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Polarization and Finite Size Effects in Correlation Functions of Dusty Plasmas

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An approach is presented to derive a pseudopotential model of interaction between dust particles that simultaneously takes into account the polarization, finite size and screening effects. The consideration starts from the assumption that the dust particles are hard balls made of a conductive material such that their mutual interaction and interaction with the electrons and ions of the buffer plasma can analytically be interpreted within the method of image charges. Then, the renormalization theory of plasma particles interaction, leading to the so-called generalized Poisson-Boltzmann equation, is applied to obtain the interaction potential of two isolated dust grains immersed into the buffer plasma of electrons and ions. After that the Ornstein-Zernike relation in the hyper-netted chain approximation (HNC) is numerically solved to study the radial distribution function and the static structure factor of the dust grains. In doing so the system of hard balls is actually replaced by a system of point-like charges with properly adjusted number density in the form of van der Waals correction. A straightforward comparison is made with the Monte-Carlo simulation to find a fairly good agreement for the radial distribution function at relatively high dust couplings.

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1 Introduction

These days strongly coupled Coulomb systems are still attracting much interest of the plasma physics community since they frequently appear in contemporary context ranging from nanotechnology [1–3] and Penning traps [4] to astrophysics [5–7]. One common feature that unifies such intrinsically various objects is strong interparticle interactions caused by the long-range electrostatic forces with the latter being responsible for notorious difficulties in theoretical description. It is, thus, rather obvious that the realm of strongly coupled plasmas cannot be theoretically covered by one single approach. Moreover, the entire apparatus of theoretical physics [8,9] and the simulation techniques [10,11] are engaged to correctly describe the whole range of phenomena occurring at such different scales.

A dusty plasma takes a very special place among the strongly coupled Coulomb systems since it is a fundamentally classical system whose behavior is readily visualized in rather sophisticated experimental researches. This provides a good opportunity to test theoretical approaches worked out for the past decades and to shed some light on what effect the strong interactions have on thermodynamic [12, 13] and transport [14, 15] properties of plasmas. Until very recently almost all investigations have been adapting the Yukawa potential to describe the interaction between the dust particles [16, 17]. As it will be shown below such an assumption implicitly implies that the dust particles are point-like charges which cannot be always true especially if the grain number density grows. This work solely focuses on the influence of finite dimensions of dust particles on such measurable macroscopic characteristics as the radial distribution function and the static structure factor.

2 Dusty plasma parameters

Let the dust particles, called grains, be merged into a two-component hydrogen plasma consisting of free electrons with the electric charge -e and the number density n_e , and free protons with the electric charge e and the number

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density n_p . It is assumed hereinafter that the dust particles are metallic hard balls of radius R and possess the negative electric charge $-Z_d e$ with Z_d being the grain charge number. Since an ordinary plasma medium must remain quasineutral, the equality $n_p = n_e + Z_d n_d$ should essentially be held with n_d being the dust particle number density.

The state of the buffer hydrogen plasma is described by the density parameter $r_s = a/a_B$, where $a_e = (3/4\pi n_e)^{1/3}$ stands for the average distance between free electrons in the buffer plasma, $a_B = \hbar^2/m_e e^2$ is the very well known first Bohr radius, \hbar designates the reduced Planck constant and m_e denotes the electron mass. The coupling parameter of the buffer plasma $\Gamma = e^2/a_e k_B T$ represents the ratio of the average Coulomb interaction and thermal kinetic energies of free electrons. Here k_B denotes the Boltzmann constant and T stands for the plasma temperature.

The interrelation between the dust component and the buffer plasma is introduced by the Havnes parameter $P = Z_d n_d/n_e$ that determines the ratio of the charge densities of the dust and electron components [18], as well as by the screening parameter $\kappa = a_d/\lambda_D$, with $\lambda_D = (k_B T/4\pi (n_e + n_p)e^2)^{1/2}$ being the Debye screening length and $a_d = (3/4\pi n_d)^{1/3}$ being the mean intergrain spacing. The main objective in the sequel is to consistently treat the finite dimensions of dust particles that are to be characterized by the grain size parameter $D = a_d/R$.

It has to be strictly emphasized that numerical values of plasma parameters, i.e. all the number densities and the plasma temperature, are simply retrieved if all magnitudes of the dimensionless parameters mentioned above are thoroughly specified.

3 Intergrain interaction model

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As it has already been mentioned above the grains are assumed to be metallic charged balls such that the interaction micropotentials between the dusty plasma constituents are found in the framework of the image charge method as follows [19]:

$$\varphi_{ee}(r) = \varphi_{pp}(r) = -\varphi_{ep}(r) = \frac{e^2}{r},$$
(1)

$$\varphi_{ed}(r) = \frac{Z_d e^2}{r} - \frac{e^2 R^3}{2r^2(r^2 - R^2)}, \ \varphi_{pd}(r) = -\frac{Z_d e^2}{r} - \frac{e^2 R^3}{2r^2(r^2 - R^2)}, \tag{2}$$

$$\varphi_{dd}(r) = \frac{Z_d^2 e^2}{R} \left[\frac{1}{\sinh \beta \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{\sinh n\beta}} - 1 \right].$$
(3)

where $\cosh \beta = r/2R$.

It is seen from (2) that the electrostatic induction results in that the interaction of a charged particle with a metallic charged ball comprises, together with the pure Coulomb interaction, an additional term corresponding to the attraction of the charged particle with an induced image charge of opposite sign. It can be learnt from formula (3) an infinite number of image charges must be taken into account in describing the interaction between two charged metallic balls.

It makes no sense to consider the penetration of the electrons and the protons into the dust particle since it only alters the grain charge already accounted for by the introduction of the grain charge number Z_d . The same can be said about the interpenetration of grains. Thus, to treat the finite size effects in interaction potentials (2) and (3) the substitutions $\varphi_{d(e,p)}(r) \rightarrow \varphi_{d(e,p)}(r+R)$, $\varphi_{dd}(r) \rightarrow \varphi_{dd}(r+2R)$ are made to imply that the distances between the particles involved are now counted from the grain surface. Such a shift in distance counting is introduced in order to correctly derive the Fourier transforms of interaction potential (2) and (3) needed for all further consideration. At the same time this means that the system of hard balls is virtually substituted by the system of point-like charges with the appropriately modified interaction potential. What other consequences such a treatment has on the collective events in plasmas is discussed in the following section. The Fourier transforms of micropotentials (1), (2) and (3) take the form:

$$\tilde{\varphi}_{ee}(k) = \tilde{\varphi}_{pp}(k) = -\tilde{\varphi}_{ep}(k) = \frac{4\pi e^2}{k^2},\tag{4}$$

$$\tilde{\varphi}_{pd}(k) = -\frac{4\pi Z_d e^2}{k^2} + \frac{4\pi Z_d e^2 R}{k} \left[\operatorname{Ci}(kR) \sin(kR) + \frac{1}{2} \cos(kR) (\pi - 2\operatorname{Si}(kR)) \right] - \frac{\pi e^2 R}{k} \times \left[2\operatorname{Ci}(kR) \sin(kR) - 2\operatorname{Ci}(2kR) \sin(2kR) + \cos(kR) (\pi - 2\operatorname{Si}(kR)) - \cos(2kR) (\pi - 2\operatorname{Si}(2kR)) \right] - \frac{1}{2} \cos(kR) \left[-\cos(kR) (\pi - 2\operatorname{Si}(kR)) - \cos(kR) (\pi - 2\operatorname{Si}(kR)) \right]$$
(5)

$$\tilde{\varphi}_{ed}(k) = \frac{4\pi Z_d e^2}{k^2} - \frac{4\pi Z_d e^2 R}{k} \left[\operatorname{Ci}(kR) \sin(kR) + \frac{1}{2} \cos(kR) (\pi - 2\operatorname{Si}(kR)) \right] - \frac{\pi e^2 R}{k} \times \left[2\operatorname{Ci}(kR) \sin(kR) - 2\operatorname{Ci}(2kR) \sin(2kR) + \cos(kR) (\pi - 2\operatorname{Si}(kR)) - \cos(2kR) (\pi - 2\operatorname{Si}(2kR)) \right] - \frac{\pi e^2 R}{k}$$
(6)

$$\tilde{\varphi}_{dd}(k) = \frac{4\pi Z_d^2 e^2}{k^2} + \frac{Z_d^2 e^2 R f(k)}{k} - \frac{8\pi Z_d e^2 R}{k} [\operatorname{Ci}(2kR) \sin(2kR) + \frac{1}{2} \cos(2kR)(\pi - 2\operatorname{Si}(2kR))],$$
(7)

where f(k) is a known interpolating function.

To account for the screening effects in the interaction of two isolated dust particles the following generalized Poisson-Boltzmann equation is applied [20]:

$$\Delta_i \Phi_{ab}(\mathbf{r}_i^a, \mathbf{r}_j^b) = \Delta_i \varphi_{ab}(\mathbf{r}_i^a, \mathbf{r}_j^b) - \sum_{c=e,p} \frac{n_c}{k_B T} \int \Delta_i \varphi_{ac}(\mathbf{r}_i^a, \mathbf{r}_k^c) \Phi_{cb}(\mathbf{r}_j^b, \mathbf{r}_k^c) d\mathbf{r}_k^c, \tag{8}$$

with n_c being the number density of particle species c. Note that in equation (8) the summation is only taken over the free electrons and protons of the buffer plasma, c = e, p, whereas the number density of dust particles is kept to be zero. It is deliberately done since of interest is the interaction of two isolated grains whose screening is realized by the electrons and protons of the buffer plasma.

Note that the generalized Poisson-Boltzmann equation can be strictly derived from the Bogolyubov hierarchy for the equilibrium distribution functions in the pair correlation approximation [21]. Moreover, in the past decade it was successfully applied to a variety of plasmas, such as semiclassical [22], partially ionized [23, 24] or even dusty plasmas in the Debye approximation [25]. Some of those results were then successfully used to neatly describe experimental data on X-ray scattering in dense plasmas [26, 27].

In virtue of (8), the microscopic potentials φ_{ab} determine the intergrain potential Φ_{dd} which takes into account the screening phenomena due to the electrons and protons of the buffer plasma by incorporating the corresponding number densities. In the Fourier space, the set of equations (8) turns into a set of linear algebraic equations whose solution for the intergrain interaction potential is found as:

$$\tilde{\Phi}_{dd}(k) = \tilde{\varphi}_{dd}(k) - \frac{A_p \tilde{\varphi}_{pd}^2(k) + A_e \tilde{\varphi}_{ed}^2(k) - A_e A_p \tilde{\varphi}_{ee}(k) [\tilde{\varphi}_{ed}^2(k) + \tilde{\varphi}_{pd}^2(k) + 2\tilde{\varphi}_{ed}(k)\tilde{\varphi}_{pd}(k)]}{1 + (A_e + A_p)\tilde{\varphi}_{ee}(k)}, \quad (9)$$

where $A_{e,p} = n_{e,p}/k_B T$.

The expression for the intergrain potential in the configuration space is utterly obtained from (9) by the inverse Fourier transform

$$\Phi_{dd}(\mathbf{r}) = \int \tilde{\Phi}_{dd}(k) \exp(-i\mathbf{k}\mathbf{r}) d\mathbf{k}.$$
(10)

It is worth noting that under the present consideration the dust particles have absolutely no effect on the interaction of the buffer plasma particles, i.e. the free electrons and protons. At the same time the well used Yukawa potential is a limiting case of the above expressions when $R \rightarrow 0$, i.e. when the dust particles are assumed to be point-like charges to entirely ignore their finite dimensions.

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As it has been mentioned above expressions (9) and (10) simultaneously take into account the finite size of grains, the shielding of their electric field due to the buffer plasma and the polarization phenomena. A theoretical analog of the present approach is the dielectric medium approximation [28] in which the screening in the intergrain interaction is accounted for by the dielectric function of the buffer plasma. The only drawback of both methods is that the dusty plasma is meant to be in equilibrium state which somehow restricts the applicability of the results to real dusty plasma experiments. Nevertheless, deviations of the particle distribution functions from the Maxwellian, caused by the so-called absorption and shadowing effects. can easily be handled to show that the Yukawa potential turns invalid at rather large distances between grains [29–31]. Moreover, under certain external conditions the free flight paths of the buffer plasma particles may turn less in magnitude than the Debye shielding length and, thus, an increasingly important role is played by interparticle collisions that result in ion trapping in the vicinity of dust particles [32] or even requires an application of hydrodynamics to correctly treat the plasma shielding effect [33]. It has to be admitted that real dust grains are hardly spherical in shape which leads to non-zero dipole moments of dust particles and, as a consequence, to anisotropic interactions between them [34]. The intergrain interaction potential can yet be determined experimentally with the aid of some theoretical arguments which, for example, was done in [35] for the rf discharge dusty plasma in the framework of the Langevin dynamics.

4 Correlation functions of dusty plasmas

It has already been stressed in the previous section that the present consideration essentially stems from the insight that the system of metallic hard balls is to be replaced by the system of point-like charges. This has immediate effect on the interaction between two particular grains since if the number density of dust particles is left unchanged, then, the average interaction energy will inevitably decrease because the distance between grains is now counted from their surfaces. Thus, the grain number density should be adjusted for the average interaction energy to stay the same which is simply achieved by the idea of van der Waals when he introduced his famous correction for the finite size of atoms into the ideal gas equation of state. In particular, the effective number density of dust particles n_d^{eff} is proposed to take the following form:

$$n_d^{eff} = \frac{n_d}{1 - \frac{4\pi n_d R^3}{3\Delta}}.$$
(11)

Here $\Delta = \pi/\sqrt{18}$ stands for the packing parameter of the hexagonal packing of hard balls which is believed to be the most compact of all possible packings in the theory of condensed matter physics. The idea is to only consider the volume available to the dust particles such that the grains should completely lose their mobility when the packing becomes the most compact and the distance between the surfaces of two adjacent dust particles turns zero. In this particular case the effective number density of dust particles turns infinite and the real average distance between them becomes equal to 2R as it should be.

Neither the number density of dust particles nor its effective counterpart does enter interaction potential (9) and (10) that virtually holds for the interaction energy of two isolated grains whose shielding is performed by the electrons and protons of the buffer plasma. It is therefore fully justified to further apply the constructed effective potential model in well-tested theoretical approaches and computer simulation techniques treating the collective events for dust particles as it is routinely done in a one-component system. One of the reliable methods for studying system correlation functions is the method of integral equations [36, 37]. In particular, the Ornstein-Zernike relation in the hyper-netted chain approximation (HNC) is numerically solved with the effective number density introduced above to obtain the radial distribution function of dust particles whose non-monotonic behavior is portrayed in Figures 1 and 2 to clearly demonstrate the short- or even long-range order formation. A comparison is also made with the Monte-Carlo simulations with the same interaction potential between grains to find a fairly good agreement at rather high values of the dust coupling.

Figures 3 and 4 show non-monotonic behavior of the static structure factor calculated within the HNC for different values of the grain size parameter. The maxima and minima, interpreted as an order formation, turn less pronounced when the polarization phenomena are properly taken into account since they always weaken repulsion between the dust particles. Analogous inference can absolutely be made in case of the decrease in

the grain size parameter *D*.Note that quite a similar behavior of the correlation function was observed in the Percus-Yewick and superposition approximations with further experimental verification for the gas-discharge plasmas [38], cf. [39, 40].



Fig. 1 Radial distribution function g_d of grains against the dimensionless distance r/a_d at $\Gamma = 0.2$, P = 5, $\kappa = 4$ and D = 2. Blue line: without polarization phenomena; red line: with polarization phenomena; circles: corresponding Monte-Carlo simulation data.



Fig. 3 Static structure factor S_{dd} of grains against the dimensionless wavenumber ka_d at $\Gamma = 0.2$, P = 5 and $\kappa = 4$ with the polarization phenomena taken into account. Red line: D = 2; blue line: D = 2; green line: D = 8.



Fig. 2 Radial distribution function g_d of grains against the dimensionless distance r/a_d at $\Gamma = 0.2$, P = 5, $\kappa = 4$ and D = 8. Blue line: without polarization phenomena; red line: with polarization phenomena; circles: corresponding Monte-Carlo simulation data.



Fig. 4 Static structure factor S_{dd} of grains against the dimensionless wavenumber ka_d at $\Gamma = 0.2$, P = 5 and $\kappa = 4$ without the polarization phenomena taken into account. Red line: D = 2; blue line: D = 2; green line: D = 8.

5 Conclusions

This paper has studied the correlation functions of dust particles starting from the original interaction model taking into account the polarization phenomena, the finite size of grains and the screening due to the buffer plasma particles. The grains have been assumed to be metallic hard balls to take into account the polarization phenomena by invoking the image charge method. Then, the generalized Poisson-Boltzmann equation has been utilized to

appropriately treat the shielding of electric fields. The main idea behind this paper is to substitute the hard ball system of interest by a system of point-like particles with the properly introduced effective number density as it is regularly done in the van der Waals equation of state of real gases. In particular, the Ornstein-Zernike relation in the hyper-netted chain approximation has been iteratively solved with the effective number density of grains and highly pronounced peaks in the curve of the radial distribution function and the static structure factor unveils the short- or even long-range order formation in the system.

It is concluded on the basis of the above stated results that the polarization effects weaken the intergrain interaction energy as compared to the case of taking into account the finite size effects only which manifests itself in that the corresponding peaks in the correlation functions decrease in height with a shift to smaller values of the distance or the wavenumber, respectively. The Monte-Carlo simulations have shown a satisfactory agreement for the radial distribution function at relatively high values of the dust coupling.

References

- [1] T. Stauber, J. Schliemann and N.M.R. Peres, Phys. Rev. B 81, 085409 (2010).
- [2] A. Scholz and J. Schliemann, Phys. Rev. B 83, 235409 (2011).
- [3] A. Scholz, T. Stauber, J. Schliemann, Phys. Rev. B 86, 195424 (2012).
- [4] D. Dubin, Phys. Rev. A 88, 013403 (2013).
- [5] R. Redmer, T. Mattsson, and N. Nettelmann, M. French, Icarus 211, 798 (2011).
- [6] J. Leconte and G. Chabrier, Nature Geoscience 6, 347 (2013).
- [7] L. Zeng and D. Sasselov, Astrophys. J., 784:96 (2014).
- [8] M.W.C. Dharma-wardana, Phys. Rev. E 86, 036407 (2012).
- [9] J. Dufty and S. Dutta, Phys. Rev. E 87, 032101 (2013).
- [10] T. School, M. Bonitz, and A. Filinov, D. Hochstuhl, J.W. Dufty, Contrib. Plasma Phys. 51, 687 (2011).
- [11] V.S. Filinov, M. Bonitz, Y.B. Ivanov, P.R. Levashov, and V.E. Fortov, Contrib. Plasma Phys. 52, 135 (2012).
- [12] B.P. Pandey, Phys. Rev. E 69, 026410 (2004).
- [13] O.S. Vaulina, X.G. Koss, Yu.V. Khrustalyov, O.F. Petrov, and V.E. Fortov, Phys. Rev. E 82, 056411 (2010).
- [14] A. Shahzad and M.-G. He, Contrib. Plasma Phys. 52, 667 (2012).
- [15] V.S. Karakhtanov, R. Redmer, H. Reinholz, and G. Röpke, Contrib. Plasma Phys. 53, 639 (2013).
- [16] T. Ott, H. Löwen, and M. Bonitz, Phys. Rev. E 89, 0.13105 (2014).
- [17] J. Goree, Z. Donko, P. Hartmann, Phys. Rev. E 85, 066401 (2012).
- [18] O. Havnes, C. Goertz, G. Morfill, E. Grün, and W. Ip, J. Geophys. Res. 92, 2281 (1987).
- [19] V.A. Saranin, V.V. Mayer, Physics-Uspekhi 53:10, 1067 (2010).
- [20] Yu.V. Arkhipov, F.B. Baimbetov, and A.E. Davletov, Phys. Rev. E 83, 016405 (2011).
- [21] Yu.V. Arkhipov, F.B. Baimbetov, A.E. Davletov, and T.S. Ramazanov, Contrib. Plasma Phys. 39, 495 (1999).
- [22] Yu.V. Arkhipov, F.B. Baimbetov, A.E. Davletov, and K.V. Starikov, J. Plasma Phys. 68, 81 (2002).
- [23] Yu.V. Arkhipov, F.B. Baimbetov, and A.E. Davletov, Phys. Plasmas 12, 082701 (2005).
- [24] Yu.V. Arkhipov, F.B. Baimbetov, and A.E. Davletov, Contrib. Plasma Phys. 43, 258 (2003).
- [25] F.B. Baimbetov, A.E. Davletov, Zh.A. Kudyshev, and E.S. Mukhametkarimov, Contrib. Plasma Phys. 51, 533 (2011).
- [26] G. Gregori, S.H. Glenzer, W. Rozmus, R.W. Lee, and O.L. Landen, Phys. Rev. E 67, 026412 (2003).
- [27] G. Gregori, S.H. Glenzer, and O.L. Landen, J. Phys. A: Math. Gen. 36, 5671 (2003).
- [28] V. Tsytovich and U. de Angelis, Phys. Plasmas 8, 1141 (2001).
- [29] S. Khrapak, B. Klumov, and G. Morfill, Phys. Rev. Lett. 100, 225003 (2008).
- [30] S. Khrapak, A. Ivlev, G. Morfill, Phys. Rev. E 64, 046403 (2001).
- [31] A. Filippov, A. Zagorodny, A. Pal', A. Starostin, and A. Momot, JETP Lett. 86, 761 (2008).
- [32] M. Lampe, R. Goswami, Z. Sternovsky, S. Robertson, V. Gavrishchaka, G. Ganguli, and G. Joyce, Phys. Plasmas 10, 1500 (2003).
- [33] P. Tolias and S. Ratynskaia, Phys. Plasmas 20, 023702 (2013).
- [34] I. Lisina and O. Vaulina, EPL **103**, 55002 (2013).
- [35] O. Vaulina, E. Lisin, A. Gavrikov, O. Petrov, and V. Fortov, Phys. Rev. Lett. 103, 035003 (2009).
- [36] C.E. Starrett and D. Saumon, High Energy Density Physics **10**, 35 (2014).
- [37] S. Dutta and J. Dufty, Phys. Rev. E 87, 032102 (2013).
- [38] V. Fortov, O. Petrov, and O. Vaulina, Phys. Rev. Lett. 101, 195003 (2008).
- [39] L.T. Erimbetova, A.E. Davletov, Zh.A. Kudyshev, and Ye.S. Mukhametkarimov, Contrib. Plasma Phys. 53, 414 (2013).
- [40] A.E. Davletov, L.T. Yerimbetova, Ye.S. Mukhametkarimov, and A.K. Ospanova, Phys. Plasmas 21, 073704 (2014).