### Analytical model of particle charging in plasmas over a wide range of collisionality

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An accurate prediction of the particle charge in plasmas is of fundamental importance for a wide range of problems from the study of dusty or complex plasmas to the controlled synthesis of nanoparticle materials in plasmas. Despite its known deficiencies, the orbital motion limited (OML) theory, which strictly applies only to collisionless plasmas, is the most widely used model to describe particle charging. This paper develops a simple, analytical model to describe the charging of particles in plasmas over a wide range of pressures and particle sizes. In spite of its simplicity, excellent agreement is found with results of a self-consistent molecular dynamics Monte Carlo model and with experimental results found in the literature. In particular, the model presented here provides significant improvements compared to the OML theory.

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## I. INTRODUCTION

The charging of particles is arguably the most important mechanism governing the interaction between plasmas and particles. Significant advances have been made in understanding charging of micron-sized particles used in complex plasma studies [1–11]. However, the situation for nanometersized particles remains surprisingly confused.

Part of the problem with the accurate description of particle charging is the prevalent use of orbital motion limited (OML) theory to describe electron and ion capture by particles. The original OML theory (see Ref. [12] for a review) assumes that the effective potential around a particle, i.e., the sum of the electrostatic and centrifugal potentials, decreases monotonically towards the particle. The simple expressions derived under this assumption are widely used in models for nanoparticle charging [13–17]. A number of shortcomings of the OML theory are now well established. As pointed out by Allen [12,18] and Daugherty et al. [19], a maximum in the effective potential can arise when the electrostatic potential varies more steeply than  $1/r^2$ , leading to a reflection of ions whose total energy is smaller than this potential barrier, an effect neglected in the original OML theory. However, for particles small compared to the Debye length, this effect is expected to be small [2,19].

More critical, however, is the OML theory's neglect of trapped ions. Trapped ions are generated by charge-exchange collisions of energetic ions with less energetic neutrals in the sheath around the particle, leading to ions with negative total energy, which are trapped around the particle. As shown by Goree [4], this effect can become important even for very low charge-exchange collision frequencies  $v_{cx}$ , since both the trapping and detrapping rate are proportional to  $\nu_{cx}$ . The molecular dynamics simulation by Zobnin et al. [3] suggest that the neglect of trapped ions causes the classical OML theory to overpredict the negative particle potential by a factor of  $\sim$ 2. Lampe and co-workers developed an elegant, largely analytical theory to describe trapped ions [1,2]. Their results were consistent with Zobnin's and showed that trapped ions can be more important than untrapped ions in screening the particle potential and for the ion flux towards the particle surface. Recent experiments performed with micron-sized particles suspended in a positive column [10,20] show good agreement with Zobnin's model [3] and confirm the OML theory's overestimation of the particle charge by a factor of 2-3. In a more recent study Rovagnati et al. [21], using a particle-in-cell Monte Carlo collision method, essentially confirmed the results of Ref. [3]. However, the authors also demonstrated the importance of considering the details of the electron-neutral and ion-neutral collision processes, which can lead to non-Maxwellian distribution functions close to the particle and to deviations from the more simple theory in [3].

In 2005 Khrapak *et al.* [10] proposed a simple analytical model based on the idea of a capture radius, i.e., a radius at which the total energy of an ion that is created in a chargeexchange collision event is smaller than  $-kT_{g}$ , with k the Boltzmann constant and  $T_g$  the gas temperature. Such ions are essentially trapped in the potential field of the charged particle and are bound to eventually be collected by the particle. Based on this simple idea, the authors derived an expression for the collision-enhanced ion current in the weakly collisional regime that was identical to the one previously obtained by Lampe [1]. In 2007 D'yachkov et al. [22] developed an analytical model that significantly expanded the range of validity in terms of the collisionality of the ion motion from the collisionless, i.e., OML regime all the way to the strongly collisional, hydrodynamic range. Different from the idea of a capture radius, the authors subdivided the solution domain for their problem into two ranges: (1) a collisionless layer around the particle of the thickness  $\lambda_{i(e)}$ , the collision mean free path of ions (electrons), in which the particle motion was described within the framework of the OML theory; and (2) the space outside of this collisionless layer, in which a hydrodynamic approach was used to describe the electron and ion transport to the particle. The authors' model successfully described the collision-induced reduction of the particle charge found in Zobnin's molecular dynamics simulations [3] and in some experiments.

One consequence of D'yachkov et al.'s [22] assumptions is that the resulting normalized particle potential exhibits no explicit dependence on the particle size but rather only on the particle Knudsen number  $Kn_a = \lambda_i / a$ , with a the particle radius. While this is an attractive feature of the model, it is not a priori clear that it correctly describes reality. Moreover, the model proposed in [22] abandons the attractive, since physically motivated, concept of a capture radius. In this paper, we demonstrate that based on the capture radius concept, an equally elegant and more accurate model as in [22] can be developed. Different from [22], this model captures the explicit dependence of the particle charge on the particle size. It will also be shown that results of the model are in good agreement with molecular dynamics simulations and that they agree better with available experimental data than the model in [22]. Furthermore, effects of high particle concentration leading to a strong depletion of the free electron density in the plasma are consistently taken into account.

### **II. MOLECULAR DYNAMICS SIMULATION**

As a benchmark for the semianalytical model proposed here, a self-consistent molecular dynamics (MD) Monte Carlo model was developed, largely following Zobnin's work [3]; details on its implementation can be found in that reference. The ion equation of motion is integrated using a velocity Verlet scheme, which is symplectic. The time step is limited by the requirement of resolving the ion motion close to the particle and it can be estimated as

$$dt \approx a \sqrt{\frac{m_i}{2e|V_{OML}|}}.$$
 (1)

Here  $m_i$  is the ion mass, and  $V_{OML}$  is the particle potential as predicted by the OML theory (see below). Our model differs from the one in [3] only in the choice of cross sections and in the inclusion of the effects of high particle concentrations. The gas considered here is argon. As the cross sections of elastic scattering and resonant charge transfer for argon ions in argon are of comparable magnitude [23], both processes are considered using the cross sections from [24]. The effect of high particle density, which leads to a reduction of the free plasma electron density, is taken into account by forcing the simulation cell to be quasineutral over the average volume occupied by a particle.

$$4\pi \int_{a}^{L_{p}} [n_{i}(r) - n_{e}(r)]r^{2}dr + Q = 0 \quad \text{and} \quad L_{p} = \sqrt[3]{\frac{3}{4\pi n_{p}}},$$
(2)

where  $n_i$ ,  $n_e$ , and  $n_p$  are the ion, electron, and particle density, respectively; r is the radius measured from the center of the particle and Q is the particle charge. While Eq. (2) has been formulated for the vicinity of one particle, it implies an infinitely extended plasma in which the overall charge balance between electrons residing on the particles, free electrons, and positive ions needs to be conserved. This condition is satisfied by adjusting the unperturbed electron density  $n_{e0}$ . In order to obtain a self-consistent solution, the Poisson equation, the analytical expression for the electron density [3], and Eq. (2) are solved iteratively.

Assuming a Maxwell-Boltzmann electron energy distribution, the electron current reaching the particle is calculated as



FIG. 1. (Color online) Normalized particle potential z as a function of the capture radius Knudsen number  $\text{Kn}_{R_0}$  for a particle with a diameter of 500 nm,  $n_{i0}=10^{10}$  cm<sup>-3</sup>,  $T_e=2.5$  eV,  $T_i=0.025$  eV, and  $n_p/n_{i0}\approx 0$ . Also plotted are the probabilities of performing zero  $(P_0)$ , one  $(P_1)$ , and more than one collision  $(P_{>1})$  inside the capture radius sphere.

$$I_e = \pi a^2 n_{e0} \left( \frac{8kT_e}{\pi m_e} \right)^{1/2} \exp\left(\frac{eV_p}{kT_e}\right),\tag{3}$$

where  $T_e$  and  $m_e$  are the electron temperature and mass, respectively, and  $V_p$  is the particle potential. While non-Maxwellian electron distribution functions have been observed in the simulations in [21], we here use the Maxwellian assumption in order to be able to compare our results with other literature results. However, the electron current (3) could easily be modified to account for non-Maxwellian electron distribution functions. While Eq. (3) represents a continuous current, the particle charge is only updated after an integer elementary charge was deposited on the particle. This can become important for small particles for which one elementary charge causes a significant change of the particle potential.

Simulations were performed for a range of background gas pressures from  $10^{-5}-10^5$  Pa, particle diameters from 10 nm-1  $\mu$ m, and fractions of negative charges residing on the particles from 0–98 %, and for two electron temperatures of 2.5 and 5.0 eV. The unperturbed ion density  $n_{i0}$  was kept constant at  $10^{10}$  cm<sup>-3</sup> and the ion temperature was 0.025 eV.

Figure 1 shows results of the molecular dynamics simulation for a particle with a diameter of 500 nm. The normalized particle potential  $z=-eV_p/kT_e$  is shown as a function of the particle Knudsen number Kn<sub>a</sub> in the insert. At high Knudsen numbers (low pressures) the MD results converge toward the classical OML theory. At high pressures and small Kn<sub>a</sub> the particle potential approaches the result of the hydrodynamic limit. At intermediate Knudsen numbers Kn<sub>a</sub>  $\approx 10^2$ , the normalized particle potential has a minimum, at  $z\approx 0.5$ , i.e., five times smaller than the potential is a result of the collision enhancement of the ion current, as already shown in [1,3,10].

However, the minimum of z occurs at  $\text{Kn}_a \approx 10^2$ . This suggests that the particle Knudsen number is not the natural

variable to describe the transition from the OML to the hydrodynamic regime. For a sensibly defined Knudsen number, the transition is expected to appear around 1. We propose that a rational Knudsen number for the problem of particle charging needs to be defined in terms of the capture radius, rather than the particle radius. Following [10], we define the capture radius  $R_0$  of an ion with kinetic energy  $E_{kin}$  through  $E_{kin}+U(R_0)=0$ , where U=U(r) is the ion potential energy, which is a priori unknown. To derive an estimate for  $R_0$ , we approximate U by a linearized Yukawa potential as follows:

$$U(r) = eV_p \frac{a}{r} \exp\left(-\frac{r-a}{\lambda_{DL}}\right) \approx eV_p \frac{a}{r} \left[1 - \frac{r-a}{\lambda_{DL}}\right], \quad (4)$$

with  $\lambda_{DL}$  the linearized Debye length, defined by  $1/\lambda_{DL}^2$ = $1/\lambda_{Di}^2 + 1/\lambda_{De}^2$  with  $\lambda_{Di}$  and  $\lambda_{De}$  the ion and electron Debye lengths, respectively [19]. The numerical investigation in [19] revealed that the Yukawa potential using the linearized Debye length is a good approximation of the actual potential as long as the particle radius is smaller than  $\lambda_{DL}$ . Defining  $R_0$ as the radius at which  $R_0$  equals the ion kinetic energy  $E_{kin}$ , we find

$$R_0(E_{kin}) = \frac{e|V_p|a\left(1 + \frac{a}{\lambda_{DL}}\right)}{E_{kin} + e|V_p|\frac{a}{\lambda_{DL}}}.$$
(5)

We now define the capture radius Knudsen number as  $\text{Kn}_{R_0} = \lambda_i / (2\alpha R_0)$ , with

$$\alpha R_0 = \int_0^\infty R_0(E_{kin}) f(E_{kin}) dE_{kin} = 1.22 R_0 \left(\frac{3}{2} k T_i\right).$$
(6)

The factor  $\alpha = 1.22$  arises from the energy dependence of the capture radius when averaged of a Maxwellian distribution f of ion energies. In the following, we denote  $R_0(3kT_i/2)$  with  $R_0$  for simplicity. As can be seen from Fig. 1, the minimum of the normalized particle potential appears at  $\text{Kn}_{R_0} \approx 1$ . This suggests that the capture radius Knudsen number is the natural variable to describe the problem. Further shown in Fig. 1 are the probabilities of an ion approaching the particle from the unperturbed plasma to perform zero, exactly one, and more than one collision [25] inside the capture radius sphere.

$$P_0 = \exp\left(-\frac{1}{\mathrm{Kn}_{R_0}}\right),\tag{7a}$$

$$P_1 = \frac{1}{\mathrm{Kn}_{R_0}} \exp\left(-\frac{1}{\mathrm{Kn}_{R_0}}\right),$$
 (7b)

$$P_{>1} = 1 - (P_0 + P_1). \tag{7c}$$

Figure 1 demonstrates that there is a strong correlation between the minimum in the normalized particle potential and the maximum in the probability of performing one collision inside  $R_0$ . This suggests that the collision-enhancement of the ion current is maximum if most ions perform one collision within the capture radius sphere. These ions become trapped and will eventually be collected by the particles, possibly after further collisions. The increase of the normalized potential when  $P_{>1}$  dominates is related to the increasing collisional inhibition of the ion transport to the particle in the hydrodynamic regime.

#### **III. ANALYTICAL MODEL**

The overall behavior of the collision probabilities in Fig. 1 suggests that  $P_0$ ,  $P_1$ , and  $P_{>1}$  are characteristic for the contributions of the OML, the collision-enhanced, and the hydrodynamic ion transport to the particle. Based on this observation, we propose an analytical model for the ion current for the entire range of  $Kn_{R_0}$  by accounting for three components, i.e., the OML, collision-enhanced, and hydrodynamic ion currents, which are weighed by  $P_0$ ,  $P_1$ , and  $P_{>1}$ , respectively. Therefore,

$$I_i = P_0 I_i^{OML} + P_1 I_i^{CE} + P_{>1} I_i^{HY}.$$
 (8)

Expressions for  $I_i^{OML}$  and  $I_i^{HY}$  were derived in [10]. The collision-enhanced ion current  $I_i^{CE}$  is estimated by the thermal flux of ions crossing a sphere around the particle defined by average capture radius.

$$I_i^{OML} = \pi a^2 v_{i,th} n_{i,0} \left( 1 - \frac{eV_P}{kT_i} \right), \tag{9a}$$

$$I_i^{CE} = \pi (\alpha R_0)^2 n_{i0} v_{i,th}, \qquad (9b)$$

$$I_i^{HY} = 4\pi a n_{i,0} \mu_i |V_p|.$$
(9c)

Here  $v_{i,th}$  is the thermal velocity of ions and  $\mu_i$  is the ion mobility.

It is obvious that the approach used in Eq. (8) correctly describes the two limiting cases for the ion current, i.e., the collisionless OML limit at very low pressures and the collisional hydrodynamic limit at large pressures. There are many examples in plasma sheath theory, where the hydrodynamic approach still yields a reasonable approximation even in the case when ions perform only a few collisions in the sheath (e.g., [26]). Hence the collision probability  $P_{>1}$  has been defined to fade in this effect already for weakly collisional cases. The rationale for including a contribution of the collision-enhanced current is to approximate the effect of ions that get collected by the particle as a result of a single collision while traveling through the capture radius sphere. As a result of this collision event, ions get transformed from initially free ions with positive total energy into trapped ions with negative total energy. These ions will eventually get collected by the particle, however, the details of the actual capture process do not need to be known. Thus in steady state, one only requires knowledge of the frequency with which ions are being trapped in the capture sphere (represented by  $P_1 I_i^{CE}$ ).

Using these arguments, the total ion current including all three components becomes,



FIG. 2. (Color online) Comparison of MD and analytical results for  $\tau$ =100, M=1.37×10<sup>-5</sup>, at low particle number density for three different particle sizes at different levels of collisionality. (*a* =250 nm:  $\eta$ =46.8; *a*=50 nm:  $\eta$ =234; *a*=5 nm:  $\eta$ =2340).

$$I_{i} = \pi a^{2} v_{i,th} n_{i,0} \left[ \left( 1 - \frac{eV_{P}}{kT_{i}} \right) + \frac{2\alpha^{3}R_{0}^{3}}{a^{2}\lambda_{i}} \right] \exp\left(-\frac{2\alpha R_{0}}{\lambda_{i}}\right) + 4\pi a n_{i,0} \mu_{i} |V_{P}| \left[ 1 - \left( 1 + \frac{2\alpha R_{0}}{\lambda_{i}} \right) \exp\left(-\frac{2\alpha R_{0}}{\lambda_{i}}\right) \right].$$

$$(10)$$

We now define some important nondimensional quantities:  $\tau = T_e/T_i$ ,  $\eta = \lambda_{DL}/a$ , and  $M = m_e/m_i$ . Equating expression (10) for the ion current with the OML electron current (8), using the Einstein relation, and remembering that the diffusion coefficient can be expressed as  $D_i = [3\pi/(16\sqrt{2})]v_{i,th}\lambda_i$ , we obtain the following equation:

$$\frac{n_{i,0}}{n_{e,0}} \sqrt{\frac{M}{\tau}} \Biggl\{ (1+\tau z) + \frac{2[2\alpha z \tau(\eta+1)]^3}{\mathrm{Kn}_a(3\eta+2z\tau)^3} \\ + \frac{3\pi}{4\sqrt{2}} \mathrm{Kn}_a \tau z \Biggl[ \exp\Biggl(\frac{4\alpha z \tau(\eta+1)}{\mathrm{Kn}_a(3\eta+2z\tau)} \Biggr) \\ - \Biggl(1 + \frac{4\alpha z \tau(\eta+1)}{\mathrm{Kn}_a(3\eta+2z\tau)} \Biggr) \Biggr] \Biggr\} \\ \times \exp\Biggl(-\frac{4\alpha z \tau(\eta+1)}{\mathrm{Kn}_a(3\eta+2z\tau)} \Biggr) \exp(z) = 1.$$
(11)

For given nondimensional parameters M,  $\tau$ ,  $\eta$ , and  $\text{Kn}_a$ , Eq. (11) is a nonlinear equation for the normalized particle potential z. While this equation could be written in a more compact form if expressed in terms of the capture radius  $R_0$  or the capture radius Knudsen number  $\text{Kn}_{R_0}$ , these parameters are a function of the particle potential and therefore not suitable to be used as independent parameters.

Figure 2 shows the comparison between the MD results for z and the values obtained with Eq. (11) for different particle sizes. For clarity, we plot the results against the capture Knudsen number  $Kn_{R_0}$ , rather than the particle Knudsen number  $Kn_a$ , which was used as an independent parameter. It is obvious that the simple analytical model proposed with



FIG. 3. (Color online) Sensitivity analysis of the importance of the definition of the capture radius  $\alpha R_0$  for particles with diameters of 100 and 1000 nm. Different values of  $\alpha$  are shown:  $\alpha$ =1.0, dotted lines; 1.22, solid lines; and 1.5, dash-dotted lines. Also shown is the solution of Eq. (13) for  $\alpha$ =1.22, which is based on the assumption of a Coulomb potential around the particle. ( $\tau$ =100, M=1.37 ×10<sup>-5</sup>, a=50 nm:  $\eta$ =234).

Eq. (11) captures the results of the MD simulation very well. Both the analytical model and the simulation yield a minimum of the normalized particle potential at  $\text{Kn}_{R_0} \approx 1$ , which corroborates that the capture radius Knudsen number is the sensible normalized variable of the problem. Different from [22], our MD simulations indicate that there is an explicit dependence of the normalized particle potential on the particle size in terms of the width of the minimum of *z*. Our analytical model equation (11) generally captures this trend very well.

As the agreement between our analytical model and the MD simulations is quite good, one may wonder whether this is due to the particular definition of the capture radius  $\alpha R_0$  defined above in Eqs. (5) and (6). Hence a sensitivity analysis was performed in which the value of  $\alpha$  was changed to test the influence of the specific definition of the capture radius. Figure 3 shows the results for two nanoparticles with diameters of 100 nm and 1000 nm. Apparently the influence of  $\alpha$  is rather small. Since the value of  $\alpha$  was defined by averaging over a Maxwellian distribution function for the ions [Eq. (6)], which may not always be accurate [21], one may conclude that the actual shape of the ion distribution function will also only have a small influence on the normalized particle charge.

For very small particles such that  $a/\lambda_{DL} \ll e|V_p|/E_{kin}$ , one can simplify the definition of the capture radius in Eq. (5) to

$$R_0(E_{kin}) = \frac{e|V_p|a}{E_{kin}} = \frac{2}{3}z\tau a,$$
 (12)

which essentially corresponds to deriving the capture radius based on the unscreened Coulomb potential. With this definition, Eq. (11) can be simplified to



FIG. 4. (Color online) Comparison between experimental results from [10] and analytical results from the present study as well as results of other analytical models. The parameters for this comparison were taken from Ref. [10].

$$\frac{n_{i,0}}{n_{e,0}} \sqrt{\frac{M}{\tau}} \left\{ (1+\tau z) + \frac{16(\alpha z\tau)^3}{27\mathrm{Kn}_a} + \frac{3\pi}{4\sqrt{2}}\mathrm{Kn}_a\tau z \left[ \exp\left(\frac{4\alpha z\tau}{3\mathrm{Kn}_a}\right) - \left(1 + \frac{4\alpha z\tau}{3\mathrm{Kn}_a}\right) \right] \right\} \exp\left(-\frac{4\alpha z\tau}{3\mathrm{Kn}_a}\right) \exp(z) = 1.$$
(13)

The solution of Eq. (13) is also shown in Fig. 3. It is in rather good agreement with the solution of the more accurate model equation (11) for the particle of 100 nm diameter, with the exception of the transitional region between the OML and collision-enhanced regime. However, as Eq. (13) eliminates any dependence on the particle radius, the agreement with the results for the 1000 nm particle is rather poor. Equation (11) is thus the more general model which needs to be used for larger particles.

In Fig. 4 we compare the results of our analytical model with experimental results reported by Khrapak and coworkers [10] for particles with 0.6  $\mu$ m radius obtained with three different methods. As the presence of a high density of particles will reduce the electron density compared to the ion density, we report results for two different situations:  $n_{i0}$  $=n_{e0}$  and  $n_{i0}=4n_{e0}$ . Obviously, our analytical model (11) describes the experimental results very well. Both the results of our model and the experimental results show a significant reduction of the normalized particle potential with respect to the OML theory, whose results are also indicated in Fig. 4. In the same figure we also compare the results of our model with the ones of other analytical models reported in the literature [3,10,22]. Our model produces results very close with the model presented by Khrapak *et al.* [10]. These two models show the best agreement with experimental results. However, the applicability of Khrapak's model is limited to the slightly collisional regime and does not include the transition to the hydrodynamic regime. The paper by Zobnin *et al.* [3] already had identified a simple analytical expression for the collison-enhanced current and suggested that it be treated as an additional component to the OML ion current. Using these expressions from Ref. [3] still yields reasonably good



FIG. 5. (Color online) Comparison between MD results and analytical predictions of normalized particle charge for a range of particle concentrations and ion collisionality.  $\tau$ =100, *M*=1.37 ×10<sup>-5</sup>,  $\eta$ =234.

agreement with the experimental data, however, not as good as the present model and the model by Khrapak *et al.* [10]. Moreover, the expressions in Ref. [3] are again limited to the weakly collisional regime. In contrast, the model derived by D'yachkov *et al.* [22] is not limited to the weakly collisional regime but applies to a wide range of pressures. However, its agreement with the experimental results is not very good, at least, for particles of the size as shown in Fig. 3. This poor agreement with experimental results was already obvious in Fig. 4 of D'yachkov's paper. Obviously, our model, based on the concept of a capture radius, yields a more accurate description of available experimental data.

Finally, Eq. (11) can be modified to account for the reduction of the electron density in the case of high particle density. Rewriting the plasma-quasineutrality condition as

$$\frac{n_{e,0}}{n_{i,0}} = 1 + \frac{n_p}{n_{i,0}} Q_p = 1 + \frac{n_p}{n_{i,0}} \frac{4\pi\epsilon_0 a V_p}{e} = 1 - 4\pi n_p \lambda_{Di}^2 \frac{\lambda_{DIZ}\tau}{\eta},$$
(14)

we can introduce the nondimensional quantity  $\delta = \lambda_{Di}^2 \lambda_{Dl} n_p$ , leading to

$$\frac{\eta}{\eta - 4\pi z \delta \tau} \sqrt{\frac{M}{\tau}} \left\{ (1 + \tau z) + \frac{2[2\alpha z \tau(\eta + 1)]^3}{\mathrm{Kn}_a(3\eta + 2z\tau)^3} + \frac{3\pi}{4\sqrt{2}} \mathrm{Kn}_a \tau z \left[ \exp\left(\frac{4\alpha z \tau(\eta + 1)}{\mathrm{Kn}_a(3\eta + 2z\tau)}\right) - \left(1 + \frac{4\alpha z \tau(\eta + 1)}{\mathrm{Kn}_a(3\eta + 2z\tau)}\right) \right] \right\} \\ \times \exp\left(-\frac{4\alpha z \tau(\eta + 1)}{\mathrm{Kn}_a(3\eta + 2z\tau)}\right) \exp(z) = 1.$$
(15)

Note that usually,  $\lambda_{Di} \ll \lambda_{De}$  and  $\lambda_{Di} \approx \lambda_{Dl}$ . Hence  $\delta = \lambda_{Dl}^3 n_p$  describes the number of particles in a cube with the length defined by the linearized Debye length.

Figure 5 shows the comparison between the MD simula-

tion results and the results of the analytical expression (13) for a wide range of collisionality and particle density. Calculations were performed for  $(n_pQ)/n_{i0}=4\pi\delta_z\tau/\eta$  = 0,0.5,0.75,0.9,0.98, i.e., situations in which between 0 and 98% of all negative charges reside on the particles. It is evident that the analytical model (15) reproduces the results of the MD simulation very well.

#### **IV. CONCLUSIONS**

We have presented a simple analytical model to describe the charging of nanoparticles in plasmas. The model covers a wide range of collisionality from the collisionless (OML) regime to the highly collisional hydrodynamic regime. The model is based on the concept of a capture radius of ions, which is defined such that ions undergoing charge-exchange collision within this radius will eventually be collected by the particle. The ion current is described as a sum of three components: the collisionless OML current, the collision-

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enhanced transition regime current, and the hydrodynamic current over the collisional regime. These three components are weighted with their respective probablilities of ions performing zero, one, and more than one collision within a sphere around the particle defined by the capture radius. Particle potentials derived based on this simple model were found to be in good agreement with results of molecular dynamics simulations and experimental results. Furthermore, the effect of high particle density was included by introducing a parameter that measures the number of particles in a volume defined by a cube with the length of the linearized Debye length. Good agreement between the analytical model and MD simulations and experimental results was found.

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