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Dynamics of the charging and motion of a macroparticle in a plasma flow

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The dynamics of motion and charging of a macroscopic ''dust'' particle in a plasma with an ion flow is investigated by employing the particle-in-cell method. It is demonstrated that the charging and motion of the dust particle levitating in an external parabolic potential is related to the ion flow. This situation is relevant for the majority of experiments on the self-organization and crystallization of colloidal dust grains in a low-temperature plasma.

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Recently, the properties of a low-temperature plasma containing charged macroscopic colloidal ''dust'' particles has been the subject of increasing interest, associated primarily with dust-plasma crystals [1] as well as with other self-organized formations such as dust clouds, ''drops,'' ''voids,'' etc. [2–4]. For typical gas discharge conditions, the macroscopic colloidal particles (with size of order of 1 μm) inserted in the plasma acquire a negative charge and, under certain conditions, levitate in the sheath or presheath region under the balance of gravitational, electrostatic (due to the sheath electric field), and plasma (such as the ion drag) forces. It was experimentally demonstrated [5] that the levitation can become unstable because of an instability associated with the charging of the dust; an analytical model suggested that fluctuations of the dust charge may also affect stability of the horizontal motions of dust grains [6]. Moreover, the problem of the experimentally observed anomalously high temperature of dust motion [1] has attracted serious attention recently [7,8]; there are good reasons to assume that it is also related to the dust charging process.

The full problem of the motion and charging of a macroscopic body in the presence of plasma flows is highly nonlinear, and therefore its numerical analysis is of major importance. In this Rapid Communication, we report the results found on the basis of a numerical particle-in-cell (PIC) simulation of the dynamics of dust charging and thermal motion, using a self-consistent model of a plasma with an ion flow. We solve Newton's equations for pointlike charged plasma particles in a box with thermal boundaries (reflecting Maxwell distributed particles). We take into account the interactions of plasma particles with the macroparticle and the effects of the Debye screening of the macroparticle by the plasma. Initially, we place the uncharged macroparticle at rest in the center of the box. The calculations of the macroparticle dynamics demonstrate that in the process of its charging it acquires a significant kinetic energy which can exceed the plasma ion and electron temperatures as well as the energy of the flowing ions.

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Although *ab initio* modeling by the molecular dynamics (MD) method is the most complete description of plasma processes [9], modern computer power is often not sufficient for a full three-dimensional (3D) study with real values of the plasma parameters even if we restrict ourselves to a system consisting of a few tens of thousands of plasma particles. Consider a fully ionized plasma (a neutral dissipative background can be added if necessary) consisting of (singly charged) ions with the charge e and mass m_i, and electrons with the charge $-e$ and mass m_e. We are interested in the temporal evolution of the system of N_e electrons and N_i ions confined in a cubic box in the center of which we place a macroscopic spherical body of radius R and initial charge $Q=-Z_0 e$ (we assume $Z_0 \geqslant 0$) and large mass $m_d \gg m_i > m_e$. The time averaged numbers of electrons and ions are chosen to satisfy the quasineutrality condition $n_i - n_e = \langle Z_d \rangle$. Here, $\langle Z_d \rangle$ is the time averaged charge of the macroparticle defined as the sum of the electron and ion charges of those plasma particles which reached the surface of the macroparticle (all electrons and ions hitting the grain surface are assumed to be attached to the macroparticle). The trajectories of the plasma particles are found by the solution of Newton's equations

$$\frac{d^2 \mathbf{r}_k}{dt^2} = \frac{\mathbf{F}_k}{m_k}, \quad \mathbf{F}_k = \frac{q_k Q(\mathbf{r}_k - \mathbf{r}_g)}{|\mathbf{r}_k - \mathbf{r}_g|^3} + \sum_{l \neq k}^{N_p} \mathbf{f}_{kl}, \tag{1}$$

where $k=1,2,\ldots,N_p$ and N_p is the total number of particles. Furthermore, in Eq. (1) $\mathbf{r}_k = \mathbf{r}_k(t)$ is the radius-vector of the particle k with the charge q_k, $\mathbf{r}_g = \mathbf{r}_g(t)$ is the radius vector of the macroparticle with the charge Q, and $\mathbf{f}_{kl}$ is the Coulomb force of interaction between the plasma particles. The full set of Eq. (1) together with the equation of motion of the macroparticle can be solved by a Runge-Kutta method of the fourth order [10–12].

In a dusty plasma, the macroscopic size of the dust grains and their charging play an important role, thus demanding long runs in systems of many particles. To take into account these effects under conditions of reasonable simulation times we employ the less (computer) power-consuming PIC method. The difference to the above outlined MD method is in a more time saving computation of the interaction forces (naturally, this comes at the cost of more approximate physics), thus allowing us to study a longer time evolution of the system. Thus, we assume

$$\mathbf{F}_k=\frac{q_k\mathbf{r}_{kg}}{|\mathbf{r}_{kg}|^3}\left(Q+\sum_{|\mathbf{r}_{lg}|<|\mathbf{r}_{kg}|} q_l\right), \tag{2}$$

where $\mathbf{r}_{kg}=\mathbf{r}_k-\mathbf{r}_g$. In Eq. (2), we take into account the macroparticle screening by plasma particles and effectively compute only interactions of plasma particles inside the Debye cloud around the macroparticle [the sum is calculated in Eq. (2) only for those plasma particles that are closer to the macroparticle than the kth particle]. The force acting on the macroparticle due to particle interactions is defined using Newton's third law, and there is an additional force proportional to the deviation of the particle position from the center of the simulation box (i.e., the macroparticle is in an external parabolic potential). This model allows us to simulate macroparticle levitation under the experimental conditions where the equilibrium is achieved under the action of gravity, the sheath electric force and the ion drag force [13,14]. In addition, the dynamics of the macroparticle takes into account the momentum transfer due to the attachment of plasma electrons and ions. To check the model we also compared the results of MD (1) [10–12] and PIC (2) simulations (for shorter times after the initial moment).

The initial particle number density distribution was chosen to be homogeneous inside the simulation box. The initial velocity distribution of plasma particles corresponds to a Maxwellian distribution at infinity. Depending on the distance to the macroparticle, the Maxwellian velocity distribution is shifted according to the interaction energy with the macroparticle. The initial distribution of the plasma particles' velocity directions is isotropic. The macroparticle is initially uncharged ($Z_0=0$); it absorbs every plasma particle hitting its surface. To account for the electron-ion recombination at the surface and preserve quasineutrality, the electrons and ions are inserted in the simulation volume after absorption by dust (thus modeling ionization effects and the dynamical character of the equilibrium when the plasma production is balanced by the electron and ion flows to the dust surface). The boundaries of the simulation box are thermostatic. Thus, the initial and boundary conditions of the problem allow us to take into account the finite size of the macroparticle as well as fluctuations of its charge.

For the simulation we have chosen a helium plasma with singly charged ions and the ion number density $n_i=2\times10^{12}$ cm^{-3}. The electron temperature is $T_e=1$ eV and the ion temperature is $T_i=0.025$ eV. The simulation time is $t_0=6.5\times10^{-8}$ s, which significantly exceeds the ion plasma period $t_{pi}=6.7\times10^{-9}$ s. The ion Debye length for such a plasma normalized to the average distance between ions is $r_{Di}n_i^{1/3}=1.06$, while for electrons we have $r_{De}n_i^{1/3}=6.6$.

In Fig. 1, we present the dependence of the macroparticle charge as a function of time. The macroparticle has a mass $m_g=10^4m_p$, where m_p is the proton mass, and radius $r_g=0.5$ μm. We present three cases: (a) a plasma without ion flow ($M^2=0$, where M is the Mach number); (b) a plasma with a subsonic ion flow ($M^2=0.6$); and (c) a plasma with a supersonic ion flow ($M^2=2.4$). The number of ions in the system corresponds to charge neutrality. The motion of the macroparticle is also defined by the external parabolic potential with a minimum in the center of the simulation box. The depth of the potential well is 20 V. We stress that for simplicity we assume that the parabolic potential does not apply to the plasma electrons and ions, i.e., it acts only on the macroparticle. An exponential fit was applied to the simulated curves, and demonstrates an extremely good fit to charging with an exponential character,

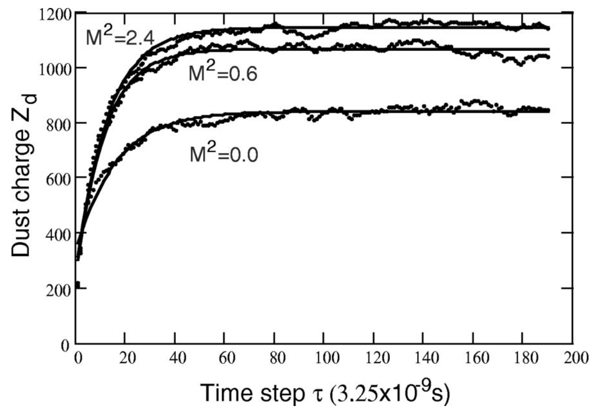

FIG. 1. Charging dynamics of the macroparticle of $m_g=10^5m_p$ with and without an ion flow. The time step is $\tau=3.25\times10^{-10}$ s; the total simulation time is $t_0=200\tau=6.5\times10^{-8}$ s. Exponential fits to the computed charging curves are presented (see also Table I). The asymptoptic charge is: (a) $Z_\infty=842$ in the absence of the ion flow, $M^2=0$; (b) $Z_\infty=1067$ for $M^2=0.6$; and (c) $Z_\infty=1146$ for $M^2=2.4$.

$$\langle Z_d\rangle(t)=Z_\infty-Z_1\exp(-\nu_0 t). \tag{3}$$

The asymptotic values of the macroparticle charge Z_∞ as well other fitting parameters (Z_1 and ν_0) are given in Table I. Note that the asymptotic dimensionless charge increases with the increase of the velocity of the ion flow; qualitatively, this can easily be understood since for more energetic ions, fewer of them participate in the macroparticle charging, which leads to a larger negative charge (i.e., larger Z_∞).

In Fig. 2, we present the time dependence of the kinetic energy of the macroparticle of the same mass as for Fig. 1 ($m_g=10^4m_p$) and for the same plasma parameters. Note that the energy level is higher for subsonic velocities of the flow. Qualitatively this can be understood by noting that the ion drag force has a maximum for flow velocities of the order of the ion thermal velocity, decreases when the velocity of the flow approaches the speed of sound, and for highly supersonic velocities it increases again (see, e.g., Ref. [3]).

Figure 3 presents the dependence on time of the kinetic energy of a more massive particle, $m_g=10^5m_p$. The simu-

TABLE I. The parameters for the exponential fit Eq. (3) of the charging dynamics of the macroparticle.

Squared Mach number	0.0	0.6	2.4
Charge Z_∞	842	1067	1146
Charge Z_1	510	838	900
Rate ν_0, 10^8 s^{-1}	1.85	2.59	2.32

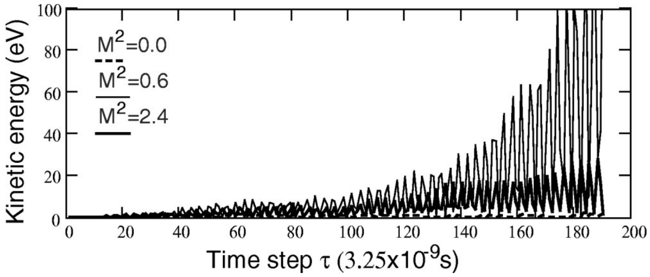

FIG. 2. Kinetic energy of the macroparticle of $m_g=10^4 m_p$ initially placed at rest in the center of the simulation box. The external parabolic potential centered in the middle of the box is 20 V. Three cases related to the absence of the ion flow ($M^2=0$) as well as to the subsonic ($M^2=0.6$) and supersonic ($M^2=2.4$) flows are presented.

lation time in this case is $t_0=2.5\times10^{-7}$ s. We see that in this case there is also an increase of the grain kinetic energy in the process of its charging. It is interesting that the kinetic energy of the macroparticle significantly exceeds the temperature of the plasma ions (noting that $T_i=0.025$ eV). The period of the energy fluctuations of the macroparticle is of the order of the ion plasma period $t_{pi}=6.7\times10^{-9}$ s. This allows us to conclude that the kinetic energy of the macroparticle is related to the kinetic energy of the plasma ions hitting its surface; on the other hand, the kinetic energy of the plasma ions at the surface of the grain is related to the floating potential of the grain and therefore to the electron temperature.

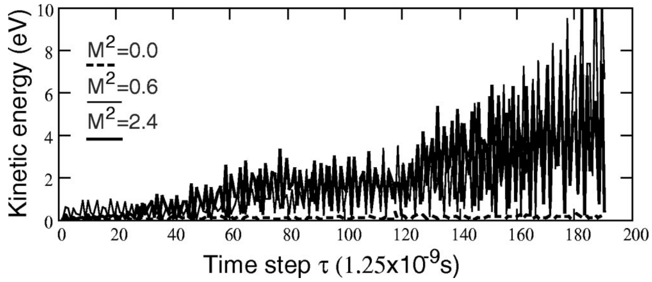

FIG. 3. The same as Fig. 2 but for a macroparticle of ten times larger mass $m_g=10^5 m_p$. The time step in this case is bigger than in Figs. 1 and 2: $\tau=1.25\times10^{-9}$ s; the total simulation time is $t_0=200\tau=2.5\times10^{-7}$ s.

The reported numerical study is the first step of a simulation from first principles of the kinetic energy of a macroparticle in the presence of an ion flow. The numerical results agree with the experimental data [1] that in a dusty plasma the dust temperature (i.e., the mean kinetic energy of the dust) is not in equilibrium with the temperature of the plasma ions. The numerical results also agree with the recent experimental findings [5] that dust grains levitating in the plasma sheath can develop oscillations in the vertical direction (i.e., the direction of the ion flow). We have demonstrated that this instability can be related to the ion flow, and is strongly dependent on the velocity of the plasma ions.

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[1] H. M. Thomas and G. E. Morfill, Nature (London) **379**, 806 (1996).
[2] D. Samsonov and J. Goree, Phys. Rev. E **59**, 1047 (1999).
[3] J. Goree, G. E. Morfill, V. N. Tsytovich, and S. V. Vladimirov, Phys. Rev. E **59**, 7055 (1999).
[4] G. E. Morfill, H. M. Thomas, U. Konopka, H. Rothermel, M. Zuzic, A. Ivlev, and J. Goree, Phys. Rev. Lett. **83**, 1598 (1999).
[5] S. Nunomura, T. Misawa, N. Ohno, and S. Takamura, Phys. Rev. Lett. **83**, 1970 (1999).
[6] A. V. Ivlev, U. Konopka, and G. Morfill, Phys. Rev. E **62**, 2739 (2000).
[7] O. S. Vaulina, A. P. Nefedov, O. F. Petrov, and S. A. Khrapak, Zh. Éksp. Teor. Fiz. **115**, 206 (1999) [JETP **88**, 1130 (1999)].
[8] R. A. Quinn and J. Goree, Phys. Rev. E **61**, 3033 (2000).
[9] R. W. Hockney and J. W. Eastwood, *Computer Simulation Using Particles* (McGraw-Hill, New York, 1981).
[10] S. A. Maiorov, A. N. Tkachev, and S. I. Yakovlenko, Phys. Scr. **51**, 498 (1995).
[11] S. A. Maiorov, Plasma Phys. Rep. **26**, 628 (2000).
[12] S. A. Maiorov, S. V. Vladimirov, and N. F. Cramer, Phys. Rev. E **63**, 017401 (2001).
[13] S. V. Vladimirov, N. F. Cramer, and P. V. Shevchenko, Phys. Rev. E **60**, 7369 (1999).
[14] S. V. Vladimirov and N. F. Cramer, Phys. Rev. E **62**, 2754 (2000).