CHARGING OF DUST PARTICLES IN COLLISIONLESS PLASMA SHEATH WITH NON-MAXWELLIAN ELECTRON ENERGY DISTRIBUTION FUNCTION

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1. Introduction

general form

The key parameter driving behavior of dust particles in plasma is their electric charge [1]. Present-day theories as well as experiments are not fully successful in determining its value [2]. Moreover, the theoretical uncertainties are increased in the plasma sheath – a think plasma layer at a wall or electrode. The standard models of dust charging in the plasma sheath usually suppose Maxwellian electron energy distribution function (EEDF) and a flux of cold ions satisfying classical Bohm criterion. In this paper we generalize this model of plasma sheath and dust charging to arbitrary EEDF with adapted Bohm criterion. We limit our considerations to collisionless or slightly collisional plasma, when the EEDF at the plasma sheath can be derived from the EEDF calculated or measured in the plasma bulk. This possibility is of practical importance as direct measurements of EEDF in the plasma sheath are questionable.

Derived theoretical formulas have been incorporated into a set of codes realized in MATLAB. The codes characterize electrical conditions in rf (radio frequency) or dc (direct current) plasma sheath as well as behavior of an isolated dust particle occurring there. Collective effects of dust particles are not investigated in this contribution. As an illustrative example of such computations we compare balancing radii of dust particles levitating above a planar electrode for three different distribution functions. Although applied model distributions in the bulk have been chosen with identical electron number density and average thermal energy, the behavior of particles confined in the sheath are noticeably different.

2. Description of electrons in quasistationary collisionless plasma sheath

We suppose *x*-axis oriented upward from the horizontally placed electrode (cathode), which is at the origin x = 0. For the plasma layer (sheath) above the electrode the Boltzmann's kinetic equation reads

$$\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} + \frac{e}{m_e} \frac{\partial U}{\partial x} \frac{\partial f}{\partial v_x} = \left(\frac{\delta f}{\delta t}\right)_c \tag{1}$$

where f is the electron distribution function in velocity space $(dn_e = f d^3v)$ and U(x,t) is potential. Supposing sheath thickness much lower than the electron mean path, we can neglect collisional term on $\left| \frac{\partial U}{\partial t} \right|$

the right-hand side. If time changes of electric potential are slow, $|\overline{v}_x| \gg \left| \frac{\partial U / \partial t}{\partial U / \partial x} \right|$, we can also neglect the first term. The solution of kinetic equation (1) with omitted collisional and time terms is of

$$f(x, v_{x}, v_{y}, v_{z}) = f^{\pm} \left(\frac{m v_{x}^{2}}{2} - e U(x), v_{y}, v_{z} \right)$$
(2)

where signs +/- distinguish between positive / negative velocities v_x , i.e. velocities from / to the electrode. We will restrict our considerations to distributions fully isotropic in velocity space (anisotropic distributions can be analyzed in similar way). Then $f = f(mv^2/2 - eU)$, where v is the magnitude of

electron velocity. Substituting energy coordinate $\varepsilon = mv^2/2$, the common form of EEDF is $g(\varepsilon, x) \sim \sqrt{\varepsilon} f(\varepsilon - eU(x))$ (d $n_e = g d\varepsilon$), hence

$$g(U,\varepsilon) = \left(1 - \frac{eV}{\varepsilon}\right)^{-1/2} g_0(\varepsilon - eV)$$
(3)

 $V \equiv U - U_0$ is voltage between a position x with local potential U(x) and some reference position x_0 with potential $U_0 = U(x_0)$, where the EEDF $g_0(\varepsilon)$ is known. As the potential monotonously increases from the electrode to the plasma bulk, we will use U as a parameter characterizing position in the sheath. The reference point could be chosen at the sheath edge x_s ($U_s = 0$ by definition) or at the plasma bulk ($U_b > 0$). Positions in the sheath in both cases satisfy $x \le x_0$ and $V \le 0$. Hereinafter the reference point will be situated in the plasma bulk.

Specially, if the EEDF at the edge x_0 is Maxwellian,

$$g_{0M}(\varepsilon) = n_0 \frac{2}{\sqrt{\pi} (kT)^{3/2}} \sqrt{\varepsilon} \exp\left(-\frac{\varepsilon}{kT}\right)$$
(4)

then the EEDF (3) inside the sheath is also Maxwellian,

$$g_{\rm M}(U,\varepsilon) = n_0 \exp\left(\frac{eV}{kT}\right) \frac{2}{\sqrt{\pi} \left(kT\right)^{3/2}} \sqrt{\varepsilon} \exp\left(-\frac{\varepsilon}{kT}\right)$$
(5)

From (3) we obtain electron number density anywhere in the sheath. The electron density at a point with potential U is

$$n_{\rm e}(U) = \int_{0}^{\infty} g(U,\varepsilon) \,\mathrm{d}\varepsilon = \int_{-eV}^{\infty} (\varepsilon + eV)^{1/2} \frac{g_{0}(\varepsilon)}{\sqrt{\varepsilon}} \,\mathrm{d}\varepsilon \tag{4}$$

Maxwellian EEDF (4) gives Boltzmann distribution

$$n = n_0 \exp\left(\frac{eV}{kT}\right) \tag{5}$$

This result is due to total reflections of electrons moving towards the cathode back to the bulk.

It is useful to compare our formula (4) with sometimes applied alternative expression

$$n_{\rm e}(U) = \int_{-eV}^{\infty} g_0(\varepsilon) \,\mathrm{d}\varepsilon \tag{6}$$

being a bit superficially justified by the argument that only electrons at the reference position with potential U_0 having energy greater than -eV ($V = U - U_0$) can overcome the potential hill at position with voltage U [4]. This expression does not relate the Maxwellian distribution to the Boltzmann one, as it should be.

Besides electron number density also electron flux influences electrical conditions and dust charging. We will derive general expressions for electron flux crossing through a planar surface parallel to the electrode ("planar" flux) and impinging on a spherical surface of a dust ("spherical" flux).

In planar case we will consider the flux of electrons towards the electrode, i.e. moving in opposite direction to the orientation of x-axis. The planar surface is situated anywhere in the plasma sheath. Number of electrons moving across a unit surface per unit time is given by integration of

 $d\gamma_e(x) = |v_x| dn_e$ for $v_x < 0$. Substituting $d\gamma_e = \sqrt{2m\varepsilon} \cos\theta g(\varepsilon) d\varepsilon$ ($\pi/2 \le \theta \le \pi$), with EEDF g at position x expressed through g_0 , we get after integration over θ

$$\gamma_{\rm e}(U) = \frac{1}{4} \int_{0}^{\infty} \sqrt{\frac{2\varepsilon}{m_{\rm e}}} g(U,\varepsilon) \,\mathrm{d}\varepsilon = \frac{1}{2\sqrt{2m_{\rm e}}} \int_{-eV}^{\infty} (\varepsilon + eV) \frac{g_0(\varepsilon)}{\sqrt{\varepsilon}} \,\mathrm{d}\varepsilon \tag{7}$$

Specially Maxwellian EEDF (4) gives the well-known formula

$$\gamma_{\rm eM} = \frac{1}{4} \sqrt{\frac{8kT}{\pi m}} n_0 \exp\left(\frac{eV}{kT}\right) \tag{8}$$

Now consider flux of electrons caught by a spherical particle of radius a and potential U_p measured relatively to the local undisturbed plasma. Number of electrons with velocity \vec{v} falling on the surface is in general

$$d\Gamma_{\rm e} = v \, dn_{\rm e}(\vec{v}) \, \pi \, a^2 \, F(U_{\rm p}, \vec{v}) \tag{9}$$

 dn_e is number of electrons in undisturbed plasma with velocity (around) \vec{v} and kinetic energy ε . Attracting/repulsing effect of the particle charge is involved in the factor F. We restrict our considerations to the orbital motion limited (OML) theory [5], for which

$$F(U_{p},\varepsilon) = \underbrace{\begin{array}{c} 1 + \frac{eU_{p}}{\varepsilon}, \quad \varepsilon + eU_{p} > 0\\ 0, \quad \varepsilon + eU_{p} \le 0 \end{array}}$$
(10)

The flux per unit area $\gamma_{\rm e} = \Gamma_{\rm e} / 4\pi a^2$ in position specified by local potential U is then

$$\gamma_{\rm e}(U, U_{\rm p}) = \frac{1}{4} \int_{0}^{\infty} \sqrt{\frac{2\varepsilon}{m_{\rm e}}} g(U, \varepsilon) F(U_{\rm p}, \varepsilon) \,\mathrm{d}\varepsilon$$
⁽¹¹⁾

or, after substitution from (3)

$$\gamma_{\rm e}(U, U_{\rm p}) = \frac{1}{2\sqrt{2m_{\rm e}}} \int_{-eV_0}^{\infty} (\varepsilon + eV_{\rm p}) \frac{g_0(\varepsilon)}{\sqrt{\varepsilon}} \mathrm{d}\varepsilon$$
(12)

where $V_p \equiv U_p + V$ is voltage between the particle and reference point x_0 and $V_0 \equiv \min(U_p, 0) + V$. If a particle is charged negatively, then the formula for spherical surface is identical to the formula (7) for planar surface, with only the plasma voltage V replaced by particle voltage V_p .

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For Maxwellian EEDF (4) the above integral gives

$$\gamma_{e}(U, U_{p}) = \frac{1}{4} \sqrt{\frac{8kT}{\pi m_{e}}} n_{0} \exp\left(\frac{eV}{kT}\right) \times \left(\begin{array}{c} \exp\left(\frac{eU_{p}}{kT}\right), & U_{p} \leq 0 \\ 1 + \frac{eU_{p}}{kT}, & U_{p} > 0 \end{array} \right)$$
(13)

3. Description of ions in quasistationary collisionless plasma sheath

As a first step we will adapt the Bohm criterion to general form of EEDF. This criterion gives ion velocity and density at the sheath boundary x_s and also specifies the plasma bulk potential U_b with regard to the sheath boundary, where by definition $U(x_s) \equiv 0$. The procedure partly follows the approach of review article [6].

Electric field in the sheath is described by Poisson equation

$$\frac{\partial^2 U(x)}{\partial x^2} = -\frac{e[n_i(x) - n_e(U)]}{\varepsilon_0}$$
(14)

where electron number density $n_e(U)$ is commonly taken Maxwellian (5). We suppose here more general distribution (3), corresponding to the collisionless sheath. Boundary conditions at the sheath edge are

$$U(x_{s}) = 0, \qquad \frac{dU(x_{s})}{dx} = 0$$
 (15)

In approximation of cold ions monoenergetic ion flux enters the sheath perpendicularly to the electrode. The ion velocity and density inside the sheath satisfy conservation of energy and continuity equation

$$\frac{m_{\rm i}v_{\rm i}(x)^2}{2} + eU(x) = \frac{m_{\rm i}v_{\rm is}^2}{2}, \qquad n_{\rm i}(x)v_{\rm i}(x) = n_{\rm is}v_{\rm is}$$
(16)

These equations give concentration and kinetic energy in dependence on potential,

$$n_{\rm i}(U) = n_{\rm is} \left(1 - \frac{eU}{\varepsilon_{\rm is}} \right)^{-1/2}, \qquad \varepsilon_{\rm i}(U) = \varepsilon_{\rm is} - eU$$
(17)

where $\varepsilon_{is} \equiv m_i v_{is}^2 / 2$ and n_{is} are (so far unknown) energy and concentration of ions at the sheath boundary. After substituting the last expression into Poisson equation, multiplying both sides by dU / dx and integrating, we obtain

$$\frac{1}{2} \left[\left(\frac{\mathrm{d}U}{\mathrm{d}x} \right)^2 \right]_{x_{\mathrm{s}}}^x = \frac{e}{\varepsilon_0} \left\{ \int_0^U n_{\mathrm{e}}(U) \,\mathrm{d}U - 2 \frac{n_{\mathrm{is}} \varepsilon_{\mathrm{is}}}{\mathrm{e}} \left[1 - \left(1 - \frac{eU}{\varepsilon_{\mathrm{is}}} \right)^{1/2} \right] \right\}$$
(18)

For the while we restrict our analysis to the vicinity of the sheath boundary, where the potential U is close to zero. After expansion of the right-hand side into Taylor series up to the terms of second order we get

$$\left(\frac{\mathrm{d}U}{\mathrm{d}x}\right)^{2} \Big|_{x_{\mathrm{s}}}^{x} = \frac{2e}{\varepsilon_{0}} \left\{ \left(n_{\mathrm{es}} - n_{\mathrm{is}}\right)U + \frac{1}{2} \left(\frac{\mathrm{d}n_{\mathrm{e}}(0)}{\mathrm{d}U} - \frac{en_{\mathrm{is}}}{2\varepsilon_{\mathrm{is}}}\right)U^{2} \right\}$$
(19)

Supposing quasineutral plasma up to the sheath boundary, we have $n_{es} = n_{is} \equiv n_s$. Taking into account the second boundary condition in (15), we get

$$\left(\frac{\mathrm{d}U}{\mathrm{d}x}\right)^2 = \frac{e}{\varepsilon_0} \left(\frac{\mathrm{d}n_{\rm e}(0)}{\mathrm{d}U} - \frac{en_{\rm s}}{2\varepsilon_{\rm is}}\right) U^2 \tag{20}$$

Hence the kinetic ion energy \mathcal{E}_{is} at the sheath edge satisfies the inequality

$$\frac{n_{\rm s}}{\varepsilon_{\rm is}} \le \frac{2}{e} \frac{\mathrm{d}n_{\rm e}(0)}{\mathrm{d}U} \quad \text{or} \quad \varepsilon_{\rm is} \ge \frac{e}{2} \left(\frac{\mathrm{d}\ln n_{\rm e}}{\mathrm{d}U}\right)^{-1} \bigg|_{U=0}$$
(21)

which represents the generalized Bohm criterion. It is conventional to take minimum value of ion kinetic energy or velocity satisfying this inequality. The conservation of energy also gives the bulk potential $U_{\rm b} = \varepsilon_{\rm is} / e$.

For Boltzmann distribution function the above formula yields classical result [7]

$$\mathcal{E}_{is} \ge \frac{kT_e}{2}, \qquad |v_{is}| \ge \sqrt{\frac{kT_e}{m_i}} \equiv v_B$$
(22)

where $v_{\rm B}$ is the Bohm (or ion acoustic) velocity.

For collisional sheath the field strength at the sheath edge is slightly negative [3], $-dU(x_s)/dx < 0$, therefore the above procedure giving inequality (21) cannot be applied. Nevertheless, its validity is still reasonable. Supposing the plasma just below the sheath edge positively charged, we get $d(n_i - n_e)/dU \le 0$ at U = 0, which in fact represents the Bohm criterion (21).

Neglecting collisions of ions and thermal component of their velocity, the ions move directly to the electrode in a monoenergetic beam with constant planar flux, $\gamma_i = n_s v_{is}$. The flux per unit spherical surface is within the OML theory

$$\gamma_{i}(U,U_{p}) = \frac{1}{4}n_{s}v_{is} \times$$

$$0, \qquad \varepsilon_{i} - eU_{p} > 0 \qquad (23)$$

4. Sheath and dust particle models

System of equations describing electric field and dust particles in the sheath are in more detail discussed in [3] or [1]. We mention here only some basic facts.

Results presented in this paper concern rf discharge (13.56 MHz) in argon plasma with the lower electrode powered. At this frequency the electrons follow instantaneous electric field whereas the ions respond to its time average. The potential at the electrode is assumed harmonic,

$$U_{0}(t) = U_{dc0} + U_{rf0} \sin(\omega_{rf} t)$$
(24)

Here U_{dc0} is the dc self bias and U_{rf0} is the amplitude of the rf potential oscillations. In capacitively coupled rf discharge the average electron current to the electrode is equal to the ion current, i.e

$$\frac{1}{T}\int_{0}^{T}\gamma_{e}(U_{0}(t))dt = \gamma_{i}$$
(25)

where T is the rf period. This condition couples U_{dc0} and U_{rf0} . The dc component is taken as optional (experimental), harmonic component is evaluated.

In asymmetric rf discharges with powered electrode much smaller than the grounded one the potential oscillations outside the sheath can be neglected [8]. It enables to define the boundary condition at the sheath edge as is usual for dc disharge, $U(t, x_s) = 0$. Formulas determining electric field, potential of plasma bulk, electron and ion characteristics (densities, energies, fluxes) including Bohm criterion have been specified in previous sections.

As the main part of rf power is primarily absorbed by electrons, the EEDF is usually far from the equilibrium Maxwell-Boltzmann distribution. A very complicated kinetic description cannot give fully satisfactory results for EEDF. Our approach enables to determine EEDF in plasma bulk directly by measurements and, if collisional processes are negligible, such experimentally determined distribution extend in some way to the sheath.

Numerous experiments in low-pressure rf discharges show two-temperature character of EEDF. In our model computations we compare equilibrium Maxwellian EEDF,

$$g_{0M}(\varepsilon) = n_0 \frac{2}{\sqrt{\pi} (kT)^{3/2}} \sqrt{\varepsilon} \exp\left(-\frac{\varepsilon}{kT}\right)$$
(26)

with two other related EEDF. Double Maxwellian EEDF is a superposition of two single Maxwellian EEDF with temperatures T_1 , T_2 and relative ratios P_1 , P_2 , $\sum P_i = 1$:

$$g_{0D}(\varepsilon) = n_0 \sum_{i} \frac{2P_i}{\sqrt{\pi} (kT_i)^{3/2}} \sqrt{\varepsilon} \exp\left(-\frac{\varepsilon}{kT_i}\right)$$
(27)

Another modification is represented by a cutoff like the two-temperature Maxwellian distribution

$$g_{0C}(\varepsilon) = \left\langle \begin{array}{c} n_0 c_1 \sqrt{\varepsilon} \exp\left(-\frac{\varepsilon}{kT_1}\right), \quad \varepsilon < \varepsilon^* \\ n_0 c_2 \sqrt{\varepsilon} \exp\left(-\frac{\varepsilon}{kT_2}\right), \quad \varepsilon \ge \varepsilon^* \end{array} \right\rangle$$
(28)

where ε^* is the threshold energy for inelastic scattering (the first excitation energy) and T_1 and T_2 are temperatures for low- and high-energy electrons, respectively. The constants c_1 and c_2 are determined from continuity of g_{0C} at $\varepsilon = \varepsilon^*$ and from normalization of g_{0C} to the given electron density n_0 at the bulk:

$$c_1 \exp\left(-\frac{\varepsilon^*}{kT_1}\right) = c_2 \exp\left(-\frac{\varepsilon^*}{kT_2}\right), \qquad \int_0^\infty g_{0C}(\varepsilon) d\varepsilon = n_0$$
(30)

By virtue of briefness we do not present here these coefficients explicitly. For the same reason we not present explicitly analytic expressions for the Bohm criterion, number density and fluxes to planar or spherical surfaces in collisionless planar sheath for each EEDF. Most of these formulas can be expressed in terms of incomplete gamma function, available in MATLAB (gammainc).

Behavior of a dust particle in the sheath is mainly determined by gravitational and electric forces. Under some assumptions about the electron Debye length the particle can be approximately considered as a spherical capacitor of the radius r_p . Its charge Q_p and potential U_p relative to the local undisturbed plasma are related by

$$Q_{\rm p} = 4\pi\varepsilon_0 r_{\rm p} U_{\rm p} \tag{31}$$

The charge or potential of the particle is a result of electron and ion currents hitting its surface. Neglecting reflections and desorptions of ions and electrons from the surface [2], the equilibrium potential U_p of the particle is determined from the formula

$$\langle \gamma_{\rm e}(U, U_{\rm p}) \rangle = \gamma_{\rm i}(U, U_{\rm p}) \tag{32}$$

balancing the average electron and ion fluxes impinging the particle. As is shown in [3], the timeaveraging can be with high accuracy realized by replacing electron number density n_e with its mean value

 $< n_{\rm e} >$.

5. Numerical results

Previous formulas have been incorporated into several codes, written in MATLAB. Specialized but cooperating modules compute electric field in the sheath, charge and potential of particles, forces acting on them, their balancing radii and resonance frequencies. Computations have been performed for collisionless rf or dc plasma sheath and several kinds of EEDF defined in the bulk.

Results presented here have been made for argon rf plasma with the same electron number density $n_0 = 1.0 \times 10^{16} \text{ m}^{-3}$ and dc component of electrode potential $U_{dc0} = -50 \text{ V}$ (Eq. 24).

Parameters for the cutoff like the two-temperature Maxwellian distribution (28) have been taken from [4]: $\varepsilon^* = 11.5 \text{ eV}, T_1 = 2.9 \text{ eV}, T_2 = T_1/10$. This data numerically correspond to the effective temperature

$$T_{\rm eff} = \frac{2}{3} < \varepsilon > = \frac{2}{3n_0} \int_0^\infty \varepsilon g_{0\rm C}(\varepsilon) d\varepsilon \approx 2.6 \,\mathrm{eV}$$
(33)

Other distributions were chosen with the same effective temperature: For single Maxwellian EEDF T = 2.6 eV and for double Maxwellian EEDF $P_1 = 0.8$, $T_1 = 2$ eV and $P_2 = 0.2$, $T_2 = 5.2$ eV.

Dust particles were supposed made of melamine formaldehyde of mass density $\rho = 1.5 \times 10^3 \text{ kg/m}^3$ and of radius of several micrometers.

As is obvious from Fig.1, the shape of EEDF influences the electric field in the sheath negligibly. Contrary to it the dust charge is sensitive to the shape of electron characteristic (Fig.2). The charge determines behavior of a particle in the sheath.

Total force acting on a particle is mainly formed by gravitational (-mg) and electric (QE) forces. Magnitudes of other possible forces (ion and neutral drag, thermophoretic force) are under conditions considered here negligible. From the condition that the total force acting on a spherical particle is zero we determine its equilibrium radius, i.e. the radius of a particle levitating at given position above the electrode. As is seen in Fig.3, the maximum radius of a particle confined in the sheath is sensitive to the shape of electron characteristics. For single and double Maxwellian EEDF heavier particles are confined in the sheath than for cutoff EEDF although effective temperature and electron number density are the same. Dust particles deflected from their unstable equilibrium position (dotted lines) will fall down to the electrode or migrate to the higher stable equilibrium positions (solid lines) above the electrode. The extent of dust-free zone at the electrode is independent on energy distribution.

Dust particles deflected from their equilibria positions perform slightly damped oscillations with frequencies, which can be directly observed. They may serve as a test of reliability for chosen theoretical model. Fig.4 demonstrates that the shape of EEDF influences resonance frequencies mainly at the sheath boundary.



Fig. 1: Average electric field versus position above the planar rf electrode for different EEDF with same effective temperatures and number densities .Origin x = 0 corresponds to the position of the electrode, dotted vertical line indicates the sheath edge.



Fig. 2: Dust potential versus position above the planar rf electrode for different *EEDF*.



Fig. 3 Equilibrium radius versus position of microparticles levitating above the planar rf electrode for different EEDF. Dotted curves indicate unstable equilibria positions (in reality dust-free zone).



Fig. 4 Resonance frequency versus height above the electrode for various EEDF.

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