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Solution of the inverse Langevin problem for open dissipative systems with anisotropic interparticle interaction

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Solution of the inverse Langevin problem is presented for open dissipative systems with anisotropic interparticle interaction. Possibility of applying this solution for experimental determining the anisotropic interaction forces between dust particles in complex plasmas with ion flow is considered. For this purpose, we have tested the method on the results of numerical simulation of chain structures of particles with quasidipole-dipole interaction, similar to the one occurring due to effects of ion focusing in gas discharges. Influence of charge spatial inhomogeneity and fluctuations on the results of recovery is also discussed. © *2015 AIP Publishing LLC*.
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I. INTRODUCTION

It is well known that a charged particle or macroobject, immersed in a flowing plasma, creates a perturbed region (a wake) behind itself.[1–11] Wakefield potential is often invoked to explain a vertical alignment of dust particles levitating in the plasma sheath of capacitive radio-frequency (RF) discharge. In such a plasma, ions have a directed velocity relative to stationary dust particles[12] which in turn acquire a significant negative charge (10^3–10^4 elementary charges) due to the higher electron mobility. This can lead to focusing of ion fluxes behind particles and, as a consequence, to difference between the interaction of dust particles in the directions perpendicular to the ion flow and parallel to it.

The first theoretical works on the interaction of dust particles in the ion flow appeared in the mid-nineties of the last century.[13–17] In Refs. 13 and 17, the wake produced by a grain in a flowing collisionless plasma was analytically investigated. It was shown that in a certain angle range the wake potential has an oscillatory structure, while outside the Mach cone the potential decays exponentially. Later on, the wake was studied both analytically and numerically as a function of the Mach number (the ion flow velocity); the electron to ion temperature ratio, which controls the Landau damping; the size and dielectric constant of the grain; plasma inhomogeneity; and the frequency of ion-neutral collisions, which decreases the directed ion velocity and restricts the dimensions of the perturbed plasma region.[18–27] Collisional processes in plasma and Landau damping can substantially suppress the oscillating structure of the wake potential behind the grain, due to which only the first maximum of the potential (so-called ion focus) is often observed. It is assumed that other dust particles interact with both the negatively charged grain and the positive ion focus, which leads to some effective attraction between the negatively charged particles. In ground based experiments with RF discharge dusty plasmas, multilayer dust structures usually have a pronounced hexagonal lattice in the horizontal direction (perpendicular to the ion flow), while in the vertical direction, particles of neighboring layers aligned in chains (strings).[28–30] Recent experimental observations of the string-like dust structures in complex plasmas are discussed in Refs. 31–34.

To date, the experimental determination of the pair interaction forces has been carried out between two horizontally aligned particles[35] and between many particles of horizontal quasi-two-dimensional monolayer[36,37] suspended in the sheath of capacitive RF discharge; as well as between heavy probe particle and dust cloud in the diffuse edge of inductive (electrodeless) RF discharge.[38] In all the cases,[35–38] the interparticle interaction can be described in the isotropic approximation.

In this paper, we analyze the possibility of experimental diagnostics of anisotropic interaction forces between dust particles in a plasma with ion flow using an improved method based on solving the inverse problem of particle motion.[39]

II. THE PROCEDURE FOR DETERMINING ANISOTROPIC INTERACTION FORCES (THE INVERSE LANGEVIN PROBLEM)

Dust subsystem in a weakly ionized plasma is an open dissipative system. Energy swapping is carried out by fluctuations of particle charges and by the work of non-potential forces. Dissipative channel is related to collisions of dust particles with neutrals. Motion of dust particles is caused by the forces of their interaction, the external force field, and by the friction forces with the neutral component of a buffer gas. This process is irreversible because of stochastic processes and energy dissipation in the system. However, in Ref. 39 it was shown that if the required forces in the system is given by some parametric functions, analyzing the dynamics of the studied system of particles within a certain (rather long) time interval τ and averaging over the ensemble of particles, allow one to eliminate under certain conditions random errors associated with the stochastic (thermal) motion of particles. Thus, when the trajectories $\vec{l}_k(t)$ of all N_p particles of a dust subsystem are well known, for correct determination of the unknown parameters of internal (interaction) and external forces (F_{int} and F_{ext}) a highly overdetermined set of motion equations

$$\frac{d^2\vec{l}_k}{\Delta t^2} = -\nu_{fr}\frac{d\vec{l}_k}{\Delta t} + \frac{1}{M}\left[\sum_j \vec{F}_{\text{int}}\left(\vec{l}_k - \vec{l}_j\right) + \vec{F}_{ext}\left(\vec{l}_k\right)\right] + \vec{g}, \quad (1)$$

consisting of $\sim N_p \times (\tau/\Delta t)$ equations, must be solved. Here, Δt is the time step related to the video registration frame rate, M is the mass of dust particles, ν_{fr} is the friction coefficient, and $\vec{g}$ is the gravitational acceleration.

Additional difficulty of a correct solution of the inverse problem (1) for strongly coupled systems is related to asymptotic behavior of the interparticle interaction forces $F_{\text{int}}(l)$, which limits the spatial range of the inverse problem solution. The maximum spatial range ($l_{\min} < l < l_{\max}$) of a correct recovery of the interparticle interaction force $F_{\text{int}}(l)$ is determined by the minimum distance between the particles $l_{\min}$ (is always less than the most probable interparticle distance l_p) and the following semi empirical condition $F_{\text{int}}(l_p)/F_{\text{int}}(l_{\max}) \leq 100$–$200$.[39] Within this spatial range, a methodic error in determining the function $F_{\text{int}}(l)$ is less than 5%.

We emphasize that when restoring forces, we do not base on any theoretical descriptions of the field distribution around the charged particles in plasmas. The unknown force can be approximated by piecewise constant functions, splines, or various combinations of power-law and exponential functions.

To recover the force of pair interparticle interaction in the anisotropic case, we use an assumption of axial symmetry of the unknown interaction force and the external field. Let the z-axis is parallel to the chosen axis of symmetry. We denote the angle between the z-axis and the vector $\vec{l}_{kj} = \vec{l}_k - \vec{l}_j$ connecting any pair of interacting particles (the particles number k and j) as θ. We divide the range of angle variation $\theta \in [0°; 180°]$ into S intervals $[\theta_s; \theta_{s+1})$, $s = 1,2,\ldots,S$. Then, the unknown parameters of the approximation functions for interparticle forces will be a set of piecewise constant functions dependent on the partition sequence number s.

Note that the vector $\vec{F}_{\text{int}}(\vec{l}_{kj})$ of the interaction forces with dipole component can generally not be parallel to the vector $\vec{l}_{kj}$. Based on the results of calculations of the ion flux focus behind dust particles, we can estimate the maximum value of the angle α between the vectors $\vec{l}_{kj}$ and $\vec{F}_{\text{int}}(\vec{l}_{kj})$. When the ion flow speed $\sim$0.5–2 Mach numbers, the concentration maximum of the ion cloud is located at a distance d less or comparable with the electron screening length λ_{De}, and estimation of the space charge of ion cloud is $\sim$5%–30% of the particle charge and may decrease with increasing the number of collisions with neutrals.[18,21,24] The ion focus between two particles aligned with the ion flow becomes noticeably weaker when the interparticle distance is less than $2d$.[21] At the considered parameters of the ion focus, deviation of the interaction force direction from the vector $\vec{l}_{kj}$ is less than $\alpha = 10°$ for $l_{kj} > 2d$ and cannot be taken into account when solving the inverse problem, which greatly simplifies the process of determining forces.

The described method is very picky about the spatial and temporal resolution of the video surveillance system.[40] In laboratory experiments, three dimensional determination of the dust particle trajectories with high spatial resolution is associated with a number of difficulties, including an insufficient depth of sharply imaged space and a simultaneous overlapping of several particle images. Therefore, in order to simplify the experimental diagnostics we propose to study the interaction of dust particles in an isolated vertically aligned dust chain. Such a quasi-one-dimensional structure can be observed in electrostatic trap, created by a glass cuvette mounted on the lower electrode.[34]

To test the proposed method, we carried out numerical simulation of dynamics of dust particles interacting via various anisotropic pair forces and forming linear chains in an external electric field.

III. NUMERICAL SIMULATION

In this work, to model the anisotropic interparticle interaction we used its quasi-dipole approximation. For this purpose, under each grain with a mass M and charge Q, a virtual charge q with the opposite sign and a zero mass were placed at a fixed distance d along the z-axis (see Fig. 1). The virtual charge acts only on the neighboring grains with the charge Q, whereas the neighboring grains themselves do not act on the virtual charges. Similar simple model has previously been used in the construction of an anisotropic distribution of the interaction forces between dust particles in plasmas, since it reflects in an adequate way the generation of a restoring force acting on the downstream particle.[16,41,42]

In our model, the force $\vec{F}_{kj}$ acting on a particle with number j and charge Q_j in the electric field created by the

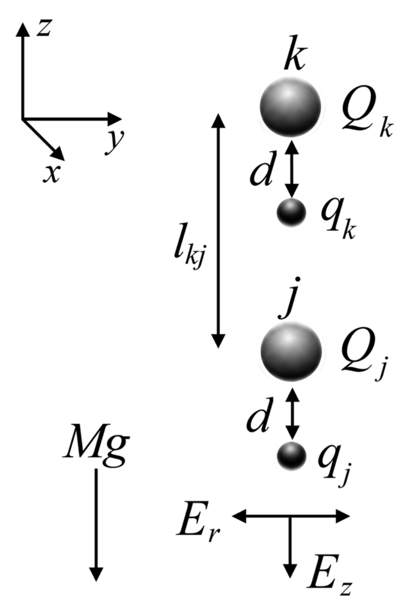

FIG. 1. Scheme of modeling a vertical chain of particles with quasi-dipole interaction, confined by a trap with cylindrical symmetry of the electric field $E(z,r)$.

particle with number k and charge Q_k together with its virtual charge q_k, can be represented as follows:

$$\vec{F}_{kj} = -Q_j(\nabla\varphi_{k_1 j} + \nabla\varphi_{k_2 j}), \tag{2}$$

$$\varphi_{k_{1,2}j} = \frac{Q_{k_{1,2}}}{l_{k_{1,2}j}}\left[\exp\left(-\kappa\frac{l_{k_{1,2}j}}{l_p}\right) + \frac{C}{l_{k_{1,2}j}^{m-1}}\right], \tag{3}$$

where $Q_{k_1} \equiv Q_k$, $Q_{k_2} \equiv q_k$, $l_{k_1 j} = |\vec{l}_k - \vec{l}_j| \equiv ({z_{kj}}^2 + {x_{kj}}^2 + {y_{kj}}^2)^{1/2}$ is the distance between particles with numbers k and j (provided that $l_{kj} > d$); $l_{k_2 j} = |\vec{l}_k + \vec{d} - \vec{l}_j|$—the distance between the virtual charge q_k of particle with number k and the main charge Q_j of the particle with number j; κ is the screening parameter; and C is a certain coefficient. Electric field potentials (3) around a charged grain as well as a virtual charge have both a Debay part, most commonly used in modeling dust particle interactions in plasmas, and a long-range power-law part ($m = 2$ or 3), predicted in many theoretical works for particles in the collisionless and collisional plasma flow.[4,7,22,23] The described interaction model is non-reciprocal, since if $q \neq 0$ and $z_{kj} \neq 0$ then $|\vec{F}_{kj}| \neq |\vec{F}_{jk}|$.

We note that in the view of recent experimental and numerical work on dust grains aligned with the ion flow, the charge of grains in the chain is reduced downstream, and the corresponding ion focus can be modified.[21,25,43,44] In order to model the vertical variation of the charges of particles, the function of the charge was specified in the form of $Q(z) = Q_0(1 + \gamma_z z)$ with such a coefficient γ_z, where a change of the particle charges was not exceed 30% within the simulated chain. Note that the numerical calculations performed for three or more particles aligned with the ion flow[25,43] predict a nonlinear dependence of $Q(z)$. However, since we study the capabilities of the method, we restrict ourselves to the linear approximation here.

Simulation of the particle motion in finite chains was carried out by Langevin molecular dynamics. The simulation technique is described in detail in Refs. 45 and 46. The following parameters of quasi-dipole interaction were considered: $d/l_p = 1/6 \div 1/2$, $q = -(0.1 \div 0.3)Q$, $\kappa = 0.5 \div 2$. Particle mass was $\mathrm{M} = 10^{-10}$ g and the number of particles N_p was ranged from 2 to 16. The system of particles was in a trap with cylindrical symmetry of the electrical field. In radial directions, particles were confined by the electric field $E_r = \alpha r$ and in the vertical direction they were in the field of gravity $F_\mathrm{g} = Mg$ compensated by the linear electric field $E_\mathrm{z} = {E_\mathrm{z}}^\mathrm{o} + \beta z$, where ${E_\mathrm{z}}^\mathrm{o} = Mg/Q_0$.

In all calculations, the effective coupling parameter of the system was $\Gamma^* = {l_p}^2\, F'_1/(2K) \sim 3\Gamma^*_\mathrm{c}$, where $\Gamma^*_\mathrm{c} \approx 100$ is the melting point of the systems with isotropic pair interaction potentials,[45] F'_1 is the averaged value of the first term derivative in Eq. (2) at the point of most probable interparticle distance l_p, and K is the characteristic kinetic energy of particles controlled by the fluctuation-dissipation theorem.[47] The ratio of characteristic frequencies ω^*/ν_fr was varied in the range from ∼0.1 to ∼10, corresponding to typical conditions of laboratory experiments,[34] here $\omega^* = (F'_1/\pi M)^{1/2}$ is the own dust frequency.[45]

In the course of modeling, the particle trajectories were recorded for the time interval $\tau \sim 100/\min[\nu_{fr}; \omega^*]$ required for a correct solution of the inverse problem (1).[39,40] Trajectories of two central particles of the chain consisting of 16 particles are shown in Fig. 2. Fig. 3 illustrates the spatial pair correlation of particles $g(l,\theta)$ in the chain consisting of 16 particles.

IV. RESULTS AND DISCUSSION

To solve the inverse problem of determining forces acting in the simulated systems, we used only the numerical data on particle trajectories $\vec{l}_j(t)$. The results of solving the inverse problem of determining anisotropic interaction forces in the chain-like structure of identical charges are shown in Fig. 4 for different angles $\theta^* = (\theta_s + \theta_{s+1},)/2$. Unknown force of interparticle interaction was found as a combination of power-law functions

$$F_\mathrm{int} = \sum_{i=1}^{5}\frac{a_{si}}{l^{i+1}} \tag{4}$$

for each angular interval $[\theta_s; \theta_{s+1})$, wherein $\int g(l,\theta)\,dl\,d\theta \neq 0$. Here, a_{si} are the sought expansion coefficients. The error in determining the values of interaction forces at small distances ($l < 0.75 l_p$) primarily associated with nonparallelism of the vectors $\vec{l}_{kj}$ and $\vec{F}_\mathrm{int}(\vec{l}_{kj})$, as well as with the lack of accumulated data on particle accelerations required to eliminate random errors caused by stochastic motion of particles. At the interparticle distances $l < 0.65 l_p$ recovery of the interaction forces is impossible in the considered chain, since the correlation function $g(l < 0.65 l_p)$ at all angles θ is zero.

Note that additional errors of the interaction force recovery may be in real experiments due to technical capabilities of the video surveillance system, such as not complete visualization of the dust cloud, and limited temporal and spatial resolution of particle motion.[39,40] The required temporal resolution (frame rate selection video recording) depends on

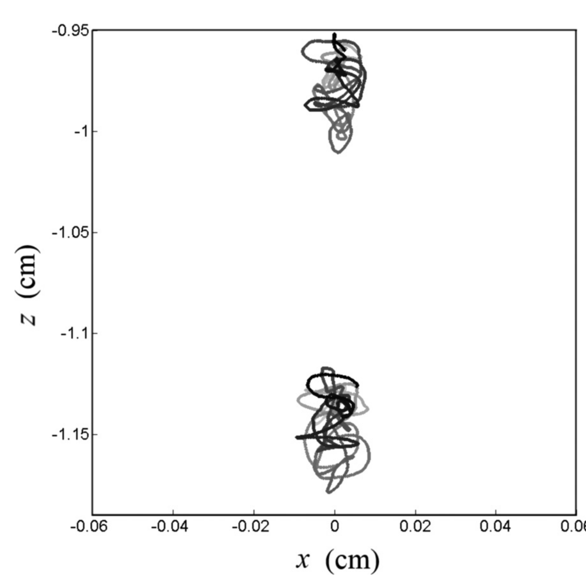

FIG. 2. Trajectories of two central particles of the chain consisting of 16 particles in the XZ-plane. Scale on the X-axis is twice larger than the Z-axis. Duration of the trajectories is $30/\omega^*$. The darker color of the trajectories corresponds to a longer time.

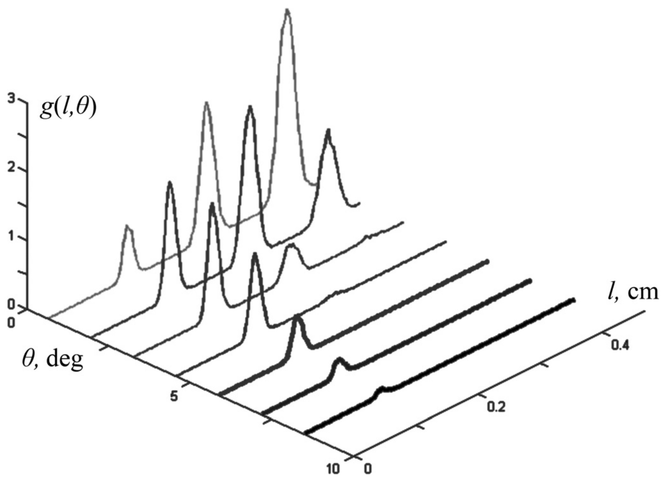

FIG. 3. Spatial pair correlation of particles $g(l,\theta)$ in the quasi-one dimensional chain consisting of 16 particles with the following parameters of quasi-dipole interaction: $\gamma_z = 0$, $q = -0.2Q$, $d/l_p = 0.3$, $\kappa = 1$, and $C = 0$.

the characteristic frequencies in the dust subsystem: the own dust frequency ω^* and the friction coefficient ν_{fr}.[39] The main influence of the spatial resolution on the results of solving the inverse problem is associated with imprecise definition of mass centers of dust particles, which depends on particle velocities, frame rate, and pixel density of video cameras, as well as on the recognition procedure.[40]

Numerical simulation allows us to estimate the maximum relative spatial variation of the particle charges in the analyzed system $\Delta Q/Q$, when the inverse problem solution is possible under the assumption of constancy of the charge magnitude. Fig. 5 shows the results of solving the inverse problem (1) for the chain systems of charged particles with such charge gradient γ_z that a change of the particle charges $\Delta Q/Q_0$ was not exceed 30% within the simulated chains. Deviation of the recovered force from the given force with $Q(z) = Q_0$ does not exceed 10% for the chains with $\Delta Q/Q_0 < 15\%$.

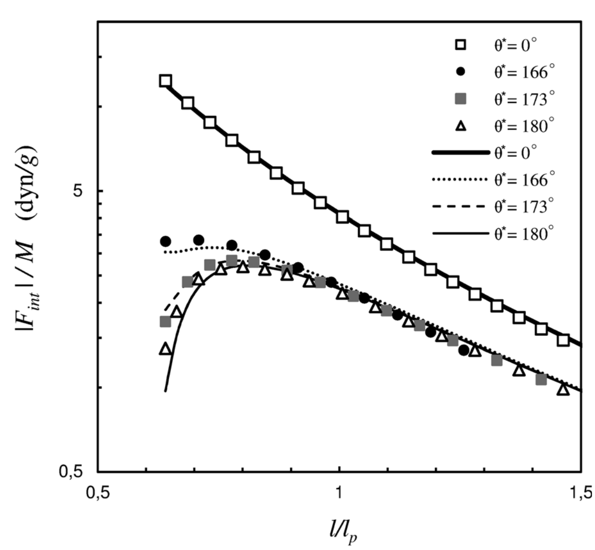

FIG. 4. The recovered spatial distribution of the force of anisotropic pair interaction $|F_{int}|/M$ between 16 particles in a quasi-one dimensional chain (symbols) with $\omega^*/\nu_{fr} = 1$. Lines denote the given force with the following parameters: $\gamma_z = 0$, $q = -0.2Q$, $d/l_p = 0.3$, $\kappa = 1$, and $C = 0$.

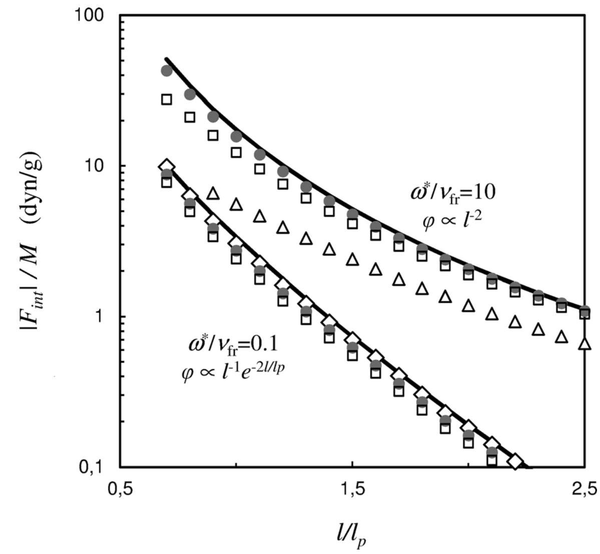

FIG. 5. The recovered force $|F(l/l_p)|$ in the chain system of 16 interacting particles with a gradient of charge: $\Delta Q/Q = 5\%$ (●); 10% (○); 15% (△); 25% (◇). Lines indicate the given pair forces calculated for $Q(z) = Q_0$ and $q = 0$.

The inverse problem (1) comprising an additional unknown functional dependence $Q(z)$ can only be solved under the assumption of simple screened Coulomb interaction between the particles. Search for a more complex spatial dependence of the interparticle interaction force leads to an ambiguous solution of the system (1). In this case, to solve such a system we need additional information, for example, on the own frequency of oscillation for each particle, containing information on the first derivative of the forces acting on the part of the nearest neighbors.

Since the particle charge is not a fixed value and is determined by local plasma parameters near the particle, under perturbations of plasma parameters the particle charge is also perturbed.[48–52] Such random fluctuations lead to fluctuations in the interaction force and the electric force acting on a particle in an external electric field. Information on the main characteristics of the fluctuations is required to quantify the effect of random fluctuations of the particle charges on the procedure of determining the unknown forces in the system. These include the amplitude δZ and characteristic correlation time τ_c of fluctuations. In Refs. 48–50, it was found that $\delta Z = \alpha\ |\langle Z\rangle|^{1/2}$, where $\langle Z\rangle$ is the equilibrium particle charge in units of electron charge e and α is the coefficient dependent on the plasma parameters. For particles of 1–10 μm size, levitating in a sheath of rf discharge, the characteristic value of the charge $\langle Z\rangle$ can be 10^3–10^4,[45] values of α are in the range from 0.4 to 0.6 (Refs. 48–50) and the characteristic correlation time of fluctuations τ_c can vary from 10^{-4} to 10^{-5} s.[50] At such parameters, the characteristic fluctuations of the interparticle interaction forces $\delta F_{int}/F_{int} \approx 2\delta Z/Z = 2\alpha/\sqrt{Z}$ caused by random fluctuations of the particle charges will be less or of the order of 1%. Next, we compare the amplitude of fluctuations $\delta F_{int}(l_p)$ with characteristic returning force ΔF_{int} when the particle displaces along the chain relative to equilibrium position by a value $\Delta l \sim \sqrt{K l_p^3/eZ}$ due to its thermal motion. Since the micron-sized grains levitating in a sheath, usually acquire kinetic energy $K \sim 0.1$–$1\,\mathrm{eV}$ and the average distance between them is $l_p \sim 0.1\,\mathrm{cm}$, then $\delta F_{\rm int}/\Delta F_{\rm int} \sim (\delta Z/Z)(l/\Delta l) \sim \alpha\sqrt{Ze^2/Kl_p} \sim 0.01$–$0.1$. Moreover, since the correlation time of fluctuations $\tau_c \ll \Delta t$, then the accelerations of particles $d^2\vec{l}_k/\Delta t^2$ (experimentally measured and used in (1)) correspond to time-averaged charges of the particles and interaction forces between them. Thus, fluctuations of dust particle charges should not significantly affect on recovery of interparticle interaction forces under the considered experimental conditions.

V. CONCLUSIONS

In this paper, we considered a possibility of experimental diagnostics of anisotropic interaction forces between dust particles in plasmas, arising due to effects of ion focusing. To recover anisotropic interparticle interaction forces, we improved the method based on solving the inverse Langevin problem. In order to simplify the experimental diagnostics, we propose to apply this method for an isolated vertically aligned dust chain which is formed in a glass cuvette mounted on the lower electrode of rf gas discharge chamber.[34]

We verified the method on the results of numerical simulation of chain structures of particles with quasidipole-dipole interaction, similar to the one occurring due to effects of ion focusing in gas discharges. It was shown that the proposed method can recover the spatial distribution of anisotropic interparticle interaction forces, and can be used for diagnostics of a laboratory dusty plasma with ion flow. For chain-like systems within which change in the charge of particles does not exceed 15%, the proposed method can be used without taking into account a spatial dependence of the particle charges. Fluctuations of the charges should not significantly affect on recovery of interparticle interaction forces at typical experimental conditions.

The results may be useful for studying dusty plasma systems with other types of anisotropic interactions, such as dusty plasmas with non-spherical grains.

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