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Advanced Statistical Physics

Non-Equilibrium Systems

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Contents

Abstract

This paper presents an introductory investigation into non-equilibrium dynamical systems within the realm of statistical physics, employing Direct Simulation Monte-Carlo (DSMC) techniques. Non-equilibrium phenomena pose intriguing challenges in understanding the behavior of complex systems far from thermal equilibrium. Through meticulous simulation methodologies, this study delves into the dynamics of such systems and the natural evolution of initial delta, uniform and Cauchy velocities' distribution to Maxwell-Boltzmann's distribution after a relaxation time τ. Furthermore, the paper explores theoretical questions such as Boltzmann's H function theorem and the evolution of average values of $\langle v^2 \rangle$ and $\langle v^4 \rangle$ moments.

1 Introduction

It is well-known that we live in a world of equilibrium: From the equations that describe how electrons and holes move within in a semiconductor to those that describe how air flows around the wings of a plane, it is no exaggeration to say that many of the technological advances of past and present are predicated on the fact that the Maxwell-Boltmzann, the Fermi-Dirac and Bose-Einstein distributions fundamentally describe reality very well.

With this in mind, this paper seeks to analyze what happens to a system that initially does not follow those distributions to understand how their evolution to stable states. More concretely, we want to study how a classical closed system of elastic hard spheres without any external forces relaxes towards equilibrium.

To do this, we will start by making some theoretical considerations from the Boltzmann equation, with the end goal of obtaining certain approximate analytical expressions for the time-evolution of some statistical moments of our distribution, focusing on the cases of $\langle v^2 \rangle$ and $\langle v^4 \rangle$. Furthermore, we will proceed to do a similar analysis to the Boltzmann H-function, closely related to the Shannon entropy of the distribution, that will also help towards understanding the underlying processes.

With the understanding obtained in the last section in hand, we will proceed to comment on the simulations done by Direct Simulation Monte Carlo (DSMC) methods and compare the results to our predictions. We will consider the evolution of three distinct initial distributions to see how well the predictions hold for each case: First, a fixed magnitude for the velocities but in random directions, which we will call a delta distribution (because this leads to a delta distribution on the magnitude of the velocities), then a uniform distribution over each direction and, finally, we will see what happens with the highly 'pathological'[1] case of a Cauchy (or Breit-Wigner) distribution to try to understand the limits of our description.

As we will see, this will provide us with a decent amount of comprehension on the road towards equilibrium in classical, closed system with very simple interactions between the particles. This is, of course, still not the full picture for the infinitude of possible systems one

[1]Statisticians may be opposed to this description as the Cauchy is not a distribution that has to be constructed with special care, but one that naturally appears and also happens to have unusual properties that make it troublesome.

can think of, but provides a decent foundation that can generalize to understand those more complex situations.

As such, we will begin Section 2 by giving a very brief overview of the main results we need from kinetic theory and prove some useful results that we will compare later with our simulations. In Section 3, we will sketch an overview of how the DSMC methods works and provide the main results of our simulation. Finally, Section 4 will be dedicated to a concise conclusion of the paper.

2 Theoretical Background

In this section we are going to study evolution of generic functions of velocity and the Boltzmann H-function in terms of the distribution function of hard spheres in the system.

In general, the dynamics of particles can be described by their positions and velocities, but by assumption we will consider homogeneous systems, which will greatly simplify the dynamics because the velocities will fully determine our system. It also implies that the density is constant, which will make a lot of calculations much easier to follow.

A general collision can be supposed inelastic with a parameter α that determines how much energy is lost in each collision. This parameter is called the normal restitution coefficient, but it alone doesn't fully describe a collision, as we also need the velocities of the two particles before colliding, the *pre-collisional velocities*, which we will denote by $\mathbf{v}_1$ and $\mathbf{v}_2$. These will allow us to find the velocities after the collision, the *post-collisional velocities*, $\mathbf{v}_1^*$ and $\mathbf{v}_2^*$ respectively, given by the expression:

$$\begin{aligned}\mathbf{v}_1^* &= \mathbf{v}_1 - \frac{1}{2}(1+\alpha)(\mathbf{v}_{12}\cdot\hat{\sigma})\hat{\sigma},\\ \mathbf{v}_2^* &= \mathbf{v}_2 + \frac{1}{2}(1+\alpha)(\mathbf{v}_{12}\cdot\hat{\sigma})\hat{\sigma},\end{aligned} \tag{1}$$

where $\mathbf{v}_{12}$ is the relative velocities of the colliding particles,$\mathbf{v}_{12} = \mathbf{v}_1 - \mathbf{v}_2$ and $\hat{\sigma}$ is a unit vector along the line of centers of the colliding spheres.

It is possible to define another velocities called *restituting velocities*, which we will denoted by $\mathbf{v}_1^{**}$ and $\mathbf{v}_2^{**}$, which can be used to obtain pre-collisional velocities, their relations are

$$\begin{aligned}\mathbf{v}_1^{**} &= \mathbf{v}_1 - \frac{1}{2}(1+\alpha^{-1})(\mathbf{v}_{12}\cdot\hat{\sigma})\hat{\sigma},\\ \mathbf{v}_2^{**} &= \mathbf{v}_2 + \frac{1}{2}(1+\alpha^{-1})(\mathbf{v}_{12}\cdot\hat{\sigma})\hat{\sigma}.\end{aligned} \tag{2}$$

Previous equations, (1) and (2), can be used to obtain useful relations between all velocities that are going to be used during the article, such as the Jacobians of both transformations, $d\mathbf{v}_1^* d\mathbf{v}_2^* = \alpha\, d\mathbf{v}_1 d\mathbf{v}_2$ and $d\mathbf{v}_1^{**} d\mathbf{v}_2^{**} = (1/\alpha)\, d\mathbf{v}_1 d\mathbf{v}_2$, relations between components of the pre-collisional and post-collisional velocities in the $\hat{\sigma}$, $\mathbf{v}_{12}^* \cdot \hat{\sigma} = -\alpha\, \mathbf{v}_{12}\cdot\hat{\sigma}$ and $\mathbf{v}_{12}^{**}\cdot\hat{\sigma} = -(1/\alpha)\,\mathbf{v}_{12}\cdot\hat{\sigma}$, and a relation between post-collisional velocities and restituting velocities in the same direction, $\mathbf{v}_i^{**}(\alpha) = \mathbf{v}_i^*(1/\alpha)$.

2.1 Evolution of average values

Since we want to calculate the time-evolution of several functions of only the velocity, it makes sense to find general expression for all of them. It is natural to begin our journey with the nonlinear Enskog-Boltzamann (E-B) equation for the single particle distribution function $f(\mathbf{r}, \mathbf{v}, t) = f(\mathbf{v}, t)$ in a homogeneous system of inelastic spheres in d-dimensions. Since we are considering a system with no external forces, the E-B equation reduces to [2, 3]:

$$\partial_t f(\mathbf{v}_1, t) = \chi \sigma^{d-1} \int d\mathbf{v}_2 \int' d\hat{\sigma} (\mathbf{v}_{12} \cdot \hat{\sigma}) \left\{ \frac{1}{\alpha^2} f(\mathbf{v}_1^{**}, t) f(\mathbf{v}_2^{**}, t) - f(\mathbf{v}_1, t) f(\mathbf{v}_2, t) \right\}, \tag{3}$$

where prime in the integral of $\hat{\sigma}$ is notation to indicate we only consider collisions where $\mathbf{v}_{12} \cdot \hat{\sigma} > 0$. In general, the expected value of a function of random variable can be calculate as $\langle \psi \rangle = (1/n) \int dv \psi(v) f(v, t)$, its time-evolution is determined by its temporal derivative,

$$\frac{d\langle \psi \rangle}{dt} = \frac{1}{n} \int d\mathbf{v}_1 \partial_t (\psi(\mathbf{v}_1) f(\mathbf{v}_1, t)) = \frac{1}{n} \int d\mathbf{v}_1 \psi(\mathbf{v}_1) \partial_t f(\mathbf{v}_1, t). \tag{4}$$

Now, equation (3) gives us an expression for $\partial_t f$, such that we can write

$$\frac{d\langle \psi \rangle}{dt} = \frac{\chi \sigma^{d-1}}{n} \int d\mathbf{v}_1 \int d\mathbf{v}_2 \int' d\hat{\sigma} (\mathbf{v}_{12} \cdot \hat{\sigma}) \psi(\mathbf{v}_1) \left\{ \frac{1}{\alpha^2} f(\mathbf{v}_1^{**}, t) f(\mathbf{v}_2^{**}, t) - f(\mathbf{v}_1, t) f(\mathbf{v}_2, t) \right\}. \tag{5}$$

This expression might give us some trouble both in actually integrating and interpreting its results due to the presence of distribution functions for pre-collsional and restituting velocities. This naturally leads to the idea of simplifying it with the expressions we discussed in the last section: First of all, we can slit in two integrals and analyze the integral with distribution functions of restituting velocities,

$$\int d\mathbf{v}_1 \int d\mathbf{v}_2 \int' d\hat{\sigma} (\mathbf{v}_{12} \cdot \hat{\sigma}) \psi(\mathbf{v}_1) \frac{1}{\alpha^2} f(\mathbf{v}_1^{**}, t) f(\mathbf{v}_2^{**}, t),$$

in which we can do a change of variables ($\mathbf{v}_i^{**} \to \mathbf{v}_i$ and $\mathbf{v}_i \to \mathbf{v}_i^*$) and the relations between them to eliminate the restituting velocities in distribution functions, obtaining

$$\int d\mathbf{v}_1 \int d\mathbf{v}_2 \int' d\hat{\sigma} (\mathbf{v}_{12} \cdot \hat{\sigma}) \psi(\mathbf{v}_1^*) f(\mathbf{v}_1^, t) f(\mathbf{v}_2, t).$$

Introducing last integral in equation (5) it is possible to rewrite it as

$$\frac{d\langle \psi \rangle}{dt} = \frac{\chi \sigma^{d-1}}{n} \int d\mathbf{v}_1 \int d\mathbf{v}_2 \int' d\hat{\sigma} (\mathbf{v}_{12} \cdot \hat{\sigma}) \Delta \psi(\mathbf{v}_1) f(\mathbf{v}_1, t) f(\mathbf{v}_2, t), \tag{6}$$

where we have define $\Delta \psi(\mathbf{v}_i) = \psi(\mathbf{v}_i^*) - \psi(\mathbf{v}_i)$ to make manifest the symmetry of the equation. It is possible to get a more symmetric equation doing the permutation of velocities involved in the collision ($\mathbf{v}_i \to \mathbf{v}_j$, $\mathbf{v}_i^* \to \mathbf{v}_j^*$ for i $\neq$ j), adding both equations and rewrite terms

$$\frac{d\langle \psi \rangle}{dt} = \frac{\chi \sigma^{d-1}}{2n} \int d\mathbf{v}_1 \int d\mathbf{v}_2 \int d\hat{\sigma} (\mathbf{v}_{12} \cdot \hat{\sigma}) \Delta [\psi(\mathbf{v}_1) + \psi(\mathbf{v}_2)] f(\mathbf{v}_1, t) f(\mathbf{v}_2, t). \tag{7}$$

At first, it may seems more difficult than the original, but this will then allow us to calculate the time-evolution of a generic function of the velocities, ψ, for inelastic collisions in d-dimensions. This, in turn, we will use to study elastic ($\alpha = 1$) collisions in 3-dimensions ($d = 3$) of a particular set of functions; namely, the moments of our distribution.

2.1.1 Particular cases

As previously mentioned, we now want to understand the evolution of the moments of our distribution, giving special attention the second,$\langle \mathbf{v}^2 \rangle$, and fourth, $\langle \mathbf{v}^4 \rangle$, moments, as they will paint a picture for our whole system.

It is important to realise that the $\Delta\psi$ term of equation (7) has to impose the conservation of energy, since our choice of α implies that $\mathbf{v}_i^{**} = \mathbf{v}_i^*$, what change $\psi(\mathbf{v}_i^{**})$ to $\psi(\mathbf{v}_i^*)$.

We continue analysing particular cases,

- Second Moment, $\langle \mathbf{v}^2 \rangle$: In this case, we take $\psi(\mathbf{v}_i) = \mathbf{v}_i^2$, and the equation (7) becomes:

$$\frac{d\langle \mathbf{v}^2 \rangle}{dt} = \frac{\chi\sigma^2}{2n} \int d\mathbf{v}_1 \int d\mathbf{v}_2 \int d\hat{\sigma} (\mathbf{v}_{12} \cdot \hat{\sigma}) \Delta[\mathbf{v}_1^2 + \mathbf{v}_2^2] f(\mathbf{v}_1, t) f(\mathbf{v}_2, t), \tag{8}$$

  we then expand $\Delta[\mathbf{v}_1^2 + \mathbf{v}_2^2]$ to obtain that:

$$\Delta[\mathbf{v}_1^2 + \mathbf{v}_2^2] = (\mathbf{v}_1^*)^2 + (\mathbf{v}_2^*)^2 - (\mathbf{v}_1)^2 - (\mathbf{v}_2)^2, \tag{9}$$

  finally, we can impose the conservation of the kinetic energy in collisions, $T^* = T$, and since all particles are the same (and thus their masses are the same), we can write that:

$$(\mathbf{v}_1^*)^2 + (\mathbf{v}_2^*)^2 - (\mathbf{v}_1)^2 - (\mathbf{v}_2)^2 = 0, \tag{10}$$

  recovering the delta therm, $\Delta[\mathbf{v}_1^2 + \mathbf{v}_2^2] = 0$, that can be introduced in equation (8) to get

$$\frac{d\langle \mathbf{v}^2 \rangle}{dt} = 0 \Longrightarrow \langle \mathbf{v}^2 \rangle = const. \tag{11}$$

  Since the moments completely characterize a distribution, this value being constant means that $\langle \mathbf{v}^2 \rangle$ must coincide with the Maxwell-Boltzmann value, $\langle \mathbf{v}^2 \rangle_{MB} = 3k_B T/m$. This in turn implies that the initial value of $\langle \mathbf{v}^2 \rangle$ determines the temperature of our system

- Fourth moment, $\langle \mathbf{v}^4 \rangle$: another interesting case is the average value of the velocity to the fourth power, $\langle \mathbf{v}^4 \rangle$, that in general will not be constant. Using the same techniques as before, we will get that:

$$\frac{d\langle \mathbf{v}^4 \rangle}{dt} = \frac{\chi\sigma^2}{2n} \int d\mathbf{v}_1 \int d\mathbf{v}_2 \int d\hat{\sigma} (\mathbf{v}_{12} \cdot \hat{\sigma}) \Delta[\mathbf{v}_1^4 + \mathbf{v}_2^4] f(\mathbf{v}_1, t) f(\mathbf{v}_2, t), \tag{12}$$

  that could be expanded in the delta therm

$$\Delta[\mathbf{v}_1^4 + \mathbf{v}_2^4] = (\mathbf{v}_1^*)^4 + (\mathbf{v}_2^*)^4 - (\mathbf{v}_1)^4 - (\mathbf{v}_2)^4. \tag{13}$$

If we use the relationships between the velocities we have to elevate now to the forth power a sum of two therms of the conservation of energy and the result is a fourth degree polynomial with mixed terms that, in the end, don't conspire to be 0, leaving us with an equation that we cannot analytically solve because we don't know the distribution function at each point in time, but qualitatively we can say that it won't, in general, be constant.

2.1.2 Approximation of the 4th moment

As we have seen previously, we cannot find an analytical expression for $\langle \mathbf{v}^4 \rangle(t)$ because we have no analytical expression for the distribution function. One way to make progress here is to use what is usually called the *relaxation time approximation*, which for a spatially homogeneous system with no external forces states that:

$$\left(\frac{\partial f}{\partial t} \right) = -\frac{f - f^0}{\tau_0}. \tag{14}$$

where we have distribution function $f = f(\mathbf{v}, t)$, which depends on the velocity of a particle and the time but its structure is unknown *a priori* for us, $f^0 = f_{MB}(\mathbf{v})$ is Maxwell-Boltzmann distribution and τ_0 is the relaxation time of our system.

We can use the approximation to the equation (4) remembering that $\psi(\mathbf{v}) = \mathbf{v}^4$ which cancels out the first integral:

$$\frac{d\langle \mathbf{v}^4 \rangle}{dt} = \frac{1}{n} \int d\mathbf{v}\, \mathbf{v}^4 \partial_t f(\mathbf{v}, t) = \frac{1}{n} \int d\mathbf{v}\, \mathbf{v}^4 \left(-\frac{f - f^0}{\tau_0} \right), \tag{15}$$

we can split the integral into two integrals, one for Maxwell-Boltzmann distribution function and another for distribution function of the system,

$$\frac{d\langle \mathbf{v}^4 \rangle}{dt} = -\frac{1}{\tau_0 n} \int d\mathbf{v}\, \mathbf{v}^4 f(\mathbf{v}) + \frac{1}{\tau_0 n} \int d\mathbf{v}\, \mathbf{v}^4 f_{MB}(\mathbf{v}), \tag{16}$$

where we can see that we have obtained to integral that are by definition the 4th moment of the our distribution and that of the Maxwell-Boltzmann, which is constant over time, which is constant over time. This allows us to write that:

$$\frac{d\langle \mathbf{v}^4 \rangle}{dt} = \frac{-\langle \mathbf{v}^4 \rangle}{\tau_0} + \frac{\langle \mathbf{v}^4 \rangle_{MB}}{\tau_0}, \tag{17}$$

And this is now something that we can easily integrate:

$$\int \frac{d\langle \mathbf{v}^4 \rangle}{\langle \mathbf{v}^4 \rangle - \langle \mathbf{v}^4 \rangle_{MB}} = -\int \frac{dt}{\tau_0}, \tag{18}$$

resulting in the following solution:

$$\langle \mathbf{v}^4 \rangle(t) = \left(\langle \mathbf{v}^4 \rangle_0 - \langle \mathbf{v}^4 \rangle_{MB} \right) e^{-t/\tau_0} + \langle \mathbf{v}^4 \rangle_{MB}, \tag{19}$$

where $\langle \mathbf{v}^4 \rangle_0 = \langle \mathbf{v}^4 \rangle(t = 0)$ is a constant fixed by initial conditions, that is, fixed by the initial distribution.

It is important to realize that the result for any moments, including $\langle \mathbf{v}^2 \rangle$ with time relaxation approximation will have the same solution, but we have seen previously that $\langle \mathbf{v}^2 \rangle$ does not change because of conservation laws, which points to possible failstates of our approximation. The solution to this is, of course, realizing that $\langle \mathbf{v}^2 \rangle = \langle \mathbf{v}^2 \rangle_{MB}$, but it should be noted that the approximation gives us no reason as to why: It is only readily apparent in the non-approximate regime.

2.2 Evolution of the Boltzmann's H function

Having seen the expressions we arrived at by considering the relaxation-time approximation for the moments of the distribution, it is natural to think that a similar technique may be employed to find such an expression for the H-function, defined as[2]:

$$H(t) \equiv \int \mathrm{d}^3\mathbf{r} \int \mathrm{d}^3\mathbf{v} f(\mathbf{r}, \mathbf{v}, t) \ln f(\mathbf{r}, \mathbf{v}, t). \tag{20}$$

To find a differential equation for $H(t)$, the most natural place to start would be by differentiating equation (20), from which we get that:

$$\frac{dH(t)}{dt} = \int \mathrm{d}^3\mathbf{r} \int \mathrm{d}^3\mathbf{v} \left(\frac{\partial f}{\partial t} \ln f + \frac{\partial f}{\partial t} \right), \tag{21}$$

where some usual considerations about Gauss' theorem coupled with the conservation of the number of particles will set the contributions of the last term to zero and simplify the first to only include the collisional part of the time derivative. Because of this, we can write:

$$\frac{dH(t)}{dt} = \int \mathrm{d}^3\mathbf{r} \int \mathrm{d}^3\mathbf{v} \left(\frac{\partial f}{\partial t} \right)_{Col} \ln f, \tag{22}$$

where we will now need to employ the relaxation-time approximation to make any further progress. By using (1), we can then get:

$$\frac{dH(t)}{dt} = \int d^3\mathbf{r} \int d^3\mathbf{v} - \left(\frac{f - f_{MB}}{\tau_0} \right) \ln(f) = \frac{1}{\tau_0} \int d^3\mathbf{r} \int d^3\mathbf{v} [f_{MB} \ln(f) - f \ln(f)], \tag{23}$$

which is as far we can get without making any further assumptions. To get there, we need deal with the $f_{MB} \ln(f)$ term, and for that we will need to further assume that our system is **close to equilibrium**, that is, that $\ln(f) \approx \ln(f_{MB}) + \left(\frac{f - f_{MB}}{f_{MB}} \right) + \mathcal{O}(f^2)$ holds to first order. If it does, the linear term will be identically 0 when integrated and leave us with:

$$\frac{dH(t)}{dt} \approx \frac{1}{\tau_0} \int \mathrm{d}^3\mathbf{r} \int \mathrm{d}^3\mathbf{v} [f_{MB} \ln(f_{MB}) - f \ln(f)] = \frac{H_{MB} - H(t)}{\tau_0} \tag{24}$$

[2]Note the similarity when compared to the Shannon entropy of a distribution. If $f(\mathbf{r}, \mathbf{v}, t)$ was normalized to unity and we added a minus sign, they'd be almost the same! Because of this, we can closely relate this function to the entropy of the system.

where we have used the definition of H(t) in (20) to greatly simplify things. This is a very familiar differential equation, which we already saw solved by equation (17), meaning we can just write:

$$H(t) = (H_0 - H_{MB})e^{-t/\tau_0} + H_{MB}. \tag{25}$$

This leads us to expect the same general convergence behaviour that we see in the moments for H.

3 Simulation Methods and Results

So far, we have employed many different analytical techniques to further our understanding of non-equilibrium systems. That, perhaps unfortunately, is not enough: In many sections, we have been forced to employ relaxation-time approximation schemes to be able to progress at all and, a priori, we have no way of knowing if these approximations fully capture the physics of our system.

Because of this, we now proceed onto the second step of this paper in which we will employ numerical schemes, in particular, a Direct Simulation Monte-Carlo (DSMC) method, to evolve our system and, at each step of this evolution, we use standard statistical estimators to calculate to infer the values of $\langle v^2 \rangle$, $\langle v^4 \rangle$, possibly any other higher order moments of the distribution, and H.

We will begin this section by a very brief overview of what these methods actually are, followed by the main results obtained from them for the different initial distributions with a brief discussion of their main features and how well the analytical methods predict them.

3.1 Direct Simulation Monte Carlo of Hard Spheres with Elastic Collisions

In general, DSMC methods can be applied in many different situations, have very broad scopes and we cannot really hope to cover them in all their generality[3] and our aim here is to merely sketch out its structure for a very simple case: That of a spatially homogeneous system with only elastic collisions.

Because of these stipulations, a lot of usual complications or finer points involved in DSMC simulations disappear: Since the only interactions we are considering are collisions and we do not wish to track the position of the particles, the only evolution of our system experiences is during its collisional phase and, because of this, we essentially do not have to care about anything else.

To talk very generally, to implement these methods we need to:

1. **Distribute the initial velocities** among N particles, according to some probability distribution, using standard sampling techniques from statistics. To fix the temperature of the system, we re-scale the velocities to fix $\langle v^2 \rangle$

[3] If one is looking for such details, [1] has a very insightful chapter on the matter.

2. Select random pairs of particles and **make them collide**, if possible, and **update their velocities** using the collision rules encoded in equation (2).
3. Estimate the moments and H-function of the distribution by **computing sample moments and the histogram** respectively.
4. Repeat steps 2 and 3 until satisfied.
5. Since this is inherently a non-deterministic process, we then repeat this process for the same initial conditions multiple times so that the **magnitudes of interest can be averaged over** many repetitions and their noise greatly reduced.

For our simulations, we have used $N = 1024$ particles, fixed $\langle v^2 \rangle = 6.25$ and did 500 repetitions for the averaging, and we also used natural units, where we have considered $k_b = m = 1$.

3.2 Results

3.2.1 Delta initial distribution

For this, we initially distribute the velocities on the unit sphere, i.e.

$$\mathbf{v} \sim Sph(1) \tag{26}$$

That is, we take $|\mathbf{v}| = 1$ and 'uniformly' sample a direction. That'll lead us, after rescaling, to initially have a delta distribution on $|\mathbf{v}|$ and thus why we call it a "delta distribution".

Figure 1 represents the results of this simulation

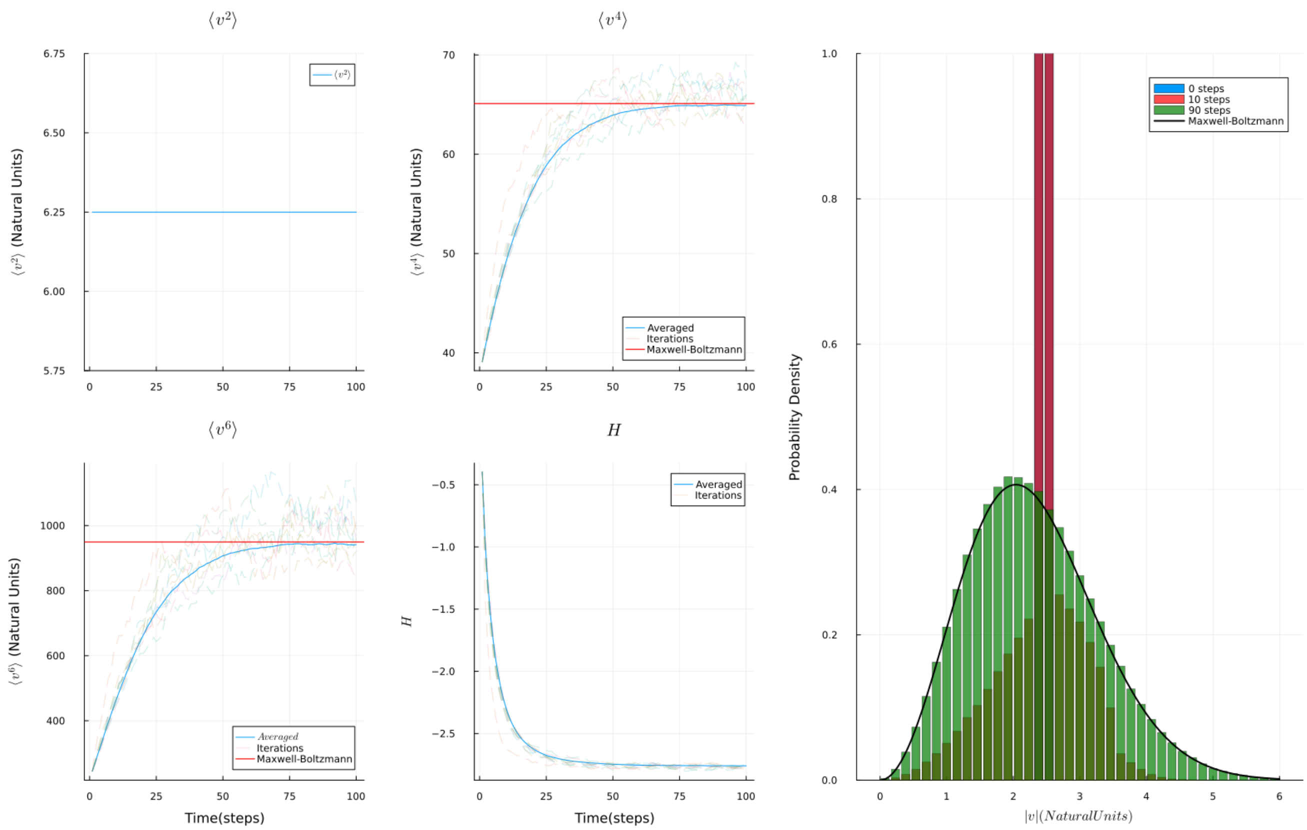

Figure 1: Left: Moments and H-function as a function of time for an initial delta-like distribution. They all converge to the MB values. Right: Evolution of the histogram for those initial conditions, converging to the MB distribution after enough time.

3.2.2 Uniform Initial Distribution

For the uniform distribution, we take each component of the velocity to be uniformly distributed between 0 and 1, that is

$$v_i \sim U(-1, 1) \tag{27}$$

The results from this simulation are represented in Figure 2, and we chose to represent the histogram of v_x instead of $|v|$:

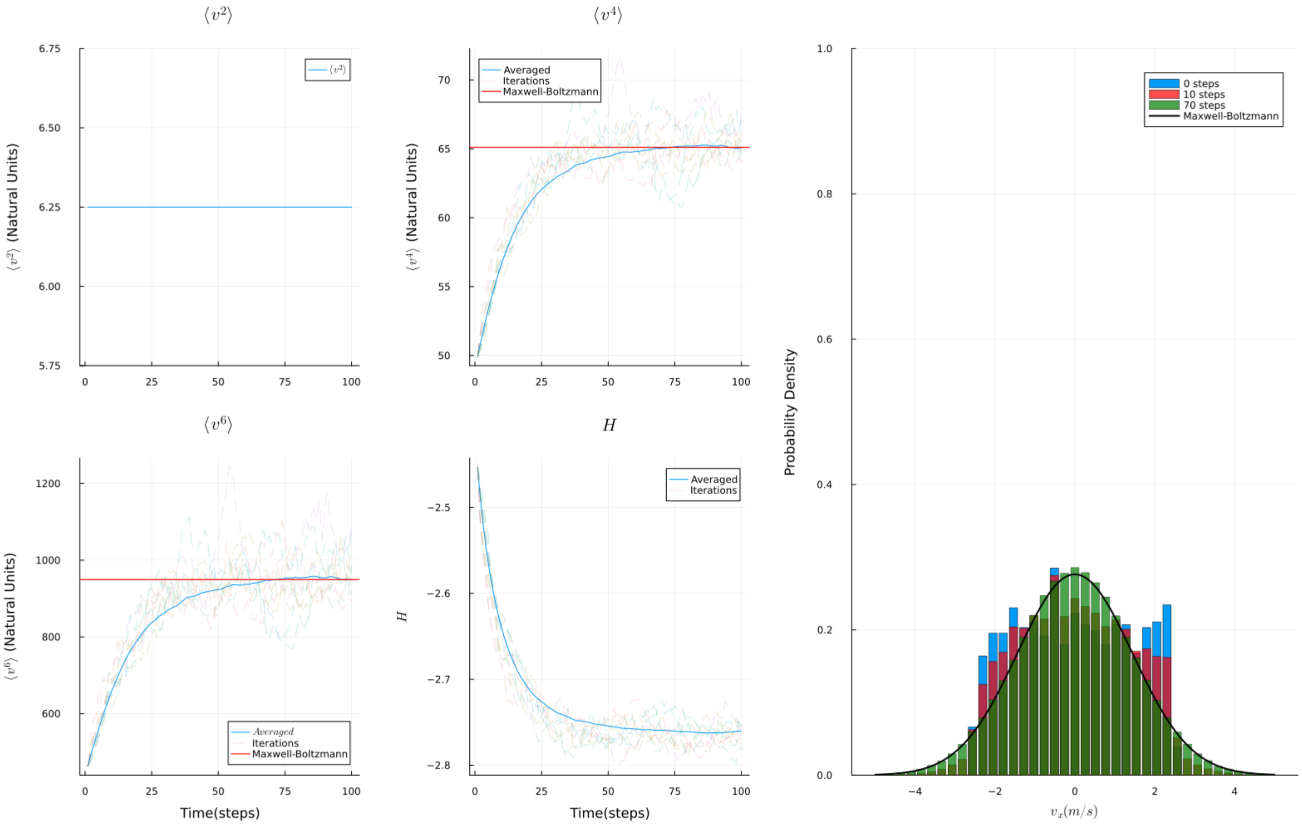

Figure 2: Left: Moments and H-function as a function of time for an initial uniform distribution Right: Evolution of the histogram for those initial conditions.

General comments on the results

In both of the previous cases, the exponential behaviour of the solutions mentioned in Sections 2.1.2 and 2.2 is readily apparent and can be used to infer the value of the relaxation time, for each of the cases. For both of them, we have found that while similar in order of magnitude, the values of τ_0 are slightly different for each of the parameters: As represented in Figure 3 for the uniform[4] initial conditions, and explicitly shown in Table 1 for each of them, we have that $\tau_{v^4} \neq \tau_{v^6} \neq \tau_H$.

	$\tau_{\langle v^6 \rangle}$	$\tau_{\langle v^4 \rangle}$	τ_H
Delta	21.0 steps	17.0 steps	7.0 steps
Uniform	17.0 steps	15.0 steps	10.0 steps

Table 1: Relaxation times for the different parameters and different innitial conditions.

More precisely, we have a similar time for the moments while the H-function's is reasonably lower. Furthermore, the H-function is the least exponential of them all, *i.e.* it is clear that

[4]The results are almost the same for the delta-like distribution, so we have decided not to represent them.

there is a slight concavity on the results, likely due to the close-to-equilibrium approximation we had to employ in that section not working very well.

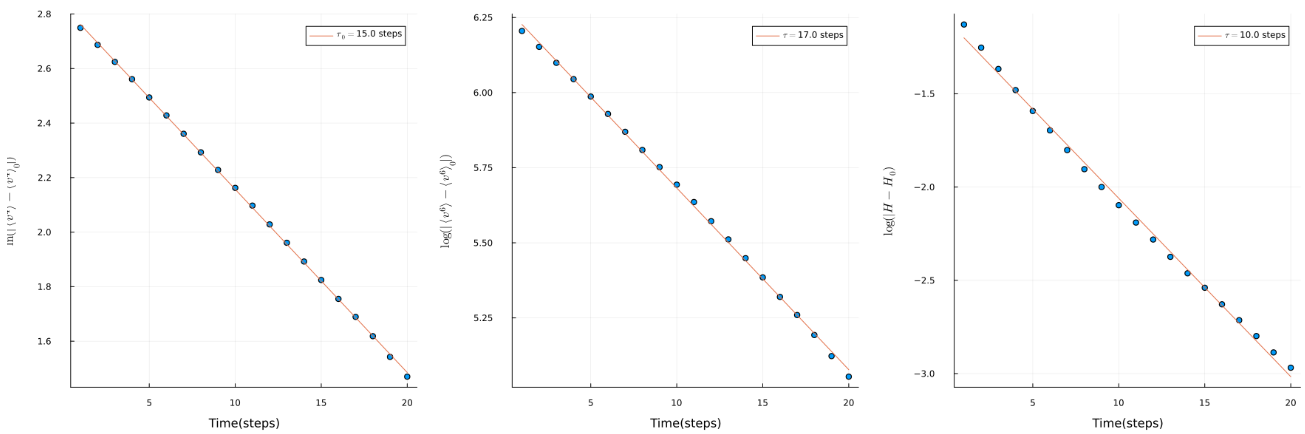

Figure 3: Least-square regressions for the different relaxation times for the uniform initial conditions.

Another remarkable feature of these cases is that they all respect Boltzmann's H-theorem, *i.e.* the H-function is a strictly decreasing function of time, which is a very good indicator that everything is working as intended.

3.2.3 Cauchy

As should be expected, we sample each velocity component from a Cauchy distribution:

$$v_i \sim Cauchy(0, 1) \tag{28}$$

The Cauchy distribution is the one where we need to take the most care to interpret the results. Firstly, we should note that fixing $\langle v^2 \rangle$ is at least a bit suspicious, since it doesn't actually have a finite moments of any kind. What it will have is finite sample moments (that don't converge to anything), and we observed that this was enough for a convergence into a Maxwell-Boltzmann distribution. This will also mean that the values of the higher sample moments (e.g. $\langle v^4 \rangle$ and $\langle v^6 \rangle$) will be unrealistically high at the beginning.

All of these results are summarized in Figure 4:

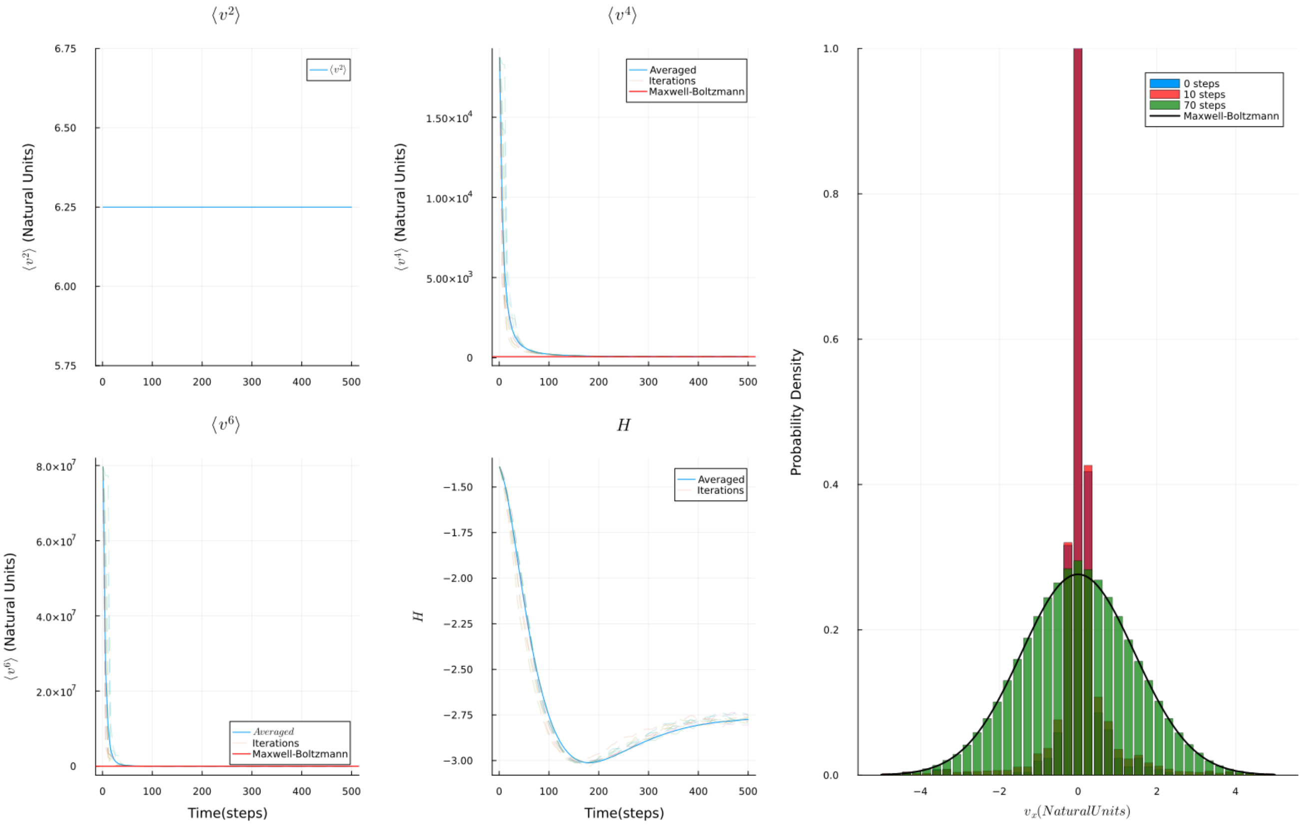

Figure 4: Left: Moments and H-function as a function of time for an initial Cauchy distribution Right: Evolution of the histogram for those initial conditions.

What works and fails on the Cauchy?

Contrary to expectations, a lot more works on the Cauchy distribution than is first expected: It converges, although it does so much slower than the other. This is unexpected! Having no defined moments, it would be expected for almost everything to fail here, but that is not the case.

Unfortunately, not all is well: As we can clearly see, since there is a minimum at around 163, the H-theorem is not respected by a Cauchy initial condition. While we don't fully understand this, we can certainly imagine it is caused by the diverging initial moments that lead to a failure in one of the presuppositions that are needed to prove the theorem or it could even be an issue related to the way we have calculate the entropy.

4 Conclusions

From both a theoretical and computational perspective, we have illustrated how the Boltzmann equation and elastic collisions naturally lead towards a relaxation towards an equilibrium state, at least in the classical context with very simple interactions.

These results also illustrate a bit of problem with the relaxation time approximation: As we have shown, it is readily obvious that they differ by significant amounts. This suggests that while these approximations may be valid for each individual parameter, they don't globally hold and, furthermore suggests that it may be a bit dubious to make such an approximation when these differences might matter.

Another thing of note is that the H-function of the Cauchy, represented in Figure 4, does not verify Boltzmann's H-theorem: There is a minimum at about 167 steps, and the function has a positive derivative from there on. The underlying causes of this could myriad: The most obvious one is a problem with the estimator we have used for H, but since it did only happen with the Cauchy, it could very well be a more technical problem regarding conditions under which the H-theorem holds which any of the pathological aspects of the Cauchy may violate.

Even with these caveats, all of our different initial distributions did converge[5], which suggests that the actual conditions necessary for convergence are quite loose: With what we observed, it would be reasonable to assume that the existence of sample moments is sufficient, but we will leave this as a mere suggestion towards a possible proof.

Data Availability

All of the code used to generate the data and its graphical representations is freely available at `https://github.com/BielUsal/BoltzmannNonEq/tree/main`.

References

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[5] While the definition of convergence here might not be immediately obvious, one could always pointwise compare the histogram with the Maxwell-Boltzmann function and define a norm in which an "error" term could be defined.