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Octupole inhomogeneity tensor of ion microfield in Debye plasma at ionized emitter

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Abstract. The first constrained moments of the microfield octupole inhomogeneity tensor at ionized emitter have been calculated for the first time. Calculations were performed for three-component Debye plasmas using cluster expansion method in Baranger-Mozer scheme.

PACS. 52.20.-j Elementary processes in plasmas – 52.25.-b Plasma properties – 32.70.Jz Line shapes, widths, and shifts

1 Introduction

For a theoretical description of the spectral line asymmetry and shift of hydrogen and hydrogen-like ions the inhomogeneity of the local ion microfield in the plasma and the second order corrections in the perturbation theory (PT) are necessary to be taken into account [1–3]. The most efficient source of this asymmetry is the emitter-(ion microfield) quadrupole interaction. The quadrupole interaction is proportional to R_0^{-3}, where R_0 is the mean ons-perturbers distance defined by the relationship $(4/15)(2\pi)^{3/2}R_0^3N_e = 1$. The quadrupole inhomogeneity tensors of the local ion microfield in the plasma, in multiparticle model, have been calculated in papers [1,2,4–15]. Terms proportional to R_0^{-4} are the second order importance source of the asymmetry and shift i.e.: the quadratic Stark effect, the second order corrections in PT for quadrupole interactions, and the first order correction in PT for the octupole interaction [2,16].

In paper [17] it is shown that in the wings of H_β line, formed in plasmas of electron concentrations $N_e > 10^{17}$ cm^{-3}, great discrepancies between calculated and measured asymmetry parameters occur. In our opinion the probable reason for these discrepancies is negligence in the calculations [17] of all terms proportional to R_0^{-4}. Substantial discrepancies occur also between the calculated and measured quantities for lines of the hydrogenic ions, as to e.g. the FWHM and shifts of the H_α line of HeII in paper [12]. In that last paper the second order corrections in PT for quadrupole interactions and the first order correction in PT for the octupole interactions have been entirely omitted, and, moreover, the quadratic Stark effect has been taken into account only partially. The physical model becomes internally consistent only when all terms proportional to R_0^{-4} are accounted, in all matrix elements of each operator occurring in the line profile formula. The contributions of the octupole interactions to the matrix elements: of the Hamiltonian, of the dipole momentum of the transition, and of the broadening operator cause symmetrical (in respect to the unperturbed line location) changes of the line profile. Furthermore, these changes indirectly affect the values of the asymmetry parameters of the line profile [18]. For a fixed spectral line the importance of the octupole interaction increases relatively with the increasing N_e, and also with the order number of the spectral line in the series. The octupole interaction gives, furthermore, an essential contribution to the lowering of the ionization energy of emitters in plasma. On the substantial role of the high order multipoles in plasma-emitter interaction see e.g. [19].

This is the second paper dealing with the problem of octupole inhomogeneity tensors of ion microfield in plasma. The first paper [15], hereafter referred to as HO, dealt with inhomogeneity tensors (in particular with quadrupole and octupole tensors) of ion microfield in a two-component Debye plasma at neutral emitter. The problem of the octupole inhomogeneity tensors at ionized emitter in three-component Debye plasma is the subject of this paper.

2 Formalism

The plasma is represented here as a collection of two kinds of (pseudo) ions with number charges Z_a and Z_b and concentrations N_a and N_b. The temperature of ions is T_i.

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Ions interact with each other through an effective shielded Coulomb potential (Debye potential). The effective potential includes the effect of the ion-electron interactions. The temperature of electrons are indicated as T_e. The number charge of an emitter is Z_e. The plasma is neutral, i.e. $Z_aN_a + Z_bN_b = N_e$. The composition parameter is $C = N_b/(N_a + N_b)$ and temperatures ratio parameter is $R_T = T_e/T_i$. For such binary plasma, the ion microfield distribution function in Baranger-Mozer [20] scheme has been calculated in paper [21]. The equations presented below are based on the formalism developed in the papers [7,15,21].

For the description of the octupole inhomogeneity tensor we have introduced, similarly as in HO, a seven-dimensional vector,

$$G = \{G_n\} \equiv \{E_{xxy}, E_{xxz}, E_{xyy}, E_{xyz}, E_{xzz}, E_{yzz}, E_{zzz}\}. \quad (1)$$

The components can be written as follows

$$E_{ijk} = \left(\frac{\partial^2 E_i(\mathbf{r})}{\partial x_j \partial x_k} - \frac{1}{5}\left[\frac{\partial}{\partial x_i}\nabla\cdot\mathbf{E}(\mathbf{r})\delta_{jk} + \frac{\partial}{\partial x_j}\nabla\cdot\mathbf{E}(\mathbf{r})\delta_{ik} + \frac{\partial}{\partial x_k}\nabla\cdot\mathbf{E}(\mathbf{r})\delta_{ij}\right]\right)\Bigg|_{\mathbf{r}=0}, \quad (2)$$

where $\mathbf{E}$ is the electric field

$$\mathbf{E} = \sum_{\alpha=1}^{n_a} \mathbf{E}^a_\alpha(\mathbf{R}^a_\alpha) + \sum_{\alpha=1}^{n_b} \mathbf{E}^b_\alpha(\mathbf{R}^a_\alpha), \quad (3)$$

at the origin (emitter) produced by n_a pointlike (pseudo) ions a located at $\mathbf{R}^a_1, \ldots, \mathbf{R}^a_{n_a}$ and n_b (pseudo) ions of b located at $\mathbf{R}^b_1, \ldots, \mathbf{R}^b_{n_b}$. In spherical coordinates (R, θ, and φ), the components of the octuople inhomogeneity tensors $G^p_{\alpha,n}$, can be written as follows:

$$G^p_{\alpha,n} = -G^p_\alpha A^{(3)}_n(\theta^p_\alpha, \varphi^p_\alpha), \quad (4)$$

where the seven functions $A^{(3)}_n$ depending on angles are given by equation (48) of HO. The upper index (3) indicates the octupole terms similarly as of HO. The radial contribution to the octupole inhomogeneity tensor is

$$G^p_\alpha = Z_p e\left[1 + 3R^p_\alpha/D + 6(R^p_\alpha/D)^2 + (R^p_\alpha/D)^2/5\right] \times \exp(-R^p_\alpha/D)/(R^p_\alpha)^4, \quad (5)$$

where $D = \sqrt{kT/(4\pi e^2 N_e)}$ is the electronic Debye length. Then, the joint probability distribution function for the ion microfield strength $\mathbf{E}$ and the microfield inhomogeneity tensor $\mathbf{G}$ is given by [7,15]

$$W(\mathbf{E}, \mathbf{G}) = \frac{1}{(2\pi)^{10}} \int d^3k\, d^7\sigma \times \exp\{-i\left[\mathbf{k}\cdot\mathbf{E} + \boldsymbol{\sigma}\cdot\mathbf{G}\right]\} F(\mathbf{k}, \sigma). \quad (6)$$

In the case of our plasma the generalized (compared to HO) Fourier transform has the form:

$$F(\mathbf{k}, \sigma) = \exp\left[\sum_{l=1}^{n_a+n_b} \sum_{m=0}^{l} \frac{N_a^m N_b^{l-m}}{m!(l-m)!} h_{m,l-m}(\mathbf{k}, \sigma)\right]. \quad (7)$$

This Fourier transform was obtained by the same method as in the case of the Fourier transform $F^{(0)}(\mathbf{k}) \equiv F(\mathbf{k}, \mathbf{0})$ of the ion microfield distribution function $W(\mathbf{E}) \equiv W(\mathbf{E}, \mathbf{0})$ calculated in [21]. The general expression for functions $h_{m,l-m}(\mathbf{k}, \sigma)$, resulting from the cluster expansion method in Baranger-Mozer scheme, is as follows:

$$h_{m,l-m}(\mathbf{k}, \sigma) = \int \Phi^a_1 \ldots \Phi^a_m \Phi^b_{m+1} \ldots \Phi^b_l \times g_{m,l-m}(\mathbf{R}^a_1, \ldots, \mathbf{R}^a_m, \mathbf{R}^b_{m+1}, \ldots, \mathbf{R}^b_l) d\mathbf{R}^a_1, \ldots d\mathbf{R}^b_l, \quad (8)$$

with

$$\Phi^p_\alpha = \exp\left[i(\mathbf{k}\cdot\mathbf{E}^p_\alpha + \boldsymbol{\sigma}\cdot\mathbf{G}^p_\alpha)\right] - 1, \quad (9)$$

where $g_{m,l-m}$ is the correlation function for m ions of type a and $(m-l)$ ions of type b. By analogy, we introduced also the following symbols

$$h^{(0)}_{m,l-m}(\mathbf{k}) \equiv h_{m,l-m}(\mathbf{k}, \mathbf{0}) \quad (10)$$

and

$$\varphi^p_\alpha = \exp(i\mathbf{k}\cdot\mathbf{E}^p_\alpha) - 1. \quad (11)$$

Calculation of the line profile using as many as 11 dimension functions $W(\mathbf{E}, \mathbf{G})$ is very burdensome. Therefore, in the Hamiltonian for an emitter emerged in plasma one uses the mean values (taken for a fixed $\mathbf{E}$ vector) of the quadrupole, octupole and higher order terms to the emitter-plasma interactions. Such an approximation is acceptable because the above-mentioned interactions are considerably smaller than the dipole term. Estimation of the accuracy of this approximation can be found in papers [10,13]. The constrained average (at an emitter) of the microfield inhomogeneity octupole tensor is defined by

$$\langle G_n\rangle_{\mathbf{E}} \equiv \int d^7 G G_n W(\mathbf{E}, \mathbf{G})/W(\mathbf{E}) \quad (12)$$

and can be calculated [22] from

$$W(\mathbf{E})\langle G_n\rangle_{\mathbf{E}} = \frac{i}{8\pi^3} \int d^3k \exp(-i\mathbf{k}\cdot\mathbf{E}) F^{(3)}_n(\mathbf{k}), \quad (13)$$

where $F^{(3)}_n(\mathbf{k})$ represents a derivate of the Fourier transform

$$F^{(3)}_n(\mathbf{k}) \equiv \left[\partial F(\mathbf{k}, \sigma)/\partial\sigma_n\right]_{\sigma=\mathbf{0}} = \left[\sum_{l=1}^{\infty} \sum_{m=0}^{l} \frac{N_a^m N_b^{l-m}}{m!(l-m)!} h^{(3)}_{(m,l-m),n}(\mathbf{k})\right] \times F^{(0)}(\mathbf{k}), \quad (14)$$

where

$$h^{(3)}_{(m,l-m),n}(\mathbf{k}) \equiv \left[\partial h_{(m,l-m)}(\mathbf{k}, \sigma)/\partial\sigma_n\right]_{\sigma=\mathbf{0}}. \quad (15)$$

However, the probability distribution function for the ion microfield strength is calculated from

$$W(\mathbf{E}) = \frac{1}{(2\pi)^3}\int d^3k \exp(-i\mathbf{k}\cdot\mathbf{E})F^{(0)}(\mathbf{k}). \qquad (16)$$

In reference [23] it was shown that in the case when the Debye potential is valid – a plasma model is internally coherent, when the group expansion terms are taken into account up to the two-body (pseudo)ion-ion correlations term. Therefore, in equations (7) and (14) the expansions can be limited to $l = 2$. Then, the Fourier transform and its derivate can be written (see Eq. (20) in [21])

$$F^{(0)}(\mathbf{k}) \cong \exp\Big[N_a h_a^{(0)}(\mathbf{k}) + N_b h_b^{(0)}(\mathbf{k}) + \frac{1}{2}N_a^2 h_{aa}^{(0)}(\mathbf{k}) + N_a N_b h_{ab}^{(0)}(\mathbf{k}) + \frac{1}{2}N_b^2 h_{bb}^{(0)}(\mathbf{k})\Big], \qquad (17)$$

and

$$F_n^{(3)}(\mathbf{k}) \cong F^{(0)}(\mathbf{k})\exp\Big[N_a h_{a,n}^{(3)}(\mathbf{k}) + N_b h_{b,n}^{(3)}(\mathbf{k}) + \frac{1}{2}N_a^2 h_{aa,n}^{(3)}(\mathbf{k}) + N_a N_b h_{ab,n}^{(3)}(\mathbf{k}) + \frac{1}{2}N_b^2 h_{bb,n}^{(3)}(\mathbf{k})\Big], \qquad (18)$$

where we introduced new symbols: $a \equiv (1,0)$, $b \equiv (0,1)$, $aa \equiv (2,0)$, $bb \equiv (0,2)$, $ab \equiv (1,1)$. The above functions $h(\mathbf{k})$ resulting from equations (8), (9) and (15) can be written as follows:

- one-body functions

$$h_p^{(0)}(\mathbf{k}) = \int g_p\ \varphi_1^p\ d^3R_1^p; \qquad (19)$$

$$h_{p,n}^{(3)}(\mathbf{k}) = i\int g_p(\varphi_1^p+1)G_{1,n}^p\ d^3R_1^p; \qquad (20)$$

- two-body functions

$$h_{pp}^{(0)}(\mathbf{k}) = \int g_{pp}\ \varphi_1^p\varphi_2^p\ d^3R_1^p d^3R_2^p, \qquad (21)$$

$$h_{ab}^{(0)}(\mathbf{k}) = \int g_{ab}\ \varphi_1^a\varphi_1^b\ d^3R_1^a d^3R_1^b, \qquad (22)$$

$$h_{pp,n}^{(3)}(\mathbf{k}) = i\int g_{pp}\left[(\varphi_1^p+1)\varphi_2^p\ G_{1,n}^a + \varphi_1^p(\varphi_2^p+1)G_{2,n}^p\right] d^3R_1^p d^3R_2^p, \qquad (23)$$

$$h_{ab,n}^{(3)}(\mathbf{k}) = i\int g_{ab}\left[(\varphi_1^a+1)\varphi_1^b\ G_{1,n}^a + \varphi_1^a(\varphi_1^b+1)G_{1,n}^b\right] d^3R_1^a d^3R_1^b, \qquad (24)$$

for $p = a$ *or* b. (Note: Eq. (41) on page 429 in HO, which is equivalent to Eq. (23), has typographical errors.) The functions $h^{(0)}(\mathbf{k})$ are the same as in [21]. In the case of the weak coupled plasma (i.e. Debye plasma), the one-body at a charged point and the two-body correlation functions (according with terminology [21]) are given by the following expression, cf. e.g. [7,9,12,21,24,25],

$$g_p = \exp\left[-Z_e Z_p R_D R_T \varGamma_e \frac{\exp(-R_1^p/D_p)}{R_1^p/D_p}\right], \qquad (25)$$

$$g_{pp} = -Z_p^2 R_D R_T \varGamma_e \frac{\exp\left(-|\mathbf{R}_1^p - \mathbf{R}_2^p|/D_p\right)}{|\mathbf{R}_1^p - \mathbf{R}_2^p|/D_p}, \qquad (26)$$

$$g_{ab} = -Z_a Z_b R_D R_T \varGamma_e \frac{\exp\left(-|\mathbf{R}_1^a - \mathbf{R}_1^b|/D_p\right)}{|\mathbf{R}_1^p - \mathbf{R}_2^p|/D_p}, \qquad (27)$$

for $p = a$ *or* b; where $\varGamma_e = \rho^3/3$ is the electronic plasma parameter, $\rho = R_0/D$ is the screening parameter, and $D_p = D/R_D$ is the plasma Debye length, whereas [21]

$$R_D = \left\{1 + R_T\left[\frac{Z_a^2 + C(Z_b^2 - Z_a^2)}{Z_a + C(Z_b - Z_a)}\right]\right\}^{1/2}. \qquad (28)$$

In the Debye plasma (where $\varGamma_e \ll 1$) higher order contributions to two-body correlation functions, as well as three-body and terms of higher number-body correlation functions are proportional to the square or higher powers of the plasma parameter ($\sim \varGamma_e^n$ at $n \geq 2$) and, therefore, they are negligible [25]. The integrals given by equations (19)–(24) have been calculated similarly as in our earlier papers [7,12,15]. There are only two essential differences in calculations of integrals in the present paper compared to HO: (i) the one-body correlation function is given by equation (25) which in HO are equal to one ($g_p = 1$), (ii) a new definition of the variable u is introduced. Namely, in HO in equation (34) we defined u as $u = \sqrt{1+Z_p}vy$, whereas in the present paper $u = R_D vy$. Other variables are the same as in HO, i.e. $y = (ke)^{-1/2}R$, $v = \rho x^{1/2}$ and $x = kE_0$, where E_0 is the normal Holtsmark field strength. Because we apply a similar calculation technique as in HO, we introduce also similar auxiliary functions $\varPsi(v)$. Then, the contributions of one-body and two-body clusters in equations (17) and (18), using the auxiliary functions, can be written:

$$\begin{aligned} N_a h_a^{(0)} + N_b h_b^{(0)} &= -x^{3/2}\varPsi_1^{(0)}(v), \\ \frac{1}{2}N_a^2 h_{aa}^{(0)} + N_a N_b h_{ab}^{(0)} + \frac{1}{2}N_b^2 h_{bb}^{(0)} &= x^{3/2}\varPsi_2^{(0)}(v), \\ N_a h_{a,n}^{(3)} + N_b h_{b,n}^{(3)} &= \frac{15}{28}\frac{E_0}{R_0^2}\varPsi_{1,n}^{(3)}(v) \times A_n^{(3)}(\theta_k,\varphi_k), \\ N_a h_{aa,n}^{(3)} + N_a N_b h_{ab}^{(3)} + N_b h_{bb,n}^{(3)} &= \frac{15}{28}\frac{E_0}{R_0^2}\varPsi_{2,n}^{(3)}(v) \times A_n^{(3)}(\theta_k,\varphi_k), \end{aligned} \qquad (29)$$

where the angles θ_k and φ_k describe the direction of the vector $\mathbf{k}$ in the coordinate system xyz.

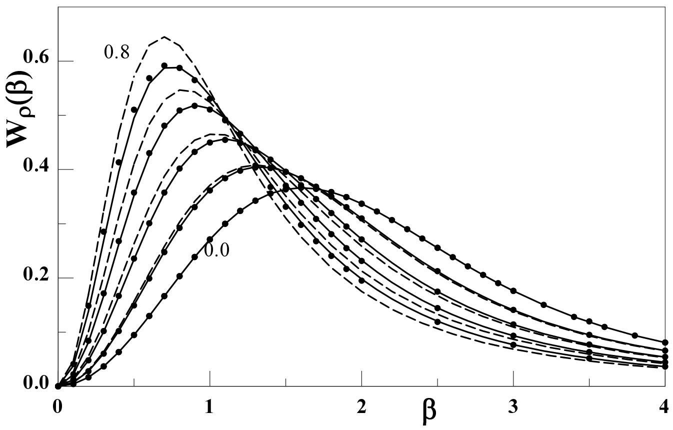

Fig. 1. The electric microfield distribution function $W_\rho(\beta)$ at a singly-charged emitter ($Z_e = 1$) in singly-ionized plasma ($Z_p = 1$) as a function of the reduced electric field β, for several values of the screening parameter $\rho = 0.0, 0.2, 0.4, 0.6$, and 0.8. The solid lines represent our results, the points represent Hooper's data [26], whereas the dashed lines represent Mozer-Baranger's [20] results.

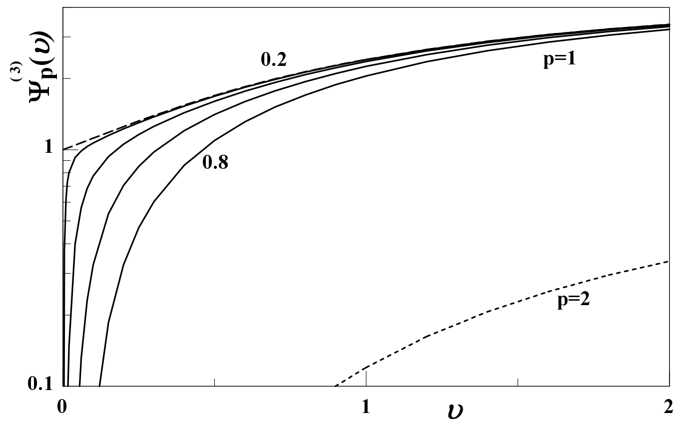

Fig. 2. Comparison of the auxiliary octopule functions at singly-charged emitter ($Z_e = 1$) and the auxiliary octopule function at a neutral emitter ($Z_e = 0$) in singly-ionized plasma ($Z_p = 1$). The solid lines represent one-body auxiliary functions at an ionized emitter, for several values of the screening parameter $\rho = 0.2, 0.4, 0.6$, and 0.8. The dashed line represents the one-body auxiliary function at a neutral emitter. The pointed line represents the two-body auxiliary functions.

Finally, the average of the component of the microfield inhomogeneity octupole tensor given by equation (12) can be written in the same from as in HO:

$$\langle G_n \rangle_{\mathbf{E}} = \frac{15}{28}\frac{E_0}{R_0^2} B_\rho^{(3)}(\beta) A_n^{(3)}(\theta_E, \varphi_E), \tag{30}$$

where the octupole function is,

$$B_\rho^{(3)}(\beta) = \frac{2}{\pi}\beta^2 / W_\rho(\beta) \int_0^\infty dx x^2 \left[\Psi_1^{(3)}(\rho x^{1/2}) + \Psi_2^{(3)}(\rho x^{1/2})\right]$$
$$\times \exp\left\{-x^{3/2}\left[\Psi_1^{(0)}(\rho x^{1/2}) - \Psi_2^{(0)}(\rho x^{1/2})\right] j_t(\beta x)\right\}, \tag{31}$$

whereas the microfield distribution function is

$$W_\rho(\beta) = \frac{2}{\pi}\beta^2 \int_0^\infty dx x^2$$
$$\times \exp\left\{-x^{3/2}\left[\Psi_1^{(0)}(a x^{1/2}) - \Psi_2^{(0)}(a x^{1/2})\right]\right\} j_0(\beta x); \tag{32}$$

both functions are given in the normalised scale $\beta = E/E_0$. The function $j_l(\epsilon)$ is the *spherical Bessel function* of order l.

3 Numerical results

The main aim of the present paper is to perform calculations of the octupole functions $B_\rho^{(3)}(\beta)$ at ionized emitter. From equation (31) we see that to calculate the octupole functions $B_\rho^{(3)}(\beta)$, the distribution functions $W_\rho(\beta)$ are needed. In Figure 1 our $W_\rho(\beta)$ function calculated at ionized emitter in the case of singly-ionized plasma with that of Hooper [26], and with the original Baranger-Mozer's one [20] are compared as an example. We find an excellent agreement between our distribution function $W_\rho(\beta)$ at ionized emitter and the Hooper's one, similarly as it was shown in [25]. Such an agreement is a positive test of a numerical code used in the present paper.

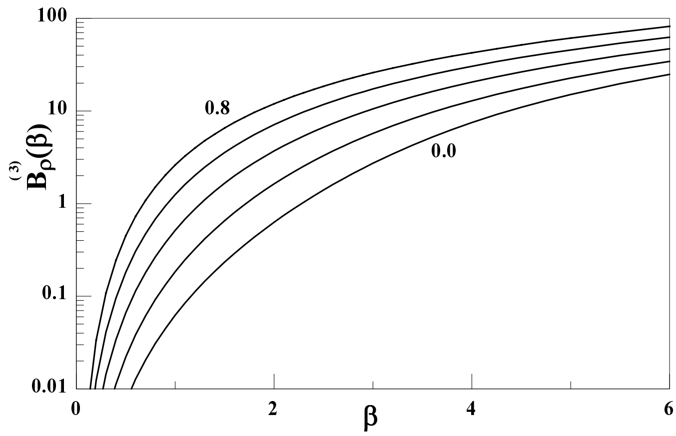

Fig. 3. The octupole function $B_\rho^{(3)}(\beta)$ at a singly-charged emitter ($Z_e = 1$) in singly-ionized plasma ($Z_p = 1$) as a function of the reduced electric field β, for several values of the screening parameter $\rho = 0.0, 0.2, 0.4, 0.6$, and 0.8.

In the next figures, as examples, our numerical results for octupole functions are presented. Figure 2 presents a comparison of the auxiliary octopule functions at ionized emitter and the auxiliary function at neutral emitter. We see that only for $v < 1$ essential differences appear between the one-body function at neutral emitter $\Psi_1^{(3)}(v, Z_e = 0)$ and the one at ionized emitter $\Psi_1^{(3)}(v, Z_e = 1)$. The two-body auxiliary functions $\Psi_2^{(3)}(v)$ are the same, because they do not depend on the number charge of the emitter.

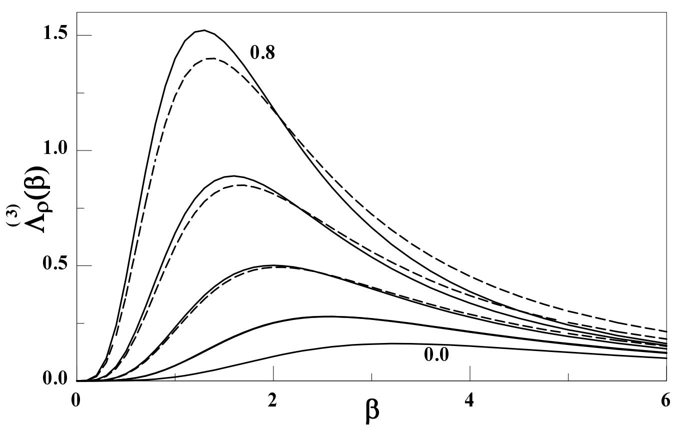

Fig. 4. Comparison the octupole function $\Lambda_\rho^{(3)}(\beta)$ at a singly-charged emitter (solid lines) and one at a neutral emitter (dashed lines) – both functions in singly-ionized plasma, for several values of the screening parameter $\rho = 0.0, 0.2, 0.4, 0.6,$ and 0.8.

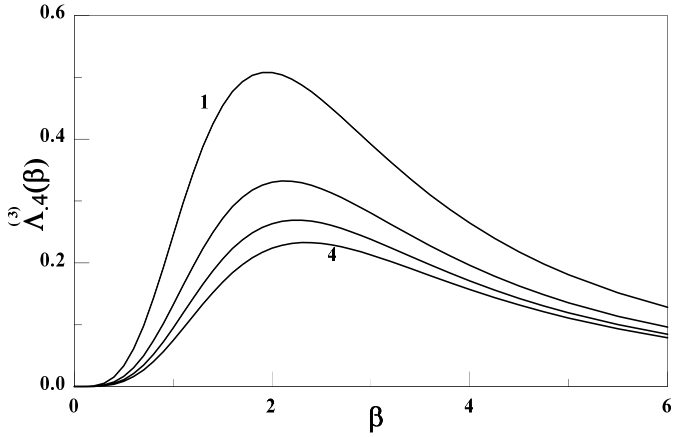

Fig. 6. The octupole function $\Lambda_{0.4}^{(3)}(\beta)$ at a doubly-charged emitter ($Z_e = 2$) in plasmas with the number charges of perturbers $Z_p = 1$ or 2 or 3 or 4.

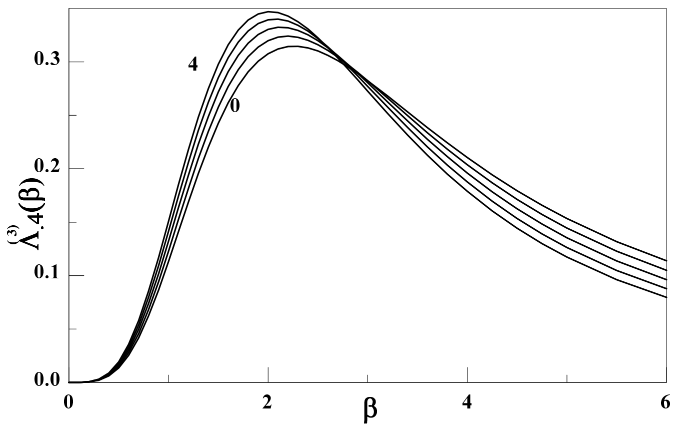

Fig. 5. The octupole function $\Lambda_{0.4}^{(3)}(\beta)$ in doubly-ionized plasma ($Z_p = 2$) at an ionized emitter for several values of the number charges of emitter $Z_e = 0, 1, 2, 3,$ and 4.

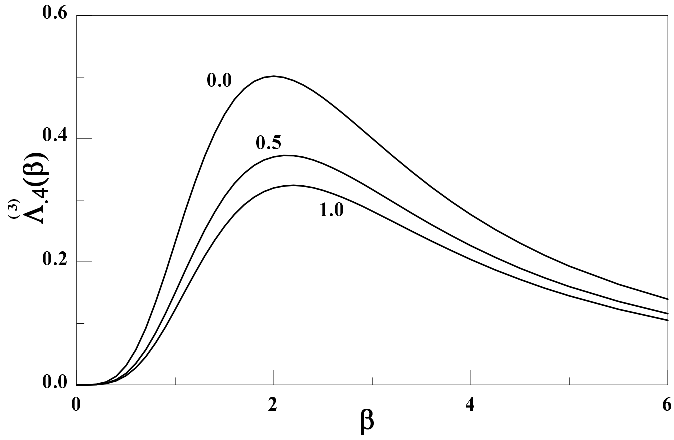

Fig. 7. The octupole function $\Lambda_{0.4}^{(3)}(\beta)$ at a singly-charged emitter ($Z_e = 1$) in plasmas of two kinds of perturbers: $Z_a = 1$ and $Z_b = 2$, for several values of the composition parameter $C = 0.0,\ 0.5,$ and 1.0.

Figure 3 shows the strong joint shielding and correlated effect (represented by the screening parameter ρ) for octupole function $B_\rho^{(3)}(\beta)$ at an ionized emitter in singly-ionized plasma. The effect can also be observed in Figure 4 for the function $\Lambda_\rho^{(3)}(\beta) = B_\rho^{(3)}(\beta)W_\rho(\beta)/\beta$. Additionally, in Figure 4 this function is compared with the function $\Lambda_\rho^{(3)}(\beta)$ at neutral emitter, both functions are calculated for singly-ionized plasma. For a fixed value of the screening parameter ρ (which represents also the physical conditions of the plasma) these functions differ slightly from each other. The function $\Lambda_\rho^{(3)}(\beta)$ conveys the influence of the emitter – (plasma) octupole interaction on the line profile better than the function $B_\rho^{(3)}(\beta)$. Thus, in the next figures the functions $\Lambda_{0.4}^{(3)}(\beta)$ are presented. In Figures 5–7 three effects are shown: the weak emitter effect, the perturber charge effect, and the composition perturber charge effect, respectively. In the last two figures the function values $\Lambda_{0.4}^{(3)}(\beta)$ are smaller for perturbers with larger Z_p. At first glance it seems that this dependency could not be correct. However we would like to emphasize that for neutral plasma of identical temperatures and identical electron densities N_e (ρ is constant) – ion densities $N_p = N_e/Z_p$ are smaller for larger Z_p values. Indeed, the distances between the emitter and perturbers are larger and the inhomogeneity of the ion microfield is therefore smaller.

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