COMPUTER SIMULATIONS OF CHARGE FLUCTUATIONS IN DUSTY PLASMAS

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Charge fluctuations in dusty plasmas (DP) are studied by means of Brownian dynamics (BD) computer simulations and within the drift-diffusion (DD) approach. For a dust grain embedded in the weakly ionized isothermal background, the statistical properties of fluctuations are found to be close to the equilibrium ones. The simulations evidence for that the correlations of fluctuations decrease exponentially with time while the correlation time is proportional to the squared Debye length. It is shown that the charge variance is close to the inverse coupling parameter, regardless of the other parameters of the problem.

1. Introduction

In the recent years, DPs have received an increasing attention as the objects with rich collective properties, capable, in particular, of forming crystal structures in the colloidal component [1, 2]. The formation of ordered structures in DP is associated with the strong coupling in the subsystem of charged grains indicating that the average potential-to-kinetic energy ratio in the dust component is much greater than unity. Such a strong coupling is the result of a very high grain charge (typically, of the order of $\simeq 10^4$ electron charges) which emerges due to the grain charging by ion and electron currents and the difference in the ion and electron diffusivity. In most of the works, including computer simulations [3—5], the theoretical studies of the processes in DP employ the assumption that the grain charge is constant. However, in actual fact, the steady grain charge experiences fluctuations near its average magnitude associated with the discrete nature of the plasma components. These fluctuations may strongly affect the properties of DP.

The charge fluctuations in DP received a considerable attention in the literature including the numerical and theoretical studies of various aspects of their properties and effects on the dust transport and a motion in DP [6—15]. One of the interesting manifestations of the charge fluctuations may be the effect of grain heating observed in the experiments with the dust particles embedded in a weakly ionized neutral gas like He or Ar. In these experiments, there has been observed the unexpectedly high temperature (up to $\simeq 50$ eV) of the kinetic grain motion [16, 17]. One of the possible explanation for this phenomenon has been suggested in [18], where the grain heating was related to the influence of the charge fluctuations.

In spite of all the above-mentioned, the properties of the charge fluctuations in DP still remain insufficienty known. In particular, this concerns the case of a strongly collisional plasma background, e.g., a weakly ionized high-pressure gas. Systems of this kind can be created as a result of the ionization induced by nuclear or UV radiation. Besides its fundamental significance, this case has also industrial aspects [19].

In our previous paper [20], we examined the basic properties of charge fluctuations in DP by means of microscopic BD computer simulations. In this paper we expand our study to a wider range of parameters and investigate the problem within the alternative DD approach in order to compare the results and obtain some important conclusions.

2. Basic Assumptions and the Methods of Simulations

Let us formulate the basic physical assumptions used and the methods of simulations. We consider a single spherical grain of radius a embedded in the weakly

ionized high-pressure isothermal plasma background with the plasma-neutral collisions playing a major role. It is assumed that there are only two oppositely charged plasma components, e.g., ions and electrons, with the equal temperatures $T_i = T_e = T$ and the charge numbers $z_{i,e} = \pm 1$. The grain charge $Q_{\rm gr} = Ze$ (with e being the absolute value of the electron charge) emerges as a result of the complete absorption of both types of plasma particles by the grain surface and the difference in electron and ion diffusivities. No recombination processes over the volume are taken into account, while the plasma sources are assumed to be far from the grain.

To study of the grain charge dynamics, we employed two approaches, the method of BD computer simulations and its continuous analogue, the DD approach. These methods have been tested earlier rather exhaustively on the problem of grain screening [21].

As for the BD simulations, we employ, following [21], the particle-in-cell (PIC) method of simulations [22] with a concentric arrangement of spherical cells which allows for the spherical symmetry of the problem. The plasma background is considered as a set of discrete particles of two kinds. The relevant equations of motion are, in general, the Langevin equations (see, for instance, [23, 24]), since the two-component plasma immersed in a neutral gas represents an example of a many-particle system moving in a thermostat. In our simulations, we employ the reduced equations of overdamped motion

$$h\frac{d\mathbf{x}_k}{dt} = -\nabla_k U + \mathbf{F}_k(t), \tag{1}$$

where the inertial forces are neglected, because it is assumed that the friction forces are much stronger due to the strong plasma-neutral collisions. Here, $\mathbf{x}_k$ is the radius vector of the k-th particle, and U is the potential energy of the configuration. The friction coefficient h and the random force $\mathbf{F}_k(t)$ are determined by the properties of the heatbath represented in this case by the high-pressure neutral gas. Random forces acting on the plasma particles are specified by the time correlator

$$\langle F_{k,\alpha}(t) F_{m,\beta}(t')\rangle = 2B\delta_{km}\delta_{\alpha\beta}\delta(t-t'), \tag{2}$$

where the indices $\alpha, \beta = x, y, z$ denote the Cartesian components of the random force, the indices k, m enumerate the plasma particles, and $B = hk_{\rm B}T$.

In BD computer simulations, Eqs.(1) have been solved numerically within the mean field approach. This means that the configurational energy was approximated by $U = \sum_k ez_k\phi(\mathbf{r})$, where the self-consistent potential ϕ was found at each time step as a numerical solution of the relevant Poisson equation. The random forces $\mathbf{F}_k(t)$ were generated in simulations to satisfy relation (2) (with the accuracy of the discrete time representation) with the Gaussian amplitude distribution

$$P(\mathbf{B}_k(\Delta t)) = \frac{1}{(4\pi h^2 D\Delta t)^{3/2}} \exp\left[-\frac{|\mathbf{B}_k(\Delta t)|^2}{4h^2 D\Delta t}\right],$$

which determines the probability for the momentum

$$\mathbf{B}_k(\Delta t) = \int_t^{t+\Delta t} \mathbf{F}_k(t)dt$$

to be transferred to the k-th plasma particle during the time span Δt. In the above relations, the quantities h and D related to the ion and electron components are different; we ommitted the relevant subscripts for simplicity.

Let us say a few words about the boundary conditions (BC). In actual simulations, we consider the system of a finite size confined in a spherical volume of radius R with a grain placed at its center. The radius R is chosen to be sufficiently large in order to satisfy the conditions $R \gg a$, $R \geq r_{\rm Deb}$ (where $r_{\rm Deb}$ is the Debye radius). The loss of plasma particles due to the absorption by the grain is compensated by the flux of particles from outside the sphere. The BC are specified by this flux of particles, which is generated so that to simulate the constant plasma density outside the volume.

The study of the stochastic grain charge dynamics is possible due to the direct monitoring of the grain charge in BD simulations.

Although the DD approach is continuous in nature, it can still provide a valuable information on the properties of charge fluctuations, since it enables one to study the relaxation processes in the system (see the next section). Within the DD approach, we solve the general time-dependent equations for the unknown ion/electron densities $n_{i,e}$ and self-consistent potential ϕ in the form

$$\frac{\partial n_{i,e}}{\partial t} = -{\rm div}\mathbf{j}_{i,e}, \tag{3}$$

$$\Delta\phi = -4\pi e(n_i - n_e). \tag{4}$$

The expression for the current densities $\mathbf{j}_{i,e}$ has the form

$$\mathbf{j}_{i,e} = -\mu_{i,e} n_{i,e}\nabla\phi - D_{i,e}\nabla n_{i,e},$$

where $\mu_{i,e}$ and $D_{i,e}$ are the ionic/electronic mobility and diffusivity, respectively. These latter are assumed to be related due to the Einstein's equation $\mu_{i,e} = z_{i,e}e_{i,e}D_{i,e}/k_{\rm B}T$, where $z_{i,e} = \pm 1$ is the ion/electron charge number.

The grain charge emerges as a result of plasma currents due to the difference in electron and ion diffusivities. The study of the grain charge dynamics within the DD approach is based on the relevant equation for the grain charge, which, with regard for spherical symmetry, reads

$$\frac{dZ}{dt} = -4\pi a^2 (j_{(r)i} - j_{(r)e}), \tag{5}$$

where the subscript (r) denotes the radial component of a current and $Z = Q_{\rm gr}/e$.

In order to formulate the BC equivivalent to the ones used in BD simulations, we admit that the system is confined in a spherical volume with a sufficiently large radius $R \simeq 50 \div 500 r_{\rm Deb}$ with a grain placed at the center. The BC are specified at the surface of this sphere and at the surface grain. The sources of plasma ionization, which compensate the loss of plasma particles due to the absorption on the grain surface, are assumed to be outside the spherical volume. The action of these sources is modeled by maintaining the constant electron and ion densities on the sphere surface, $n_i = n_e = n_0$. According to this, we write the BC for the densities $n_{i,e}$ at $r = R$ in the form

$$n_{i,e} = n_0 \quad \text{at } r = R.$$

At the grain surface, we have, for the potential,

$$\frac{\partial \phi}{\partial r} = -\frac{Z(t)e}{a^2} \quad \text{at } r = a,$$

and we use the BC of [21] for the densities:

$$n_{i,e} = 0 \quad \text{at } r = a,$$

which is appropriate in the case of a strongly collisional background.

Note that there is a relation connecting the friction coefficient, diffusivity, and temperature, namely $D_{i,e} = k_{\rm B}T/h_{i,e}$, which enables one to establish the correspondence with the continuous DD approach and microscopic BD simulations. A detailed presentation of the issues concerning BD and its relation to the continuous probabilistic approaches, such as Fokker–Planck and Smoluchowski equations, can be found in [23, 24]. Here we point out that the overdamped BD represents a direct microscopic analogue to the DD approach, since the latter can be derived from the Smoluchowski equations for one-particle distributions (i.e., within the additional mean field approximation).

3. Numerical Simulations. Results and Conclusions

In order to present the results of numerical simulations, we use below the dimensionless charge number Z and the dimensionless time τ, which are measured in the units of the electron charge e and the time unit a^2/D_i, respectively.

The simulations have been performed mainly for the following range of parameters: the ratio of diffusivities $A \equiv D_e/D_i = 2, 10, 1000$, the dimensionless Debye radius $x_{\rm Deb} \equiv r_{\rm Deb}/a = 2 \div 10$. The coupling parameter defined as

$$\chi \equiv e^2/k_{\rm B}Ta \tag{6}$$

was within the range $0.1 - 0.01$. Note that a is here the grain radius rather than the interparticle distance. Selected runs were performed for $A = 5$; $x_{\rm Deb} = 30$; 70; $\chi = 0.005$. These values qualitatively correlate with the typical experimental numbers $x_{\rm Deb} \simeq 10 \div 100$, $\chi \simeq 0.01 \div 0.001$, $A \simeq 2 \div 1000$. The lower values of A are possible in the case of two-component ion-counterion plasmas with no free electrons present. The number of particles in BD simulations was within the range $N \simeq 500 \div 3000$. It was kept sufficiently large to ensure that the number of particles in the Debye sphere must be no less than 20.

The results of simulations are presented in the figures. Fig. 1 illustrates the charging processes of an initially neutral grain embedded in the weakly ionized plasma at the moment $\tau = 0$. As is seen, the results obtained within the DD approach and BD simulations correlate well. The system tends to its steady state with the grain charge fluctuating near its average magnitude.

The dynamical behavior of the charge $Z(\tau)$ in the steady state obtained in BD simulations can be used in straightforward calculations of the correlation function $\langle \delta Z(0) \delta Z(\tau) \rangle$ for the charge fluctuations, by the time averaging. As one would expect [18], the typical behavior of the charge autocorrelation function obtained in simulations suggests the exponential decrease of the charge correlations with time, Fig. 2. Note that this correlates with the general theory of equilibrium fluctuations [25], although we deal here with a non-equilibrium case. The equilibrium theory predicts as well the form

$$\langle \delta Z(0) \delta Z(\tau) \rangle = \langle \delta Z^2 \rangle \exp\left(-\frac{|\tau|}{\tau_{\rm corr}}\right) \tag{7}$$

for the correlator. As is seen from the above relation, the statistical properties of charge are determined by the

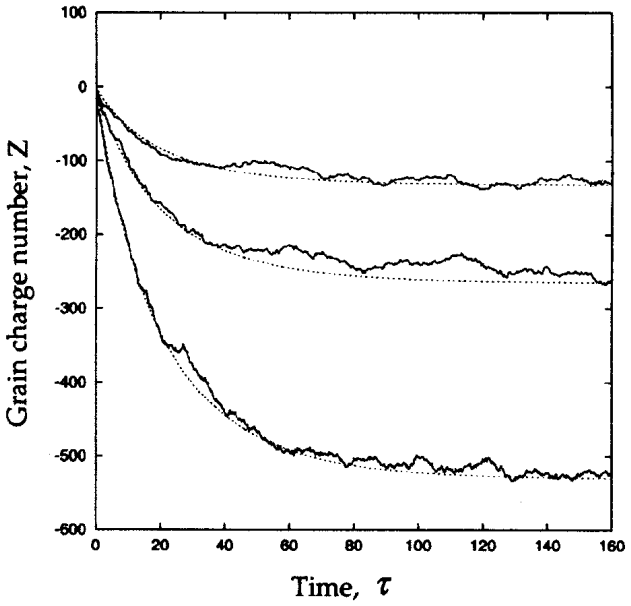

Fig. 1. Typical dynamics of the grain charge for the initially neutral grain embedded in a weakly ionized gas obtained in BD simulations (irregular curves) and within the DD approach (smooth dashed lines) for three different sets of plasma parameters

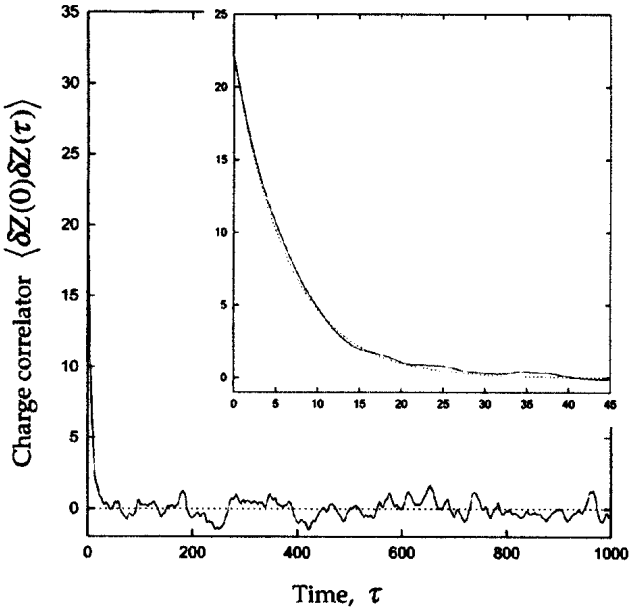

Fig. 2. Typical behavior of the charge correlator $\langle \delta Z(0) \delta Z(\tau) \rangle$ obtained in a straighfoward manner in BD simulations. The dashed line in the insert gives the relevant exponential fit

charge variance $\langle \delta Z^2 \rangle$, and the correlation time $\tau_{\rm corr}$ is dependent on the parameters of the problem.

The computations have revealed that, within the accuracy of BD simulations, the charge variance can be fitted, regardless of the other parameters, by the relation

$$\langle \delta Z^2 \rangle = \frac{1}{\chi}. \tag{8}$$

The results are given in Fig. 3.

It is important to note that this relation can be regarded as a consequence of the fluctuation-dissipation theorem. Really, we can consider the plasma in the spherical volume as an electric circuit extending from $r = a$ to $r = R$. Then, Eq.(8) can be obtained from the well-known Nyquist formula under the assumption that the static capacity of the grain is equal to its radius, $C(\omega = 0) = a$. This indicates that, although we deal here with the non-equilibrium system, its statistical properties in the steady state are close to the equilibrium ones.

It should be noted that result (8) also correlates with the results of other works [8,26] (based on the Fokker–Planck approach) which predict as well proportional dependence of the type (8), though with the coefficients slightly different from the unity.

In Fig. 4, we give the relative charge variance obtained in BD simulations. The computations evidence for that this quantity depends on the ratio of diffusivities A only, and its magnitude is $\sigma = \langle \delta Z^2 \rangle / Z \simeq 0.6$ and 1.1 for $A = 10$ and 2, respectively. We note that paper [7] reports the value $\sigma \simeq 0.5$ obtained in realistic computer simulations for a wide range of parameters provided that $Z \gg 1$, $A \gg 1$.

Admitting the exponential behavior of the charge correlation function obtained in BD simulations, one can evaluate the correlation time by the slope of this function at the point $\tau = 0$. The DD approach provides another possibilty to evaluate the correlation time. The idea of computations, which is commonly used for this purpose [9], is to study the relaxation of a system to the steady state. Actually, it is based on the assumption that the relaxation of a perturbed system to its steady state is identical to the relaxation of small fluctuations. Strictly speaking, this statement is formulated for equilibrium systems only and is known as Onsager's hypothesis. Thus, in the case of non-equilibrium systems, we deal with its generalization. It can be easily shown that, in this case, the relaxation time of a perturbed system is equal to the correlation time of fluctuations.

The computations performed in the above-described manner have demonstrated a very good agreement between the results for correlation times obtained within the DD approach and in BD simulations, Fig. 5. The

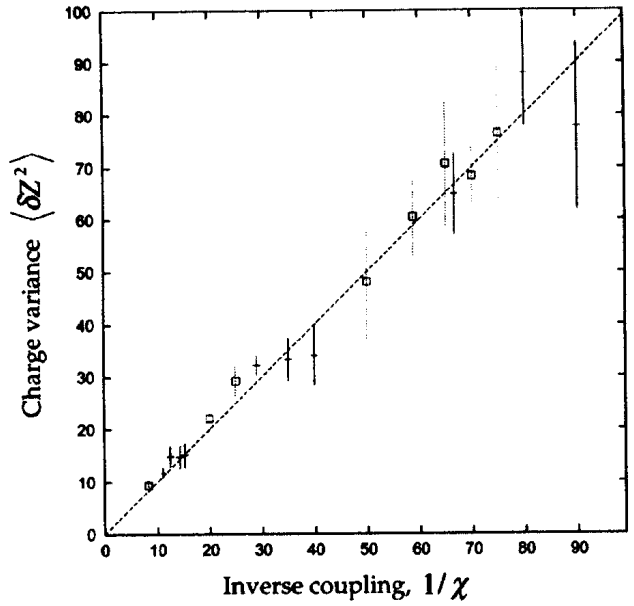

Fig. 3. Charge variance as a function of the inverse coupling. The dashed line gives the relation $\langle \delta Z^2 \rangle = 1/\chi$. Different points are obtained in BD simulations with different (arbitrary) ratios $r_{\rm Deb}/a$ within the range $2-10$ for $A = 10$(crosses) and $A = 2$ (squares). The error bars indicate the standard deviation

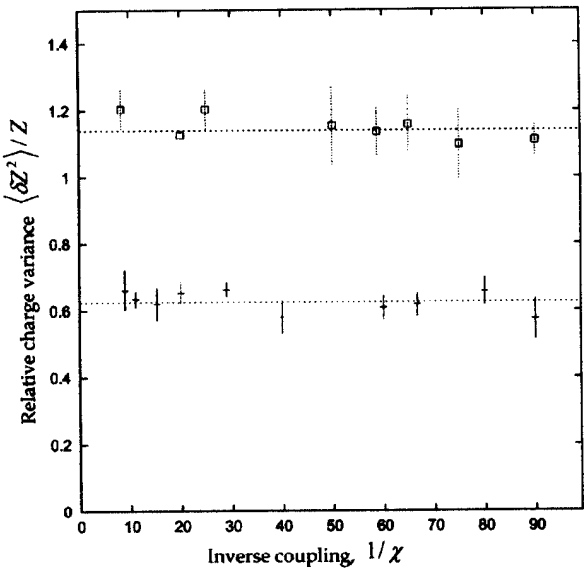

Fig. 4. The same as in Fig. 3, but for the relative charge variance

simulations evidence for that the correlation time for a fixed parameter A is determined by the Debye length only. In Fig. 5, we present the results obtained for various values of the coupling parameter within the range $\chi = 0.1 \div 0.01$ for the ratios $A = 2, 10, 1000$. Since the BD simulations for a high asymmetry with $A = 1000$ encounter serious computational difficulties, we do not present them in the figure. As is seen from the figure, within the accuracy of simulations, the function $\tau_{\rm corr}(x_{\rm Deb})$ can be fitted by the relation

$$\tau_{\rm corr} = \alpha x_{\rm Deb}^2. \qquad (9)$$

The dependence $t_{\rm corr} \sim r_{\rm Deb}^2$ is in agreement with the results of [8] based on the Fokker—Planck approach. Note that this relation can be also substantiated by the dimensionality-based reasons, since it looks in the dimensional form as $t_{\rm corr} = \alpha r_{\rm Deb}^2/D_i$. In general, the dimensionless proportionality coefficient α is a function of A. For the cases $A = 2$, 10, 1000 given in Fig. 5, we found $\alpha = 1.5$,0.8, 0.3, respectively.

It should be mentioned that relation (9) yields rather long correlation times for high-pressure weakly ionized gases. For instance, in the case of dust particles immersed in Ar at room temperature and the atmospheric pressure with the typical value $r_{\rm Deb} \simeq 100$

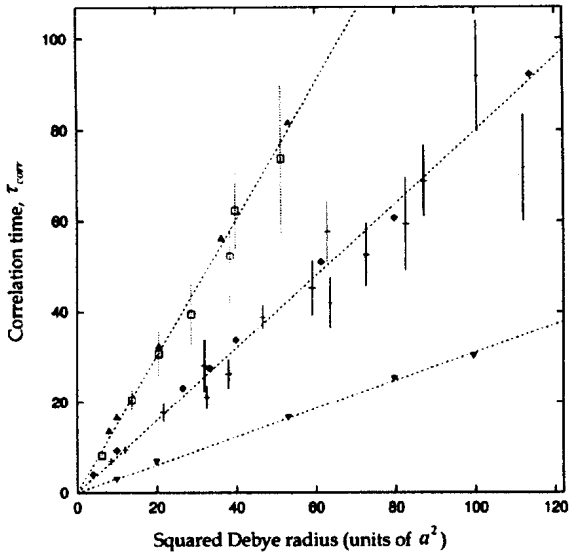

Fig. 5. Correlation time as a function of the squared Debye length $x_{\rm Deb}^2$ for $A = 2$ (top; squares); 10 (middle; crosses); and 1000 (bottom). Different points with error bars are obtained in BD simulations for different (arbitrary) values of the coupling within the range $0.1 - 0.01$. The dashed lines give the relation $\tau_{\rm corr} = \alpha x_{\rm Deb}^2$ with $\alpha = 1.5$ (top), 0.8 (middle), 0.3 (bottom). The filled symbols (triangles and rhombs) represent the results of simulations (respectively, with the relevant parameters) based on the DD approach

μm, one obtains $t_{\rm corr} \simeq 0.01$ sec. This justifies the applicability of the overdamped BD which is valid on the time scales $t \gg m/h$ (here, m is the mass of a plasma particle). It can be verified that the above inequality is satisfied within a rather wide range of parameters including the pressure $\simeq 0.001$ atm. and the temperature $k_{\rm B}T \simeq 1$ eV. This means that, in fact, the above-presented method of BD simulations, as well as its continuous analogue, the DD approach, has a rather wide range of applicability.

We have studied the charge fluctuations of a dust grain embedded in the weakly ionized isothermal background by means of BD computer simulations and within the DD approach. The statistical properties of the system (charge variance, correlation time, and charge correlator) are shown to be close to the equilibrium ones. The simulations evidence for that the correlations of fluctuations decrease exponentially with time while the correlation time is proportional to the squared Debye length. Within the accuracy of simulations, the charge variance is found to be close to the inverse coupling parameter, regardless of the other parameters.

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КОМП'ЮТЕРНЕ МОДЕЛЮВАННЯ ФЛУКТУАЦІЙ ЗАРЯДУ В ЗАПОРОШЕНІЙ ПЛАЗМІ

О. Бистренко, Т. Бистренко, А. Загородній

Р е з ю м е

Флуктуації заряду в запорошеній плазмі вивчаються шляхом комп'ютерного моделювання методом броунівської динаміки та в рамках дифузійно-дрейфового наближення. Показано, що для порошинки, що перебуває в слабкоіонізованій ізотермічній плазмі, статистичні властивості флуктуацій близькі до рівноважних. Моделювання свідчить, що кореляції флуктуацій зменшуються з часом експоненціально, а час кореляцій пропорційний квадрату радіуса Дебая. Показано, що дисперсія заряду близька до оберненої константи зв'язку незалежно від інших параметрів задачі.