Localization area, fractal dimension and phase transitions in dissipative two-dimensional Yukawa systems: Numerical simulation

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Abstract. In the present work, the dynamic entropy of an extensive dissipative system with Yukawa interaction is studied numerically. Two parameters defining the state of a system—the coupling parameter and the scaling parameter—were varied in the wide range (from disordered to highly-ordered state of a system). For each state, the dynamical entropy of a system was calculated; the fractal dimension of trajectories of grains and the size of their localization area were found. Two latter parameters appeared to have critical points in the vicinity of $\Gamma^*_c = 98$, that complies with the results obtained by the pair correlation function method.

1. Introduction

Today, the study of laws of statistics is almost purely theoretical, because it is hard to find an experimental system that would be easy to follow the motion of its particles on a kinetic level. Nevertheless, there is a unique object that allows it—the structures formed by micron-sized grains in plasma. They gain sufficiently high electrical charge ($\sim 10^2$–$10^5$ of elementary charge) under the flows of plasma particles or in the emission processes [1]. These charged grains effectively interact with each other as well as with external electrical and magnetic (if they are present) fields. The action of external forces and forces of interparticle interaction combined with dissipative mechanisms in these systems can lead to the self-organization of the system, resulting in formation of quasi-stationary dusty plasma systems as well as to complex oscillatory or chaotic regimes [2]. An essential characteristic of dust structures in laboratory gas discharges is that these systems are far from equilibrium—for the existence of the discharge (i.e. for the levitation of particles) a constant energy supply is needed; during the experiment this energy dissipates on the surrounding plasma particles.

Note that ordered dynamic systems, in spite of their stationarity, almost always are non-equilibrium (because in equilibrium state the entropy reaches its maximum). Due to this, the attempts to describe them with the help of classical equilibrium thermodynamics often lead to inconsistencies like one described in [3]. Because of this, the dynamic entropy approach is especially important for the description of the state of these systems. The connection between the kinetic characteristics of the system and the ergodic theory was proved for several dynamic systems almost three decades ago [4]. Namely, there was established a fundamental correlation
between the diffusion coefficient, the maximum Lyapunov exponent and Kolmogorov–Sinai entropy for Lorentz gas. And in a number of works [5, 6] the maximum Lyapunov exponent was used as an indicator of the phase transition in a dynamic system.

To study phase transitions in small system of dust particles in plasma, the concept of mean first-passage time dynamic entropy was used in our work—a simple approximation of Kolmogorov–Sinai entropy [7, 8]. The main idea here is that the change of a phase state is essentially the way from the ordered to the chaotic state and back, and all approaches to the measurement of degree of chaotization of open systems are reduced to the determination of their entropy [9].

In present work, the dynamic entropy of a two-dimensional extensive system with Yukawa interaction is studied numerically. Two parameters defining the state of a system—the coupling parameter and the scaling parameter—were varied in the wide range (from disordered to highly-ordered state of a system). For each state, the dynamic entropy of a system was calculated, the fractal dimension of trajectories of grains and the size of their localization area were found.

2. Numerical simulation
Simulation of particle dynamics in extended homogeneous monolayer structure was carried out using Langevin molecular dynamics method, for parameters close to the conditions in laboratory dusty plasmas. The simulation procedure is detailed in [10,11]. The molecular dynamics method is based on solution of equations of motion and gives a good description of changes in transport properties of the system while it is approaching to equilibrium state. Besides that, Langevin approach takes into account the dissipation of stochastic kinetic energy of dust particles due to viscous friction with the buffer gas, and the statistical equilibrium in the system is maintained by energy exchange with the thermostat. Accordingly, Langevin molecular dynamics method is used to study such physical phenomena as phase transitions, thermal diffusion of macroparticles, viscosity and thermal conductivity, nonequilibrium dynamics of particle system, etc. When integrating the equations of motion, an important issue is how to control the integration time step gently, and to define the characteristic equilibration time correctly [12]. The correct choice of integration time step depends on characteristic frequencies of the physical process under consideration. In our case, the time step of the integration was $\Delta t = 1/(100 \max\{\nu_{fr}, \omega^*\})$; we took the time of the system relaxation to the equilibrium state no less than $10^3/(\max\{\nu_{fr}, \omega^*\})$ and the duration of analyzed particle trajectories was greater than $1.5 \times 10^3/(\max\{\nu_{fr}, \omega^*\})$. Here $\nu_{fr}$ is the coefficient of friction of dust particles against neutrals of the surrounding gas, and $\omega^*$ is the characteristic frequency of interparticle interactions.

Calculations were performed for the system consisting of identical particles of mass $M = 10^{-10}$ grams and charge $Q = 5 \times 10^3 e$ interacting with Yukawa (screened Coulomb) potential,

$$U(r) = Q^2 \exp(-\kappa r/l_p)/r, \quad (1)$$

with screening parameter $\kappa \equiv l_p/\lambda = 1$, where $l_p$ is the average interparticle distance and $\lambda$ is the screening length. The periodic boundary conditions were applied in the horizontal directions (x and y). The number of particles in the central simulation cell was $N_p = 400$; the potential cut-off length was $\sim 10l_p$. The assigned temperature $T$ of particles was valued to provide the effective coupling parameter $\Gamma^* = l_p^2 (U^{(2)}/(2T))$, where $U^{(2)} = Q^2 [2(1 + \kappa^2/2) \exp(-\kappa)/l_p^3]$ is the second derivative of the expression (1) at the average interparticle distance $l_p$. The coupling parameter was changed from $\Gamma^* = 10$ to $\Gamma^* = 150$, the scaling factor $\xi = \omega^*/\nu_{fr}$ was changed from $\xi \sim 0.5$ to $\xi \sim 10$; here $\omega^* = (U^{(2)}/\pi M)^{1/2}$. For a system of particles interacting via screened Coulomb potential these parameters (with screening parameter $\kappa < 6$) define mass transfer processes and phase state of the system regardless of the interaction parameters [13]. Trajectories of particles in a fragment of central cell of 2D systems for time $t = 7 \times 10^3 \Delta t\nu_{fr}$,
with $\kappa = 1$, $\xi = 1$ and for different values of effective coupling parameter $\Gamma^* (50, 90, 110, 150)$ are shown in figure 1.

We used the pair correlation function in order to measure the translational order in the system of interacting particles. The pair correlation function $g(r)$ is the normalized radial distribution function of particle concentration which tends toward a uniform value of 1 for large values of $r$ for isotropic liquid state and for the crystal state at zero temperature $g(r)$ is a series of $\delta$-functions with positions determined by particles separation [14]. We obtained pair correlation functions from calculation of the positions of particles registered in simulation for different parameters of simulated 2D systems. In the simulation the functions $g(r)$ (see figure 2) were averaged over 5000 timesteps and over a finite number of particles for correct calculation. The calculations also showed that the order in the system of particles is practically independent on friction.

The dependence of the first maximum $g_{\text{max}}$ of pair correlation functions $g(r/l_p)$ on coupling parameter $\Gamma^*$ is shown in figure 3. The deviation of the magnitude $g_{\text{max}}$ for different $\xi$ is less than 7%. We can easily see a singular point for $\Gamma^*_c \sim 98 \pm 5$ (the dashed line in the figure 3). This critical point may be related to the liquid–hexatic transition. The obtained results for our 2D calculations are in agreement with the numerical study of properties for collisionless ($\xi \rightarrow \infty$) and weakly collisional 2D systems presented in [15–17].

3. Results and discussion

3.1. Mean first-passage time dynamic entropy method

To calculate the dynamic entropy, we use the simple approximation [7,18,19]. For each particle of the two-dimensional structure, we draw the circle of radius $\varepsilon$ around the particle in the moment $t = 0$, and then find the moment of time $\tau$, when the trajectory first passes the threshold value $\varepsilon$. Averaging this mean first-passage time, MFPT, $\tau(\varepsilon)$ over all the particles of the system, we obtain the “MFPT dynamic entropy” $S(\varepsilon)$ [8,19]:

$$S(\varepsilon) = \frac{1}{\tau(\varepsilon)}.$$ (2)

For all values of $\xi$ and $\Gamma^*$ under study we have plotted the dependences of the dynamic entropy $S$ from the normalized coarsening parameter $\varepsilon/l_p$, where $l_p$ is the mean distance between the particles. It appeared that for each simulated particle there existed a limiting circle, that contains the whole trajectory of the particle; the grain never leaves it. The radius of this circle $\varepsilon_0^*$ represents the localization area of the grain. Another informative parameter in the dependence $S(\varepsilon^*)$ is its slope, i.e. the derivative $\Delta(\varepsilon^*) \equiv \frac{d(\log[S(\varepsilon^*)])}{d(\log[\varepsilon^*])}$. For small values of $\varepsilon^*$
Figure 2. Dependence of pair correlation functions \( g(r/l_p) \) on effective coupling parameter \( \Gamma^* \) for 2D system with parameters: \( \kappa = 1 \) and \( \xi = 2 \).

Figure 3. Maximum of pair correlation functions \( g_{\text{max}} \) versus effective coupling parameter \( \Gamma^* \) for 2D system with parameters: \( \kappa = 1 \), \( \xi = 2 \) (diamonds) and \( \xi = 0.5 \) (bold line). The dashed line depicts the singular point for \( \Gamma^*_c = 98 \).

(in the ballistic regime of motion) \( \Delta(\varepsilon^*) \approx -1 \); for distances approaching the limiting circle \( (\varepsilon^* \to \varepsilon^*_0) - \Delta(\varepsilon^*) \to \Delta_f \)—the value corresponding to the fractal dimension of the trajectory of a grain. Fractal dimension is a specific measure of a self-similar object (fractal), a concept that was coined by Benoit Mandelbrot [20]. Unlike the “familiar”, spatial dimension, the fractal dimension does not have to be an integer. For example, the spatial dimension of a flat curve is 1, but the fractal dimension of a trajectory of the Brownian particle on a plane (representing a fractal), is 2. So, the fractal dimension of a pattern shows its space-filling capacity.

3.2. Results
The method of mean first-passage time dynamic entropy allows following and analyzing the motion of each particle of a system under study. From the coordinates of 100 grains of each numerical experiment the dynamic entropy \( S(\varepsilon^*) \) and its logarithmic derivative were calculated. Examples of \( S(\varepsilon^*) \) and \( \Delta(\varepsilon^*) \) functions are shown in figure 4 with the illustration of the average fractal dimension of trajectory of grains \( \Delta_f \) and the size of its localization area \( \varepsilon^*_0 \).

The values of \( \varepsilon^*_0 \) and \( \Delta_f \) were averaged over all studied grains. The dependencies of these parameters on the effective coupling parameter \( \Gamma^* \) are shown in figures 5 and 6, correspondingly.

The parameter \( \varepsilon^*_0 \) is the localization area of the grain, i.e. the size of the region that the particle never leaves. For the smallest explored value of coupling parameter \( \Gamma^* = 10 \varepsilon^*_0 = 13.15 \) (for various values of \( \xi \)); with increase of \( \Gamma^* \), the size of localization area diminishes down to \( \varepsilon^*_0 \approx 1.3 \) for \( \Gamma^* \sim \Gamma^*_c = 98 \). Then, crossing the point \( \Gamma^* = \Gamma^*_c \pm 5 \), it experiences the jump, and for higher \( \Gamma^* \) the localization area takes values not higher than 0.63. That means that the grains move within the circles smaller than the inter-grain distance, and their trajectories do not intersect. This conclusion is completely verified visually by figure 1: for \( \Gamma^* = 50, 90 \) the trajectories look more or less mixed, while for \( \Gamma^* = 110, 150 \) they represent an organized structure.
Figure 4. Mean first-passage time dynamic entropy $S(\varepsilon^*)$ (a) and its logarithmic derivative $\Delta(\varepsilon^*)$ (b) for arbitrary 5 grains of a simulated system with $\Gamma^* = 110$, $\xi = 0.5$. Dashed lines illustrate the definition of parameters $\Delta_f$ and $\varepsilon_0^*$.

Figure 5. Dependence of the size of localization area $\varepsilon_0^*$ on the coupling parameter $\Gamma^*$ for the systems with $\xi = 0.5$ (black circles) and $\xi = 2$ (gray squares). Dotted line indicates the critical effective coupling parameter $\Gamma^*_c = 98$.

Figure 6. Dependence of the size of average fractal dimension of the trajectories of grains $\Delta_f$ on the coupling parameter $\Gamma^*$ for the systems with $\xi = 0.5$ (black circles) and $\xi = 2$ (gray squares). Dotted line indicates the critical effective coupling parameter $\Gamma^*_c = 98$.

As for the value of fractal dimension $\Delta_f$, for small $\Gamma^*$ it is close to 1 (describing the deterministic motion). With the increase of $\Gamma^*$ it monotonically grows, reaching $\Delta_f \approx 2$ (the Hausdorff dimension of Brownian trace [20]) in the vicinity of $\Gamma^* = \Gamma^*_c$. Then, crossing the point
$\Gamma^* = \Gamma^* \pm 5$, it experiences the jump, and for higher $\Gamma^*$ it fluctuates around $\Delta_f \approx 4$. This kind of motion corresponds to the antipersistent fractal Brownian motion. The antipersistent system changes more quick than a random one; it has frequent but small alterations.

4. Conclusion

We have carried out the numerical simulation of a homogeneous dissipative monolayer of grains interacting with Yukawa potential. Two parameters of simulation defining the state of a system—the coupling parameter and the scaling parameter—were varied in the wide range (from disordered to highly-ordered state of a system), corresponding to the parameters of laboratory dusty plasma. The phase state of a system was determined using the method of pair correlation functions. Then, the dynamical entropy of this system was found, as well as the fractal dimension of trajectories of grains and the size of their localization area. Two latter parameters appeared to have critical points in the vicinity of $\Gamma^*_c = 98$, that complies with the results obtained by the pair correlation function method.

Acknowledgments

This work was supported by the Russian Science Foundation (project No. 14-12-01440).

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