CPP
Contributions to Plasma Physics

www.cpp-journal.org

WILEY-VCH

REPRINT

Contrib. Plasma Phys. **52**, No. 3, 182 – 185 (2012) / **DOI** 10.1002/ctpp.201100070

Velocity Autocorrelation Functions and Diffusion Coefficient of Dusty Component in Complex Plasmas

K. N. Dzhumagulova*, **T. S. Ramazanov,** and **R. U. Masheeva**

IETP, Al Farabi Kazakh National University, al Farabi 71, Almaty, 050038, Kazakhstan

Received 13 October 2011, revised 14 January 2012, accepted 18 January 2012
Published online 11 April 2012

Key words Langevin dynamics, dusty plasma, dust particles, diffusion, velocity autocorrelation function

The velocity autocorrelation functions of dust particles were calculated by the Langevin dynamics. It was indicated that their oscillations decay more rapidly with increase in the friction parameters. The dependencies of the dust particles diffusion coefficient on the friction coefficient at the different values of various parameters were obtained by the Green-Kubo relation and mean square displacements. The validity of the Einstein relation at small values of coupling parameter was shown.

1 Introduction

Now many physicists know what is a so-called dusty plasma. This is the plasma containing solid particles of the size far larger then the size of atoms. Dusty plasma is often found in nature, especially in astrophysical objects such as planetary rings, comet tails, etc. [1]. Moreover, in terrestrial conditions dusty plasma is formed in many installations using plasma technology. In such installations the dust is formed by sputtering of the walls surfaces adjacent to the plasma flows, as well as by the formation of reactive radicals in the working gases, leading to condensation and subsequent agglomeration of dust particles (grains) [2, 3]. Now, many works are carried out to eliminate the harmful effects of dusty plasma in plasma installations and its practical use. The spectrum of practical applications can be quite wide, so, these are the micro-electronics, medicine, chemical catalysis, etc.

In connection with all above mentioned the study of the fundamental properties of dusty plasmas is of particular importance. Considerable attention is paid to numerical simulations. The method of the Langevin dynamics found its recent wide application in studies of dusty plasma properties.

Part 2 contains short description of the main equation of the Langevin dynamics and results on the velocity autocorrelation function of the dust particles.

In Part 3, the dependencies of the diffusion coefficient on the friction parameter for different values of coupling parameter were obtained by the Green-Kubo relation as well as by the mean square displacements. Some conclusions were maid.

2 Langevin dynamics method and the velocity autocorrelation functions of the dust particles

The method of the Langevin dynamics found its recent wide application in studies of dusty plasma properties. This method was described in works [4-6]. Simulation of the dust particles space-time trajectories was maid on the basis of the following equations:

$$m_d \frac{d^2 \vec{r}_i}{dt^2} = \sum_j F_{int}(r_{ij}) \frac{\vec{r}_i - \vec{r}_j}{|\vec{r}_i - \vec{r}_j|} - m_d \nu_{fr} \frac{d\vec{r}_i}{dt} + \vec{F}_{br}(t), \tag{1}$$

where $F_{int}(r_{ij}) = -\partial\Phi/\partial r$ is a force imposed on a selected i-th particle due to interaction with j-th particle, $r_{ij} = |\vec{r}_i - \vec{r}_j|$ is a distance between two grains, $\vec{F}_{br}(t)$ is the stochastic force due to interactions with neutrals,

* Corresponding author. E-mail: dzhumagulova.karlygash@gmail.com, Phone: +00 772 737 73405, Fax: +00 772 729 24988

ν_{fr} is the friction coefficient dependent on buffer plasma pressure, m_d is mass of a dust particle. The Yukawa potential was chosen as interaction potential; in the dimensionless form it looks as:

$$\Phi(R) = \frac{\Gamma}{R} e^{-\kappa R} \tag{2}$$

here $\Gamma = (Z_d e)^2/(a k_B T_d)$ is the coupling parameter, $\kappa = a/r_D$ is the screening parameter, $a = (3/4\pi n_d)^{1/3}$ is the average distance between dust particles.

Set of 1024 dust particles were randomly distributed within a 3D cubic cell that was extended by periodical boundary conditions. Time is taken in the units of reverse plasma frequency of dust component $\omega_d = (4\pi n_d (Z_d e)^2/m_d)^{1/2}$. Number of the time steps $N_t = 30000$. Some performed tests of the temporal characteristics showed the validity of these parameters. The dimensionless friction parameter is $\theta = \nu_{fr}/\omega_d$. Simulations were performed for the dust particles system according to usual scheme [5]- [7].

One of the important dynamical characteristic of the system is a velocity autocorrelation function (VAF) of the particles:

$$A_{vv}(t) = \langle \vec{v}(t)\vec{v}(0) \rangle \tag{3}$$

where the brackets denote averaging over the ensemble and over various initial times. Velocity autocorrelation function demonstrates decay which is characterized by the relaxation time τ [7]. It is well known, that with increase of the coupling parameter and decrease of the screening parameter the relaxation time decreases [7, 8].

Fig. 1 presents autocorrelation functions obtained on the basis of the Langevin dynamics for various values of κ and θ at constant values of other parameters. It also represents the line, when autocorrelation functions reduced by a factor e. As one can see from this figure the time of relaxation increases with decrease in θ and increase in screening parameter.

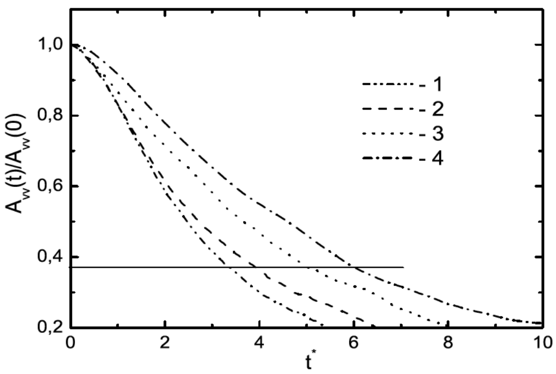

Fig. 1 VAFs obtained for different κ and θ at $\Gamma = 1$. 1) $\theta = 0.05$, $\kappa = 0.1$, 2) $\theta = 0.05$, $\kappa = 0.5$, 3) $\theta = 0.05$, $\kappa = 2$, 4) $\theta = 0.001$, $\kappa = 2$. Here $t^* = t\omega_d$.

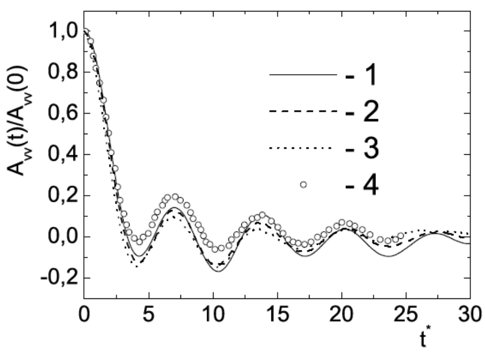

Fig. 2 VAFs obtained for different θ at $\Gamma = 50$ and $\kappa = 0.1$. 1) $\theta = 0.001$, 2) $\theta = 0.05$, 3) $\theta = 0.1$, 4) MD [9]. Here $t^* = t\omega_d$.

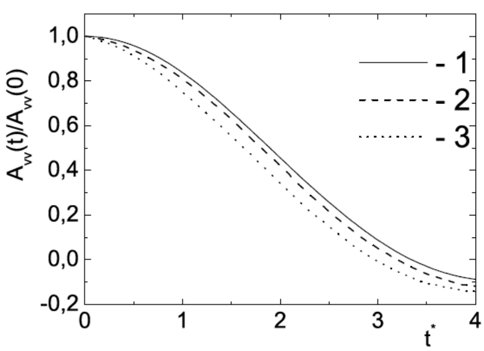

Fig. 3 VAFs from fig.2 focused on the first decay. 1) $\theta = 0.001$, 2) $\theta = 0.05$, 3) $\theta = 0.1$. Here $t^* = t\omega_d$.

The comparisons with results of MD simulation [8, 9] are given in Fig. 2. From this figure one can see that at the same Γ and κ but different θ the oscillations decay more rapidly with increase in θ. In Fig. 3 the same VAFs focused on the first decay are presented.

3 Diffusion coefficient

On the basis of the obtained values of the microstates one can obtain the diffusion coefficient by the well known relation connecting the diffusion coefficient with mean square displacements of the particles

$$D_{msd} = \lim_{t\to\infty} (\langle \vec{r}(0) - \vec{r}(t) \rangle^2 / 6t) \tag{4}$$

On the other hand, the transport coefficients can be calculated with Green-Kubo relations, for diffusion coefficient in three dimensional case it is written as:

$$D_{G-K} = \frac{1}{3}\int_0^\infty A_{vv}(t)dt \,, \tag{5}$$

here $A_{vv}(t)$ is the velocity autocorrelation function (3).

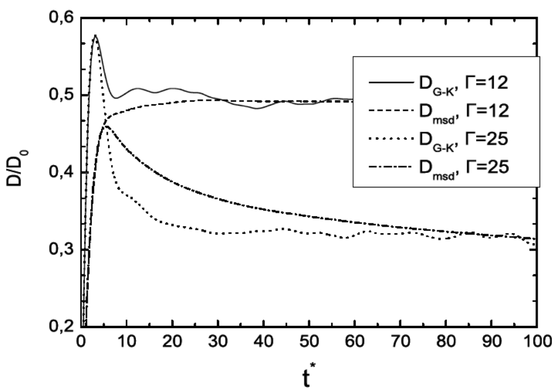

Fig. 4 The reduced values of $D(t)/D_0$ at different values of the coupling parameter Γ. Here $t^* = t\omega_d$.

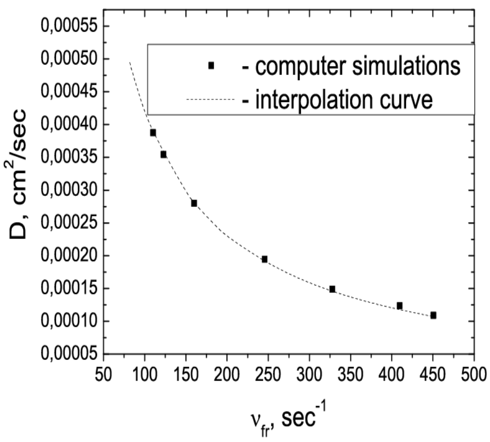

Fig. 5 Diffusion coefficient for $\Gamma = 80$

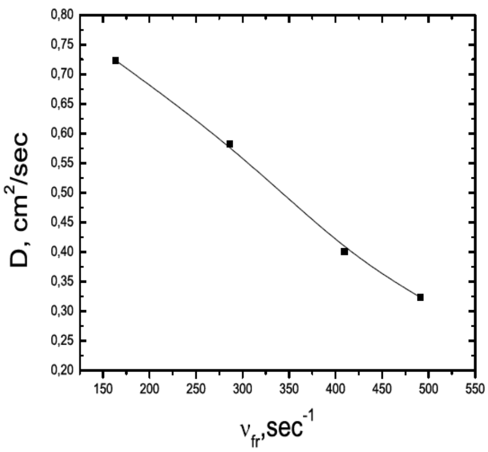

Fig. 6 Diffusion coefficient for $\Gamma = 0.1$

In Fig. 4 the time evolutions of $D_{msd}(t) = \langle \vec{r}(0) - \vec{r}(t) \rangle^2 / 6t$ and $D_{G-K}(t) = \frac{1}{3}\int_0^t A_{vv}(t)dt$ in units of $D_0 = k_B T/(\nu_{fr} m_d)$ (Einstein relation for diffusion coefficient of noninteracting particle in liquids) are given. As one can see from Fig. 4 the D_{G-K} converges more quickly then D_{msd}. In Figs. 5,6 the dependencies of the diffusion coefficient on the friction coefficient ν_{fr} obtained by means of eq.(5) for $Z_d = 5000$, $\kappa = 2$ and different values of Γ are given. Here the diffusion coefficient is given in dimensional form because some dimensional estimations were made. At $\Gamma = 80$ the following interpolation formula, which is in good agreement with computer simulation, was obtained:

$$D = \frac{0.24 k_B T_d}{(\nu_{fr} + 20) m_d} \tag{6}$$

For other values of Γ, Z_d computer simulations were performed, and the generalized formula for a wide range of parameters will be presented in the next work.

For $\Gamma = 0.1$ the dependence is almost inversely proportional to the friction coefficient, and D has the values very near to D_0. For example, at pressure $P = 70\,Pa$ and $m_d = 1.72 * 10^{-11}\,g$ other parameters are $k_B T_d = 2.88 * 10^{-9}\,erg$, $\nu_{fr} = 286\,sec^{-1}$, so, $D_0 = 0.58\,cm^2/sec$. Calculations indicated that $D/D_0 = 1$ at $\Gamma < 0.2$ with acceptable accuracy for a wide region of ν_{fr}. This fact proves the validity of the Einstein relation for the case of the low coupling parameters.

Acknowledgements This work was supported by Grants FI-13.6 and MP-1 of Ministry of Education and Science of RK.

References

[1] V. Ye. Fortov, A. G. Khrapak, S. A. Khrapak, V. I. Molotkov, and O. F. Petrov, Uspekhi Fizicheskikh Nauk, 174 (2004).
[2] V. N. Tsytovich and J. Winter, Uspekhi Fizicheskikh Nauk, 899 (1999).
[3] L. Boufendi and A. Boushole, Plasma Sources Sci. Technol. **3**, 262 (1994).
[4] O. S. Vaulina, X. G. Adamovich, O. F. Petrov, and V. E. Fortov, Phys. Rev. E **77**, 066403 (2008).
[5] T. S. Ramazanov and K. N. Dzhumagulova, Contr. Plasma Phys. **48**, 357 (2008).
[6] F. B. Baimbetov, T. S. Ramazanov, K. N. Dzhumagulova, E. R. Kadyrsizov, O. F. Petrov, and A. V. Gavrikov, J. Phys. A: Math. Gen. **39**, 4521 (2006).
[7] J.-P. Hansen and I.R. McDonald, Theory of simple liquids (Academic Press, New York, 1976).
[8] Z. Donkó and B.Nyiri, Phys. Plasmas **7**, 45 (2000).
[9] Z. Donkó and P. Hartmann, Phys. Rev. E. **69**, 016405 (2004).

