Divergence of dust particles trajectories in dusty plasma model

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Divergence of dust particles trajectories in dusty plasma model

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Abstract. The description of the properties of the plasma–dust system can be improved by using elements of thermodynamics. Divergence of the dusty particles trajectories allows us to estimate Krylov–Kolmogorov–Sinai entropy for a system of dust particles in plasma. In this way, we can verify if the behavior of the K-entropy of the dusty plasma subsystem in the partial equilibrium is close to the physical entropy. A picture of the divergence of trajectories for the dusty plasma model is obtained. The memory time of the model is estimated. The dependence of K-entropy on the number of dust particles and on the average kinetic energy of the dust particles are presented. The similarity of the behavior of the K-entropy parameter in the plasma–dust system and in the classical molecular-dynamic gas model is shown. The possibility of using this parameter for the description of dusty plasma is discussed.

1. Introduction

The thermodynamics (the entropy and the thermostat model), statistical physics, concepts of equilibrium and partial equilibrium are crucial for dusty plasma description [1–7]. The problem of estimation of dusty plasma entropy has been under consideration for several years [8, 9]. All approaches of this research are based on analytical and theoretical approach, and also on molecular dynamics simulation of dusty plasma system. The divergence of trajectories of dusty plasma model system allows to calculate K-entropy (Krylov–Kolmogorov–Sinai entropy) [10,11]. Henri Poincare showed that the classical dynamical systems of many particles belong to systems with strong local instability [12]. In physics, these representations introduced N S Krylov in the book [13]. In connection with molecular dynamics method, this fact was brought to the attention of E E Shnol [14]. The analysis of the results of elucidating the exponential runaway of particle trajectories in the Lennard-Jones system is performed in [11]. The connection between Krylov–Kolmogorov–Sinai entropy and physical entropy is discussed many times [15–17]. The value of $K$ is also equal to averaged maximum Lyapunov exponent and entropy growth rate since reciprocal is an important relaxation time. Furthermore, predictability time is studied. This time characterizes the time interval, during this interval future behavior of a dynamic system based on the initial conditions and deterministic dynamical equations can be predicted. The time of trajectories divergence in the molecular dynamics simulation might be different in different directions, so the partial equilibrium subsystem can be observed in the system. In this paper estimations for the characteristic time of divergence in different directions of dust particles...
motion are presented for the case of detailed model of dusty plasma. The estimates of the time of dynamic memory are discussed and conclusions are drawn about the effect of model features on dynamic memory and on the entire system. The method for entropy is verified for conditions of standard laboratory experiment on dusty plasma. The dependence of K-entropy on the number of dust particles and on the average kinetic energy of the dust particles are presented. The similarity of the behavior of the K-entropy parameter in the plasma–dust system and in the classical molecular-dynamic gas model is shown. The possibility of using this parameter for the description of dusty plasma is discussed.

2. Dusty plasma model
Author considers the three-dimensional system with dust particles of a few micrometers in gas-discharge plasma conditions. The number of dust particles $N$ differs from one up to several hundreds. The screened Coulomb potential is selected as the interaction potential \[ U_{ij}(r_i - r_j) = Q_i Q_j \exp\left(-\kappa |r_i - r_j|/|r_i - r_j|\right), \] (1)
where $Q_i$ is a charge of $i$-th dust particle, $r_i$ is radius vector of $i$-th dust particle, $\kappa$ is a screening parameter. This potential is chosen as the first step, and in the future it is planned to check and develop the obtained results using more detailed interaction potentials [22, 23] and taking into account the effect of ion heating in cryogenic conditions [24]. The interaction potential gives us the dust particles interaction force $F_{\text{int}}$. Dust particles move near the height where the electric field balances the force of gravity: $F_{\text{gr}} = m g = \langle F_{\text{el}} \rangle = \langle Q E(z) \rangle$, where $m$ is a particle mass, $g$ is a free fall acceleration, $Q$ is a dust particle charge, $z$ is vertical coordinate, triangular brackets mean averaging. The force of friction $F_{\text{fr}}$ is modeled by the Langevin thermostat. Trap potential is considered to be parabolic and gives us the linear force $F_{\text{trap}}$. Thus, the system of equations of motion of the dust particles is given by
\[ m \ddot{r}_i = F_{\text{int}} + F_{\text{fr}} + F_{\text{trap}} + F_{\text{gr}} + F_{\text{el}}, \quad i = \overline{1, N}. \] (2)

In equation (2) the dependence of particle charge $Q$ on the coordinates and time is taken into account. Charge is determined by the equilibrium of electron and ion fluxes onto the surface of dust particle. Dust particle charge fluctuations are due to fluctuations of these flows and local plasma parameters near the particle. Hence, the dust particle charge fluctuates on time. In the sheath gas-discharge electron and ion densities vary considerably in height. That leads to the charge dependence on vertical coordinate. Dust particles in the gas-discharge plasma acquire big charge and affect the surrounding plasma. Thus, two adjacent dust particles charge depend on the distance between each other. The Lorentz forces, the interaction of particles with each other and with the trap include the expression $Q_i = Q_i[t, z(t), r_{ij}(t)]$. Joint consideration of all these factors leads to the effects, which are discussed below.

The parameters of the system are chosen to be close to the conditions of standard laboratory experiment: screening radius is 0.025 cm, average charge is $10^4 e$, parameter of trap potential is 0.08 CGS units, friction coefficient is 3.0 s$^{-1}$, step of numerical integration is equal to $10^{-6} \text{ s}$.

3. Divergence of trajectories
All points on the MD trajectory are described by floating-point number with finite mantissa, where the bit depth is determined by the computer characteristics. Points on the trajectories are mostly irrational, since they belong to the exact solutions of the system of Newton’s equations. Therefore, each subsequent point of the trajectory, obtained by numerical integration of Newton’s equations, belongs to different solutions of the system of Newton’s equations. In itself, this fact is obvious for any numerical method, but these solutions remain in a small neighborhood of the exact trajectory in the phase space [11]. However, due to the Lyapunov instability, the Newtonian trajectories, calculated from the initial conditions that are close to
Figure 1. Divergence of particle velocity for two MD trajectories with similar initial conditions and slightly different steps of numerical integration: black curve—the result of numerical simulation; red curve—the approximation of numerical results in the stage of exponential growth of the run-off magnitude.

The initial point, but which do not coincide with it, exponentially diverge with time. The same runaway character with the same value of the exponent can be expected on the average for MD trajectories wandering along Newton trajectories.

There is an assumption that the entropy of a system as a whole can be estimated with the use of the concept of the Krylov–Kolmogorov–Sinai entropy. K-entropy is a measure of chaos and instability; it is related to the average running-off velocity of trajectories close at the initial instant. Moreover, the K-entropy is larger for the faster scatter of trajectories, which means the greater instability of trajectories and the more chaotic system.

There is only a general statement about the scattering of Newtonian trajectories. Then one can verify the trajectories divergence in simulation directly. Let us consider two trajectories calculated from the same initial conditions, but with different steps of numerical integration $\Delta t$ and $\Delta t'$. The first and second trajectories let us denote as $(r_i(t), v_i(t))$ and $(r'_i(t), v'_i(t))$. The difference in the coordinates (velocities) of the first and second trajectories averaged over the trajectory should be calculated by formulas

$$
\langle \Delta r^2(t) \rangle = \frac{1}{N} \sum_{i=1}^{n} ((r_i(t) - r'_i(t))^2), \quad \langle \Delta v^2(t) \rangle = \frac{1}{N} \sum_{i=1}^{n} ((v_i(t) - v'_i(t))^2).
$$

(3)

It turned out that these values increase exponentially with time:

$$
\langle \Delta r^2(t) \rangle = A \exp (Kt), \quad \langle \Delta v^2(t) \rangle = B \exp (Kt).
$$

(4)

This formula is valid for time in the range from the time between collisions to the memory time.

K-entropy is equal to the parameter $K$ in the formulas. We can formulate that K-entropy is a rate of exponential divergence of particle trajectories. The molecular-dynamic trajectories, calculated for the described model of a dusty plasma, scatter in the expected manner in figure 1 and allow us to estimate the time of memory and K-entropy of the system under consideration. It appears to be close to 0.05 s, that is 6 times smaller than inverse of friction coefficient. Thus, we can conclude that charge fluctuations, the effect of a neutral gas and others have a significant effect on the rate of forgetting by trajectories of its prehistory. Picture of divergence
Figure 2. The dependence of K-entropy on number of dusty particles in model.

Figure 3. The dependence of K-entropy on average kinetic energy of dusty particles in model.

It is found that the K-entropy $K$ depends on the number of dust particles $N$ in the model in figure 2. It looks logical, because the increase in the number of particles changes the structure of the system and its ordering. With an increase in the number of particles greater than 6, the slope of the curve decreases and the curve already resembles a straight line, which leads to an analogy with classical thermodynamics, when the entropy is proportional to the number of particles.

The dependence of the K-entropy on the average kinetic energy $T$ of the dust particles shows a linear dependence on the logarithm of temperatures in figure 3 when the dust system begins
to lose a strict structure. In the chosen temperature range, the dust particle system undergoes a transition from a crystalline state to a fluid-like state. In this case, the K-entropy behaves similarly to a thermodynamic system in the process with preservation of the characteristic, for example, in an isochoric or isobaric process.

4. Conclusion

The equations of dust particles motion in gas discharge are formulated with account of charge fluctuations and features of near-electrode layer. The method of the K-entropy calculation for dusty plasma model is tested. The form of the dependence of the runaway of the trajectories on time turned out to be identical to the form of this dependence for the classical molecular-dynamic model of the Lennard-Jones gas. The memory time of the model is 6 times less than the inverse coefficient of friction. Thus, we can conclude that charge fluctuations, the effect of a neutral gas and others components of model have a significant effect on the rate of forgetting by trajectories of its prehistory. The dependence of the K-entropy on the kinetic temperature of the dust particles turns out to be very similar to the dependence for the classical thermodynamic system under the conditions of the constancy of one parameter, for example, volume or pressure. The dependence of the K-entropy on the number of particles confirms the additivity rule observed for the entropy of classical thermodynamic systems. These moments allow us to assume that the K-entropy of the plasma–dust subsystem in the partial equilibrium behaves similarly to the behavior of the entropy of the equilibrium system for the parameters under consideration. The K-entropy can be used as one of the parameters in thermodynamics description of dusty plasma subsystem in partial equilibrium.

Acknowledgments

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