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Abstract Systems of particles with long range interactions present two phases in their evolution: first, the formation of Quasi-Stationary states (such as galaxies) in a process called *violent relaxation* and, second, the much slower relaxation towards thermal equilibrium, in a process called *collisional relaxation*. In this contribution we focus on the last process and we present the first exact calculations of diffusion coefficients performed for non-homogeneous configurations.

1 Introduction

In Statistical Physics, we call systems with long range interactions those in which all the particles interact significantly. If they interact through a pair potential, this potential decreases with distance slower than $u(r \to \infty) \sim 1/r^d$, where d is the dimension of space. There are many such systems in nature: self-gravitating systems such as galaxies, globular clusters or the large scale structure of the Universe, cold trapped atoms, colloids at surface interfaces, active particles, etc. The long range nature of these systems results in the apparition of "exotic" collective effects compared with short range systems. They have different manifestations: formation of Quasi-Stationary

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states via the mechanism of "violent relaxation" (such as a galaxy, which is a quasi-stable structure but completely out of thermodynamic equilibrium), "collisional" slow relaxation towards thermodynamic equilibrium in a time scaling with the number of particles, the possibility of negative specific heat at thermodynamic equilibrium, etc. In this contribution we will focus on the process of "collisional" slow relaxation of a long range system towards thermodynamic equilibrium. An example of such a process is the evaporation of stars in a galaxy or a globular cluster. This process is driven by the finiteness of the number of particles, which causes fluctuations ("noise") in the (mean-field) potential generated by the system. The effect of these fluctuations can be modeled, as it is usually done in Statistical Physics, through a Fokker-Planck or Langevin equation. There are, however, two important difficulties: *(i)* the noise has to be modeled very precisely taking into account, accurately, the orbit of each particle and *(ii)* the motion of the particles perturbs, in turn, the mean-field potential giving rise to collective effects. In general this results in very difficult perturbative calculations. We will present the first (to our knowledge) exact calculations of diffusion coefficients for spatially inhomogeneous systems, performed for a simplified one-dimensional long range model, the Hamiltonian Mean Field model (HMF). The material presented in this contribution can be found, in an extended format, in [1].

2 Kinetic theory

The natural framework to describe these kinds of out-of-equilibrium systems, composed by a large number of particles N, is kinetic theory. We start from the discrete distribution function $f_d(\mathbf{r},\mathbf{v},t)$, which contains all the information of the state of the system at a given time t,

$$f_d(\mathbf{r},\mathbf{v},t) = m\sum_{i=1}^{N}\delta[\mathbf{r}-\mathbf{r}_i(t)]\delta[\mathbf{v}-\mathbf{v}_i(t)]. \tag{1}$$

This function has too much information to study the system. Averaging over initial conditions (denoted by the operator $\langle\ldots\rangle$) we define the smoothed distribution function $f(\mathbf{r},\mathbf{v},t) = \langle f_d(\mathbf{r},\mathbf{v},t)\rangle$, which is the equivalent of taking the limit $N\to\infty$ for a single realization. The fluctuations are defined with $f_d(\mathbf{r},\mathbf{v},t) = f(\mathbf{r},\mathbf{v},t) + \delta f(\mathbf{r},\mathbf{v},t)$. It is possible to show that the smoothed distribution function obeys the Vlasov-Boltzmann equation [1]:

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}} - \frac{\partial \phi}{\partial \mathbf{r}}\cdot\frac{\partial f}{\partial \mathbf{v}} = \frac{\partial}{\partial \mathbf{v}}\cdot\langle \delta f\frac{\partial \delta\phi}{\partial \mathbf{r}}\rangle, \tag{2}$$

The above equation gives the evolution of the smooth distribution due to correlation between its own fluctuations and the fluctuation of the smooth potential $\phi(\mathbf{r},t)$, determined by $\phi_d(\mathbf{r},t) = \phi(\mathbf{r},t) + \delta\phi(\mathbf{r},t)$, where

$$\phi(\mathbf{r},t) = \int u(|\mathbf{r}-\mathbf{r}'|) f(\mathbf{r}',\mathbf{v}',t)\,\mathrm{d}\mathbf{r}'\,\mathrm{d}\mathbf{v}' \tag{3}$$

$$\delta\phi(\mathbf{r},t) = \int u(|\mathbf{r}-\mathbf{r}'|) \delta f(\mathbf{r}',\mathbf{v}',t)\,\mathrm{d}\mathbf{r}'\,\mathrm{d}\mathbf{v}', \tag{4}$$

where $u(r)$ is the inter-particle potential.

The strategy to solve Eq. (2) at first order in δf (which is an excellent approximation) consists in linearizing equation (2), to obtain,

$$\frac{\partial \delta f}{\partial t} + \mathbf{v}\cdot\frac{\partial \delta f}{\partial \mathbf{r}} - \frac{\partial \delta\phi}{\partial \mathbf{r}}\cdot\frac{\partial f}{\partial \mathbf{v}} - \frac{\partial \phi}{\partial \mathbf{r}}\cdot\frac{\partial \delta f}{\partial \mathbf{v}} = 0. \tag{5}$$

The evolution of the system can be computed by solving the system of equations (2) and (5).

2.1 *Homogeneous systems*

We will first give a brief derivation of the kinetic equations for the spatially homogeneous case. It is technically simpler than the inhomogeneous one while sharing the same ideas. In this case $f = f(\mathbf{v},t)$, so equations (2) and (5) become

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial \mathbf{v}}\cdot\langle \delta f \frac{\partial \delta\phi}{\partial \mathbf{r}}\rangle, \tag{6a}$$

$$\frac{\partial \delta f}{\partial t} + \mathbf{v}\cdot\frac{\partial \delta f}{\partial \mathbf{r}} - \frac{\partial \delta\phi}{\partial \mathbf{r}}\cdot\frac{\partial f}{\partial \mathbf{v}} = 0. \tag{6b}$$

In this case it is (relatively) simple to solve Eq. (6b) because f does not depend on the space variable $\mathbf{r}$. Therefore the unperturbed orbits are straight lines with constant velocity. Moreover, applying a Fourier-Laplace transform to the variables t and $\mathbf{r}$ does not introduce a convolution in the last term of Eq. (6b).

Defining $\widetilde{\delta f}(\mathbf{k},\mathbf{v},\omega) = \frac{1}{(2\pi)^d}\int \mathrm{d}\mathbf{r}\int_0^\infty \mathrm{d}t\, e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\delta f(\mathbf{r},\mathbf{v},t)$ and $\widetilde{\delta\phi}(\mathbf{k},\omega) = \frac{1}{(2\pi)^d}\int \mathrm{d}\mathbf{r}\int_0^\infty \mathrm{d}t\, e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\delta\phi(\mathbf{r},t)$ and taking the Fourier-Laplace transform of Eq. (6b), we obtain

$$\widetilde{\delta f} = \underbrace{\frac{\mathbf{k}\cdot\frac{\partial f}{\partial \mathbf{v}}\widetilde{\delta\phi}(\mathbf{k})}{\mathbf{k}\cdot\mathbf{v}-\omega}}_{\substack{\text{collective}\\\text{effects}}} + \underbrace{\frac{\widehat{\delta f}(\mathbf{k},\mathbf{v},0)}{i(\mathbf{k}\cdot\mathbf{v}-\omega)}}_{\substack{\text{initial}\\\text{conditions}}}, \tag{7}$$

where $\widehat{\delta f}(\mathbf{k},\mathbf{v},0) = \int \frac{\mathrm{d}\mathbf{r}}{(2\pi)^d} e^{-i\mathbf{k}\cdot\mathbf{r}}\delta f(\mathbf{r},\mathbf{v},0)$ is a Fourier transform. The first term of the r.h.s. of Eq. (7) corresponds to collective effects, which are a generic feature of long range systems. The second term corresponds to the initial fluctuations because of the finiteness of the number of particles N.

The next step in the derivation consists in expressing the Fourier transform of the fluctuation of the potential $\widetilde{\delta\phi}(\mathbf{k},\omega)$ as a function of the fluctuation $\widetilde{\delta f}(\mathbf{k},w)$. To do so, we integrate equation (7) over $\mathbf{v}$, and using the Fourier transform of equation (4), we get

$$\int_{-\infty}^{\infty}\mathrm{d}\mathbf{v}\widetilde{\delta f}(\mathbf{k},\mathbf{v},\omega) = \frac{1}{\epsilon(\mathbf{k},\omega)}\int_{-\infty}^{\infty}\mathrm{d}\mathbf{v}\frac{\widehat{\delta f}(\mathbf{k},\mathbf{v},0)}{i(\mathbf{v}\cdot\mathbf{k}-\omega)}, \tag{8}$$

where we have defined the plasma response dielectric function $\epsilon(\mathbf{k},\omega) = 1-\hat{u}(\mathbf{k})\int \mathrm{d}\mathbf{v}\frac{\mathbf{k}\cdot\partial f(\mathbf{v})/\partial\mathbf{v}}{\mathbf{v}\cdot\mathbf{k}-\omega}$. Using again equations (4) and (8), we get $\widetilde{\delta\phi}(\mathbf{k},\omega)$. After some algebra, we obtain the Lenard-Balescu equation [2]:

$$\begin{aligned}\frac{\partial f}{\partial t} = \pi(2\pi)^d m\sum_{i,j=1}^{d}\frac{\partial}{\partial v_i}\int \mathrm{d}\mathbf{k}\,\mathrm{d}\mathbf{v}' k_i k_j \frac{\hat{u}(\mathbf{k})^2\delta[\mathbf{k}\cdot(\mathbf{v}-\mathbf{v}')]}{|\epsilon(\mathbf{k},\mathbf{k}\cdot\mathbf{v})|^2}\\ \times\left(\frac{\partial}{\partial v_j}-\frac{\partial}{\partial v_j'}\right) f(\mathbf{v},t)f(\mathbf{v}',t).\end{aligned} \tag{9}$$

When collective effects are not taken into account, the first term of the r.h.s. of equation (7) is neglected, which is equivalent to set $\epsilon(\mathbf{k},\omega)=1$. The Lenard-Balescu equation is called in this case the Landau equation.

2.2 *Inhomogeneous systems*

In inhomogeneous systems, new difficulties appear: (*i*) the unperturbed orbits are much more complicated than in the homogeneous case and (*ii*) in the last term of (6b) f depends also in the position $\mathbf{r}$, and taking the Laplace-Fourier transform would give a convolution term. The strategy to solve the difficulty (*ii*) consists in "homogenizing" the equations, using an appropriate change of variables. These new variables are the angle-action $(\mathbf{w},\mathbf{J})$ corresponding to the Hamiltonian $\mathcal{H}$ of smooth dynamics (i.e., the one corresponding to the limit $N \to \infty$) [3]). Using these variables, particles described by the Hamiltonian $\mathcal{H}$ keep their action $\mathbf{J}$ constant during the dynamic and their angle evolves with time as $\mathbf{w} = \Omega(\mathbf{J})t + \mathbf{w}_0$ where $\mathbf{w}_0$ is the angle at $t = 0$ and $\Omega(\mathbf{J}) = \partial\mathcal{H}/\partial\mathbf{J}$ is the angular frequency [4].

The equations for the evolution of the smooth distribution function f and its fluctuation δf are [5,6]

$$\frac{\partial f}{\partial t} = \frac{\partial}{\partial \mathbf{J}} \cdot \left\langle \delta f \frac{\partial \delta\phi}{\partial \mathbf{w}} \right\rangle, \tag{10a}$$

$$\frac{\partial \delta f}{\partial t} + \Omega(\mathbf{J}) \cdot \frac{\partial \delta f}{\partial \mathbf{w}} - \frac{\partial \delta\phi}{\partial \mathbf{w}} \cdot \frac{\partial f}{\partial \mathbf{J}} = 0. \tag{10b}$$

Despite these equations seeming as simple as Eqs. (7), the difficulty (*i*) described in the first paragraph of this section is not solved; the complexity of the unperturbed orbits is hidden in the change of variables, which makes the expression of the potential very complicated.

Following the same procedure as the one described in the homogeneous case, we get the Lenard-Balescu-type kinetic equation in action-angle variables [6,7],

$$\frac{\partial f}{\partial t} = \pi(2\pi)^d m \frac{\partial}{\partial \mathbf{J}} \cdot \sum_{\mathbf{k},\mathbf{k}'} \int d\mathbf{J}' \mathbf{k} \frac{\delta[\mathbf{k}\cdot\Omega(\mathbf{J}) - \mathbf{k}'\cdot\Omega(\mathbf{J}')]}{|D_{\mathbf{k},\mathbf{k}'}(\mathbf{J},\mathbf{J}',\mathbf{k}\cdot\Omega(\mathbf{J}))|^2} \times \left(\mathbf{k}\cdot\frac{\partial}{\partial \mathbf{J}} - \mathbf{k}'\cdot\frac{\partial}{\partial \mathbf{J}'}\right) f(\mathbf{J},t) f(\mathbf{J}',t) \tag{11}$$

where

$$\frac{1}{D_{\mathbf{k},\mathbf{k}'}(\mathbf{J},\mathbf{J}',\omega)} = \sum_{\alpha,\alpha'} \hat{\Phi}_\alpha(\mathbf{k},\mathbf{J}) (\epsilon^{-1})_{\alpha,\alpha'}(\omega) \hat{\Phi}^\star_{\alpha'}(\mathbf{k}',\mathbf{J}'), \tag{12}$$

and $\epsilon_{\alpha\alpha'}(\omega)$ is the dielectric tensor

$$\epsilon_{\alpha\alpha'}(\omega) = \delta_{\alpha\alpha'} + (2\pi)^d \sum_{\mathbf{k}} \int d\mathbf{J} \frac{\mathbf{k}\cdot\partial f/\partial\mathbf{J}}{\mathbf{k}\cdot\Omega(\mathbf{J}) - \omega} \times \hat{\Phi}^\star_\alpha(\mathbf{k},\mathbf{J}) \hat{\Phi}_{\alpha'}(\mathbf{k},\mathbf{J}). \tag{13}$$

The indices (α,α') are labels for a bi-orthogonal basis $\{\rho_\alpha, \Phi_\alpha\}$ for the density and the potential [8]. , where $\rho(\mathbf{r}) = \int f(\mathbf{r},\mathbf{v},t)\,\mathrm{d}\mathbf{v}$, which satisfies [8]

$$\int u(|\mathbf{r}-\mathbf{r}'|)\rho_\alpha(\mathbf{r}')\,\mathrm{d}\mathbf{r}' = \Phi_\alpha \tag{14}$$

$$\int \rho_\alpha(\mathbf{r})\Phi^\star_{\alpha'}(\mathbf{r})\,\mathrm{d}\mathbf{r} = -\delta_{\alpha,\alpha'}. \tag{15}$$

The terms $\hat{\Phi}_\alpha$ are the Fourier transforms of the potential in the bi-orthogonal representation with respect to the angles $\hat{\Phi}_\alpha(\mathbf{k},\mathbf{J}) = \frac{1}{(2\pi)^d}\int \mathrm{d}\mathbf{w} e^{-i\mathbf{k}\cdot\mathbf{w}}\Phi_\alpha(\mathbf{w},\mathbf{J})$. The Lenard-Balescu equation (11) gives the evolution of f due to the inclusion of a finite-N correction to the collision-less (Vlasov) kinetic equation. From equation (11), we see that the evolution, which slowly deforms the orbits of constant $\mathbf{J}$, is driven by resonances between orbital frequencies, $\mathbf{k}\cdot\Omega(\mathbf{J}) = \mathbf{k}'\cdot\Omega(\mathbf{J}')$. This differs from the homogeneous case, equation (9), where f evolves due to the resonances $\mathbf{v} = \mathbf{v}'$.

From the Lenard-Balescu-type equation (11) it is possible to compute diffusion coefficients, defined as $D^{ij}_{dif}(\mathbf{J},t) = \lim_{\Delta t\to 0}\langle \Delta J_i(t)\Delta J_j(t)\rangle/\Delta t$:

$$D^{ij}_{dif}(\mathbf{J},t) = \pi(2\pi)^d m \sum_{\mathbf{k},\mathbf{k}'} \int \mathrm{d}\mathbf{J}' k_i k_j \frac{\delta[\mathbf{k}\cdot\Omega(\mathbf{J}) - \mathbf{k}'\cdot\Omega(\mathbf{J}')]}{|D_{\mathbf{k},\mathbf{k}'}(\mathbf{J},\mathbf{J}',\mathbf{k}'\cdot\Omega(\mathbf{J}'))|^2} f(\mathbf{J}',t). \tag{16}$$

When collective effects are not considered, we have $\epsilon_{\alpha\alpha'} = \delta_{\alpha\alpha'}$.

3 Kinetic equations for the Hamiltonian Mean-Field model

We will compute explicitly the diffusion coefficients for the HMF model [9]. It is given by the Hamiltonian

$$H = \sum_{i=1}^{N} \frac{p^2}{2} - \frac{1}{2N}\sum_{i,j=1}^{N} \cos(\theta_i - \theta_j). \tag{17}$$

This model corresponds to a simplified model of one-dimensional gravity, in which only the first harmonic of a Fourier expansion on the potential is considered. This model is widely studied because many calculations can be performed analytically. The energy of one particle can be written as

$$h(\theta,p) = \frac{p^2}{2} + \phi(\theta) = \frac{p^2}{2} - \frac{1}{N}\sum_{i=1}^{N}\cos(\theta_i - \theta). \tag{18}$$

The potential $\phi(\theta) = -1/N\sum_i \cos(\theta_i - \theta)$ can be rewritten as

$$\phi(\theta) = -\frac{\sum_{i=1}^{N}\cos\theta_i}{N}\cos\theta - \frac{\sum_{i=1}^{N}\sin\theta_i}{N}\sin\theta = -M_x\cos\theta - M_y\sin\theta \tag{19}$$

where $\mathbf{M} = (M_x, M_y)$ is the magnetization vector. Its modulus M quantifies how bunched, or clustered, the particles are. From Eq. (19) we can see that, when M_x and M_y are approximately constant, the particles motion corresponds to a real pendulum. The action variables can be computed analytically:

$$J(\kappa) = \frac{4\sqrt{M_0}}{\pi} \begin{cases} 2\left[\mathrm{E}(\kappa) - (1-\kappa^2)K(\kappa)\right], & \kappa < 1 \\ \kappa \mathrm{E}\left(\frac{1}{\kappa}\right), & \kappa > 1 \end{cases} \tag{20}$$

where M_0 is the magnetization of the Quasi-Stationary state, $E(x)$ is the complete Legendre elliptic integral of the second kind and $\kappa = \sqrt{(1+h/M_0)/2}$. The angular frequency can be computed analytically,

$$\Omega(\kappa) = \pi\sqrt{M_0} \begin{cases} \frac{1}{2K(\kappa)}, & \kappa < 1 \\ \frac{\kappa}{K\left(\frac{1}{\kappa}\right)}, & \kappa > 1, \end{cases} \tag{21}$$

where $K(x)$ is the complete elliptic integral of the first kind. It is also possible to compute analytically the bi-orthogonal basis, which is composed by only two family of functions in this case. We will call them $c_l(\kappa)$ and $s_l(\kappa)$ (see [1] for detailed expressions). This permits us to express all the quantities of interest analytically, except the dielectric tensor, for which numerical integrals have to be performed:

$$\epsilon_{cc/ss}(\omega) = 1 + 2\pi \sum_{\ell=-\infty}^{\infty} \int_0^{\infty} \mathrm{d}\kappa \frac{g_\ell^{cc/ss}(\kappa)}{\Omega(\kappa) - \omega/\ell}, \tag{22}$$

where

$$g_\ell^{cc}(\kappa) = |c_\ell(\kappa)|^2 \partial f/\partial\kappa \tag{23a}$$

$$g_\ell^{ss}(\kappa) = |s_\ell(\kappa)|^2 \partial f/\partial\kappa. \tag{23b}$$

The final expression for the diffusion coefficient is

$$D_{dif}(\kappa) = \frac{2\pi^2}{N} \sum_{n,n'=\infty}^{\infty} \sum_{\kappa^\star} \frac{n^2 |\partial J/\partial\kappa|_{\kappa^\star}}{|D_{nn'}(\kappa, \kappa^\star, n\Omega(\kappa))|^2} \frac{f(\kappa^\star, t)}{\left| n' \frac{\partial\Omega}{\partial\kappa'} \right|_{\kappa^\star}} \tag{24}$$

where $\kappa^\star$ are the roots of the equation $m\Omega(\kappa) - m'\Omega(\kappa') = 0$ and

$$\frac{1}{D_{nn'}(\kappa, \kappa', \omega)} = \frac{c_n(\kappa)c_{n'}(\kappa')}{\epsilon_{cc}(\omega)} - \frac{s_n(\kappa)s_{n'}(\kappa')}{\epsilon_{ss}(\omega)}. \tag{25}$$

It is usually necessary to take a only few terms of the sum over n and n' in Eq. (24) to obtain accurate results (see [1]).

4 Numerical checking

In this section we check the diffusion coefficients (24) with molecular dynamics (MD) simulations. The details can be found in [1]. In Figure 1 we show an excellent agreement between theory and simulations for Quasi-Stationary states with different values of the magnetization M_0 (which measures the clusterization of the system). We performed simulations suppressing the collective effects (top panels) and with collective effects (bottom panels). Row (a) corresponds to high magnetization (very clustered states), row (b) to intermediate magnetization and row (c) low magnetization (quasi-homogeneous configuration). A very good agreement between theory and simulations is observed in all cases.

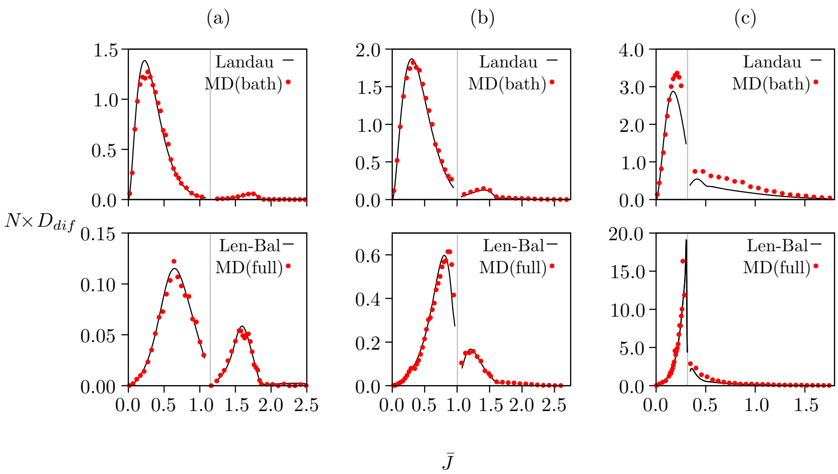

Fig. 1 Diffusion coefficients calculated by molecular dynamics, compared to the theoretical results, for an equilibrium distribution with magnetization (a) $M_0 = 0.816$, (b) $M_0 = 0.622$ and (c) $M_0 = 0.06$. On the bottom, MD simulations without collective effects, with the prediction of the Landau equation ($\epsilon_{ss} = \epsilon_{cc} = 1$). On the top, MD simulations with collective effects with the theoretical curve predicted by the Lenard-Balescu (Len-Bal) equation, and the molecular dynamics given by the regular HMF model – MD(full).

References

1. F. P. C. Benetti and B. Marcos. Collisional relaxation in the inhomogeneous Hamiltonian mean-field model: Diffusion coefficients. *Phys. Rev. E*, **95**:022111, 2017.

2. P. H. Chavanis. Kinetic theory of spatially homogeneous systems with long-range interactions: I. General results. *The European Physical Journal Plus*,**127**:19, 2012.
3. J. Binney and S. Tremaine. *Galactic Dynamics*. Princeton University Press, 2008.
4. H. Goldstein. *Classical Mechanics*. Pearson Education, 2002.
5. J. F. Luciani and R. Pellat. Kinetic equation of finite Hamiltonian systems with integrable mean field. *Journal de Physique*, **48**:591–599, 1987.
6. P.-H. Chavanis. Kinetic theory of long-range interacting systems with angle-action variables and collective effects. *Physica A*, **391**:3680, 2012.
7. J. Heyvaerts. A Balescu-Lenard-type kinetic equation for the collisional evolution of stable self-gravitating systems. MNRAS, 407, 2010.
8. A. J. Kalnajs. Dynamics of Flat Galaxies. II. Biorthonormal Surface Density-Potential Pairs for Finite Disks. *Astrophysical Journal*, 205:745, 1976.
9. Mickael Antoni and Stefano Ruffo. Clustering and relaxation in hamiltonian long-range dynamics. *Phys. Rev. E*, **52**:2361–2374, Sep 1995.