and Markov processes. In section 3 we present a kinetic description of diluted granular gases and some results about the H-theorems for such a systems in particular limits. Section 4 treats numerical simulation of the granular gases in different regimes. In section 5 the reader can find some conclusion. The appendices are devoted to few technical details.

2. Monotonic approach to invariant probability

For completeness we briefly review, in this section, two known H-theorems.

2.1. Boltzmann equation for elastic isolated gases

For the sake of notational simplicity we consider the case where the states of the system are discrete. Let us call $P_i(t)$ the probability of observing a state $i$ at time $t$. Assuming
the validity of the molecular chaos assumption, its evolution is governed by the following non-linear equation:

$$\frac{dP_i(t)}{dt} = \sum_{k,l,j} \left[ W^{(2)}_{(k,l)\rightarrow(i,j)} P_k(t)P_l(t) - W^{(2)}_{(i,j)\rightarrow(k,l)} P_i(t)P_j(t) \right],$$

where $W^{(2)}_{(k,l)\rightarrow(i,j)}$ denotes the transition rate of the ‘collision’ from the states $k$ and $l$ to the states $i$ and $j$. By invariance under time inversion one has the following property:

$$W^{(2)}_{(k,l)\rightarrow(i,j)} = W^{(2)}_{(i,j)\rightarrow(k,l)}$$

so that (1) takes the form

$$\frac{dP_i(t)}{dt} = \sum_{k,l,j} W^{(2)}_{(k,l)\rightarrow(i,j)} \left[ P_k(t)P_l(t) - P_i(t)P_j(t) \right].$$

Using such a structure it is easy to show the H-theorem, i.e. the $H_G(t)$ function

$$H_G(t) = \sum_i P_i(t) \ln P_i(t)$$

is monotonically decreasing:

$$\frac{dH_G(t)}{dt} \leq 0$$

and reaches its minimum $P_j = \Pi_j$ when the PdF corresponds to the Maxwell–Boltzmann distribution.

### 2.2. Markov processes

An H-theorem also holds under rather general hypothesis [6] for processes governed by a master equation of the form

$$\frac{dP_i(t)}{dt} = \sum_{k \neq i} \left[ W^{(1)}_{k\rightarrow i} P_k(t) - W^{(1)}_{i\rightarrow k} P_i(t) \right].$$

Here $W^{(1)}_{k\rightarrow i}$ is the transition rate from the state $k$ to the state $i$.

In this case indicating with $\{\Pi_i\}$ the invariant probabilities, which are the solutions of the equation

$$\Pi_i = \frac{1}{\gamma_i} \sum_{k \neq i} W^{(1)}_{k\rightarrow i} \Pi_k$$

where $\gamma_i = \sum_{k \neq i} W^{(1)}_{i\rightarrow k}$,

one has that the function $H_C(t)$

$$H_C(t) = \sum_i P_i(t) \ln \frac{P_i(t)}{\Pi_i}$$

is non-increasing, i.e.

$$\frac{dH_C(t)}{dt} \leq 0$$

doi:10.1088/1742-5468/2013/08/P08003
and attains its minimum when $P_j = \Pi_j$. Let us note that $-H_C$ is the conditional entropy, also known as Kullback-Leibler or relative entropy [13].

In the case of continuous variables it is sufficient to replace the probability $P_i(t)$ with the probability density $p(x,t)$ (where $x$ is a state in a continuous space, e.g. velocity of a particle) and the sums with the integrals. The $H_C$ function becomes

$$H_C(t) = \int p(x,t) \ln \frac{p(x,t)}{\Pi(x)} \, dx.$$ 

### 2.3. Some remarks

Notice that $H_C$ is an intrinsic property, that is switching to a new variable $y(x)$, if the transformation between $x$ and $y$ is invertible, $H_C$ is invariant, whereas $H_G$ is not [13, 14].

Moreover, for certain classes of Markov processes it is possible to show [15] a result stronger than the monotonic behavior of $H_C(t)$: there exists a constant $\gamma > 0$ such that

$$H_C(t) \leq e^{-\gamma t} H_C(0).$$

Finally, one may wonder if $H_C$ is non-increasing also in the case of the (elastic) Boltzmann case, equation (3). It is immediate to verify that it is true. Indeed,

$$H_C(t) = H_G(t) - \sum_i P_i(t) \ln \Pi_i$$

and given that $\ln \Pi_i$ is a linear combination of conserved quantities, the second term of the right-hand side is constant, so that $dH_C/dt = dH_G/dt$.

In appendix A we report two derivations, necessary for the proof of result (14) below. Such derivations are nothing but the well known proofs of equations (5) and (7): the reader may verify that, by replacing $f_i(t)$ with $P_i(t)$ and $A_{i,j,k,l}$ with $W_{(i,j)\rightarrow(k,l)}^{(2)}$ in section A.2, one obtains the proof of the Boltzmann H-theorem, and, replacing $dH_C/dt|_M$ with $dH_C/dt$ in section A.1, the H-theorem for Markov processes is proved.

We conclude this section citing some recent works about an H-theorem for economic models based upon non-linear Boltzmann equations [16] also at discrete time [17], that is with an evolution law of the kind

$$P_{n+1}(v) = \int P_n(v_1)P_n(v_2)K(v, v_1, v_2) \, dv_1 \, dv_2.$$

### 3. Granular gases with homogeneous energy injection

In the case of dilute granular gases interactions are dissipative (e.g. inelastic hard-core collisions) and the property in equation (2) does not hold. One of the consequences of energy dissipation is that the Boltzmann equation [18] without any external energy input has usually a trivial asymptotic state (e.g. the velocities of all particles vanish). Among the many models of energy injection [19]–[21], experiments [12, 22] have shown the relevance of a mechanism where all particles are coupled with a random energy reservoir [7]: such a simple mechanism well reproduces the effect of an interaction of all the particles with rough vibrating boundaries of the container.

In this model, under the hypothesis of molecular chaos and in the discrete representation introduced above, the probability $P_i(t)$ obeys the following
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'Boltzmann–Fokker–Planck' (BFP) equation:

\[ \frac{dP_i(t)}{dt} = \sum_k \left[ W_{k \rightarrow i}^{(1)} P_k(t) - W_{i \rightarrow k}^{(1)} P_i(t) \right] + \sum_{k,l,j} \left[ W_{(k,l) \rightarrow (i,j)}^{(2)} P_k(t) P_l(t) - W_{(i,j) \rightarrow (k,l)}^{(2)} P_i(t) P_j(t) \right]. \] (9)

As anticipated, when collisions are inelastic the time inversion symmetry, equation (2), does not hold, i.e. \( W_{(k,l) \rightarrow (i,j)}^{(2)} \neq W_{(i,j) \rightarrow (k,l)}^{(2)} \). Notice that, in general, the existence of a solution satisfying detailed balance with respect to the Markov rates \( W^{(1)} \) is not required to guarantee a stationary state of equation (9). However in the literature detailed balance with respect to \( W^{(1)} \) has been often assumed [7] and, for this reason, it is customary to consider such an energy injection mechanism equivalent to coupling the gas with a heat bath.

For continuous variables equation (9) is replaced by an evolution equation for the density \( p(x,t) \):

\[ \frac{\partial}{\partial t} p(x,t) = L_{FP} p(x,t) + C_B(p,p), \] (10)

where \( L_{FP} \) is a linear Fokker–Planck operator and \( C_B(p,p) \) is a bilinear integral operator (the inelastic Boltzmann-collision integral [18]). The first operator describes the interaction of the system with the heat bath necessary to render the system stationary, while the second describes the collisions between the particles: the combination of the two operators produce a non-trivial velocity distribution. To our knowledge, for equation (9) (or its counterpart with continuous velocities, equation (10)), no kind of ‘H-theorem’ is known. The failure of the usual ‘H-theorem’, that for the \( H^C \) functional, has been verified in [8].

Notice that, assuming a relaxation toward equilibrium, i.e. \( P_i(t) \rightarrow \Pi_i \), then it is easy to show that at large times \( H^C \) is non-increasing. In fact, by writing \( P_i(t) = \Pi_i + \delta P_i(t) \) with \( \delta P_i \) small, one has

\[ H^C(t) = \sum_i \left( \Pi_i + \delta P_i(t) \right) \ln \left( 1 + \frac{\delta P_i(t)}{\Pi_i} \right) \approx \sum_i \frac{\delta P_i(t)^2}{\Pi_i}. \] (11)

We also mention that, for particular granular models, it is possible to prove that equation (10) in the elastic limit becomes equivalent to a Fokker–Planck equation: in that case the H-theorem for the \( H^C \) functional is obviously verified [23].

3.1. The elastic limit

Let us analyze a particular limit of the previous model where the collisions are elastic, so that \( W_{(k,l) \rightarrow (i,j)}^{(2)} = W_{(i,j) \rightarrow (k,l)}^{(2)} \). The governing equation reads

\[ \frac{dP_i}{dt} = \sum_k \left[ W_{k \rightarrow i}^{(1)} P_k - W_{i \rightarrow k}^{(1)} P_i \right] + \sum_{k,l,j} W_{(k,l) \rightarrow (i,j)}^{(2)} \left[ P_k P_l - P_i P_j \right] \] (12)

and in addition we assume that the invariant probability \( \{ \Pi_i \} \) is a stationary solution of both the linear master equation and the non-linear Boltzmann equation: i.e. for the \( \{ \Pi_k \} \)
satisfying equation (6), one has
\[ \Pi_i \Pi_j = \Pi_k \Pi_l \] (13)
if the \((i, j) \rightarrow (k, l)\) collision is allowed.

It is important to realize that, even if the invariant probability is somehow trivial, the dynamics is not, since it depends upon the interplay between the bath and the collisions which may happen, for instance, on different timescales. The example discussed in section 4.1, see figure 2, well illustrates this point, by showing the non-trivial dynamics of \(H_G\) which is non-monotonic.

In such a system one shows that
\[ \frac{dH_C(t)}{dt} \leq 0. \] (14)
In fact, we can write
\[ \frac{dH_C(t)}{dt} = \frac{dH_C}{dt} \bigg|_M + \frac{dH_C}{dt} \bigg|_B \] (15)
where
\[ \frac{dH_C}{dt} \bigg|_M = \sum_{i,k} [W^{(1)}_{k \rightarrow i} P_k - W^{(1)}_{i \rightarrow k} P_i] \left( \ln \frac{P_i(t)}{\Pi_i} + 1 \right) \] (16)
and
\[ \frac{dH_C}{dt} \bigg|_B = \sum_{i,k,l,j} W^{(2)}_{(k,l) \rightarrow (i,j)} [P_k P_l - P_i P_j] \ln \frac{P_i(t)}{\Pi_i}. \] (17)
Since \(\Pi_i \Pi_j = \Pi_k \Pi_l\) we can rewrite \(dH_C/dt\)\bigg|_B as
\[ \frac{dH_C}{dt} \bigg|_B = \sum_{i,k,l,j} W^{(2)}_{(k,l) \rightarrow (i,j)} \Pi_k \Pi_l \left( \frac{P_k P_l}{\Pi_k \Pi_l} - \frac{P_i P_j}{\Pi_i \Pi_j} \right) \ln \frac{P_i(t)}{\Pi_i}. \] (18)
It is now easy to show that both \(dH_C/dt\)\bigg|_M and \(dH_C/dt\)\bigg|_B are negative: it is enough to follow the standard proofs of the H-theorems for the master equation and for the Boltzmann equation separately: those proofs are reported in appendix A for completeness.

### 3.2. Granular Maxwell model

We discuss now an inelastic Maxwell model, a variation upon a theme, originally proposed by Ulam [24, 25] to study the approach to equilibrium, introduced by Ben Naim and Kaprivski, as a minimal kinetic model for granular gases [26–28]. The advantage of this model is that all moments can be explicitly computed [29]. In the 1D thermostatted version of the model, equation (10), takes the form

\[
\partial_t p(v, t) = \Gamma \left( \partial_v v p(v, t) \right) + D \left( \partial^2_v p(v, t) \right) \\
+ \frac{1}{\tau_c} \left( \frac{2}{1 + \alpha} \int \frac{du}{\Pi} p(u, t) p \left( \frac{2v - (1 - \alpha)u}{1 + \alpha}, t \right) - p(v, t) \right),
\] (19)

doi:10.1088/1742-5468/2013/08/P08003
where $\alpha \leq 1$ is the restitution coefficient (when $\alpha = 1$ the collisions are elastic), the first term in the right-hand side describes the effect of the heat bath at temperature $D/\Gamma$ and corresponds to $\mathcal{L}_{\text{FP}}$, while the last term represents the non-linear collisional term, which is the sum of a gain term and a loss term.

In general it is not possible to write explicitly $p(v, t)$. However, it is possible to obtain the evolution law of its moments defined as $\mu_n(t) = \int_{-\infty}^{\infty} dv v^n p(v, t)$ and prove that the high velocity tails of the PdF are Gaussian. The evaluation of the $H$-function requires the PdF, so that we use an approximation which correctly reproduces all moments up to a given order and displays the correct high velocity tails. To achieve that, we consider the following Sonine–Hermite representation of $p(v, t)$:

$$f(c, t) = \frac{1}{\sqrt{\pi}} e^{-c^2} \left[ 1 + \sum_{n=1}^{\infty} a_n(t) S_n(c^2) \right], \quad (20)$$

where $c^2 = v^2/(2\mu_2(t))$ is the non-dimensional velocity squared and $f(c, t)$ is the scaled PdF related to $p(v, t)$ by the transformation

$$p(v, t) = \frac{1}{\sqrt{2\mu_2(t)}} f(c, t). \quad (21)$$

For the sake of simplicity we assumed that the distribution is an even function of the velocity so that all its odd moments vanish. The $S_n(c^2)$ are the Sonine polynomials of order $2n$, given by the formula [30]

$$S_n(c^2) = \sum_{p=0}^{n} \frac{\Gamma(n + 1/2)(-c^2)^p}{\Gamma(p + 1/2)(n - p)!p!}$$

having the property

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi}} e^{-c^2} S_n(c^2) S_m(c^2) = N_n \delta_{mn} = \frac{1}{\sqrt{\pi}} \frac{\Gamma(n + 1/2)}{\Gamma(n + 1)} \delta_{mn} \quad (22)$$

and the $a_n(t)$ are coefficients of the expansion related to the moments $\mu_n(t)$ as shown in the appendix. They can be calculated from the averages

$$a_n(t) = \frac{1}{N_n} \int_{-\infty}^{\infty} dc f(c, t) S_n(c^2). \quad (23)$$

Since the evaluation of the moments of a given order requires only the knowledge of the moments of lower order one can proceed without excessive difficulty to any desired order. In practice, we carried on our calculation up to the eighth moment.

We can now evaluate the $H$-function for the Maxwell model using the Sonine representation of $p(v, t)$ by performing numerically the following integral:

$$H_C(t) = \int_{-\infty}^{\infty} dv p(v, t) \ln \left( \frac{p(v, t)}{\Pi(v)} \right), \quad (24)$$

where the asymptotic stationary distribution is obtained by inserting in equation (21) the asymptotic values of the moments $\mu_n(\infty)$, which are readily computed using equation (B.2)
in appendix B:

\[
\Pi(v) = \frac{1}{\sqrt{2\pi \mu_2(\infty)}} e^{-v^2/2\mu_2(\infty)} \left[ 1 + \sum_{m=2}^{\infty} a_m(\infty) S_m \left( \frac{v^2}{2\mu_2(\infty)} \right) \right].
\]  

(25)

Explicitly \( H_C \) reads

\[
H_C(t) = \int_{-\infty}^{\infty} dc \frac{1}{\sqrt{\pi}} e^{-c^2} \left[ 1 + \sum_{m=2}^{\infty} a_{l,m}(c) S_{l,m} \right] \left\{ -\frac{1}{2} \ln \left( \frac{\mu_2(t)}{\mu_2(\infty)} \right) - c^2 \left( 1 - \frac{\mu_2(t)}{\mu_2(\infty)} \right) \right\}.
\]

In figure 1 we display the behavior of the \( H_C \) and \( H_G \) functions together with the evolution of the second moment of the PdF for two different initial conditions but having the same steady state. In the first case the second moment decreases toward its asymptotic value, while the \( H_C \) function also decreases, whereas the \( H_G \) function increases. In the second case instead the \( \mu_2(t) \) increases and both \( H_C \) and \( H_G \) decrease in time. The two examples show that it is necessary to always consider \( H_C \), while \( H_G \) is not always monotonically decreasing.

A fast and simple way to prove numerically the hypothesis that the \( H_C(t) \) function is always decreasing is to consider its evolution for a short time interval \( \Delta t \) starting from a distribution \( p_{\text{init}}(v) = p(v,0) \) of the form (21) at the instant \( t = 0 \) generated assuming initial values of the moments arbitrarily with the only constraint that this PdF is everywhere non-negative. We then compute the evolution of the PdF over a small time interval, \( \Delta t \), using the governing equations for the moments \( \mu_n(t) \) and finally calculate the variation \( \Delta H_C(t) = H_C(t+\Delta t) - H_C(t) \). For all possible choices of the initial values we have found that such a variation turns out to be always non-positive. It is worth mentioning that it is not necessary to follow the system evolution over a longer time interval in order to verify the persistence of the sign of \( \Delta H_C(t) \). In fact, any possible distribution \( p(v,t^*) \) which can be reached at time \( t^* > 0 \) by the dynamics starting from the distribution \( p_{\text{init}}(v) \) can be a good candidate as initial distribution, whose choice is arbitrary. We have sampled a large number of initial conditions \( p_{\text{init}}(v) \) of the form equation (21) randomly generated and verified that \( H_C(t+\Delta t) - H_C(t) \leq 0 \).

We conclude this section by saying that although we cannot prove analytically that for the inelastic Maxwell there exists an H-theorem, our numerical results provide strong evidence that this is the case. The results of this section should be compared with those obtained for other granular systems, as discussed in section 4.

### 4. Numerical evidence for other examples of granular systems

#### 4.1. Granular gases with discrete states

We present here the simulation of a discrete BFP equation (9) for a choice of (conservative or non-conservative) collisions and with the presence of a thermal bath. In particular we have assumed that each state \( i \in [0,M] \) represents a possible value of the single particle energy \( \epsilon_i \), for instance \( \epsilon_i = i\delta E \) where \( \delta E \) is some amount of energy. Collisions have been
assumed to mix energy between colliding particles and, optionally, to dissipate a part of it, in order to reproduce the inelasticity in granular gases.

The collision model we have adopted assigns the following collision rule to transform colliding energies \( i, j \) into post-collision energies \( i', j' \):

\[
\begin{align*}
    i' &= j + 1 - \Delta \\
    j' &= i - 1 - \Delta,
\end{align*}
\]

with \( \Delta \geq 0 \) being the amount of dissipated energy and with the additional condition \( i' \geq 0, j' \geq 0 \) enforced. For simplicity we assume that the probability of two particles being chosen for a collision is independent of the relative velocity, as occurs in the so-called Maxwell models previously discussed [25, 27, 28]. The single particle mean free time between collision is defined as \( \tau_c \). The stated collision model determines the rates \( W^{(2)}_{(k,l)\rightarrow(i,j)} \) in the equation (9). To avoid cumbersome expressions we do not reproduce such rates here.
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Figure 2. Elastic collisions with characteristic time $\tau_c = 1$ combined with a thermal bath (characteristic time $\tau_b = 10$ and temperature $T_b = 10$). (A) Evolution of $P_i(t)$, (B) evolution of the average energy $e = \sum_i i P_i$, (C) evolution of the Boltzmann $H_G$ function, and (D) evolution of the $H_C$ function.

The action of the heat bath is taken into account through the *linear* part of equation (9). In particular we have assumed that

$$W_{k \rightarrow i}^{(1)} = \frac{1}{\tau_b} e^{-i/2T_b}$$

where we have introduced $\tau_b$, the characteristic bath time, and $T_b$, the bath temperature. Rates $W_{k \rightarrow i}^{(1)}$ satisfy detailed balance with respect to the ‘equilibrium’ stationary distribution $\Pi_i^{eq} = c e^{-i/T_b}$ with $c$ a normalization constant. Such equilibrium stationary distribution is attained when collisions are switched off (i.e. $\tau_c \rightarrow \infty$) as well as when they are elastic (i.e. $\Delta = 0$).

We have simulated equation (9) with the rates discussed above by means of a fourth-order Runge–Kutta integration.

In Figure 2 we show that when the collisions are elastic ($\Delta = 0$) but a thermal bath acts on each particle, one has a monotonic decrease of $H_C(t)$ but not of $H_G(t)$. Note that both mechanisms (elastic collisions and thermal bath), separately, guarantee the existence of an equilibrium steady state: however, the thermal bath enforces a well-defined temperature $T_b$, while elastic collisions do not (the temperature, in the absence of the bath, would be chosen by initial conditions, i.e. initial average energy). When the two mechanisms act together, the final temperature is that of the bath, $T_b$. Panel (A) of Figure 2 shows the evolution of $P_i$ (from initial conditions concentrated uniformly between $i = 39$ and 49).
In figure 3 we report the results for the case with dissipation ($\Delta > 0$), in the presence of a thermal bath in order to guarantee the attainment of a steady state. In this case the knowledge of $\Pi_i$ is not known \textit{a priori}, therefore a first long run of the simulation is used to obtain it. A second run is then used to measure $H_C$. We have repeated the simulation for three different initial conditions, as detailed in the figure caption. The evolution of the probability distribution for the particular case starting with $P_i(0)$ concentrated between $i = 39$ and $49$ is shown in panel (A) of the figure: it reaches an asymptotic distribution (the same for all initial conditions) different from the equilibrium one. In panel (B) we observe the average energy $e(t)$ which settles to a value smaller than the bath temperature $T_b$ because of the inelasticity of collisions. Panels (C) and (D) show that, while $H_G$ does not always verify the H-theorem, the validity of the H-theorem for $H_C(t)$ is always verified.

doi:10.1088/1742-5468/2013/08/P08003
4.2. Granular gases with continuous states through the direct simulation Monte Carlo

Direct simulation Monte Carlo (DSMC) [4, 31] is usually considered an effective ‘solver’ for Boltzmann equations and has been frequently used in the study of the kinetics of granular gases. It is a so-called ‘particles method’, since a finite number \( N \) of particles is evolved stochastically: the statistics of those \( N \) particles approximates, as \( N \to \infty \), the solution of the corresponding Boltzmann equation. For the purpose of this paper, therefore, the study of the evolution of \( H_C \) during the DSMC dynamics, with non-conservative interactions and with the presence of a heat bath, is meaningful as \( N \) becomes larger and larger.

Here we use the DSMC algorithm discarding any spatial information. However the algorithm is often used with spatial coordinates, by dividing space in small cells. Our choice is equivalent to considering the space-homogeneous version of the BFP equation (10). In the algorithm time is advanced in time steps of length \( \delta t \). At each time step two sub-steps are performed: (1) the heat bath step, where the velocity of each particle \( i \) is advanced, from \( t \) to \( t + \delta t \), by the discretized solution of an Ornstein–Uhlenbeck stochastic process, i.e.

\[
v_i(t + \delta t) = e^{-\delta t/\tau_b}v_i(t) + \sqrt{T_b(1 - e^{-2(\delta t/\tau_b)})}\phi_i(t),
\]

where \( \phi_i(t) \) is a random variable extracted from a normal distribution (different \( t \) and different \( i \) are all independent), \( T_b \) is the bath temperature and \( \tau_b \) is the typical interaction time of a particle with the bath; (2) collisions are performed by choosing random couples \( i, j \) of particles and changing their velocities by the rule

\[
v_i' = v_i - \frac{1 + \alpha}{2}(v_i - v_j), \quad v_j' = v_j + \frac{1 + \alpha}{2}(v_i - v_j),
\]

and the rate of collision per particle is fixed at \( 1/\tau_c \). The parameter \( \alpha \leq 1 \) represents the restitution coefficient, when \( \alpha = 1 \) collisions are elastic, otherwise they dissipate part of the kinetic energy. Note that in this version of the DSMC the random choice of particles is done uniformly: this is equivalent to solving a Boltzmann equation with a collision probability independent from the relative velocity of the colliding particle, as happens in the Maxwell models discussed in section 3.2.

The results of the DSMC dynamics for a case with inelastic with heat bath are shown in figure 4. In panel (A) we have reported the evolution of the probability distribution, which is started from a Gaussian distribution and \( T_0 \gg T_b \). In panel (B) the evolution of the average energy is shown, demonstrating that the initial temperature is forgot and the system attains a stationary state with an average kinetic energy (also called granular temperature) \( T_g < T_b \), because of inelastic collisions. In frame (C) and (D) we have reported the evolution of

\[
H_{G,N,M}^{N,M}(t) = \sum_{i=1}^{M} P_i(t) \ln P_i(t)
\]

and

\[
H_{C,N,M}^{N,M}(t) = \sum_{i=1}^{M} P_i(t) \ln \frac{P_i(t)}{\pi_1}
\]

doi:10.1088/1742-5468/2013/08/P08003
Figure 4. DSMC simulation of inelastic collisions ($\tau_c = 1$ and $\alpha = 0.6$) and thermal bath ($T_b = 1$ and two different cases $\tau_b = 1$ or $\tau_b = 10$), with $N = 10^5$ and $M = 10^2$. (A) Evolution of $P_i(t)$ in the case $\tau_b = 10 \tau_c$, (B) evolution of the average energy $e = \sum_i P_i$, (C) evolution of the Boltzmann $H_G$ function and (D) evolution of the $H_C$ function.

where $P_i(t)$ and $\pi_i$ are the empirical velocity probability and its long time limit respectively: the empirical probability at instant $t$ is obtained by choosing a velocity interval $[-v_{\text{max}}, v_{\text{max}}]$ with $v_{\text{max}} = 10\sqrt{T_b}$ and dividing it in $M$ sub-intervals, and taking $P_i(t)$ to be the number of particles with velocity in the $i$th sub-interval. For $N \gg 1$ and $M \gg 1$, we have $P_i(t) \simeq p(-v_{\text{max}} + i\delta v, t)\delta v$ where $\delta v = 2v_{\text{max}}/M$, so that

$$\int p(v,t) \ln p(v,t) dv \simeq H_{N,M}^G(t) - \ln(\delta v)$$

$$\int p(v,t) \ln \frac{p(v,t)}{\Pi(v)} \simeq H_{N,M}^C(t).$$

The results reported in frame (C) and (D) of figure 4 demonstrate the failure of the usual Boltzmann H-theorem (the one for $H_{N,M}^G$) together with the validity of $(d/dt)H_{N,M}^C \leq 0$.

It is interesting to notice that in the examples shown in figures 2–4, the $H_G$ functional has a behavior constituted by a first decrease followed by an increase. This seems a consequence of the relatively fast action of collisions superimposed to a slower action of the heat bath: collisions (even if inelastic) do not change dramatically the energy and therefore mainly contribute to 'equilibrate' the initial distribution, so that $H_G$ satisfies the original H-theorem $(dH_G/dt < 0)$ at the beginning; when the heat bath action becomes dominant, the distribution is near to the equilibrium one, i.e. $H_G \approx -\langle v^2 \rangle$ and the effect

doi:10.1088/1742-5468/2013/08/P08003
of the bath (a Ornstein–Uhlenbeck process which, being linear, conserves the Gaussian shape), is mainly a decrease of energy (initiated higher than \( T_b \)), implying \( dH_G/dt > 0 \).

We mention that the numerical results presented in this section are not restricted to the Maxwell model, but they are observed also for inelastic hard spheres.

4.3. The connection between the \( \Gamma \) space and the \( \mu \) space

It is interesting to notice that the DSMC algorithm is a Markov process. As discussed in section 2.2 for such processes with a finite number of states under very general conditions an H-theorem holds, therefore it is natural to expect the same result for the DSMC. Nevertheless the DSMC is a Markov process for an \( N \)-dimensional vector, i.e. in the so-called ‘\( \Gamma \) space’, while the BFP equation (10) governs the evolution of \( p(v, t) \) i.e. the single particle velocity distribution, i.e. it lives in the ‘\( \mu \) space’.

By defining \( P(v_1, \ldots, v_N, t) \) the probability density at time \( t \) in the \( N \)-dimensional space, we know that for the DSMC it obeys a master equation of the kind

\[
\frac{\partial P(v_1, \ldots, v_N, t)}{\partial t} = L_N P(v_1, \ldots, v_N, t)
\]

and it is customary to assume that it reaches a stationary state \( \Pi(v_1, \ldots, v_N) \). Therefore the \( H_C \) function

\[
H_C(t) = \int P(v_1, \ldots, v_N, t) \ln \frac{P(v_1, \ldots, v_N, t)}{\Pi(v_1, \ldots, v_N)} \, dv_1 \cdots dv_N,
\]

is a non-increasing function of time, i.e. \( dH_c/dt \leq 0 \).

Let us discuss the connection between the DSMC and equation (10) for our particular model. A more general and rigorous proof can be found, for the elastic Boltzmann equation, in [32].

In the case of the DSMC discussed above, which includes the interaction with an external energy injection mechanism and pairwise collisions, one may separate

\[
L_N = \sum_{i=1}^{N} L_{FP}(v_i) + \sum_{j=1}^{N} \sum_{i \neq j} T(v_i, v_j),
\]

where \( L_{FP} \) is the operator representing the single-particle master equation, in our case that for the Ornstein–Uhlenbeck process (the first term in the right-hand side of equation (19)), while

\[
T(v_i, v_j) = \frac{1}{\alpha} b^{-1}(v_i, v_j) - 1
\]

is the operator for the collision between the \( i, j \) particles, where \( b^{-1}(v_i, v_j) \) operates on a function of \( v_1, v_2, \ldots, v_N \) by mapping \( v_i, v_j \) into \( v_i^*, v_j^* \) which are the pre-collisional velocities, obtained by inverting equation (30). For non-space-homogeneous systems and hard-core interactions, the collisional operator is different (for instance it enforces the condition of contact among particles, as well as the velocity dependence of the scattering probability, etc), see for instance [33].

By marginalizing equation (35) and assuming molecular chaos, i.e. \( p_2(v_1, v_2, t) = p(v_1, t)p(v_2, t) \) for pre-collisional velocities, it is simple to get the BFP equation (10) for the case of the Maxwell collision model.

doi:10.1088/1742-5468/2013/08/P08003
We conclude with some speculative considerations. Let us notice that, by assuming a stronger version of molecular chaos, valid for all velocities (i.e. not only the pre-collisional ones)

$$P(v_1, \ldots, v_N, t) = \Pi_{i=1}^N P(v_i, t),$$

(39)

it is immediate to get

$$\mathcal{H}_c(t) = N \int dv P(v, t) \ln \frac{P(v, t)}{\Pi(v, t)},$$

(40)

which implies

$$\frac{d\mathcal{H}_c}{dt} \leq 0.$$

(41)

We stress however that such a stronger form of molecular chaos is usually violated in spatially homogeneous [34] as well as inhomogeneous granular gases [12, 22].

5. Conclusions

In this paper we have offered several examples of Boltzmann–Fokker–Planck (BFP) models with conservative and non-conservative interactions, where an H-functional of the kind

$$H_C(t) = \sum P_i(t) \ln \frac{P_i(t)}{\Pi_i}$$

(42)

appears to be non-increasing for the whole evolution from arbitrary initial conditions toward the asymptotic steady state $\Pi_i$. The only case where we are able to prove such a conjecture is the elastic BFP case, where the proof is a ‘superposition’ of the proofs of the two different H-theorems for the elastic Boltzmann equation and for Markov processes: notwithstanding the simplicity of the proof and the triviality of the steady state, the elastic BFP model has a non-trivial dynamics where collisions and thermostat may act on different timescales, as demonstrated by the non-monotonous behavior of the Boltzmann $H_G(t)$ functional. Establishing the monotonicity of $H_C(t)$ or other entropic functionals for a rather general class of models is certainly a challenge for future research [9, 35]. In a remark concluding the last section, we have recalled that the BFP equation may be obtained by marginalizing a master equation for the Markovian evolution of the many-particle vector in $\Gamma$ space: this remark, which is behind the operating principle of DSMC schemes, could stimulate further investigations on this complex and fascinating subject. It is interesting to observe that some of the problems associated with the marginalization discussed above already appear at the elastic level, as observed in [36].

Acknowledgments

The authors acknowledge useful discussions with A Baldassarri. They also acknowledge the support of the Italian MIUR under the PRIN 2009 grant no. 2009PYYZM5. AP acknowledges the support of the Italian MIUR under the grant FIRB-IDEAS no. RBID08Z9JE.
Appendix A. H-theorem in the case of conservative interactions and under the action of a heat bath

A.1. Master equation contribution

Let us introduce the variables \( f_i(t) = P_i(t)/\Pi_i \) and \( B_{ik} = W_{k\rightarrow i}^{(1)}\Pi_k \). It is also useful to define the function \( F(x) = x \ln x \), so that \( F'(x) = 1 + \ln x \). It is easy to verify that

\[
\left. \frac{dH_C}{dt} \right|_M = \sum_{i,k} F'(f_i)(B_{ik}f_k - B_{ki}f_i) = \sum_{i,k} B_{ik}[f_kF'(f_i) - f_kF'(f_k)], \tag{A.1}
\]

where we have exchanged the indices in the second part of the sum, in order to collect \( B_{ik} \). Then one notices that for a set of numbers \( \psi_i \) the following relation holds:

\[
\sum_{i,k} B_{ik}(\psi_i - \psi_k) = 0, \tag{A.2}
\]

which is a consequence of stationarity for \( \Pi_i \). Adding equation (A.2) to the last line of equation (A.1), and choosing \( \psi_n = F(f_n) - f_n F'(f_n) \), one gets

\[
\left. \frac{dH_C}{dt} \right|_M = \sum_{i,k} B_{ik}[(f_k - f_i)F'(f_i) + F(f_i) - F(f_k)]. \tag{A.3}
\]

Now, since \( F''(x) > 0 \), it is immediate to see that

\[
[(f_k - f_i)F'(f_i) + F(f_i) - F(f_k)] \leq 0, \tag{A.4}
\]

and therefore \( \left. \frac{dH_C}{dt} \right|_M \leq 0 \). The proof shown here is that found in [37].

A.2. Boltzmann equation contribution

Here it is useful to introduce the variable \( A_{i,j,k,l} = W_{(i,j)\rightarrow(k,l)}^{(2)}\Pi_i\Pi_j \). The symmetry between collisions \((k,l) \rightarrow (i,j)\) and \((k,l) \rightarrow (j,i)\) implies the identities \( A_{k,l,i,j} = A_{i,j,k,l} = A_{l,k,i,j} = A_{i,l,k,j} \), so that

\[
\left. \frac{dH_C}{dt} \right|_B = \frac{1}{2} \sum_{i,j,k,l} A_{i,j,k,l}\{f_k(t)f_i(t) - f_l(t)f_j(t)\}\ln[f_i(t)f_j(t)],
\]

and by means of the symmetry between \((k,l) \rightarrow (i,j)\) and \((i,j) \rightarrow (k,l)\) one gets

\[
\left. \frac{dH_C}{dt} \right|_B = -\frac{1}{4} \sum_{i,j,k,l} A_{i,j,k,l}\{f_i(t)f_j(t) - f_k(t)f_l(t)\}\{\ln[f_i(t)f_j(t)] - \ln[f_k(t)f_l(t)]\}.
\]

We notice that \( A_{i,j,k,l} > 0 \). Furthermore, since \((\ln x - \ln y)(x - y) \geq 0\) for every \( x > 0 \) and \( y > 0 \), we finally get \( \left. \frac{dH_C}{dt} \right|_B \leq 0 \). The equality holds only when the \( \{f_i\} \) are identically 1, i.e. \( P_i = \Pi_i \). The above proof is the standard one contained in any textbook and is due to Ludwig Boltzmann [1].

Appendix B. Time evolution of the moments for the Maxwell model

We provide here some details regarding the calculations presented in the main text. Applying the Fourier transform to equation (19), we obtain the following governing
equation for characteristic function $\hat{P}(k,t) = \int_{-\infty}^{\infty} dv \, e^{ikv} p(v,t)$:

$$
\partial_t \hat{P}(k,t) = -Dk^2 \hat{P}(k,t) - \Gamma k \partial_k \hat{P}(k,t) - \frac{1}{\tau_c} [\hat{P}(k,t) - \hat{P}(\gamma k,t) \hat{P}(1-\gamma k,t)]
$$

(B.1)

with $\gamma = (1+\alpha)/2$. Substituting the representation $\hat{P}(k,t) = \sum_{n=0}^{\infty} ((ik)^n/n!) \mu_n(t)$ in (B.1) and equating the coefficients of the same power of $k$ we derive a set of ordinary differential equations describing the evolution of the moments, whose integration is straightforward and leads to expressions of the type

$$
\mu_n(t) = e^{-K_n t} \mu_n(0) + e^{-K_n t} \int_0^t dt' R_n(t') e^{K_n t'}
$$

(B.2)

with

$$
K_n = n \Gamma - \frac{d_n}{\tau_c}
$$

(B.3)

where the coefficients $d_n$ are

$$
d_n = -1 + [\gamma^n + (1-\gamma)^n]
$$

(B.4)

and

$$
R_2 = 2D, \quad R_4(t) = A\mu_2(t)^2 + 12D\mu_2(t),
$$

$$
R_6(t) = B\mu_2(t)\mu_4(t) + 30D\mu_4(t), \quad R_8(t) = C_1\mu_2(t)\mu_6(t) + C_2\mu_4(t)^2 + 56D\mu_6(t),
$$

where the coefficients have the following expressions:

$$
A = 6\frac{[\gamma(1-\gamma)]^2}{\tau_c}, \quad B = 15\frac{\gamma^2(1-\gamma)^2[\gamma^2 + (1-\gamma)^2]}{\tau_c}
$$

and

$$
C_1 = 28\frac{\gamma^2(1-\gamma)^2[\gamma^4 + (1-\gamma)^4]}{\tau_c}, \quad C_2 = 70\frac{\gamma^4(1-\gamma)^4}{\tau_c}.
$$

Notice that $A,B,C_1,C_2,d_n$ vanish in the elastic limit $\gamma \rightarrow 1$ as the elastic collisions do not affect the PdF nor its moments. Since in equation (B.2) the evolution of the moment of order $n$ is coupled only to the evolution of moments of order smaller than $n$, the solution is very simple and can be achieved recursively.

In order to construct the PdF we have to use the Sonine–Hermite expansion and compute the coefficients $a_n(t)$ which are proportional to the cumulants of the distribution. In terms of the moments we find

$$
a_2(t) = \left[ -1 + \frac{1}{3} \frac{\mu_4(t)}{\mu_2(t)^2} \right]
$$

(B.5a)

$$
a_3(t) = \left[ -2 + \frac{\mu_4(t)}{\mu_2(t)^2} - \frac{1}{15} \frac{\mu_6(t)}{\mu_2(t)} \right]
$$

(B.5b)

$$
a_4(t) = \left[ -3 + \frac{2}{5} \frac{\mu_4(t)}{\mu_2(t)^2} - \frac{4}{15} \frac{\mu_6(t)}{\mu_2(t)^2} + \frac{1}{105} \frac{\mu_8(t)}{\mu_2(t)} \right].
$$

(B.5c)

Notice that $a_2,a_3,a_4$ being proportional to the cumulants vanish for the Gaussian distribution, but not for the granular gas.

doi:10.1088/1742-5468/2013/08/P08003

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