Calvin Alexandre Fracassi Farias

Entropy production and the validity of the Vlasov equation for self-gravitating systems

(Produção de entropia e a validade da equação
de Vlasov para sistemas auto-gravitacionais)

December, 2018

Calvin Alexandre Fracassi Farias

Entropy production and the validity of the Vlasov equation for self-gravitating systems

(Produção de entropia e a validade da equação de Vlasov para sistemas auto-gravitacionais)

Master's thesis[1] elaborated under the supervision of Prof. Yan Levin, co-supervision of Prof. Renato Pakter and presented to the Institute of Physics at UFRGS in partial fulfillment of the requirements for obtaining the title of Master of Physics.

Universidade Federal do Rio Grande do Sul – UFRGS
Instituto de Física
Postgraduate Program in Physics

Supervisor: Yan Levin
Co-supervisor: Renato Pakter

December, 2018

[1] Project financed by the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq).

There are many people whom I should, in different manners, express my gratitude. In particular, two among many, deserve it whole just for them.

I couldn't ever possibly write this if not for my parents. Henceforward all is dedicated to them.

"(...) there were people fighting each other.
For what I would suggest, is this:
in the interest of us together as a community
of human beings of this fragile planet,
creating a future for our children
and their children, and successive generations.
We gonna have to find some way
of figuring out how to use our fighting prowess
to fight the [redacted] *PIGS, not each other!"*
Roger Waters.

Abstract

The evolution of self-gravitating systems to out-of-equilibrium stationary states occurs through the mechanism of violent relaxation, a process by which particles exchange energy by moving in a time-changing potential. It's commonly well accepted that this stage's dynamics is governed by the Vlasov equation – a kinetic equation whose evolution conserves the system's entropy. This dissertation goes through the formulation of kinetic theories until the Vlasov equation is defined within the limit $N \to \infty$. The entropy production of finite self-gravitating systems – during the process of violent relaxation – is investigated using molecular dynamics simulations. The author then determines that the entropy is produced on a timescale that grows with N^α, $\alpha > 0$, diverging in the thermodynamic limit and therefore, keeping the entropy constant. In addition, the dynamics of a few observables in mean-field models based on the Vlasov equation are identical to those obtained from molecular dynamics simulations, corroborating the validity of the Vlasov equation even for finite models.

Key-words: Long-range interacting systems. Vlasov equation. Entropy production.

Resumo

A evolução dos sistemas auto-gravitacionais para estados estacionários fora de equilíbrio ocorre através do mecanismo de relaxação violenta, um processo pelo qual partículas trocam energia por estarem se movendo em um potencial dependente do tempo. É comumente aceito que a dinâmica dessa fase seja governada pela equação de Vlasov – uma equação cinética cuja evolução conserva a entropia do sistema. Esta dissertaçao estende-se desde a formulação de teorias cinéticas até a definição da equação de Vlasov no limite $N \to \infty$. A produção de entropia em sistemas auto-gravitacionais finitos – durante o processo de relaxação violenta – é investigada usando simulações de dinâmica molecular. O autor então determina que a entropia é produzida em uma escala de tempo que cresce com N^{α}, $\alpha > 0$, divergindo no limite termodinâmico e, portanto, mantendo a entropia constante. Além disso, a dinâmica de alguns observáveis em modelos de campo médio baseados na equação de Vlasov são idênticos àqueles obtidos de simulações de dinâmica molecular, corroborando a validade da equação de Vlasov mesmo para modelos finitos.

Palavras-chave: Sistemas com interações de longo-alcance. Produção de entropia. Equação de Vlasov.

Contents

I Introduction 11
1 Conventions . . . 13
2 Long-range interacting systems . . . 15

II Literature review 19
3 Dynamical properties of LRI systems . . . 21
3.1 Kinetic theory and reduced distribution functions . . . 21
3.2 Deduction of the Vlasov equation from Klimontovich's . . . 23
3.3 Kac's prescription . . . 26
4 Gravitational systems . . . 27
4.1 SGS in one and two dimensions . . . 27
4.1.1 Reduced Poisson equation . . . 27
4.1.2 Virial conditions for SGS . . . 28
4.1.3 Molecular dynamics simulations . . . 29
4.2 SGS in three dimensions . . . 30
4.2.1 Fine and coarse-grained entropy in three-dimensional SGS . . . 31

III Final considerations 33
5 Conclusion . . . 35
Bibliography . . . 37

APPENDIX A Solutions of Green's function for the Poisson equation . . . 39
ANNEX A Published paper on the subject . . . 41

Part I

Introduction

1 Conventions

It is interesting to define, at first, some conventions utilized by the author in this dissertation. The most outstanding ones are as follow:

- The full distribution function is denoted by $f^{(N)}$ and the one-particle DF is denoted by f, for simplicity, as it was done in the author's attached paper;
- The Eulerian vector is denoted by $\vec{x} = (\vec{q}, \vec{p})$, in contrast to the attached paper, where vectors are distinguished using a bold font, as in $\mathbf{w} = (\mathbf{q}, \mathbf{p})$;
- The set of vectors $(\vec{x}_1, \ldots, \vec{x}_N)$ is denoted by $\{\vec{x}_i\}$;
- The Laplacian is denoted by Δ, instead of ∇^2 or $\nabla \cdot \nabla$.
- The partial derivative of a function f with respect to a variable x may appear represented as $\partial_x f$.

2 Long-range interacting systems

Long-range interacting (LRI) system is a denomination for those systems whose potential decays as a power of the inverse of the distance with an exponent smaller than the dimensionality of the embedding space. These systems distinguish themselves from short-ranged ones as the contributions to its internal energy from any sub-part of the system cannot be neglected – including the interface, which isn't clearly defined. These conditions make LRI systems non-additive. Furthermore, the collisionless aspect of its interactions makes them converge to non-equilibrium *quasi*-stationary states – whose lifetime is often macroscopic, possible diverging in the thermodynamic limit – instead of stationary ones [1]. Due to its long-range (LR) forces, these systems are also known as *non-integrable*, e.g., let the interaction potential ψ be

$$\psi(r) \propto \frac{\mathcal{J}}{r^\gamma} \tag{2.1}$$

where $\mathcal{J}$ is the coupling constant and r is the distance in the configuration space. Let the internal energy ε of a particle placed at the center of a homogeneously density filled d-dimensional (hyper-)sphere of radius R be equal to

$$\varepsilon = \int_\delta^R \mathrm{d}^d r\, \rho \frac{\mathcal{J}}{r^\gamma} \tag{2.2}$$

$$= \rho \mathcal{J} \Omega_d \int_\delta^R \mathrm{d}r\, r^{d-1-\gamma} \tag{2.3}$$

$$= \frac{\rho \mathcal{J} \Omega_d}{d-\gamma} \left[R^{d-\gamma} - \delta^{d-\gamma} \right] \tag{2.4}$$

where ρ is the density, Ω_d is the volume of a d-dimensional (hyper-)sphere and δ is an arbitrarily small radius whereupon we neglect the contributions from within. As the radius R of the sphere is made to increase, the energy ε remains finite only if $\gamma > d$, otherwise the energy diverges. Hence, the definition of *non-integrable* for LRI systems. $\delta \to$ *zero*.

The outcome of N-body systems' study typically relies on statistical mechanics. The derivation of macroscopic quantities – and in particular thermodynamic properties – from a probabilistic analysis is one of the most successful and solid achievements in physics. However, one can inquire about the applicability of thermodynamic and statistical mechanics for certain research fields. The study of non-neutral plasma or self-gravitating systems (SGS) isn't trivial, as these are LRI systems (to cite only the most researched areas within the concern of LR interactions). The non-integrability of the potential makes that the total energy grows superlinearly with the volume (at constant density), which leads to non-extensivity, although it can be recovered by redefining the coupling constant $\mathcal{J}$ as $\mathcal{J} V^{\sigma/d-1}$. In particular, the Kac's prescription corresponds to the case where $\sigma = 0$, and it's usually applied for mean-field models. It's worth to note at this point that in

the models studied in this dissertation, the volume extends to infinity and, the Kac's prescription is the equivalent of $\mathcal{F} \to \mathcal{F}/N$, leading to a well defined thermodynamic limit as $N \to \infty$ [1, 2]. Nonetheless, the LR nature of the interaction forces still presents an issue, as the system's internal energy is non-additive, and there's no such mechanism as re-scaling to restore it. The lack of additivity is, indeed, the principal cause that leads to non-traditional results of statistical mechanics of long-range interacting systems – foremost non-equivalence of ensembles and negative specific heat – though, undoubtedly, it is possible to have a well understanding of it [3].

An alternative to statistical mechanics is to work out the results from a dynamical perspective relying on kinetic theories, even if it makes matters more complicated since one must figure out a closed equation for the one-particle distribution function $f^{(1)}$ (see section 3.1). The Boltzmann transport equation (BTE) is paramount in dealing with short-range interacting systems:

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \frac{\vec{p}}{m} \cdot \nabla_{\mathrm{q}} f - \nabla_{\mathrm{q}} \psi \cdot \nabla_{\mathrm{p}} f = \left(\frac{\partial f}{\partial t} \right)_{coll} \tag{2.5}$$

where $f = f^{(1)}(\vec{x}, t)$ is the one-particle distribution function (DF), $\vec{x}_i = (\vec{q}_i, \vec{p}_i)$ is the Eulerian vector of, respectively, the generalized coordinate and momentum of the i'th particle, m is the mass of the particle, and $\left(\frac{\partial f}{\partial t}\right)_{coll}$ is the collisional term, also known as relaxation term.

Because that the lifetime of collisions is supposedly very short with respect to the average time between collisions; because that the particles interact only through binary collisions within a short range of the potential; and because that the molecular chaos hypothesis holds; then, the distribution function converges to the well known Maxwell-Boltzmann distribution and the system achieves equilibrium. Contrarily, LRI systems do not hold these assumptions, and thus the time evolution mechanism of the distribution function $f = f^{(1)}(\vec{x}, t)$ must be made anew. To introduce mean-field potentials into the transport equation is a realistic choice once Kac's prescription is performed – considering the thermodynamic limit. The forces acting over an individual particle depends on the large-scale structure of the system and, with the increasing number $N \to \infty$, the particles' correlation vanishes. The full distribution function, $f^{(N)}$, is then expected to reflect the behavior of the one-particle distribution function, $f^{(1)}$. Its exact evolution, however, depends on the two-body distribution function. Hopefully, given satisfactory assumptions, one can get rid of it (or replace it by the collisional term, as in the case of the BTE), making it a closed equation [2].

In the following, the author intends to present its study of the dynamical properties of self-gravitating systems, a well known and studied LRI system, and in particular, its entropy production during the process of violent relaxation to out-of-equilibrium steady states. The key objective is to corroborate Vlasov equation's validity during this process by means of its entropy production. The author's published work on the subject [4] is

attached to the end of the dissertation and contain most of the reasoning, while the body of the dissertation presents the necessary mathematical deductions and basis theories – a literature review, so to speak. Vlasov equation is a mean-field model, which can be introduced within the context of the kinetic theory, as it was seen above. In the remaining of this chapter, the published paper's main line of thought will be briefly reproduced, showing how Vlasov equation fulfill any essential requisites to describe self-gravitating systems (in the thermodynamic limit), including the violent-relaxation phase, as well as the reasons why its entropy production not in the least invalidate its applicability.

Long-range interacting systems achieve *quasi*-stationary states instead of converging to thermodynamic equilibrium, as it has already been stated. Particularly, SGS reach it by the mechanism of *violent relaxation*, a process characterized by parametric resonances in which particles exchange energy by moving in a time-changing potential. In order to study its dynamic, it's fairly common to take advantage of the LRI nature of SGS and reduce the $2dN$-dimensional Γ phase space to the $2d$-dimensional μ phase space, containing N points. The concept behind it is as follow: the correlation functions $g^{(s)}$ become null at the thermodynamic limit $N \to \infty$ because of Kac's prescription (see section 3.1), and then the reduced distribution functions $f^{(s)}$ can be well approximated by a product of one-particle distribution functions, i.e.,

$$f^{(s)}(\vec{x}_1, \ldots, \vec{x}_s, t) = \prod_{i=1}^{s} f(\vec{x}_i, t) \tag{2.6}$$

where $f^{(s)}$ is the s-particle distribution function. The physical meaning of this factorization is clear. The full distribution function, $f^{(N)}$, can be written as Eq. 2.6 and thus, its dynamic must mimic the one-particle DF's behavior. Also, the interaction forces between particles tend to zero because the $1/N$ term in the potential. These – satisfactory – assumptions makes Vlasov equation an appropriate choice for the kinetic equation[1]. The collisionless Boltzmann transport equation, also know as the Vlasov equation, is

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \frac{\vec{p}}{m} \cdot \nabla_{\mathrm{q}} f - \nabla_{\mathrm{q}} \psi \cdot \nabla_{\mathrm{p}} f = 0. \tag{2.7}$$

The time-reversibility of Vlasov equation, however, presents another issue. Since the equation has the form of $\mathrm{d}f/\mathrm{d}t = 0$, the distribution function evolves as an incompressible fluid over the phase space, and then its entropy, as well as any local integral of the DF, must remain constant [5]. Naturally, the fine-grained entropy remains constant as the volume held by the particles in the phase space cannot increase, yet its dynamic never ceases. On a coarse-grained scale, however, the system's evolution may appear to reach a stationary state – despite the continuum evolution – as the distribution function stretches and folds over an extended volume of the μ phase space (see figure 1). In this case, the coarse-grained entropy of the system will increase until the apparent stationary state is achieved. Nonetheless, molecular dynamic simulations *shall* display some entropy

[1] Even if its 'discreteness' doesn't strictly classify it as a kinetic equation.

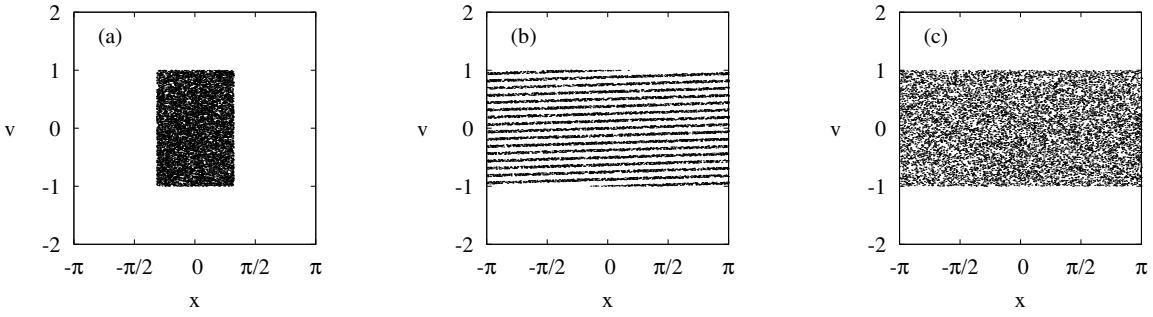

Figure 1 – Snapshots of the phase space of a one-dimensional system composed of $N = 131072$ non-interacting particles. The configuration space has periodic boundary conditions. The distribution function evolves through the process of filamentation and phase-mixing, and at some point, the resolution is no longer sufficient to perceive the dynamics and the system appears to be stationary. The times of the snapshots are: (a) t = 0; (b) t = 50 and (c) t = 1000.

production due to its coarse-grained nature, even if the entropy estimator is a fine-grained one. That's because the limited resolution of computers, or experiments for all that matter, doesn't allow the full fine-grained evolution to be seen. Take Gibbs entropy, for instance

$$S_G = -k_B \int f^{(N)}(\{\vec{x}_i\}, t) \ln f^{(N)}(\{\vec{x}_i\}, t) \mathrm{d}^N\vec{x} \tag{2.8}$$

where $f^{(N)}(\{\vec{x}_i\}, t)$ is the full DF for a system composed of N particles and $\mathrm{d}^N\vec{x} = \mathrm{d}\vec{x}_1 \ldots \mathrm{d}\vec{x}_N$. Since N must be finite, there would be some residual correlation between the particles and the system's entropy will eventually increase and reach a maximum. It should not invalidate Vlasov equation though, unless it is proven that the entropy production observed doesn't have relation with the number of particles in the simulation, i.e., that the entropy grows regardless of the *finite-number-of-particle's-residual-correlation*. Otherwise, it could be demonstrated that the entropy production scales with N^α, diverging in the thermodynamic limit and, implying that the fine-grained entropy will remain constant as it is required by Vlasov dynamics. The timescale of the relaxation time for many different systems is briefly discussed by [1], while the timescale of the entropy production in SGS is discussed by the author in the attached paper [4].

Part II

Literature review

3 Dynamical properties of LRI systems

Statistical mechanics, despite its successfulness for short-range interacting systems, is by no means 'traditional' in which concern LRI systems. Nonetheless, any system at equilibrium, for which the constraints are known, will provide the value of observables if they average computation over the appropriate distribution function at the Γ phase space is allowed. Still, this procedure has no indication of transient states or the timescale in which the process takes places, and therefore, in order to study out-of-equilibrium dynamics, specifically its approach of (*quasi-*) stationary states, one must make use of kinetic theories. In the next sections, the basis of kinetic theory and the deduction of the Vlasov equation will be presented.

3.1 Kinetic theory and reduced distribution functions

The solution of a kinetic equation determines the dynamical state of the distribution function of one single particle. Consequently, the kinetic equation must be a closed equation of the one-particle DF. Usually, two approaches can be used to derive a kinetic equation, the first is the BBGKY hierarchy – proposed almost simultaneously by Bogoliubov (1946), Born and Green (1949), Kirkwood (1946) and Yvon (1935) – which is largely used in the Boltzmann transport equation derivation. The second one is more simple, relying on Klimontovich's equation, and will be seen at the next chapter.

In order to reduce the distribution function, one can start with the Liouville equation and estimate how the chosen procedure will affect the dynamic or the value of the observables. Consider a system composed of N identical particles interacting by a pairwise potential $V_{ij} = V\left(|\vec{q}_i - \vec{q}_j|\right)$. Its Hamiltonian is written as,

$$\mathscr{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N} V\left(|\vec{q}_i - \vec{q}_j|\right) \tag{3.1}$$

where m is the mass of the particles and $\vec{q}_i$ and $\vec{p}_i$ are, respectively, the generalized coordinate and momenta. Let its distribution function $f^{(N)}(\vec{x}_1, \ldots, \vec{x}_N)$ be governed by the continuity equation. The Liouville equation is

$$\frac{\partial f^{(N)}}{\partial t} + \sum_{i=1}^{N} \frac{\vec{p}_i}{m} \cdot \nabla_i f^{(N)} - \sum_{i=1}^{N}\sum_{j\neq i}^{N} (\nabla_i V_{ij}) \cdot \frac{\partial f^{(N)}}{\partial \vec{p}_i} = 0 \tag{3.2}$$

at which point it was inserted, into the continuity equation, the Hamiltonian's equations of motion and the usual notation $\nabla_i = \partial/\partial\vec{q}_i$ was adopted.

As both Hamiltonian and Liouville equations are invariant with respect the permutation of any two particles, any reasonable DF must also satisfy this condition. In particular,

the reduced s-particle distribution function is defined by the partial integration of the full DF, i.e.,

$$f^{(s)}(\vec{x}_1, \ldots, \vec{w}_s) = \frac{N!}{(N-s)!} \int \mathrm{d}w_{s+1} \ldots \mathrm{d}w_N f^{(N)}(\vec{x}_1, \ldots, \vec{x}_N, t). \tag{3.3}$$

And as it is guaranteed that $f^{(N)}$ is completely symmetric with respect to the exchange of any two particles, there's no dilemma to which set of $(N-s)$ particles will be integrated to obtain the reduced s-particle DF. Further assuming that the full DF $f^{(N)}$ is normalized to 1, will made $f^{(s)}$ normalized to

$$\int \mathrm{d}\vec{x}_1 \ldots \mathrm{d}\vec{x}_s \, f^{(s)} = \frac{N!}{(N-s)!}. \tag{3.4}$$

The time evolution of the s-particle DF can be calculated by performing the corresponding partial integration in the Liouville equation. Then, by also requiring that $f^{(N)}$ vanishes at the boundary of the defined domain, i.e.,

$$\int \mathrm{d}\vec{x}_i \, \frac{\vec{p}_i}{m} \cdot \nabla_i f^{(N)} = 0 \ \text{ and} \tag{3.5}$$

$$\int \mathrm{d}\vec{x}_i \, (\nabla_i V_{ij}) \cdot \frac{\partial f^{(N)}}{\partial \vec{p}_i} = 0, \tag{3.6}$$

the time evolution will be given by

$$\begin{aligned} \frac{\partial f^{(s)}}{\partial t} = &- \sum_{i=1}^{s} \frac{\vec{p}_i}{m} \cdot \nabla_i f^{(s)} + \sum_{i=1}^{s} \sum_{j \neq i}^{s} (\nabla_i V_{ij}) \cdot \frac{\partial f^{(s)}}{\partial \vec{p}_i} \\ &+ \sum_{i=1}^{s} \int \mathrm{d}\vec{x}_{s+1} \, (\nabla_i V_{i,s+1}) \cdot \frac{\partial f^{(s+1)}}{\partial \vec{p}_i}, \end{aligned} \tag{3.7}$$

for $s = 2, \ldots, N-1$. If $s = 1$ the above equation holds true without the second term of the right-hand side. Together, equations 3.2 and 3.7 (including the condition for $s = 1$) constitute what is known as the BBGKY hierarchy: a set of N coupled integro-differential equations, in which the time evolution of each $f^{(s)}$ is coupled to $f^{(s+1)}$, except by Liouville equation itself, which is a closed equation for $f^{(N)}$.

So far, the BBGKY hierarchy doesn't provide a closed equation for any reduced s-particle DF. However, one can hope that cutting the hierarchy at some small value of s could be sustained by the introduction of some degree of approximation. For certain 'families' of observables, the knowledge of the first few DFs $f^{(s)}$, even if not exact, can be sufficient for the computation of its observables' expectation values. For example, suppose that some observable O is the sum of identical one-particle functions a,

$$O(\vec{x}_1, \ldots, \vec{x}_N) = \sum_{i=1}^{N} a(\vec{x}_i). \tag{3.8}$$

Its expectation value $\langle O \rangle$ is given by

$$\langle O \rangle(t) = \int \mathrm{d}\vec{x}_1 \ldots \mathrm{d}\vec{x}_N \, O(\vec{x}_1, \ldots, \vec{x}_N) \, f^{(N)}(\vec{x}_1, \ldots, \vec{x}_N, t) \tag{3.9}$$

$$= \int \mathrm{d}\vec{x}_1 \ldots \mathrm{d}\vec{x}_N \sum_{i=1}^{N} a(\vec{x}_i) \, f^{(N)}(\vec{x}_1, \ldots, \vec{x}_N, t). \tag{3.10}$$

Reducing to the one-particle DF (see equation 3.3) and recalling the conditions of normalization and permutation of the reduced s-particle DF, the expected value is given by

$$\langle O\rangle(t) = \sum_{i=1}^{N} \int \mathrm{d}\vec{x}_i a(\vec{x}_i) \int \mathrm{d}\vec{x}_1 \ldots \mathrm{d}\vec{x}_{i-1}\mathrm{d}\vec{x}_{i+1} \ldots \mathrm{d}\vec{x}_N \, f^{(N)}(\vec{x}_1, \ldots, \vec{x}_N, t) \tag{3.11}$$

$$= \sum_{i=1}^{N} \int \mathrm{d}\vec{x}_i a(\vec{x}_i) \frac{(N-1)!}{N!} f(\vec{x}_i, t) \tag{3.12}$$

$$= \int \mathrm{d}\vec{x}_1 a(\vec{x}_1) f(\vec{x}_1, t). \tag{3.13}$$

Notwithstanding the expected value being written in terms of the one-particle DF, it is still dependent on $f^{(2)}$. To make a closed equation for f further approximations will be necessary, though these will depend on the type of the system under consideration. A common expression that facilitates additional approximations of $f^{(2)}$ is

$$f^{(2)}(\vec{x}_1, \vec{x}_2, t) = f(\vec{x}_1, t)\, f(\vec{x}_2, t) + g^{(2)}(\vec{x}_1, \vec{x}_2, t) \tag{3.14}$$

where $g^{(s)}$, $s = 2$ in the above equation, is the correlation function of the s-particle DF and is related to the deviation from the complete DF in its uncorrelated form. The time evolution (equation 3.7) for the one-particle DF is then, written as

$$\begin{aligned} &\frac{\partial}{\partial t} f(\vec{x}_1, t) + \frac{\vec{p}_1}{m} \cdot \nabla_1 f(\vec{x}_1, t) - (\nabla_1 V[f, t]) \cdot \frac{\partial}{\partial \vec{p}_1} f(\vec{x}_1, t) \\ &\qquad = \int \mathrm{d}\vec{x}_2 \, (\nabla_1 V_{12}) \cdot \frac{\partial}{\partial \vec{p}_1} g^{(2)}(\vec{x}_1, \vec{x}_2, t) \end{aligned} \tag{3.15}$$

where $V[f, t]$ is the averaged two-particles interaction potential:

$$V[f, t] = \int \mathrm{d}\vec{x}_2 V_{12} f(\vec{x}_2, t). \tag{3.16}$$

A common approximation is to set $g^{(2)} = 0$ when at the thermodynamic limit – it was the one utilized by the author in the introduction, recall equation 2.6. This is satisfactory in the limit $N \to \infty$ because as $f^{(2)}$ grows with N^2, $g^{(2)}$ grows slowly, with N. Analogous evaluations can be done for $s > 2$ arriving at similar results [2]. This last procedure finally allows one to produce a kinetic equation, be it by setting $g^{(2)} = 0$ or substituting the right-hand side by the collisional term (as was also mentioned in the introduction).

3.2 Deduction of the Vlasov equation from Klimontovich's

This section is dedicated to derive Vlasov equation in a more straightforward procedure than to derive it from BBGKY hierarchy. The deductions presented here will be limited to a one-dimensional systems with periodic boundary conditions in the configuration space. Although, it can easily be expanded for two or three dimensions.

Let the Hamiltonian of a system composed of N particles be

$$\mathscr{H} = \sum_{j=1}^{N} \frac{P_j}{2} + U(\{\Theta_j\}) \tag{3.17}$$

where Θ_j and P_j are, respectively, the canonical coordinate and momenta of the j'th particle. Let the system be periodic in space with $\Theta_j \in [0, 2\pi)$ and the potential to be a sum of pair interactions

$$U(\Theta_1, \ldots, \Theta_N) = \frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} V(\Theta_i - \Theta_j). \tag{3.18}$$

The *discrete* time-dependent density function of the above system is described by

$$f_d(\theta, p, t) = \frac{1}{N} \sum_{i=1}^{N} \delta(\theta - \Theta_j(t))\, \Theta(p - P_j(t)) \tag{3.19}$$

where δ denotes the Dirac 'delta' function and $(\theta,\, p)$ are the Eulerian coordinates in the phase space. By differentiating with respect to time, the density function assumes the following form

$$\begin{aligned} \frac{\partial}{\partial t} f_d(\theta, p, t) = &-\frac{1}{N} \sum_{i=1}^{N} P_j \; \frac{\partial}{\partial \theta} \Big(\delta(\theta - \Theta_j(t))\, \delta(p - P_j(t)) \Big) \\ &+ \frac{1}{N} \sum_{i=1}^{N} \frac{\partial U}{\partial \Theta_j} \; \frac{\partial}{\partial p} \Big(\delta(\theta - \Theta_j(t))\, \delta(p - P_j(t)) \Big), \end{aligned} \tag{3.20}$$

at which point was introduced the Hamiltonian's equations of motion. Using the following property of the delta function: $a\delta(a-b) = b\delta(a-b)$, equation 3.20 can also, be written as

$$\begin{aligned} \frac{\partial}{\partial t} f_d(\theta, p, t) = &-\frac{1}{N} \sum_{i=1}^{N} p \; \frac{\partial}{\partial \theta} \Big(\delta(\theta - \Theta_j(t))\, \delta(p - P_j(t)) \Big) \\ &+ \frac{1}{N} \sum_{i=1}^{N} \frac{\partial v}{\partial \theta} \; \frac{\partial}{\partial p} \Big(\delta(\theta - \Theta_j(t))\, \delta(p - P_j(t)) \Big), \end{aligned} \tag{3.21}$$

where

$$v(\theta, t) = N \int \mathrm{d}\theta' \mathrm{d}p' V(\theta - \theta') f_d(\theta', p', t). \tag{3.22}$$

After rearranging the terms, the formal expression for the Klimontovich equation is obtained. It's also important to note that this derivation is exact even for a finite number N of particles.

$$\frac{\partial f_d}{\partial t} + p \frac{\partial f_d}{\partial \theta} - \frac{\partial v}{\partial \theta} \frac{\partial f_d}{\partial p} = 0. \tag{3.23}$$

The Klimontovich equation is the equivalent of the Hamiltonian's equations of motion, i.e., it contains the information on the orbit of each and every particle, making it very difficult (if not impractical) to solve for a system of many particles. Alternatively, starting with

an well defined set of initial conditions, all of them close to the same macroscopic state, one could define an averaged one-particle distribution function, denominated f_0, and performed over the density of such initial macroscopic state, denominated $f_{in}(\{\Theta_i(0)\},\{P_i(0)\},t)$.

$$f_0(\theta,p,t) = \langle f_d(\theta,p,t)\rangle \tag{3.24}$$

$$= \int \prod_i \mathrm{d}\Theta_i(0)\mathrm{d}P_i(0) f_{in}(\{\Theta_i(0),P_i(0)\}) f_d(\theta,p,t). \tag{3.25}$$

In contrast to the equation 3.19 which is discrete, f_0 is smooth, and its time evolution is given again by an average over f_{in}. It's necessary to note at this point that the fluctuations δf around the smooth distribution is defined as

$$f_d(\theta,p,t) = f_0(\theta,p,t) + \frac{1}{\sqrt{N}}\delta f(\theta,p,t) \tag{3.26}$$

The physical interpretation of the above equation is that, after integrating the quantity δf, i.e., the difference between a singular distribution function containing Dirac 'delta' functions and the smooth distribution function, over a region large enough to contain many particles but small compared to the total available space, its result will be of the order $1/\sqrt{N}$. That said, the introduction of the above equation (3.26) into equation 3.22 will result into the following

$$v(\theta,t) = \langle v\rangle(\theta,t) + \frac{1}{\sqrt{N}}\delta v(\theta,t) \tag{3.27}$$

where the first term is an average over f_{in} and the second defines δv. Introducing the last two expression (equations 3.26 and 3.27) into the Klimontovich equation (3.20) will result in

$$\begin{aligned}&\frac{\partial f_0}{\partial t} + p\frac{\partial f_0}{\partial \theta} - \frac{\partial\langle v\rangle}{\partial\theta}\frac{\partial f_0}{\partial p}\\ &\quad = -\frac{1}{N}\left(\frac{\partial \delta f}{\partial t} + p\frac{\partial\delta f}{\partial\theta} - \frac{\partial\delta v}{\partial\theta}\frac{\partial f_0}{\partial p} - \frac{\partial\langle v\rangle}{\partial\theta}\frac{\partial\delta f}{\partial p}\right) + \frac{1}{N}\frac{\partial\delta v}{\partial\theta}\frac{\partial\delta f}{\partial p}.\end{aligned} \tag{3.28}$$

After averaging it over f_{in}, the result will be

$$\frac{\partial f_0}{\partial t} + p\frac{\partial f_0}{\partial\theta} - \frac{\partial\langle v\rangle}{\partial\theta}\frac{\partial f_0}{\partial p} = \frac{1}{N}\left\langle\frac{\partial\delta v}{\partial\theta}\frac{\partial\delta f}{\partial p}\right\rangle. \tag{3.29}$$

because any average over f_{in} by the terms containing δf or δv will yields zero, as these depends on *all of* the Lagrangian variables of the initial state. Equation 3.29 is the equivalent of equation 3.15 and it's exact. The right-hand side of it usually correspond to – after a suitable approximation – the collisional term of the Boltzmann transport equation if short-ranged forces are acting. Otherwise, as the right-hand side is of order $1/N$, at the thermodynamic limit it can be neglected, leading to the Vlasov equation

$$\frac{\partial f_0}{\partial t} + p\frac{\partial f_0}{\partial\theta} - \frac{\partial\langle v\rangle}{\partial\theta}\frac{\partial f_0}{\partial p} = 0. \tag{3.30}$$

In the next section, it will be seen what are the effects in the system's dynamics of the introduction of terms like $1/\sqrt{N}$, as in the equations 3.26 and 3.27.

3.3 Kac's prescription

The Kac's prescription was first introduced in chapter 2 in the context of a re-scale of mean-field models as a factor of 1/N into the potential, N being the number of particles. The absolute weight of the mean-field term in Vlasov's equation (third in the left-hand side of equation 3.30) does depend on Kac's re-scaling, however it affects only the dynamics's timescale. To clarify this, take as an example the following generic equation of motion

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} = \frac{1}{N}F(q_1, \ldots, q_N) \tag{3.31}$$

where F has the Kac's scaling $1/N$ term. Now, if the system's dynamics – governed by 3.31 – reach some final (*quasi-*) stationary state within a timescale that doesn't depend on N, it's obvious that with the Kac's re-scaling the system will achieve the same final state, going through all the transient states, but $\sqrt{N}$ faster. The consequence of this statement is that for a system whose dynamic's timescale doesn't depend on N, its intensive thermodynamic quantities (e.g., temperature, energy per particle) also doesn't depend on N, after all, Kac's prescription does restore the system's extensivity. It becomes clearer if the substitution done to the time variable were to be made with the Hamiltonian $\mathscr{H} \to N\mathscr{H}$, i.e., getting rid of the $1/N$ term in the potential would be at the coast of measuring the energy in units of $N\mathscr{H}$.

In conclusion, the Kac's prescription is an appropriate mathematical tool in dealing with LRI interacting systems and the results derived from performing it are easily transformed quantitatively to find out what they would be if the prescription were not performed.

4 Gravitational systems

4.1 SGS in one and two dimensions

The study of gravitational systems in one and two dimensions, apart from the natural understanding from simplified toy models, can, sometimes, give insights into 3d gravitational structures – disk-like galaxies, for instance, are also reproduced in two-dimensional simulations. They have the advantage of a infinite upper bound of the potential, preventing the particles to escape its gravitational pull, and also avoiding the singularity of 3d Newtonian forces. Besides the interest in self-gravitating systems (SGS) by itself, simple dimensionality-reduced SGS constitute an ideal ground for studying statistical mechanics of long-range interacting (LRI) systems, or in the case of this dissertation, to corroborate the interpretation of the entropy production enunciated at the introduction.

4.1.1 Reduced Poisson equation

In order to study the entropy production of one- and two-dimensional SGS, it is convenient to define dimensionless variables, essentially to decrease numerical errors in molecular dynamics (MD) simulations, as well as to obtain an appropriate timescale. The Poisson equation, in one dimension, after re-scaling the mass, length, velocity, potential, mass density, and energy, respectively by the total mass of the system M, the arbitrary length scale L_0, the velocity unit $V_0 = (2\pi GML_0)^{1/2}$, the potential unit $\psi_0 = 2\pi GML_0$, the mass density unit $\rho_0 = M/L_0$, and the energy unit $\varepsilon_0 = MV_0^2$, is then, reduced to

$$\Delta\psi(x,t) = 2\rho(x,t) \tag{4.1}$$

where ρ is the mass density. These re-scales are the equivalent to set the gravitational constant G and the total mass of the system M to 1. Therefore, the dynamical time is defined as

$$\tau_d = (2\pi G\rho_0)^{1/2}\,. \tag{4.2}$$

The one-dimensional SGS system derived from the 1d Poisson equation (4.1) consists of N sheets of mass $m = M/N$ uniformly distributed in the yz-plane moving in the x-axis, free to pass one another. The extensivity of its internal energy is guaranteed by the constant value of the system's total mass, even in the thermodynamic limit $N \to \infty$, i.e., defining the mass of each particle as $m \propto N^{-1}$ is the equivalent of the Kac re-scaling.

In two dimensions, the re-scale done to the Poisson equation is analogous to the one made in one dimension, as it's also the equivalent to set the gravitational constant G and the total mass M to unity. The individual mass of the particles was kept as $m = M/N$, as

well as the arbitrary length scale L_0 and the energy unity $\varepsilon_0 = MV_0^2$, although the velocity unit changed to $V_0 = (2GM)^{1/2}$ and the potential unit changed to $\psi_0 = 2GM$. Then, the reduced Poisson equation, considering only systems with azimuthal symmetry, is

$$\Delta\psi(\vec{r}, t) = 2\pi\rho(\vec{r}, t) \tag{4.3}$$

where $\rho(\vec{r}, t)$ is the mass density, obtained after integrating the one-particle DF over the velocity space. The dynamical time is defined as

$$\tau_d = \frac{L_0}{\sqrt{2GM}}. \tag{4.4}$$

The solutions of the one- and two-dimensional Poisson equation (respectively, the equations 4.1 and 4.3) are easily obtained using Green's function (see appendix A), as for each one, the mass density of one single particle is a function of the Dirac 'delta' function. The solution of Green's function for one and two dimensions, together with the reduced Poisson equations, leads to the Hamiltonian for each model, which is utilized in MD simulations. It is as follow [1, 6]

The one-dimensional reduced Hamiltonian is

$$\mathscr{H}(x, p) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{m^2}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} |x_i - x_j| \,. \tag{4.5}$$

And the two-dimensional reduced Hamiltonian is

$$\mathscr{H}(\vec{r}, \vec{p}) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{m^2}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} \ln |\vec{r}_i - \vec{r}_j| \,. \tag{4.6}$$

4.1.2 Virial conditions for SGS

It's well known that the virial theorem imposes that systems at equilibrium must suffice some requirements of equipartition of energy. In what follows, for generic self-gravitating systems, the virial condition will be the demonstrated. Consider the following generic Hamiltonian of a sytem composed of N particles,

$$\mathscr{H} = \sum_{i=1}^{N} \frac{\vec{p}_i}{2m} + \frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} V(\vec{r}_i - \vec{r}_j) \tag{4.7}$$

where $\vec{q}$ and $\vec{p}$ are, respectively, the generalized coordinate and momentum and $V(\vec{r}_i - \vec{r}_j)$ is the pair interaction potential. Let the function I be defined as the virial function:

$$I = \left\langle \sum_{i=1}^{N} \vec{r}_i \cdot \vec{p}_i \right\rangle_t \tag{4.8}$$

where the brackets $\langle \circ \rangle_t$ denote a time average. For a system at equilibrium, it's desired that $\mathrm{d}I/\mathrm{d}t = 0$, then

$$\frac{\mathrm{d}}{\mathrm{d}t} \left\langle \sum_{i=1}^{N} \vec{r}_i \cdot \vec{p}_i \right\rangle_t = \left\langle \sum_{i=1}^{N} \frac{p_i^2}{m} \right\rangle_t - \left\langle \sum_{i=1}^{N} \vec{r}_i \cdot \nabla_i \tilde{V} \right\rangle_t = 0 \tag{4.9}$$

where $\tilde{V} = \sum_{k<j}^{N} V(\vec{r}_j - \vec{r}_k)$ is the second term of the right-hand side in the Hamiltonian (equation 4.7). If $\tilde{V}$ is a homogeneous function of order p, then

$$p\tilde{V} = \sum_{i=1}^{N} \vec{r}_i \cdot \nabla_i \tilde{V}. \tag{4.10}$$

The insertion of the above equation into equation 4.9 yields

$$2K - pU = 0, \tag{4.11}$$

where K and U are denoted as $K = \frac{1}{N}\left\langle \sum_{i=1}^{N} \frac{p_i^2}{2m} \right\rangle_t$ (the average of the kinetic energy per particle) and $U = \frac{1}{N}\left\langle \tilde{V} \right\rangle_t$ (the average of the potential energy per particle), both at a stationary state.

In the one-dimensional SGS model presented in the previous section, the potential is a homogeneous function of order $p = 1$. While for the two-dimensional SGS model presented, the potential is logarithm and need some manipulation to turn it homogeneous of order $p = 0$ [7]. The virial number R_0 is a defined quantity that, when equals to unity, guarantees that these conditions are fulfilled. For the SGS models described above, the definitions of R_0 is:

$$R_0 \equiv \frac{2K}{U} \qquad \text{if } d = 1 \text{ and,} \tag{4.12a}$$

$$R_0 \equiv 2\langle v^2 \rangle \qquad \text{if } d = 2 \tag{4.12b}$$

where, besides the already mentioned denotations of K and U, $\langle v^2 \rangle$ is the average velocity squared per particle, also at some stationary state.

Given that the initial distributions suffice the conditions 4.12, its expected that the system reaches a *quasi*-stationary state (qSS) as fast as it is possible. Otherwise, if the initial distribution does not satisfy these condition, the system will undergo strong oscillations, slowly approaching the qSS.

4.1.3 Molecular dynamics simulations

The simulations of self-gravitating systems were performed using molecular dynamics. The collisional nature of MD is a fundamental condition, given the hypothesis of residual correlation between the particles. In other words, if the entropy produced through the evolution shall be related to the residual interactions, these must exist in the simulations. In this regard, the methodology benefits from the Hamiltonian's equations of motion, which can be obtained from section 4.1.1, since these contain explicit interactions between the pairs of particles.

In the beginning, the particles are distributed accordingly to the waterbag distribution, satisfying the virial conditions 4.12. These distributions should be as close as possible to equilibrium, rapidly reaching a *quasi*-stationary state, avoiding loss of resolution due to

numerical imprecision resulting from strong oscillations. The initial particle distribution has the form

$$f(\vec{q},\vec{p}) = \eta\Theta(q_{\mathrm{M}} - |\vec{q}|)\Theta(p_{\mathrm{M}} - |\vec{p}|) \tag{4.13}$$

where q_{M} and p_{M} are the boundary limits to the coordinates and momenta into the μ phase space, Θ is the Heaviside function, and η is a constant of normalization whose value is $\eta = 4q_{\mathrm{M}}p_{\mathrm{M}}$ in one dimension and $\eta = (\pi q_{\mathrm{M}}p_{\mathrm{M}})^{-2}$ in two dimensions. The expected energy per particle ε_0, at the time $t = 0$, for these distributions are $\varepsilon_0 = \frac{p_{\mathrm{M}}^2}{6} - \frac{1}{3}$ in one dimension and $\varepsilon_0 = \frac{p_{\mathrm{M}}^2}{4} - \frac{1}{8}$ in two dimensions. The virial conditions reduces to $p_{\mathrm{M}} = 1$ for all dimensions.

The results of one- and two-dimensional MD simulations and the analysis of its entropy production are described in the author's attached paper.

4.2 SGS in three dimensions

The relaxation to *quasi*-stationary states of three-dimensional self-gravitating systems is extremely difficult to study with MD simulations. Newton's gravitational potential has a characteristic form – with no lower bound but with an upper one – which allows particles to gain enough energy to escape its gravitational pull. Furthermore, considering the singularity of the potential when the distance $|\vec{r}_i - \vec{r}_j| \to 0$, there's no limit to the number of particles that can escape. Nonetheless, for initial distributions satisfying the virial number $R_0 = -2K/U$ and considerable short simulation's time, its dynamic can be reasonable well represented by MD simulations.

Recalling section 4.1, the three-dimensional reduced Poisson equation is

$$\Delta\psi(\vec{r},t) = 4\pi\rho(\vec{r},t) \tag{4.14}$$

where, one more time, the mass density $\rho(\vec{r},t)$ is obtained after integrating the one-particle DF over the velocity space. These re-scaling to dimensionless variables results in a dynamical time τ_d equals to

$$\tau_d = \left(\frac{L_0^3}{GM}\right)^{1/2} \tag{4.15}$$

where, once again, L_0 is an arbitrary length scale, G is the gravitational constant and $M = mN$ is the total mass of the system. The reduced Hamiltonian is

$$\mathscr{H}(\vec{q},\vec{p}) = \sum_{i=1}^{N}\frac{p_i^2}{2m} + \sum_{i=1}^{N}\sum_{j\neq i}^{N}\frac{m^2}{|\vec{r}_i - \vec{r}_j|} \tag{4.16}$$

with an average potential energy per particle $\varepsilon_0 = \frac{3p_{\mathrm{M}}^2}{10} - \frac{3}{5}$, at the time $t = 0$, for the waterbag distribution 4.13 with a constant of normalization equal to $\eta = (4\pi/3)^{-2}(q_{\mathrm{M}}p_{\mathrm{M}})^{-3}$.

4.2.1 Fine and coarse-grained entropy in three-dimensional SGS

The entropy produced in three-dimensional molecular dynamics simulations, as in the one- and two-dimensional cases, is discussed in the author's attached paper. It's determined in there that the entropy production is originated from residual correlations between the finite number of particles [4]. However, one may ask about accuracy by reproducing an estimate of fine-grain entropy, after all, the estimator has been described as a coarse-grained.

In order to establish a reference, the entropy produced during the MD simulations of the three-dimensional model introduced in this chapter (equation 4.16) was also estimated by a fine-grained entropy estimator, besides the coarse-grained one mentioned in the attached paper. The fine-grained version is described in [8], where the entropy production for three-dimensional SGS has a different interpretation. Figure 2 compare both of the entropy estimators. It is worth noting that while the fine-grained estimator ($\hat{s}$) is Shannon's entropy, the coarse-grained one ($\bar{s}_G$) is Gibbs's entropy. They differ only by the Boltzmann constant.

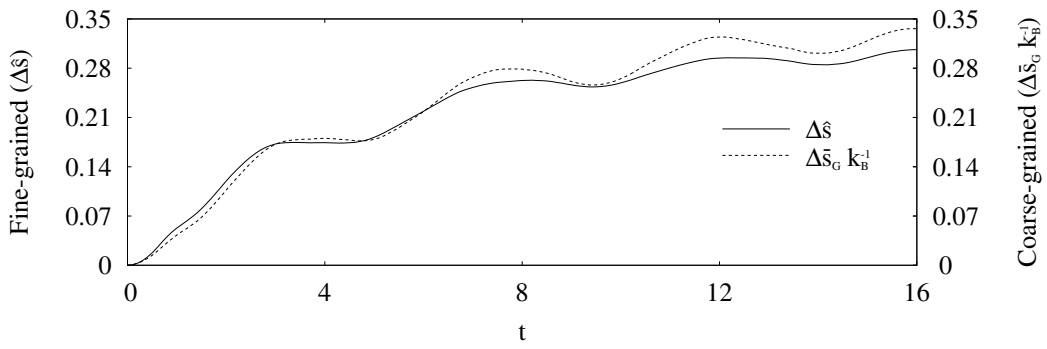

Figure 2 – Entropy production during the MD simulation of the three-dimensional SGS model (equation 4.16). The entropy is estimated using two different methods. Note that both curves are very similar, mostly if the slope is considered. The parameters of the simulation are $N = 131072$ and $R_0 = 1$.

Part III

Final considerations

5 Conclusion

The role of the entropy production in the out-of-equilibrium dynamics of self-gravitating systems was explored. In Chapter 3 it was seen the basis for which the kinetic theory was built and even with a solid understanding of it, the solution of kinetic equations depends too much on assumptions. Despite reproducing many observed physical phenomena with success, one may question if the current acceptable approach for some theory really is correct. Recently it was inferred that the Vlasov equation isn't adequate to reproduce the dynamics of self-gravitating systems because of its entropy production during the violent relaxation phase. The authors of the attached paper went over the entropy production for the initial stages of the evolution of SGS in one, two and three dimensions. They have determined that the entropy observed does not invalidate the Vlasov equation, on the contrary, its timescale was associated with a power law of the number of particles – N^{α}, where α assumes the values 0.10, 0.15 and 0.20 for respectively three, two and one dimension, though it's not clear at which conditions determines the value of the exponent α. This last statement strongly implies that at the thermodynamic limit, when $N \to \infty$, the correlations will vanish and the lifetime of the entropy production will be infinite, meaning it has to be conserved as is required by Vlasov dynamics. Nonetheless, molecular dynamics simulations of SGS *do* display some entropy production due to its residual correlations and one may question if reliable models of Vlasov dynamics could afford not to keep the entropy constant through the evolution. This could implicate that for models far from the thermodynamic limit, some observables derived from a coarse-grained procedure within the Vlasov's formalism could be wrong. The authors compared the evolution of observables from simulations with both collisional and collisionless methods. They observed no significant difference between the two. As collisionless simulations are effective solutions to Vlasov's equation, it's a clear evidence of the equivalence between the averages over fine- and coarse-grained distribution functions.

Bibliography

[1] Yan Levin, Renato Pakter, Felipe B. Rizzato, Tarcísio N. Teles, and Fernanda P.C. Benetti. Nonequilibrium statistical mechanics of systems with long-range interactions. *Physics Reports*, 535(1):1–60, February 2014. Cited 4 times on pages 15, 16, 18, and 28.

[2] Alessandro Campa, T Dauxois, D Fanelli, and Stefano Ruffo. *Physics of long-range interacting systems*. Oxford University Press, Oxford, 2014. OCLC: 984800545. Cited 2 times on pages 16 and 23.

[3] Freddy Bouchet and Julien Barré. Statistical mechanics of systems with long range interactions. *Journal of Physics: Conference Series*, 31:18–26, March 2006. Cited on page 16.

[4] Calvin Alexandre Fracassi Farias, Renato Pakter, and Yan Levin. Entropy production and Vlasov equation for self-gravitating systems. *Journal of Physics A: Mathematical and Theoretical*, October 2018. Cited 3 times on pages 16, 18, and 31.

[5] P. H. Chavanis and F. Bouchet. On the coarse-grained evolution of collisionless stellar systems. *Astronomy & Astrophysics*, 430(3):771–778, February 2005. Cited on page 17.

[6] Alessandro Campa, Thierry Dauxois, and Stefano Ruffo. Statistical mechanics and dynamics of solvable models with long-range interactions. *Physics Reports*, 480(3-6):57–159, September 2009. Cited on page 28.

[7] Tarcísio N Teles, Yan Levin, Renato Pakter, and Felipe B Rizzato. Statistical mechanics of unbound two-dimensional self-gravitating systems. *Journal of Statistical Mechanics: Theory and Experiment*, 2010(05):P05007, 2010. Cited on page 29.

[8] Leandro Beraldo e Silva, Walter de Siqueira Pedra, Laerte Sodré, Eder L. D. Perico, and Marcos Lima. The Arrow of Time in the Collapse of Collisionless Self-gravitating Systems: Non-validity of the Vlasov–Poisson Equation during Violent Relaxation. *The Astrophysical Journal*, 846(2):125, September 2017. Cited on page 31.

[9] University of Cambridge, England and Richard Chapling. A Hypergeometric Integral with Applications to the Fundamental Solution of Laplace's Equation on Hyperspheres. *Symmetry, Integrability and Geometry: Methods and Applications*, August 2016. Cited on page 39.

APPENDIX A – Solutions of Green's function for the Poisson equation

A Green's function is the *impulse response* of a non-homogeneous linear differential operator $\mathcal{L}$ acting over a subset of $\mathbb{R}^{\mathrm{N}}$. In other words, it is any solution of

$$\mathcal{L}G(\vec{x},\vec{x}_0) = \delta(\vec{x}-\vec{x}_0) \tag{A.1}$$

where $\vec{x}$ is a vector of dimension $d = \mathrm{N}$ and $\delta(\vec{x}-\vec{x}_0)$ is the Dirac delta function in d dimensions. In particular, the Green's function for the Poisson equation requires it to be harmonic in $\vec{x}$ everywhere but $\vec{x}_0$, and zero on the boundary ∂D of the domain D, i.e.,

$$\begin{cases} \Delta G(\vec{x},\vec{x}_0) = \delta(\vec{x}-\vec{x}_0) \\ G_{\partial D} = 0 \end{cases} \tag{A.2}$$

where Δ is the Laplacian. Let $\vec{x}_0 = 0$ and then, $G(\vec{x},0) \equiv G(|\vec{x}|)$. Integrating it over the space S of a (hyper-)sphere of radius ε, $S = \vec{x} : r = |\vec{x}| < \varepsilon$, yields

$$\begin{aligned} &\int_{|\vec{x}|<\varepsilon} \Delta G(r)\mathrm{d}^d\vec{x} \equiv \int_{|\vec{x}|=\varepsilon} \nabla G(r)\mathrm{d}^{d-1}\vec{x} \\ &\equiv S_{d-1}\varepsilon^{d-1}\left.\frac{\partial G}{\partial r}\right|_{r=\varepsilon} = 1 \end{aligned} \tag{A.3}$$

at which point was applied the Green's theorem and the right-hand side of equation A.2 was integrated to 1. S_{d-1} is defined as the 'surface area' of the $(d-1)$-dimensional (hyper-) sphere [9]. Solving the above equation (A.3) for $G(r)$, recalling that $\lim_{r\to\infty} G(r) = 0$, results in

$$G(\vec{x},\vec{x}_0) = \frac{-1}{(d-2)S_{d-1}\left|\vec{x}-\vec{x}_0\right|^{d-2}}. \tag{A.4}$$

In one dimension, the solution of the Green's function for the Laplace operator is trivial and can be obtained just substituting the values in equation A.4 (the surface of a 0-sphere has length $S_0 = 2$), resulting in

$$G(x,x_0) = \frac{1}{2}\left|x-x_0\right|. \tag{A.5}$$

While for two dimensions, the solution needs to be worked from equation A.3. $S_1 = 2\pi$ and then,

$$G(\vec{x},\vec{x}_0) = \frac{1}{2\pi}\ln\left|\vec{x}-\vec{x}_0\right| \tag{A.6}$$

because $\partial_r G(r)$ needs to be equal to $(2\pi r)^{-1}$. Note that the solutions, both for one and two dimensions, are distinctly different from the familiar three-dimensional gravitational

potential. The particles attract each other more as they get further apart. For three dimensions, $S_2 = 4\pi$, and just substituting the values in equation A.4 results in

$$G(\vec{x}, \vec{x}_0) = \frac{-1}{4\pi \left|\vec{x} - \vec{x}_0\right|}. \tag{A.7}$$

Notice that all of the performed solutions match its reduced Poisson equation (subsection 4.1.1 and section 4.2) so that the constants are dropped. Using Green's function second identity, the generic Poisson equation, $\Delta\psi(\vec{x}) = f(\vec{x})$, can be solved as

$$\begin{aligned} &\int G(\vec{x}, \vec{x}_0)\Delta\psi(\vec{x})\mathrm{d}^d\vec{x} \equiv \int \psi(\vec{x})\Delta G(\vec{x}, \vec{x}_0)\mathrm{d}^d\vec{x} \\ &= \int G(\vec{x}, \vec{x}_0) f(\vec{x})\mathrm{d}^d\vec{x} \end{aligned} \tag{A.8}$$

so that, the Poisson equation solution is

$$\int \psi(\vec{x})\delta(\vec{x} - \vec{x}_0)\mathrm{d}^d\vec{x} = \int G(\vec{x}, \vec{x}_0) f(\vec{x})\mathrm{d}^d\vec{x} \tag{A.9}$$

$$\psi(\vec{x}) = \int G(\vec{x}_0, \vec{x}) f(\vec{x}_0)\mathrm{d}^d\vec{x}_0 \tag{A.10}$$

where the property $G(\vec{x}_0, \vec{x}) = G(\vec{x}, \vec{x}_0)$ has been used. And because $f(\vec{x}_0)$ usually is a function of the mass density written as the Dirac delta function, the Poisson equation solution is just the product of $G(\vec{x}, \vec{x}_0)$ with the constants of $f(\vec{x})$.

ANNEX A – Published paper on the subject

In this last part of the dissertation, the author's accepted manuscript of the published paper on the subject, named "Entropy production and Vlasov equation for self-gravitating systems" is attached. In there, it is to be found all of the development that leads to the conclusion.

Entropy production and Vlasov equation for self-gravitating systems

Calvin A. Fracassi Farias, Renato Pakter, and Yan Levin*
Instituto de Física, Universidade Federal do Rio Grande do Sul.

(Dated: November 21, 2018)

The evolution of a self-gravitating system to a non-equilibrium steady state occurs through a process of violent relaxation. In the thermodynamic limit the dynamics of a many body system should be governed by the Vlasov equation. Recently, however, a question was raised regarding the validity of Vlasov equation during the process or violent relaxation. In this paper we will explore the entropy production during the relaxation process using N-body molecular dynamics simulations. We will show that the entropy production time grows as N^α, with $\alpha > 0$ and in the limit $N \to \infty$, entropy will remain constant, consistent with the Vlasov equation. Furthermore, we will show that the mean field dynamics constructed on the basis of the Vlasov equation is in excellent agreement with the full molecular dynamics simulations, justifying the applicability of Vlasov equation during the violent relaxation phase of evolution.

I. INTRODUCTION

Long range (LR) interacting systems are distinct from systems which interact through short-range forces. While the latter achieve thermodynamic equilibrium irrespective of the initial condition, the final state to which LR interacting systems evolve depends strongly on the initial condition. Self-gravitating systems (SGS) are paradigmatic of systems with LR interactions. It is known that SGS reach their *quasi*-stationary states (qSS) by process of violent relaxation [1–4], in which some particles gain energy from the rest of the system through parametric resonances [4–7]. The process usually results in a violent relaxation to a qSS. It has been well accepted that in the thermodynamic limit the dynamical evolution of the one-particle distribution function (DF) should be described by the Vlasov equation. Recently, however, this belief has been questioned [8] based on the investigation of the entropy production during the process of violent relaxation. The authors of the reference [8] observed for many different initial conditions a strong entropy increase during the process of violent relaxation which can not be accounted for in the framework of Vlasov equation, which requires that entropy must remain constant during the dynamical evolution.

For a d-dimensional system of particles interacting through a LR force, most of the contribution to the force acting on a given particle comes from the interaction with distant particles. In the thermodynamic limit, when $N \to \infty$, the pairwise interaction with the nearby particles can be neglected and the total force acting on a particle can be calculated using the mean-field potential. The probability DF of a many particle system can then be written in terms of a product on one-particle DFs

$$f^{(N)}(\{\mathbf{w}\},t) = \prod_{i=1}^{N} f(\mathbf{w}_i,t) \tag{1}$$

which satisfy the collisionless Boltzmann, or Vlasov, equation [9–12],

$$\left(\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m}\cdot\nabla_{\mathrm{q}} - \nabla_{\mathrm{q}}\psi\cdot\nabla_{\mathrm{p}}\right) f(\mathbf{q},\mathbf{p},t) = 0 \tag{2}$$

where $\mathbf{q}$ and $\mathbf{p}$ are respectively the generalized coordinate and momentum, m is the particle's mass, f is the one-particle DF, and $\psi \equiv \psi(\mathbf{q},t)$ is the mean-field interaction potential. The advantage of working with LR systems is that the $2dN$-dimensional phase space of systems with short range interactions effectively collapses to a $2d$-dimensional μ phase space which can be more easily visualized and studied. Since Vlasov equation is time-reversible, its microscopic dynamics needs to be reconciled with the Clausius second law of thermodynamics. In fact, Boltzmann solved a similar problem for systems with short-range interacts by postulating that the entropy is a logarithm of the total number of microstates compatible with a given macrostate, irrespective of whether these microstates can be reached from a given initial condition or not [13]. On the other hand, the Gibbs entropy,

$$S_G = -k_B \int f^{(N)}(\{\mathbf{w}\},t)\ln f^{(N)}(\{\mathbf{w}\},t)\,\mathrm{d}^N\mathbf{w} \tag{3}$$

where the integral is performed over all the phase space and $\mathrm{d}^N\mathbf{w} \equiv \{\mathrm{d}\mathbf{w}_1,...,\mathrm{d}\mathbf{w}_N\}$, is conserved by the Liouville/Vlasov dynamics. Since the Liouville and Vlasov equations can be written as $\mathrm{d}f^{(N)}/\mathrm{d}t = 0$, the probability DF evolves as an incompressible fluid over the phase space, and any local integral of DF is conserved by the flow [14]. The evolution of the probability DF never stops, continuing on smaller and smaller length scales. Therefore, only on a coarse-grained scale it is possible to say that a system evolves to a stationary state and that the entropy "increases" [15–17]. This behavior is illustrated in Figure 1, which shows the evolution of μ phase space of a one dimensional system of non-interacting particles confined in a box with periodic boundary conditions, starting from an initial waterbag distribution.

* levin@if.ufrgs.br

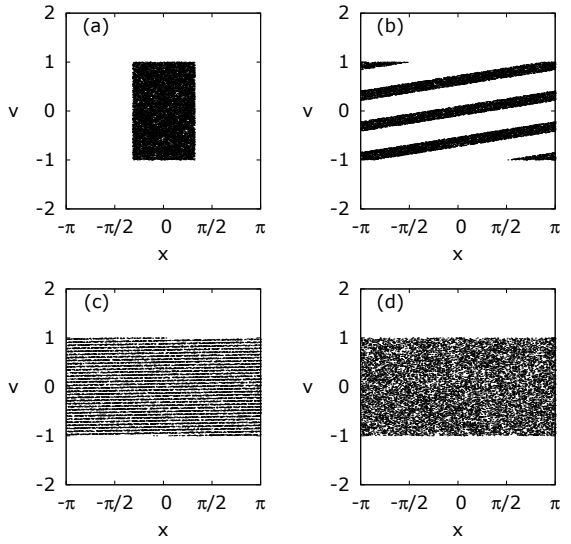

FIG. 1. Snapshots of the phase space of a one dimensional system of $N = 131072$ non-interacting particles with periodic boundary conditions: the fine-grained probability DF evolves through the process of filamentation and phase-mixing. At some point the resolution is no longer sufficient to perceive dynamics, and the system appears to be stationary. The times of plots are: (a) $t = 0$, (b) $t = 10$, (c) $t = 100$ and (d) $t = 1000$.

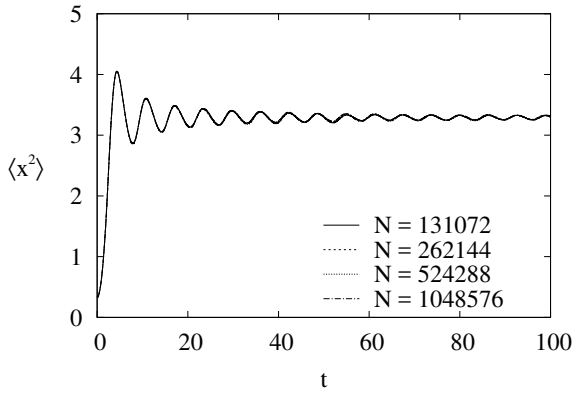

FIG. 2. Violent relaxation of the second moment of the particle distribution, from initial to final stationary state. Note that for sufficiently large system sizes, the relaxation time is independent of the number of particles in the system.

Clearly for this non-interacting system there is no doubt of validity of Vlasov equation. The initial distribution is seen to evolve through a process of filamentation and phase space mixing. During the dynamics, the initial distribution stretches and folds over an extended volume of the μ phase space, (Figures 1b and 1c). On a fine-grained scale the phase space volume occupied by the particles remains constant. On a coarse-grained scale, however, it appears that the evolution reaches a stationary state (Figure 1d), in which phase space volume occupied by the particles is larger than the volume of the original distribution. In Figure 2 we also show the "violent relaxation" of the second moment of the particle distribution function as it evolves to equilibrium from $t = 0$. Note that the violent relaxation time does not depend on the number of particles, for sufficiently large system sizes, as was also observed for systems of interacting particles [18].

For LR systems the entropy can be rewritten in terms of one-particle distribution function, Eq. 1, and can be calculated using an entropy estimator [19–21]

$$\bar{s}_G k_B^{-1} = \frac{1}{N}\sum_{i=1}^{N} \ln\left(N r_i^{2d} V_{2d}\right) + \gamma \qquad (4)$$

where r_i is the distance in the μ phase space from particle i to its nearest neighbor, V_{2d} is the volume of a hypersphere of $2d$ dimensions, γ is the Euler-Mascheroni constant, k_B is the Boltzmann constant and N the number of particles. The quantity $\bar{s}_G k_B^{-1}$ is, in fact, a coarse-grained estimator of Shannon entropy per particle, which is distinguished from Gibbs entropy by the constant k_B. This facilitates comparison with [8], which also estimates Shannon entropy.

Figure 3a shows the entropy production (per particle) for a one dimensional non-interacting particle system of Fig. (1) with various number of particles N. As expected, in spite of the system dynamics being governed by Vlasov equation, the coarse-grained entropy is not to conserved. On the other hand if the time is rescaled with $N^{1/2}$ we see that the entropy productions curves all collapse onto a universal curve. Figures 4a and 5a show the entropy production for a system of non-interacting particles in two and three dimensions, respectively. A perfect data collapse is again found, if time is rescaled with N^{α}, where the exponent α is $\alpha = 1/2d$. Therefore, the entropy production time for non-interacting particles in d dimensions scales as $\tau_\times \sim N^{1/2d}$, and diverges in the thermodynamic limit, implying that the fine-grained entropy will remain constant, as is required by the Vlasov equation. The fact that the coarse-grained entropy increases with time, does not invalidate in any sense Vlasov equation which is exact for these no-interacting systems. Indeed, as we already saw in Figure 2 a calculation of observables such as $\langle x^2\rangle$ can be equally well performed using either a fine-grained distribution function or a coarse-grained one, in spite of the fact that coarse-grained entropy increases with time.

In the remaining of this paper the entropy production of SGS will be investigated. The objective is to verify that in the thermodynamic limit, Vlasov equation does describe the dynamical evolution of a self-gravitating system, including the violent relaxation phase. The paper is organized as follow: Sec. II gives a brief review of one and two dimensional SGS; Sec. III focuses on three dimensional SGS, the entropy production, and others observables; Sec. IV discuses the results and presents the

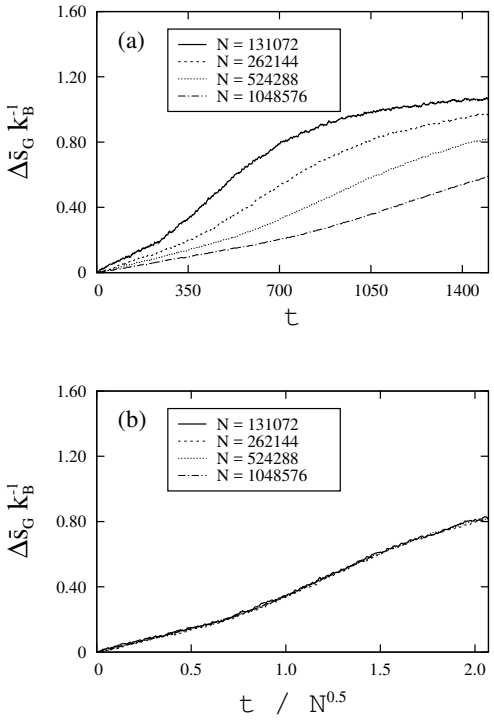

FIG. 3. (a) Entropy production per particle in a one dimensional system of non-interacting particles of Figure 1; and (b) is the data collapse. For this non-interacting system the collapse appears to be exact, showing that the entropy production time scales with N^α, $\alpha = 0.5$. Therefore, in the limit $N \to \infty$, the entropy will remain constant, as is required by Vlasov equation.

conclusions.

II. ENTROPY PRODUCTION IN SELF-GRAVITATING SYSTEMS

The difficulty with studying three dimensional self-gravitating systems is that they are intrinsically unstable. Since the Newton gravitational potential is unbounded from below and is bounded from above, some particles can gain enough energy from the rest of the system to completely escape its gravitational attraction [16, 22]. This makes it very difficult to perform any kind of statistical analysis of the 3d gravitational clusters, except for very special virial initial conditions, studied in Section III [16]. Therefore, most of our analysis will be performed using one and two dimensional self-gravitating systems, for which the gravitational potential is unbounded from above, preventing particle evaporation. The SGS MD simulations were performed in CUDA/C++ language, at constant energy, with rescaled dimensionless variables, i.e., the equivalent of considering the system's total mass and the gravitational constant equals to unity. For one dimensional SGS, the numerical method applied was a fourth order implementation of the symmetric B3A method of Runge-Kutta-Nystroem with six stages from the C++ BOOST/odeint library [23]. The error in energy was kept smaller than 2.0×10^{-7} %. For two and three dimensional SGS, it was applied the CUDA algorithm of clustering tiles into thread blocks [24] with the improvement of loop unrolling. The numerical method was a fourth order symplectic integrator from [25] and the error in the energy was kept smaller than 1.0×10^{-3} %.

A. Virial condition

To study entropy production, all the MD simulations start with initial waterbag distribution which satisfies the virial condition, $\mathcal{R}_0 = 2K/(2-d)U = 1.0$, where K is the initial kinetic energy, U is the gravitational potential energy, and d is the space dimension. Such distributions are expected to be as close to stationary as possible, without being an exact solution of Vlasov equation [11, 26],

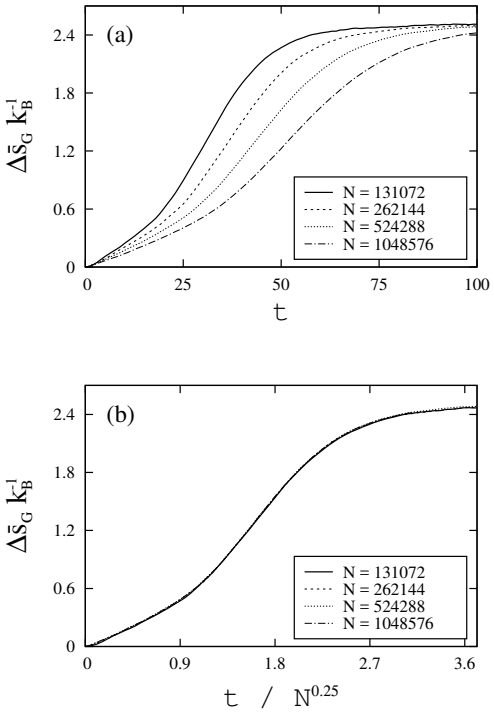

FIG. 4. (a) Entropy production in a two dimensional system of non-interacting particles in a box with periodic boundary conditions; and (b) is the data collapse. Like Figure 3, the collapse appears to be exact, showing that the entropy production time scales with N^α, $\alpha = 1/4$. Therefore, in the limit $N \to \infty$, the entropy will remain constant, as is required by Vlasov equation.

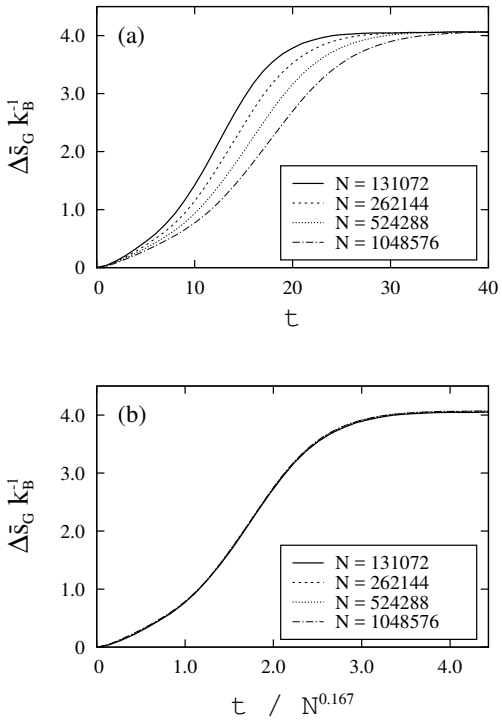

FIG. 5. (a) Entropy production for a three dimensional system of non-interacting particles inside a box with periodic boundary conditions; and (b) is the data collapse. If the entropy production time is scaled with N^α, $\alpha = 1/6$ a perfect data collapse is observed.

and should rapidly relax to the qSS [27]. This allows us to reduce the loss of resolution due to numerical imprecision resulting from strong oscillations and diminishes the system size necessary to observe the finite size scaling of the entropy production time. The initial particle distribution has the form,

$$f(\mathbf{q},\mathbf{p}) = \eta\,\Theta(\mathrm{q}_M - |\mathbf{q}|)\,\Theta(\mathrm{p}_M - |\mathbf{p}|) \qquad (5)$$

where q_M and p_M are, respectively, the boundary limits of coordinates and momenta in the μ phase space, η is a constant of normalization whose value in 1d is $\eta = (4\mathrm{q}_M\mathrm{p}_M)^{-1}$; in 2d is $\eta = (\pi\mathrm{q}_M\mathrm{p}_M)^{-2}$; in 3d $\eta = (4\pi/3)^{-2}(\mathrm{q}_M\mathrm{p}_M)^{-3}$, and Θ is the Heaviside function. In this paper, the distances will be measured in units of q_M, mass of particles in the units of total mass M, and the time in the units of dynamical time τ_d, so as to make equations of motion dimensionless. This is equivalent to setting $\mathrm{q}_M = 1.0$, total mass to $M = 1$, and the Newton gravitational constant to $G = 1$. The energy per particle at time $t = 0$ is then $\epsilon_0 = \frac{p_M^2}{6} + \frac{1}{3}$ in one dimension, $\epsilon_0 = \frac{p_M^2}{4} - \frac{1}{8}$ in two dimensions, and $\epsilon_0 = \frac{3p_M^2}{10} - \frac{3}{5}$ in three dimensions, and the virial condition reduces to $\mathrm{p}_M = 1$ for all d, see [6, 28].

B. Gravitation in one dimension

One dimensional SGS consists of point particles of mass m moving along the x-axis, free to pass through one another. The reduced Poisson equation assumes the following form

$$\nabla^2\psi(x,t) = 2\,\rho(x,t) \qquad (6)$$

where $\psi(x,t)$ is the reduced gravitational potential and $\rho(x,t)$ is the reduced mass density. The reduced variables are: the dynamical time scale $\tau_d = \sqrt{2\pi G\rho_0}$ where G is the Newton gravitational constant; $\rho_0 = M/L_0$ is the mass density; L_0 is an arbitrary length scale which we take to be $q_M = 1$; $M = mN$ is the system's total mass, which we set to 1; and $V_0 = \sqrt{2\pi GML_0}$ is a velocity scale. The mass density of the i'th particle is $\rho(x,x_i) = m\delta(x - x_i)$. The reduced gravitational potential at position x produced by N particles is

$$\psi(x,t) = \frac{1}{N}\sum_i^N |x - x_i| \qquad (7)$$

Note that the binary interaction between any two particles vanishes as $1/N^2$. In the thermodynamic limit, therefore, the dynamics of a 1d SGS should be governed by the Vlasov equation. The evolution of the particle distribution over the reduced μ phase space is shown in Figure 6. Once again we see the characteristic filamentation structure, which results in an effective gain of the phase space volume accessible to the particles, in the coarse-grained sense. The evolution of the coarse-grained entropy is shown in Figure 7a for different system

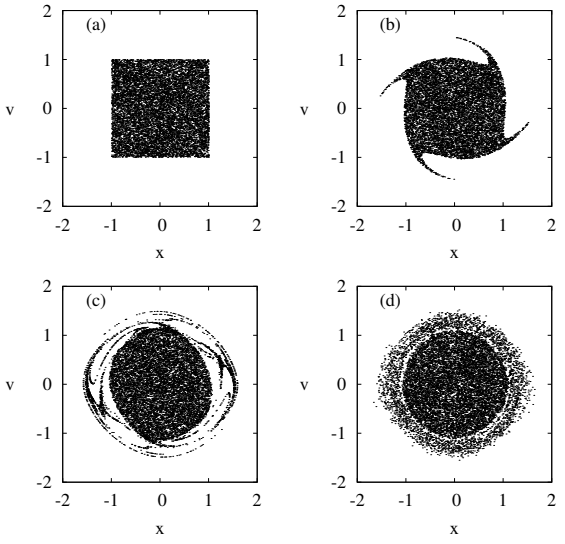

FIG. 6. Snapshots of the phase space of a 1d self-gravitating system of section II B. $N = 131072$ and $R_0 = 1.0$. The times are: (a) $t = 0$, (b) $t = 10.0$, (c) $t = 100.0$ and (d) $t = 1000.0$.

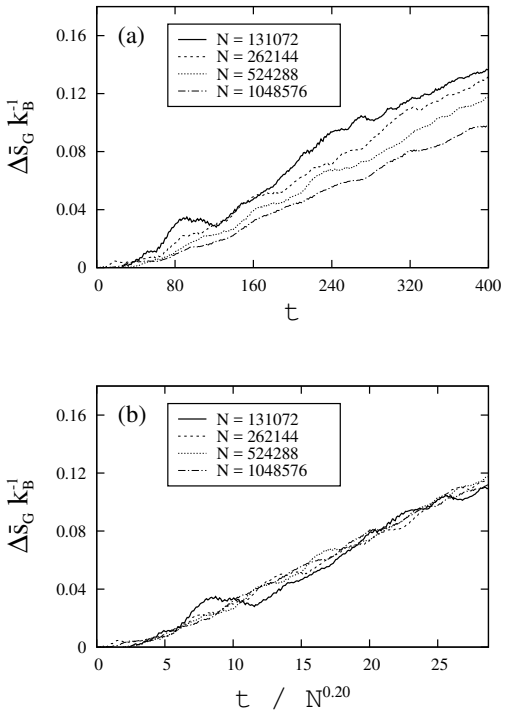

FIG. 7. (a) Entropy production for a 1d self-gravitating system of section II B; and (b) is the time rescale. The early stages evolution indicate that the entropy production time grows as N^α, $\alpha = 0.20$, therefore taking an infinite amount of time when $N \to \infty$. Different from non-interacting particles, scaling with N appears to hold only at early times.

sizes. In Figure 7b we show that if the time is rescaled with N^α, with $\alpha = 0.2$, we can collapse the entropy production onto a single curve. This implies that in the thermodynamic limit $N \to \infty$, the time scale for the entropy production will diverge, and the entropy will remain constant consistent with the Vlasov dynamics. This is similar to what was found for non-interacting particles, however, in the case of SGS the exponent α is smaller, implying that for systems with not too many particles the loss of fine-grained resolution happens very fast, leading to rapid entropy production.

C. Gravitation in two dimensions

For a two dimensional SGS, the dimensionless Poisson equation is

$$\nabla^2\psi(\mathbf{r},t) = 2\pi\,\rho(\mathbf{r},t) \tag{8}$$

where $\psi(\mathbf{r},t)$ is the two dimensional gravitational potential and $\rho(\mathbf{r},t)$ is the mass density. The dynamical time scale is $\tau_d = L_0/\sqrt{2GM}$, where once again, G is the Newton gravitational constant; M is the system's total mass, which we set to 1; and L_0 is an arbitrary length scale which we set to $q_M = 1$. The mass density $\rho(\mathbf{r},t)$ is obtained by integrating the probability DF over the momentum. For N particle system the gravitational potential at position $\mathbf{r}$ is given by the solution of Poisson equation

$$\psi(\mathbf{r},t) = \frac{1}{N}\sum_i^N \ln|\mathbf{r}-\mathbf{r}_i|\,. \tag{9}$$

The evolution of the configuration space is shown in Figures 8 and of coarse-grained entropy and its rescaled form are shown in Figures 9a and 9b. Once again we obtain a reasonable data collapse for early times, with the exponent $\alpha = 0.15$.

D. Entropy production in 3d

It is very difficult to study entropy production in 3d SGS because of a very rapid loss of resolution, which requires a very large number of particles to detect the scaling structure of the entropy production time. Nevertheless, in Fig. 10a we see that if the dynamical time is rescaled by N^α, the early time region of the entropy production curves collapses onto a single curve, showing that, at least in the early stages of the simulation, i.e., during the period of violent relaxation, there is a reasonably good scaling of entropy with the number of particles. The exponent $\alpha \approx 0.1$ for 3d systems, however, is lower than for 1d and 2d SGS. Nevertheless, in

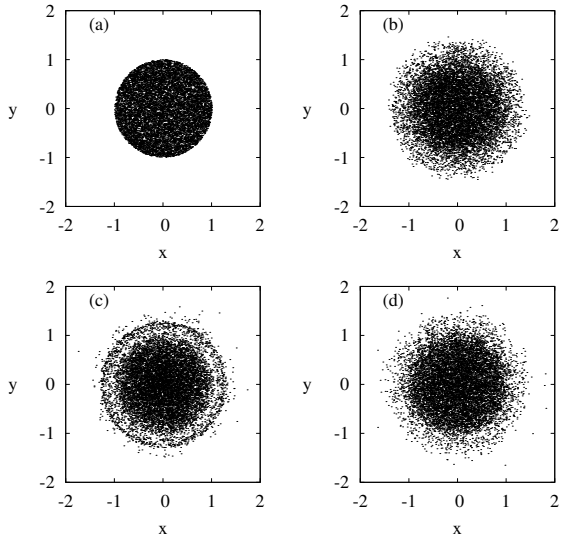

FIG. 8. Snapshots of the configuration space of a 2d self-gravitating system of section II C. $N = 131072$ and $R_0 = 1.0$. The times are: (a) $t = 0$, (b) $t = 10.0$, (c) $t = 32.0$ and (d) $t = 100.0$.

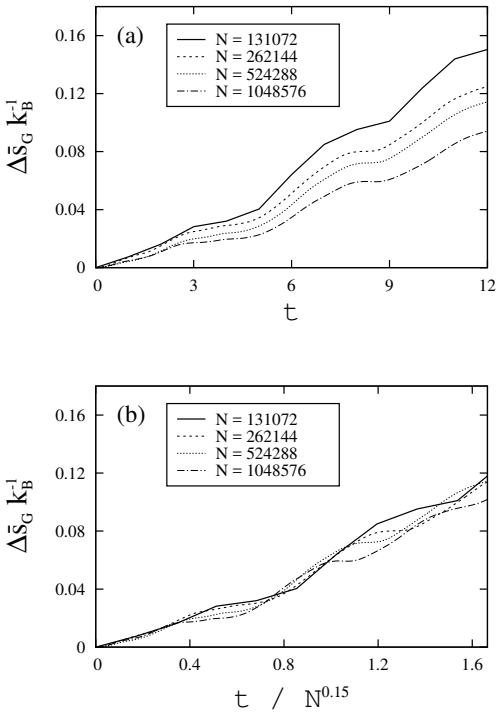

FIG. 9. (a) Entropy production in a 2d self-gravitating system with N particles, section II C; and (b) if the time is rescaled with N^α, $\alpha = 0.15$, the curves can be reasonably collapsed to a single curve for short times. In the thermodynamic limit, therefore, the entropy production will be zero, consistent with the Vlasov equation.

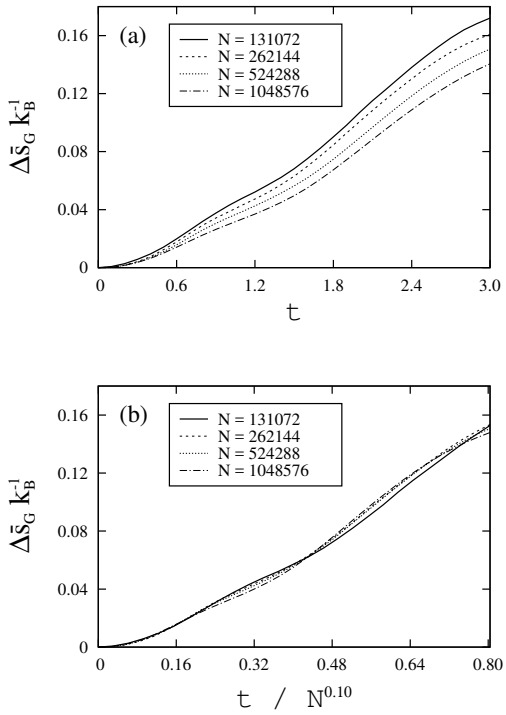

FIG. 10. (a) Entropy production in a three dimensional self-gravitating system and (b) its dynamical time rescale, $\alpha = 0.10$.

the limit $N \to \infty$ the entropy production will require infinite amount time, consistent with the Vlasov dynamics.

III. 3D SGS: EVOLUTION OF OBSERVABLES

In view of the very fast loss of resolution and rapid entropy production in 3d SGS, the authors of Ref. [8] argued that Vlasov equation is not appropriate to describe the violent relaxation of these systems. Based on our finite size analysis, however, we see that this conclusion is incorrect, since in the infinite N limit, the time for the entropy production diverges, and the fine-grained entropy will remain constant as is required by the Vlasov equation. Nevertheless, one might question whether for systems with large, but finite N, Vlasov dynamics can provide an accurate description of the temporal evolution of 3d SGS and, in particular their relaxation to the qSS. Unfortunately, it is very difficult to explicitly solve the Vlasov equation for 3d SGS, however, we can explore the validity of the assumptions underlying Vlasov equation by performing simulations in which each particle interacts with the mean gravitational potential produced by all other masses. Such simulations will eliminates the correlational (or collisional) effects and provides an indirect way of solving the Vlasov equation. We shall call such simulations "collisionless MD". For spherically symmetric particle distributions, the mean-field can be easily calculated by replacing each particle by a spinning spherical shell of radius and angular momentum same as the real particle. For the shell system, the force is purely radial, so that the angular momentum of each shell is conserved. The dynamics of each shell then reduces to its radial coordinate, and the force on each shell can be easily calculated using the Gauss law [6]. Clearly if both collisional (simulation which is based on explicit binary interaction between the particles) and collisionless simulations will result in the same dynamical evolution of observables of a system, it will provide a very clear indication of validity of Vlasov dynamics for systems with large but finite number of particles, in spite of the entropy production.

One particularly relevant quantity to study in MD simulations is the evolution of the "envelope" of the particle distribution defined in terms of the root-mean-squared

(rms) of the particle coordinates [6]

$$r_e = \sqrt{\frac{5}{3}\langle \mathbf{r}\cdot\mathbf{r}\rangle}\,. \tag{10}$$

The factor of 5/3 is included so that at t_0, the envelope is precisely q_M. The other interesting quantity to consider is the average kinetic energy of the particles. We will compare the evolution of both the envelope and the kinetic energy using both collisional and collisionless MD simulations for initial distribution with virial number $R_0 = 0.5$ and a number of particles $N = 131072$. This virial number was chosen to force the system to undergo strong oscillations, rapid entropy production, while preserving the spherical symmetry of the initial distribution [28]. Figure 11 shows the time evolution of the envelope, while Figure 12 shows the evolution of the kinetic energy per particle. We see that both collisional and collisionless simulations lead to almost identical evolution of both observables, in spite of a rapid entropy production. A small deviation in the final qSS, is due to slightly different initial conditions, due to random number generator.

Therefore, we conclude that for 3d SGS the relevant observables can be equally well calculated using either the exact fine-grained distribution $f(\mathbf{p},\mathbf{q},t)$ obtained from the solution of the Vlasov equation, or an effective coarse-grained distribution in which the $f(\mathbf{p},\mathbf{q})$ is coarse-grained over some microscopic length scale,

$$f_{cg}(\mathbf{q},\mathbf{p},t) = \frac{1}{(\Delta p\Delta q)^d}\int_{\Delta p,\Delta q} f(\mathbf{q}',\mathbf{p}',t)\,\mathrm{d}\mathbf{q}'\mathrm{d}\mathbf{p}'\,. \tag{11}$$

While the entropy calculated using the fine-grained distribution is strictly conserved, the entropy calculated using the coarse-grained distribution will grow and saturate

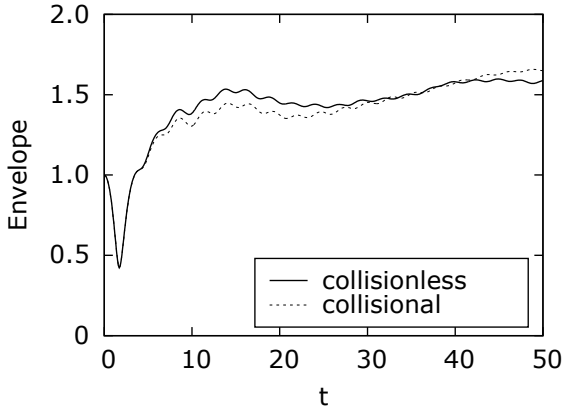

FIG. 11. Envelope of the particle distribution. Both collisional and collisionless simulations follow identical dynamical evolution, implying that Vlasov equation accounts perfectly well for the violent relaxation phase, $N = 131072$ and $R_0 = 0.5$.

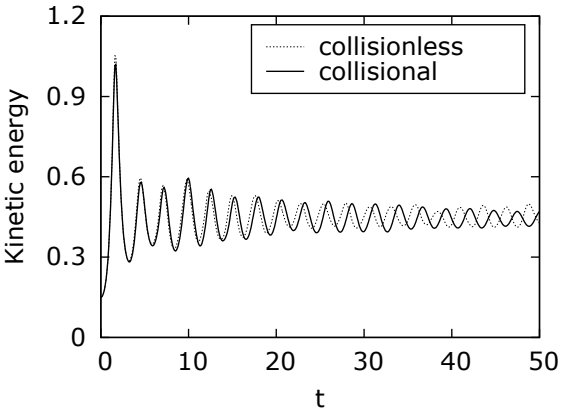

FIG. 12. Kinetic energy per particle. Both collisional and collisionless simulations have almost identical dynamics. A small difference between the curves is due to slightly different initial conditions in the two simulations verified using different seeds for the pseudo-random number generator in the MD simulations. $N = 131072$ and $R_0 = 0.5$.

as is observed in the collisional MD simulations. The role of "coarse-graining" in the MD simulations comes from the residual correlations between the masses and the numerical error. Nevertheless, the agreement between collisionless and collisional simulations implies that the average of observables calculated using either fine-grained or coarse-grained distributions are identical in the thermodynamic limit,

$$\langle O(t)\rangle = \int O(\mathbf{q},\mathbf{p}) f(\mathbf{q},\mathbf{p},t)\mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p} = \int O(\mathbf{q},\mathbf{p}) f_{cg}(\mathbf{q},\mathbf{p},t)\mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p}. \tag{12}$$

The fine-grained distribution function obtained from the solution of the Vlasov equation can, therefore, be used to account for the violent relaxation in SGS with large but finite number of particles.

IV. CONCLUSIONS

We have explored the entropy production in SGS in one, two, and three dimensions. We find that the entropy production time scales as $N \to \infty$, with $\alpha = 0.20$, 0.15, and 0.1, respectively. It is not clear what precisely determines the value of the exponent α, it decreases with the dimensionality of configuration space and may also be related to the Lyapunov spectrum. [29] The loss of resolution happens very fast for 3d SGS. Contrary to the suggestion of reference [8], this however does not imply a failure of Vlasov equation to describe the process of violent relaxation. Indeed Vlasov dynamics is entropy conserving. This, however, is only valid in the limit $N \to \infty$. For finite systems, therefore, there will be a rapid loss of

resolution which can be associated with the entropy production. Indeed within the Vlasov formalism, we can define a coarse-graining procedure, associated with the loss of resolution, which will also result in the growth of entropy. Such coarse-graining is very similar to the Boltzmann definition of entropy which counts the total number of microstates compatible with a given macrostate, irrespective of whether these microstates can be reached from a given initial condition or not. Comparing the collisionless and collisional MD simulations we saw that the dynamics of observables in systems with relatively small number of masses N is equally well described by either of the two simulation methods. The collisionless simulations are effectively a solution of the Vlasov equation, while collisional simulations include residual correlations which lead to the entropy production in a finite N system, the equivalence of the two methods implies that the evolution of the observables in SGS can be equally well calculated either using exact fine-grained distribution function or using its coarse-grained version. The same conclusion was also reached by analyzing non-interacting particle systems for which Vlasov equation is exact. We thus conclude that conservation of fine-grained entropy by Vlasov equation does not invalidate it in any way from providing an accurate description of violent relaxation dynamics that leads to quasi stationary states with increased coarse-grained entropy.

ACKNOWLEDGMENTS

This work was partially supported by the CNPq, National Institute of Science and Technology Complex Fluids INCT-FCx, and by the US-AFOSR under the grant FA9550-16-1-0280.

[1] D. Lynden-Bell. Statistical mechanics of violent relaxation in stellar systems. *Monthly Notices of the Royal Astronomical Society*, 136(1):101–121, may 1967.

[2] Alessandro Campa, Thierry Dauxois, and Stefano Ruffo. Statistical mechanics and dynamics of solvable models with long-range interactions. *Physics Reports*, 480(3-6):57–159, sep 2009.

[3] Ana C. Ribeiro-Teixeira, Fernanda P. C. Benetti, Renato Pakter, and Yan Levin. Ergodicity breaking and quasistationary states in systems with long-range interactions. *Physical Review E*, 89(2), feb 2014.

[4] Fernanda P. C. Benetti, Ana C. Ribeiro-Teixeira, Renato Pakter, and Yan Levin. Nonequilibrium stationary states of 3d self-gravitating systems. *Physical Review Letters*, 113(10), sep 2014.

[5] Fernanda P. da C. Benetti, Tarcísio N. Teles, Renato Pakter, and Yan Levin. Ergodicity breaking and parametric resonances in systems with long-range interactions. *Physical Review Letters*, 108(14), apr 2012.

[6] Yan Levin, Renato Pakter, Felipe B. Rizzato, Tarcísio N. Teles, and Fernanda P.C. Benetti. Nonequilibrium statistical mechanics of systems with long-range interactions. *Physics Reports*, 535(1):1–60, feb 2014.

[7] Robert L. Gluckstern. Analytic model for halo formation in high current ion linacs. *Physical Review Letters*, 73(9):1247–1250, aug 1994.

[8] Leandro Beraldo e Silva, Walter de Siqueira Pedra, Laerte Sodré, Eder L. D. Perico, and Marcos Lima. The arrow of time in the collapse of collisionless self-gravitating systems: Non-validity of the vlasov–poisson equation during violent relaxation. *The Astrophysical Journal*, 846(2):125, sep 2017.

[9] James Binney and Scott Tremaine. *Galactic Dynamics*. Princeton Series in Astrophysics. Princeton University Press, 2nd edition, 2008.

[10] Herbert Spohn. *Large Scale Dynamics of Interacting Particles*. Springer Berlin Heidelberg, 1991.

[11] W. Braun and K. Hepp. The vlasov dynamics and its fluctuations in the 1/n limit of interacting classical particles. *Communications in Mathematical Physics*, 56(2):101–113, jun 1977.

[12] A. Gabrielli and M. Joyce. Gravitational force in an infinite one-dimensional poisson distribution. *Physical Review E*, 81(2), feb 2010.

[13] Joel L. Lebowitz. Boltzmann's entropy and time's arrow. *Physics Today*, 46(9):32–38, sep 1993.

[14] P. H. Chavanis and F. Bouchet. On the coarse-grained evolution of collisionless stellar systems. *Astronomy & Astrophysics*, 430(3):771–778, jan 2005.

[15] Scott Tremaine, Michel Hénon, and Donald Lynden-Bell. H-functions and mixing in violent relaxation. *Monthly Notices of the Royal Astronomical Society*, 219(2):285–297, mar 1986.

[16] Yan Levin, Renato Pakter, and Felipe B. Rizzato. Collisionless relaxation in gravitational systems: From violent relaxation to gravothermal collapse. *Physical Review E*, 78(2), aug 2008.

[17] Renato Pakter and Yan Levin. Entropy production in systems with long range interactions. *Journal of Statistical Mechanics: Theory and Experiment*, 2017(4):044001, apr 2017.

[18] Julien Barré, Freddy Bouchet, Thierry Dauxois, Stefano Ruffo, and Yoshiyuki Y. Yamaguchi. The vlasov equation and the hamiltonian mean-field model. *Physica A: Statistical Mechanics and its Applications*, 365(1):177–183, jun 2006.

[19] R. L. Dobrushin. A simplified method of experimentally evaluating the entropy of a stationary sequence. *Theory of Probability & Its Applications*, 3(4):428–430, jan 1958.

[20] N. N. Leonenko L. F. Kozachenko. Sample estimate of the entropy of a random vector. *Probl. Peredachi Inf.*, 23:9–16, 1987.

[21] Harshinder Singh, Neeraj Misra, Vladimir Hnizdo, Adam Fedorowicz, and Eugene Demchuk. Nearest neighbor estimates of entropy. *American Journal of Mathematical and Management Sciences*, 23(3-4):301–321, feb 2003.

[22] T. Padmanabhan. Statistical mechanics of gravitating systems. *Physics Reports*, 188(5):285–362, apr 1990.

[23] Karsten Ahnert, Mario Mulansky, Theodore E. Simos, George Psihoyios, Ch. Tsitouras, and Zacharias Anas-

tassi. Odeint – solving ordinary differential equations in C++. AIP, 2011.

[24] Lars Nyland, M Harris, and Jan Prins. Fast n-body simulation with cuda, 01 2009.

[25] Haruo Yoshida. Construction of higher order symplectic integrators. *Physics Letters A*, 150(5-7):262–268, nov 1990.

[26] Tarcísio N Teles, Yan Levin, Renato Pakter, and Felipe B Rizzato. Statistical mechanics of unbound two-dimensional self-gravitating systems. *Journal of Statistical Mechanics: Theory and Experiment*, 2010(05):P05007, may 2010.

[27] Yoshiyuki Y. Yamaguchi and Shun Ogawa. Conditions for predicting quasistationary states by rearrangement formula. *Physical Review E*, 92(4), oct 2015.

[28] Renato Pakter, Bruno Marcos, and Yan Levin. Symmetry breaking ind-dimensional self-gravitating systems. *Physical Review Letters*, 111(23), dec 2013.

[29] Felipe L. Antunes, Fernanda P. C. Benetti, Renato Pakter, and Yan Levin. Chaos and relaxation to equilibrium in systems with long-range interactions. *Physical Review E*, 92(5), nov 2015.