

Rotational kinetics of absorbing dust grains in neutral gas

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We study the rotational and translational kinetics of massive particulates (dust grains) absorbing the ambient gas. Equations for microscopic phase densities are deduced resulting in the Fokker-Planck equation for the dust component. It is shown that although there is no stationary distribution, the translational and rotational temperatures of dust tend to certain values, which differ from the temperature of the ambient gas. The influence of the inner structure of grains on rotational kinetics is also discussed.

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I. INTRODUCTION

Recently there has been growing interest in the investigation of composite media, called dusty plasmas, consisting of aerosol particles in a gas discharge. Besides numerous industrial applications dusty plasmas provide ample opportunities in studying *in situ* phase transitions in the dust component, intergrain interactions, grain charging, etc.

One of the peculiar features of dusty plasmas is that the average kinetic energy of the dust component, i.e., its translational temperature, may be considerably higher than the temperature of the ambient plasma. In detail the problem was studied in the recent papers by Quinn and Goree [1,2], where in parallel with the experiments a model of the Brownian motion explaining anomalous kinetic temperature was developed.

The kinetic description of dusty plasma was discussed in numerous theoretical studies [3–9]. Generally, there are two ways plasma particles interact with dust grains: first, the scattering of a particle by grain electric field and, second, the direct impact of a particle on a grain surface. The latter process results in grain charging due to the higher mobility of electrons, it may change grain mass, heat its surface, etc. In other words, as it is well understood nowadays, the adequate statistical description of the dust component should take into account inner degrees of freedom, the most important among which is the grain charge. Kinetic consideration of charging process shows that absorption of small plasma particles by grains can result in inequality of the grain temperature and the temperatures of the light components even for the case of equal temperatures of electrons and ions [3,4]. To avoid confusion it should be noted that since the system is open there is no conflict of the latter result with thermodynamics.

Under the conditions of experiments on fine grain synthesis [10,11] or etching [12] grain mass should also be treated as a dynamic variable [13–15]. Thermophoretic [16] and radiometric [17] forces provided by inhomogeneous heating of the grain surface may also play an important role, under microgravity especially [18], which may necessitate inclusion of the temperature distribution inside grains into the

kinetic description. Recent experiments on rodlike particulates [19] demonstrated complicated rotational motion of dust grains. Vladimirov and Tsoy developed the theory of corresponding oscillation modes [20]. In more general context, the rotation is also of importance for Brownian motion of the particles with energy supply [21]. Although the rotation of spherical grains is hardly observable experimentally, it is of interest since it may influence translational motion and heating of the grain surface.

Being not quite complete, the above list of various processes indicates that the dimension of the phase space required for the kinetic description of the dust component may be rather large: it tends to a value of the order of 20.

The main purpose of the present paper is to develop the kinetic theory of the aerosol component taking into account the mass growth and the rotation of grains. Although our main impetus is dusty plasma, here we ignore the process of grain charging. In other words, we treat the ion component as a neutral gas and neglect the influence of electrons. Usually, a grain in a partially ionized gas is charged negatively due to the higher mobility of electrons that results in attraction of ions and corresponding increase of inelastic ion-dust cross sections. The latter is characterized by a numeric factor, which is typically of the order of five and tends to unity if the size of grains exceeds the Debye length of the ambient plasmas. Since the effects discussed in the present paper are the consequences of plasma absorption by the grain, we expect that taking into account the grain charging would enhance these effects. Another reason for accepting this simplification is that we are able to study the problem both analytically and by molecular dynamics simulation: computations with charged moving grains are on the brink of or beyond contemporary computer capabilities.

Thus, we adopt here a following toy model of the aerosol component absorbing the ambient gas. The dust component consists of spherical rotating grains with variable mass and, consequently, size and moment of inertia. Every atom hitting the grain surface is absorbed by it, transferring, therefore, its momentum, changing the mass of the grain and its angular velocity. The process is inelastic since a part of projectile atom energy is spent for heating the grain surface. It is assumed that the size of grains is small compared to the mean free path of the ambient gas, however, the gas distribution

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generally depends on the dust component. Our main finding is that although there is no stationary state of this system, the average kinetic and rotational energies of dust eventually tend to certain fixed values, which differ from each other and the temperature of the ambient gas.

The paper is organized as follows. In Sec. II A we discuss the process of the elementary collision. Microscopic phase densities and corresponding equations generalizing Newtonian dynamics are introduced in Sec. II B, the latter are used in Sec. II C to derive the Fokker-Planck Eq. (20) describing the evolution of the dust distribution. In Sec. II D we obtain the homogeneous solution of the Fokker-Planck equation and evaluate the effective temperatures. The numeric algorithms are described in Sec. III A, then we discuss various laws of collision used for simulations (Sec. III B). The results of simulations, which are in fairly good agreement with the analytical theory, are summarized in Sec. III C.

II. ANALYTIC THEORY

A. Elementary collision

We consider the dust component consisting of a number of spherical grains of variable masses M and of mass dependent radii $a(M)$. Since we are interested in both translational and rotational degrees of freedom, the state of a grain is described by the ten-dimensional vector, $\Gamma = (\mathbf{R}, \mathbf{P}, \mathbf{G}, M)$, where \mathbf{P} is the grain's linear momentum and \mathbf{G} is the angular momentum relative to its center of inertia \mathbf{R} . The angles describing the rotation are irrelevant due to the sphericity of grains. The only collision process taken into account is the absorption of an ambient gas by grains, i.e., every atom colliding a grain is assumed to attach to the grain surface transferring its linear momentum, angular momentum, and mass.

We assume that the process of collision elapses in two stages. At the first stage the atom attaches to the grain surface. Let \mathbf{r} and \mathbf{p} be the projectile atom coordinate and, respectively, the momentum at the instant of collision; evidently, $|\mathbf{r} - \mathbf{R}| = a(M)$. The net angular momentum of the projectile atom and the grain prior to the collision is written as $\mathbf{M} = \mathbf{r} \times \mathbf{p} + \mathbf{R} \times \mathbf{P} + \mathbf{G}$, while after the collision $\mathbf{M} = \mathbf{R}' \times \mathbf{P}' + \mathbf{G}'$. Since after the attachment the center of inertia of the grain changes

$$\mathbf{R}' = \frac{m\mathbf{r} + M\mathbf{R}}{M + m} \quad (1)$$

and $\mathbf{P}' = \mathbf{P} + \mathbf{p}$, the conservation of angular momentum requires that

$$\mathbf{G}' = \mathbf{G} + \frac{(\mathbf{r} - \mathbf{R}) \times (M\mathbf{p} - m\mathbf{P})}{M + m}.$$

It should be noted that both \mathbf{G} and \mathbf{G}' are independent of the reference frame.

In what follows we combine the above expressions in the convenient short-hand notation for the process of collision:

$$\begin{aligned} \Gamma \rightarrow \Gamma' &= \Lambda(\Gamma, \mathbf{r}, \mathbf{p}) \\ &= \left(\frac{m\mathbf{r} + M\mathbf{R}}{M + m}, \mathbf{P} + \mathbf{p}, \mathbf{G} \right. \\ &\quad \left. + \frac{(\mathbf{r} - \mathbf{R}) \times (M\mathbf{p} - m\mathbf{P})}{M + m}, M + m \right). \end{aligned} \quad (2)$$

The leap of the center of inertia (1) results in the nonconservative character of the mapping (2): one can easily verify that its Jacobian

$$\det \frac{\partial \Lambda(\Gamma)}{\partial \Gamma} = \frac{M^3}{(M + m)^3} \quad (3)$$

is less than unity.

Strictly speaking, the attachment of the atom to the grain surface makes the new composite grain nonspherical. To avoid complications with nonspherical grains we assume that at the second stage of the collision some inner forces redistribute the grain mass in such a way that the grain shapes into a sphere. Evidently, this does not alter the grain phase variable Γ . Although this assumption seems a fairly natural simplification, it may result in nonphysical behavior because it leaves out the energy required for the mass redistribution.

Since the process (2) is inelastic, a part of the net mechanical energy is spent for heating the grain surface, which evidently should be positive. (The grain heating is of importance if one is going to consider the aerosol processes like thermophoresis.) Abandoning for a moment the presumption of sphericity, the amount of heat released in the asymmetric grain is written as

$$\begin{aligned} \Delta E &= \frac{1}{2} \{ \tilde{m}v^2 + G_i I_{ij}^{-1} G_j - (\mathbf{G} + \tilde{m}[\boldsymbol{\rho} \times \mathbf{v}])_i I'_{ij}{}^{-1} \\ &\quad \times (\mathbf{G} + \tilde{m}[\boldsymbol{\rho} \times \mathbf{v}])_j \}, \end{aligned} \quad (4)$$

where $\mathbf{v} = \mathbf{p}/m - \mathbf{P}/M$ is the atom velocity in the grain reference frame, $\tilde{m} = mM/(M + m)$ is the reduced mass, $\boldsymbol{\rho} = \mathbf{r} - \mathbf{R}$, I_{ij} and $I'_{ij} = I_{ij} + \tilde{m}(\rho^2 \delta_{ij} - \rho_i \rho_j)$ are the grain tensors of inertia prior and, respectively, after the collision. Expanding Eq. (4) in powers of the small mass ratio, m/M , we obtain that $\Delta E = m(\mathbf{v} - \boldsymbol{\Omega} \times \boldsymbol{\rho})^2/2 \geq 0$, where $\Omega_i = I_{ij}^{-1} G_j$ is the grain angular velocity. In other words, the energy conservation does not debar the mass absorption.

On the other hand, assuming the grain shapes into a sphere, the tensor of inertia is isotropic and depends on the grain mass only, $I_{ij} = I(M) \delta_{ij}$, $I'_{ij} = I(M + m) \delta_{ij}$, and analyzing Eq. (4) one can find that ΔE is always positive if $dI(M)/dM > a^2(M)$. However, it is easy to verify for an arbitrary spherically symmetric mass distribution that the latter inequality never holds. This means that some energy is required for the grain to shape into a sphere and there exist a certain range of impact parameters, such that the available mechanical energy is insufficient for the mass redistribution. It should be noted that similar phenomena are also known in nuclear physics (e.g., Ref. [22]).

Simple estimation shows that the assumption of sphericity results in the violation of the energy conservation for atoms moving with characteristic velocities of the order of $a\Omega$. In the following we assume that the energy of rotation is of the order of the gas temperature and the mass ratio, m/M , is small, i.e., the discussed effect is relevant for a very small group of projectile atoms with velocity less than $\sqrt{m/M}v_T$, where v_T is the gas thermal velocity. We ignore the influence of deviation from sphericity for this reason. Nonetheless, the discussed effect may play an important role for small clusters and, perhaps, it explains the complex structure of fine grains grown in a gas discharge.

B. Microscopic phase densities

In order to obtain the desired kinetic equation describing the grain motion we generalize the well-known Klimontovich approach [23]. To describe the whole system the microscopic phase densities are introduced,

$$N_d(\Gamma, t) = \sum_{\alpha} \delta(\Gamma - \Gamma_{\alpha}(t)), \quad (5)$$

$$N_n(\mathbf{p}, \mathbf{r}, t) = \sum_i \delta(\mathbf{p} - \mathbf{p}_i(t)) \delta(\mathbf{r} - \mathbf{r}_i(t)), \quad (6)$$

where the indices α and i are used to enumerate grains and atoms, respectively.

The equations governing the microscopic phase densities are written as

$$\begin{aligned} \frac{dN_d(\Gamma, t)}{dt} &\equiv \left(\frac{\partial}{\partial t} + \frac{\mathbf{P}}{M} \frac{\partial}{\partial \mathbf{R}} + \mathbf{F}_d \frac{\partial}{\partial \mathbf{P}} + \mathbf{K}_d \frac{\partial}{\partial \mathbf{G}} \right) N_d(\Gamma, t), \\ &= I_d(\Gamma, \mathbf{R}), \end{aligned} \quad (7)$$

$$\frac{dN_n(\mathbf{p}, \mathbf{r}, t)}{dt} \equiv \left(\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m} \frac{\partial}{\partial \mathbf{r}} + \mathbf{F}_n \frac{\partial}{\partial \mathbf{p}} \right) N_n(\mathbf{p}, \mathbf{r}, t) = I_n(\mathbf{p}, \mathbf{r}). \quad (8)$$

Here F_d and F_n are external forces acting upon grains and neutral atoms and K_d is the external torque. The collision terms in the right-hand sides of Eqs. (7) and (8) account for gas absorption by dust grains; similar terms were introduced in Ref. [4]. The convenient short-hand forms of these terms are

$$\begin{aligned} I_d(\Gamma) &= \int d\mathbf{p} d\mathbf{r} d\Gamma' N_n(\mathbf{p}, \mathbf{r}) N_d(\Gamma', \mathbf{R}) \\ &\quad \times \sigma \left(\mathbf{r} - \mathbf{R}, \frac{\mathbf{p}}{m} - \frac{\mathbf{P}'}{M'}, M' \right) \\ &\quad \times [\delta(\Gamma - \Lambda(\Gamma', \mathbf{r}, \mathbf{p})) - \delta(\Gamma - \Gamma')], \end{aligned} \quad (9)$$

$$I_n(\mathbf{p}, \mathbf{r}) = - \int d\Gamma \sigma \left(\mathbf{r} - \mathbf{R}, \frac{\mathbf{p}}{m} - \frac{\mathbf{P}}{M}, M \right) N_n(\mathbf{p}, \mathbf{r}) N_d(\Gamma), \quad (10)$$

where the function $\Lambda(\Gamma, \mathbf{r}, \mathbf{p})$ is given by Eq. (2). The effective cross section $\sigma(\mathbf{r}, \mathbf{v}, M)$ introduced here is

$$\sigma(\mathbf{r}, \mathbf{v}, M) = -2(\mathbf{r} \cdot \mathbf{v}) \theta(-\mathbf{r} \cdot \mathbf{v}) \delta(a^2(M) - \mathbf{r}^2) \quad (11)$$

and $\theta(x)$ is the Heaviside step function.

The collision terms (9) and (10) are arranged in the following way. Suppose there is a trajectory described by a time-dependent radius vector $\mathbf{r}(t)$. If the trajectory crosses the sphere of radius a at the instant t_0 , i.e., $r(t_0) = a(M)$, then

$$\sigma(\mathbf{r}, \dot{\mathbf{r}}, M) = \delta(t - t_0). \quad (12)$$

The step function in Eq. (11) guarantees that the incoming intersection point, such that $\mathbf{r}(t_0) \cdot \dot{\mathbf{r}}(t_0) < 0$, is only taken into account.

Substituting the definitions of the microscopic phase densities (5) and (6) to Eqs. (9) and (10) and making use of Eq. (12) one can verify that the collision terms are proportional to the sum of $\delta(t - \tau_{i\alpha})$, where $\tau_{i\alpha}$ is the instant of collision of the i th atom with the α th grain. At the time intervals between the collisions Eqs. (7) and (8) describe plain Newtonian dynamics. However, at the instant of collision the microscopic phase densities change abruptly,

$$N_n(\mathbf{p}, \mathbf{r}, \tau_{i\alpha} + 0) - N_n(\mathbf{p}, \mathbf{r}, \tau_{i\alpha} - 0) = -\delta(\mathbf{p} - \mathbf{p}_i) \delta(\mathbf{r} - \mathbf{r}_i), \quad (13)$$

that is, the i th atom annihilates. Simultaneously, the α th grain changes its position in the phase space as prescribed by the conservation laws (2)

$$\begin{aligned} N_d(\Gamma, \tau_{i\alpha} + 0) - N_d(\Gamma, \tau_{i\alpha} - 0) \\ = \delta(\Gamma - \Lambda(\Gamma_{\alpha}, \mathbf{r}_i, \mathbf{p}_i)) - \delta(\Gamma - \Gamma_{\alpha}). \end{aligned} \quad (14)$$

C. Fokker-Planck equation

The purpose of this section is to expand Eqs. (9) and (10) in powers of the small mass ratio, m/M . Averaging over the ensemble and ignoring binary correlations, we may treat $N_d(\Gamma, t)$ and $N_n(\mathbf{p}, \mathbf{r}, t)$ as smooth one-particle distribution functions; in details the procedure was discussed in Ref. [4]. Then we integrate over Γ' in Eq. (9) and take into account Eq. (3) that results in

$$\begin{aligned} I_d(\Gamma) &= \int d\mathbf{p} d\mathbf{r} \left\{ \sigma \left(\mathbf{r}, \frac{M}{M-m} \mathbf{v}, M-m \right) N_d \left(\mathbf{R} - \frac{m}{M} \mathbf{r}, \right. \right. \\ &\quad \left. \left. \mathbf{P} - \mathbf{p}, \mathbf{G} - m\mathbf{r} \times \mathbf{v}, M-m \right) N_n \left(\mathbf{p}, \mathbf{R} + \frac{M-m}{M} \mathbf{r} \right) \right. \\ &\quad \left. - \sigma(\mathbf{r}, \mathbf{v}, M) N_d(\Gamma) N_n(\mathbf{p}, \mathbf{R} + \mathbf{r}) \right\}, \end{aligned} \quad (15)$$

where

$$\mathbf{v} = \frac{\mathbf{p}}{m} - \frac{\mathbf{P}}{M} \quad (16)$$

is the relative velocity. Evaluating Eq. (15) we have also performed the change of variables in the integrand (9): $\mathbf{r} \rightarrow \mathbf{R} + [(M-m)/M]\mathbf{r}$ in the first term and $\mathbf{r} \rightarrow \mathbf{R} + \mathbf{r}$ in the second term.

The next step is the expansion of Eq. (15) in powers of the grain radius $a(M)$ and mass ratio $\epsilon = m/M$. Assuming that $p/P \sim mav/G \sim \epsilon^{1/2}$ and making use of the integrals

$$\int d\mathbf{r}\sigma(\mathbf{r},\mathbf{v},M) = \pi a^2(M)v, \quad (17)$$

$$\int d\mathbf{r}\sigma(\mathbf{r},\mathbf{v},M)\mathbf{r} = -\frac{2}{3}\pi a^3(M)\mathbf{v}, \quad (18)$$

$$\int d\mathbf{r}\sigma(\mathbf{r},\mathbf{v},M)r_i r_j = \frac{\pi}{4}a^4(M)v\left(\delta_{ij} + \frac{v_i v_j}{v^2}\right), \quad (19)$$

we finally arrive at the Fokker-Planck equation for $N_d(\Gamma)$,

$$\begin{aligned} \frac{dN_d(\Gamma)}{dt} = & \frac{\partial}{\partial P_i} \left\{ -s_i N_d(\Gamma) + \kappa_{ij} \frac{\partial N_d(\Gamma)}{\partial P_j} \right\} \\ & + \frac{\partial}{\partial G_i} \left(\eta_{ij} \frac{\partial N_d(\Gamma)}{\partial G_j} \right) + \frac{\partial}{\partial R_i} \left\{ \gamma_i N_d(\Gamma) \right. \\ & \left. - \varepsilon_{ijk} \sigma_k \frac{\partial N_d(\Gamma)}{\partial G_j} - \Pi_{ij} \frac{\partial N_d(\Gamma)}{\partial P_j} \right\} - \frac{\partial J N_d(\Gamma)}{\partial M}, \end{aligned} \quad (20)$$

where ε_{ijk} is the unit skew-symmetric tensor. Here the following kinetic coefficients are introduced:

$$\begin{aligned} J(\Gamma) &= \pi a^2(M)m \int d\mathbf{p}v N_n(\mathbf{p},\mathbf{R}), \\ s_i(\Gamma) &= \pi a^2(M) \int d\mathbf{p}v p_i N_n(\mathbf{p},\mathbf{R}), \\ \kappa_{ij}(\Gamma) &= \frac{1}{2} \pi a^2(M) \int d\mathbf{p}v p_i p_j N_n(\mathbf{p},\mathbf{R}), \\ \gamma_i(\Gamma) &= \frac{2m}{3M} \pi a^3(M) \int d\mathbf{p}v_i N_n(\mathbf{p},\mathbf{R}), \\ \eta_{ij}(\Gamma) &= \frac{m^2}{8} \pi a^4(M) \int d\mathbf{p}v (\delta_{ij}v^2 - v_i v_j) N_n(\mathbf{p},\mathbf{R}), \\ \sigma_i(\Gamma) &= \frac{m^2}{4M} \pi a^4(M) \int d\mathbf{p}v v_i N_n(\mathbf{p},\mathbf{R}), \\ \Pi_{ij}(\Gamma) &= \frac{2m}{3M} \pi a^3(M) \int d\mathbf{p}v_i p_j N_n(\mathbf{p},\mathbf{R}), \end{aligned} \quad (21)$$

and \mathbf{v} is given by Eq. (16).

The physical meaning of most of the coefficients (21) and corresponding terms in Eq. (20) is fairly obvious. J is the mass flow at the grain surface, the last term in Eq. (20) provides the mass growth of the dust component. The coef-

ficient s_i is the drag force acting upon a grain, the quantities κ_{ij} and η_{ij} characterizes the diffusion in the momentum space. The term proportional to Π_{ij} is just the Archimedean force in a nonuniform gas.

Since in the process of collision the angular momentum transferred to the grain is independent of its angular velocity, there is no drag torque analogous to the first term in Eq. (20). This is the evident consequence of the adopted model. The drag torque may appear if one takes into account the non-sphericity of grains or inelastic scattering of atoms by the grain surface. Within the present model the drag torque is provided by spatial gradients and it is characterized by the coefficient σ_i . Since in the low velocity limit, $P/M \ll p/m$, σ_i is proportional to s_i , the drag torque may appear if the curl of the drag force is nonzero.

Of interest is the term proportional to γ_i in Eq. (20). It is nonvanishing if the grain moves relative to the ambient gas and it arises due to the change of the center of inertia in the process of collision (1) or, in other words, γ_i describes the migration of the center of inertia due to the asymmetric bombardment of the grain by gas atoms. Comparing the left-hand side of Eq. (7) with this term we see that γ_i appears as an addition to the grain velocity, \mathbf{P}/M . It often happens that an ambient medium exerts some forces on a particulate, an example is the drag force s_i . In this case one may say that a medium modifies Newton's second law. Here we face the example of Newton's first law altered by an ambient gas.

By the order of magnitude the drag force s_i is proportional to $\epsilon^{1/2}$, the effective torque $\sigma_i \sim \epsilon^{3/2}$, all other coefficients are of the order of ϵ .

In the lowest-order approximation the kinetics of the gas component is reduced to the absorption. The corresponding kinetic equation is readily obtained from Eq. (10),

$$\frac{dN_n(\mathbf{p},\mathbf{r},t)}{dt} = - \int d\Gamma \pi a^2(M) \frac{p}{m} N_n(\mathbf{p}) N_d(\Gamma) + I_a(\mathbf{p},\mathbf{r}), \quad (22)$$

where $I_a(\mathbf{p},\mathbf{r})$ stands for other dissipative processes, which were excluded from the above derivation. These may be, e.g., interatomic collisions, gas creation by external source, etc.

D. Effective temperature

Suppose that the gas distribution $N_n(\mathbf{p})$ is homogeneous and isotropic. Since we assume that grain velocity is small compared to the gas thermal velocity, we neglect the momentum dependence in all kinetic coefficients (21) but the drag force s_i for which the first-order term of expansion in powers of \mathbf{P}/M should be kept. Therefore, there are only three nonzero kinetic coefficients (21), which are expressed in terms of mass flow J and normalized energy flow α ,

$$\begin{aligned} s_i &= -\frac{J}{3M} P_i, \\ \kappa_{ij} &= \delta_{ij} J \alpha, \end{aligned} \quad (23)$$

$$\eta_{ij} = \delta_{ij} \frac{1}{2} a^2(M) J \alpha,$$

where

$$\alpha = \frac{a^2(M)}{6mJ} \int d\mathbf{p} p^3 N_n(\mathbf{p}). \quad (24)$$

The Fokker-Planck equation (20) is now reduced to

$$\begin{aligned} \frac{\partial N_d(\Gamma)}{\partial t} &= \frac{\partial}{\partial P_i} \left(\frac{J}{3M} P_i N_d(\Gamma) + \alpha J \frac{\partial N_d(\Gamma)}{\partial P_i} \right) \\ &+ \frac{1}{2} \alpha a^2(M) J \frac{\partial^2 N_d(\Gamma)}{\partial G_i \partial G_i} - \frac{\partial J N_d(\Gamma)}{\partial M}. \end{aligned} \quad (25)$$

Suppose there is no dispersion over the grain mass. Then we seek the solution to Eq. (25) in the form of

$$N_d(\Gamma) = \delta(M - \mu(t)) f(\mathbf{P}, \mathbf{G}, \mu(t)). \quad (26)$$

Evidently, if all the grains are of the same mass and of the same mass growth rate, we are able to use the current value of mass, $\mu(t)$, to parametrize temporal evolution in the phase space. Substituting the latter ansatz to Eq. (25) we find that

$$\frac{d\mu(t)}{dt} = J, \quad (27)$$

$$\frac{\partial f}{\partial \mu} = \frac{1}{3\mu} \frac{\partial P_i f}{\partial P_i} + \alpha \Delta_{\mathbf{P}} f + \frac{1}{2} a^2(\mu) \alpha \Delta_{\mathbf{G}} f, \quad (28)$$

where $\Delta_{\mathbf{P}}$ and $\Delta_{\mathbf{G}}$ stand for the Laplacian operators acting on the corresponding variables.

It should be noted here that the normalized energy flow α is formally independent of mass M . However, it may depend on μ due to the possible time variation of the atom distribution $N_n(\mathbf{p}, t)$.

Equation (28) is reduced to the diffusion equation by changing the variable $\mathbf{P} \rightarrow \mathbf{x} = \mu^{1/3} \mathbf{P}$. The latter is readily solved resulting in

$$\begin{aligned} f(\mathbf{P}, \mathbf{G}, \mu) &= \int d\mathbf{P}' d\mathbf{G}' \frac{\mu f_0(\mathbf{P}', \mathbf{G}')}{(2\pi)^3 [k_1(\mu) k_2(\mu)]^{3/2}} \\ &\times \exp \left[-\frac{(\mu^{1/3} \mathbf{P} - \mu_0^{1/3} \mathbf{P}')^2}{2k_1(\mu)} - \frac{(\mathbf{G} - \mathbf{G}')^2}{2k_2(\mu)} \right], \end{aligned} \quad (29)$$

where

$$k_1(\mu) = 2 \int_{\mu_0}^{\mu} \alpha(\mu) \mu^{2/3} d\mu, \quad (30)$$

$$k_2(\mu) = \int_{\mu_0}^{\mu} \alpha(\mu) a^2(\mu) d\mu, \quad (31)$$

μ_0 is the value of mass at $t=0$, and $f_0(\mathbf{P}, \mathbf{G})$ is the corresponding initial distribution.

As follows from Eq. (29), $f(\mathbf{P}, \mathbf{G}, \mu)$ eventually tends to the Maxwellian distribution. In order to obtain the parameters of asymptotic distribution one has to evaluate the moments of $f(\mathbf{P}, \mathbf{G}, \mu)$. First, it is readily checked that the dust density, $n_d = \int d\mathbf{P} d\mathbf{G} f(\mathbf{P}, \mathbf{G}, \mu)$, is independent of μ . Then, we evaluate the linear momentum dispersion $\Delta_t(\mu)$ and the angular momentum dispersion $\Delta_r(\mu)$,

$$\begin{aligned} \Delta_t(\mu) &= \frac{1}{3n_d} \int d\mathbf{P} d\mathbf{G} P^2 f(\mathbf{P}, \mathbf{G}, \mu) \\ &= \left(\frac{\mu_0}{\mu} \right)^{2/3} \Delta_t(\mu_0) + \frac{k_1(\mu)}{\mu^{2/3}}, \end{aligned} \quad (32)$$

$$\Delta_r(\mu) = \frac{1}{3n_d} \int d\mathbf{P} d\mathbf{G} G^2 f(\mathbf{P}, \mathbf{G}, \mu) = \Delta_r(\mu_0) + k_2(\mu). \quad (33)$$

Explicitly, the asymptotic distribution is given by

$$\begin{aligned} f_{\infty}(P, G, \mu) &= \frac{n_d}{(2\pi)^3 [\Delta_t(\mu) \Delta_r(\mu)]^{3/2}} \\ &\times \exp \left(-\frac{P^2}{2\Delta_t(\mu)} - \frac{G^2}{2\Delta_r(\mu)} \right). \end{aligned} \quad (34)$$

It is a matter of direct substitution to verify that the latter distribution satisfy Eq. (25) subject to relations (32) and (33).

Now we introduce the translational temperature, $T_t(\mu) = \Delta_t(\mu)/\mu$, and the rotational temperature, $T_r(\mu) = \Delta_r(\mu)/I(\mu)$, where $I(\mu)$ is the moment of inertia of a grain. Hereafter we will ignore the dependence of the normalized energy α on μ : this will be the case of particular examples discussed below. Then, as it follows from Eq. (32), the translational temperature tends to a fixed value

$$T_t|_{\mu \rightarrow \infty} \rightarrow \frac{6}{5} \alpha. \quad (35)$$

The evolution of the rotational temperature is sensitive to the dependence of its moment of inertia on the mass, i.e., by the inner structure of a grain. Of interest are two cases. Suppose that the grain radius is independent of its mass: this will be referred to as a spongy grain. Then, $I = \frac{2}{5} \mu a^2$ and Eq. (33) results in

$$T_r|_{\mu \rightarrow \infty} \rightarrow \frac{5}{2} \alpha. \quad (36)$$

Another case is a grain with an arbitrary spherically symmetric mass distribution, $\rho(r)$. In particular, $\rho(r) = \text{const}$ for a solid grain and $\rho(r) \propto r^{D-3}$ for a D -dimensional mass fractal. Since

$$I(\mu) = \frac{8\pi}{3} \int_0^{a(\mu)} dr r^4 \rho(r), \quad (37)$$

the integral in Eq. (31) is expressed in terms of the moment of inertia only: $k_2(\mu) = (3/2)\alpha(I(\mu) - I(\mu_0))$. Therefore, the asymptotic value of the rotational temperature is independent of the mass distribution,

$$T_r|_{\mu \rightarrow \infty} \rightarrow \frac{3}{2}\alpha. \quad (38)$$

It should be noted that strictly speaking our derivation of kinetic equations is applicable to solid grains only.

Now we turn to evaluation of the normalized energy α Eq. (24). Although generally the solution of the kinetic equation (22) is time dependent and can deviate from the Maxwellian distribution, there are reasons to ignore this deviation. Suppose as an example, that the collision term I_a in Eq. (22) is represented by a sum of the Boltzmann integral describing interatomic collisions and let us assume some source term balancing the gas loss. Then, with the dominating role of elastic interatomic collisions, the deviation from Maxwellian distribution becomes negligible. Assuming that N_n is the Maxwellian distribution with the temperature T_0 , we get $\varepsilon = 2/3T_0$, i.e.,

$$T_t \rightarrow \frac{4}{5}T_0, \quad (39)$$

$$T_r \rightarrow \begin{cases} \frac{5}{3}T_0; & \text{spongy grain} \\ T_0; & \text{solid grain.} \end{cases} \quad (40)$$

Of interest is that the dust kinetic temperature obtained under the same approximations but in neglecting the mass growth [4] is $2T_0$. Therefore, the mass growth results in appreciable cooling of the dust component.

At lower gas pressure interatomic collisions are negligible and we have to take into account the deviation of the ambient gas distribution from Maxwellian. Suppose there is some bulk source of a Maxwellian gas, i.e., I_a in Eq. (22) is given by

$$I_a(p) = \nu_0 f_M(p) = \nu_0 \frac{n_0}{(2\pi m T_0)^{3/2}} \exp\left(-\frac{p^2}{2mT_0}\right). \quad (41)$$

Assuming that the rate of the dust mass growth (27) is smaller than the rate of gas creation, i.e., $mn_0/\mu n_d \ll 1$, we neglect the time derivative in Eq. (22), that results in

$$N_n(p) = \frac{m\nu_0}{\xi p} f_M(p), \quad (42)$$

where $\xi = \int d\Gamma \pi a^2(M) N_d(\Gamma)$. Obviously, this distribution differs from Maxwellian due to the accumulation of slow atoms. Evaluating the integrals we get $\varepsilon = \frac{1}{2}T_0$, that is, in the case of high dust density

$$T_t \rightarrow \frac{3}{5}T_0, \quad (43)$$

$$T_r \rightarrow \begin{cases} \frac{5}{4}T_0; & \text{spongy grain} \\ \frac{3}{4}T_0; & \text{solid grain.} \end{cases} \quad (44)$$

The main results of this section may be summarized as follows. The momentum distribution of the dust component absorbing the ambient gas tends to Maxwellian. Although the average value of momenta are always growing, the corresponding temperatures tend to certain fixed values, which differ from each other. Moreover, the rotational temperature depends on the inner structure of dust grains.

In ignoring the mass growth, i.e., the last term in Eq. (25), the dust translational temperature in the Maxwellian gas tends to $2T_0$ [4]. However, due to the absence of the friction torque within the adopted model, there is no steady behavior with respect to the rotational degrees of freedom.

These conclusions were gathered assuming the mass dispersion is negligible. However, the same inferences also follow from the general nonstationary solution of Eq. (25), which may be obtained in a similar way but is too cumbersome to be adduced here.

III. NUMERIC SIMULATIONS

A. An algorithm

Prior to discussing the implemented algorithm we have to fix the relation between physical and computational units. The only natural length scale within the accepted model is the size of a grain. In numeric simulations, therefore, the choice of initial size is a matter of convenience. According to Eq. (27), the natural time scale is the characteristic time of the mass growth $\tau_M = M/J$. Since τ_M depends on mass as $M^{1/3}$, it is more convenient to fix the time scale by the initial value of τ_M . Finally, the mass scale is the mass of a single atom, m .

The simulations of the Brownian kinetics of a single grain were performed in a following way. The computational area was a three-dimensional cube of unit length on edge in contact with the unbounded equilibrium gas. This contact was simulated by point atoms, which were randomly injected inside the cube from all of its faces and could freely leave the computational area. For each atom leaving the cube, another atom with the random velocity was injected from the random point of the random cube face. The distribution function of the injected atoms was semi-Maxwellian. Since there were no forces acting upon atoms, their trajectories were straight lines.

It was verified that in the absence of dust grains the bulk distribution inside the cube was Maxwellian with the prescribed temperature T_0 . The average number of atoms depended on the thermal velocity; in most runs it fluctuated around 10 000. We also checked that our results were insensitive to the actual value of the gas temperature. By reducing T_0 we could increase the average number of atoms inside the computational area up to 10^6 . However, this did not affect the average value of the grain energy normalized to T_0 .

The grain was represented by a movable sphere of a radius small compared to the cube edge; typically, its initial size was $a_0=0.01$ and its initial mass was $M_0=1000$. If an atom hit the grain surface then it transferred a part of its momenta to the grain according to some prescribed rules, which are discussed below. In the case of the absorbing grain, no new atom was injected into the cube after the collision that resulted in some reduction of density. Since the grain was initially small, a very little part of atoms might have experienced the collisions. The equations of motion for both translational and rotational degrees of freedom of the grain were solved; the time step was small compared to the average time between the collisions.

It was observed that some spurious force arose when the grain approached the faces of the cube. To minimize the influence of this computational effect the grain was confined near the center of the cube with the help of the auxiliary spherically symmetric parabolic potential well. The parameters of the well were chosen in so that even with the kinetic energy of about $100 T_0$ the grain could not approach the faces of the cube. Evidently, such confinement resulted in multiplication of the grain distribution by a Boltzmannian factor and could not alter the distribution over the kinetic energy. Moreover, in application to the dusty plasma the confinement appears in a natural way. The imposed auxiliary potential did not influence the motion of atoms.

It is worth noting that although the mass of the grain could be as large as of the order of 10^6 atomic masses, its mobility was crucial for our simulations. We had the temptation to avoid the solution of the grain equations of motion by simply counting down the energy and momentum transferred to the immobile grain. However, this way led nowhere: the grain temperature was permanently increasing without any saturation.

The main goal of our simulations was to accumulate enough data in order to reconstruct the grain distribution function over its kinetic and rotational energy. The translational or rotational energy axis, say, $0 < E < 20 T_0$, was split in a number of subbands (usually, 50). Two methods of averaging were used. First, we could trace the energy variation of the single grain and evaluate time it spent in each energy subband. Then, these time intervals were summed up resulting in time-averaged distribution function.

Another method of averaging was the simulation of the canonical Gibbs ensemble. Initially, the grain was situated at the center of the cube, its rotational and kinetic energies were chosen randomly using the random-number generators of Maxwellian distributions with corresponding initial kinetic T_{t0} and rotational T_{r0} temperatures. The evolution of the grain energies was recorded for the time period $0 < t < t_{max}$. The obtained dependence represented a single sample from the Gibbs ensemble. The whole procedure was repeated many times with varied random initial energies but the same initial temperatures. By counting down a number of samples in each energy subband for a given time instant we were able to reconstruct the time evolution of the energy distribution function.

It should be noted that reconstruction of the distribution over both kinetic and rotational energies, $f(E_t, E_r)$ requires

too many samples or too long integration time. For this reason we could evaluate only the distribution over kinetic $f(E_t)$ or rotational $f(E_r)$ energy separately.

B. Atom-grain collisions

As it was mentioned, for test (and fun) purposes we have used various laws of interaction of an atom with the grain surface.

Specular reflections. The atom experiences the specular reflection in the grain reference frame,

$$\begin{aligned} \mathbf{p}' &= \mathbf{p} - \Delta \mathbf{p}, \\ \mathbf{P}' &= \mathbf{P} + \Delta \mathbf{p}, \\ \mathbf{G}' &= \mathbf{G}, \\ M' &= M, \end{aligned} \quad (45)$$

where the transferred momentum is

$$\Delta \mathbf{p} = 2\mathbf{n} \left(\mathbf{n} \cdot \mathbf{p} - \frac{m}{M} \mathbf{n} \cdot \mathbf{P} \right)$$

and $\mathbf{n} = (\mathbf{r} - \mathbf{R})/a$ is a unit vector.

Absorbing grain. The grain momenta change according to Eq. (2). We were able to use various dependencies $a(M)$.

The “cold grain” is also described by Eqs. (2) but its mass remains unchanged; the same law of collision was used in Ref. [4]. Physically, this corresponds to the diffuse scattering with the complete energy accommodation at the cold surface, when the net atom momentum is transferred to the grain and the influence of the scattered atom is negligible.

C. Simulation results

The simulations with specular reflections (45) were used to check the overall operation of the code. Both averaging methods described above were used. It was observed that for the relatively heavy grain ($M/m=100$) after some thousands of collisions the distribution function over the kinetic energy eventually tended to the Maxwellian distribution. The dust temperature was equal to T_0 with the accuracy less than 1%, as expected for the system in the thermodynamic equilibrium. There was no relaxation in rotational degrees of freedom because there was no coupling between translational and rotational motions.

Another series of runs was performed with the absorbing solid grain, i.e., $a(M) \propto M^{1/3}$. Although the computer facilities allowed us to monitor the motion of the grain for a very long time, up to tens of millions of collisions, it was found that no statistically significant result could be obtained with the time-averaging method. The reason is fairly evident: with growing mass the grain motion slowed down, and it took more and more time for the grain to migrate from one energy subband to another.

The ensemble averaging yielded more meaningful results. Several typical energy distributions in logarithmic scale are depicted in Fig. 1. The fit curves there correspond to Max-

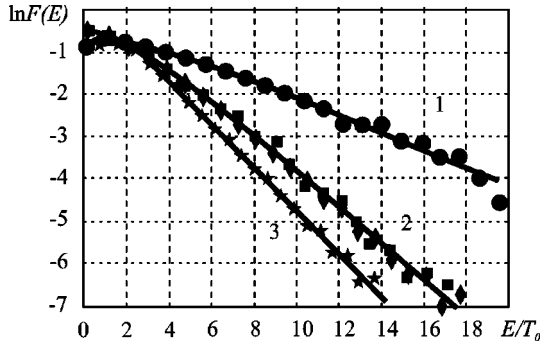


FIG. 1. Energy distributions for various kinds of atom-grain interactions. The distributions over kinetic energy are plotted for the cold grain (\bullet), for the specular reflections given by Eqs. (45) (\blacksquare) and for the absorbing grain (\star). The distribution over rotational energy is shown for the case of the absorbing grain (\blacklozenge). The solid curves correspond to Maxwellian distributions with $T/T_0=2$ (1), $T/T_0=1$ (2), and $T/T_0=4/5$ (3).

wellian distributions, i.e., $F(E) \propto \sqrt{E} \exp(-E/T)$. Figure 2 shows the temporal evolution of translational (solid line) and rotational (dashed line) temperatures. The initial temperatures are $T_{r0} = 0.8 T_0$ and $T_{r0} = 1.3 T_0$. The time in Fig. 2 is measured in the units of characteristic time of the mass growth, τ_M . The averaging was performed over the ensemble consisting of 10^4 samples.

There was the sharp drop in translational temperature evolution at the beginning of the computation. It originated due to the parabolic potential well, in which the grain was kept. Initially the grain was situated at the bottom of the well, so its potential energy was zero. Then, according to the virial theorem, half of its kinetic energy was transferred to the potential one. Since the potential well did not influence the grain rotation, there was no rotational energy drop.

Eventually the dust translational temperature tends to $\approx 0.75T_0$, that is, near the value given by Eqs. (39). The rotational temperature is also close to the value (40). Since there was only one small grain, the distribution of projectile atoms was essentially Maxwellian and we were unable to reproduce the solutions (43) and (44).

The simulations with the “cold grain” also confirmed the analytical solution: the translational temperature tends to $2T_0$ while the rotational temperature is always growing.

IV. CONCLUSION

Although the simple model of the atom-grain inelastic collisions accepted in this paper ignores some essential pro-

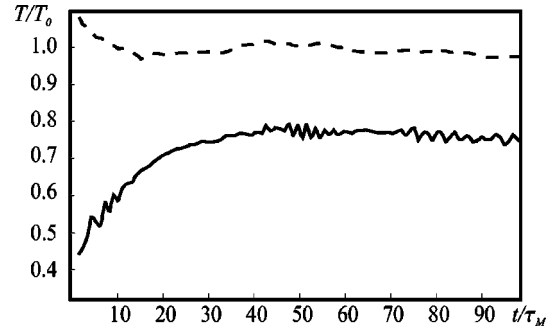


FIG. 2. Temporal dependence of translational (solid line) and rotational (dashed line) temperatures.

cesses, it demonstrates many interesting features. We confirmed that the translational temperature of the dust component differs from the temperature of the ambient gas. However, we demonstrated that the “equilibrium” temperature is highly sensitive to the details of the inelastic collision. In particular, taking into account the grain mass growth results in appreciable reduction of the dust temperature. It should be noted that the difference between various collision laws discussed above numerically is very small. The discrepancies in energy balance of the order of a fraction of a tiny mass ratio are accumulated and eventually result in a considerable effect. It is also worth pointing out that the rotational temperature is sensitive even to details of inner structure of a grain.

The important lesson, which may be drawn from the above discussion, is that there is no thermodynamic equilibrium between dust and ambient gas. The statement itself is fairly evident since a dusty plasma is an open system. However, this indicates the inapplicability of the fluctuation-dissipation theorem, which is the basement of the Langevin approach to the theory of Brownian motion. Therefore, the problem of deducing the Langevin equation applicable to dusty plasmas arises.

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- [1] R.A. Quinn and J. Goree, *Phys. Plasmas* **7**, 3904 (2000).
 [2] R.A. Quinn and J. Goree, *Phys. Rev. E* **61**, 3033 (2000).
 [3] A.G. Zagorodny, P.P.J.M. Schram, and S.A. Trigger, *Phys. Rev. Lett.* **84**, 3594 (2000).
 [4] P.P.J.M. Schram, A.G. Sitenko, S.A. Trigger, and A.G. Zagorodny, *Phys. Rev. E* **63**, 016403 (2001).
 [5] V.N. Tsytovich and U. de Angelis, *Phys. Plasmas* **6**, 1093

- (1999).
 [6] V.N. Tsytovich and O. Havnes, *Comments Plasma Phys. Control. Fusion* **15**, 267 (1993).
 [7] V.N. Tsytovich, U. de Angelis, R. Bingham, and D. Resendes, *Phys. Plasmas* **4**, 3882 (1997).
 [8] A.G. Sitenko, A.G. Zagorodny, Yu.I. Chutov, P.P.J.M. Schram, and V.N. Tsytovich, *Plasma Phys. Controlled Fusion* **38**, A105

- (1996).
- [9] A.M. Ignatov, Plasma Phys. Rep. **24**, 677 (1998).
- [10] M.A. Childs and A. Gallagher, J. Appl. Phys. **87**, 1076 (2000).
- [11] A. Gallagher, Phys. Rev. E **62**, 2690 (2000).
- [12] W.W. Stoffels, E. Stoffels, G.H.P.M. Swinkels, M. Boufnichel, and G.M.W. Kroesen, Phys. Rev. E **59**, 2302 (1999).
- [13] A.M. Ignatov and S.A. Trigger, W. Ebeling, and P.P.J.M. Schram, Phys. Lett. A **293**, 141 (2002).
- [14] S.A. Trigger, Contrib. Plasma Phys. **41**, 331 (2001).
- [15] A.M. Ignatov, S.A. Trigger, W. Ebeling, and P. P. J. M. Schram, Phys. Lett A **293**, 141 (2002).
- [16] G.M. Jellum, J.E. Daugherty, and D.B. Graves, J. Appl. Phys. **69**, 6923 (1991).
- [17] A.M. Ignatov and Sh.G. Amiranashvili, Phys. Rev. E **63**, 017402 (2001).
- [18] G.E. Morfill, H.M. Thomas, U. Konopka, H. Rothermel, M. Zuzic, A. Ivlev, and J. Goree, Phys. Rev. Lett. **83**, 1598 (1999).
- [19] B.M. Annaratone, A.G. Khrapak, A.V. Ivlev, G. Sollner, P. Bryant, R. Sutterlin, U. Konopka, K. Yoshino, M. Zuzic, H.M. Thomas, and G.E. Morfill, Phys. Rev. E **63**, 036406 (2001).
- [20] S.V. Vladimirov and E.N. Tsoy, Phys. Rev. E **64**, 035402(R) (2001).
- [21] U. Erdmann, W. Ebeling, and V. Anishchenko (unpublished).
- [22] G. Shanmugam and V. Selvam, Phys. Rev. C **62**, 014302 (2000).
- [23] Yu.L. Klimontovich, *Statistical Physics* (Harwood Academic Publishers, New York, 1986).