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Inhomogeneity tensors of ion microfield in Debye plasma at neutral emitter

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Abstract. A method of calculation of inhomogeneity microfield tensors in Debye plasma, using the Mayer-Mayer cluster expansion, is presented. The octupole inhomogeneity tensor of the ion microfield at a neutral emitter has been calculated for the first time. The quadrupole inhomogeneity tensor of the ion microfield at a neutral emitter has been recalculated. We have performed numerical calculations for plasma consisting of atoms, electrons and singly or doubly charged ions.

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

1 Introduction

The main source of asymmetry of the hydrogen spectral line shapes formed in plasma is the inhomogeneity of the ion microfield. Kudrin and Sholin [1,2] noticed the fact for the first time. They considered this problem in the nearest neighbour approximation. In the Holtsmark approximation, in order to describe the gradient of the local ion microfield, Demura and Sholin [3] adapted the Chandrasekhar and von Neumann function $B(\beta)$, which originally was introduced in [4] for the description of the gravitational field produced by groups of stars. The gradients of microfield strength in plasma, with the inclusion of screening effects characteristic of plasma, was calculated in papers [5,6]. However in papers [7–13] the screening and the ion-ion correlation effects were taken into account simultaneously. As regards the importance in the line-asymmetry formation, the second great part is played by the quadratic Stark effect, for which correction to the energy eigenvalues of the emitter in plasma is proportional to R_0^{-4}, where R_0 is the mean ions-perturbers distance. References [2,14] show that the second order correction in the perturbation theory (PT) for the quadrupole interaction and the first order correction in PT for the octupole interaction are proportional to R_0^{-4}. For this reason, to obtain correct description of the profile asymmetry of the hydrogen and hydrogen-like ion, the Hamiltonian of the emitter, immersed in plasma, should also include the octupole interactions.

The main aim of the present paper is calculation of the inhomogeneity of the octupole tensor $E^{(3)}_{ijk}$ for the ion microfield in plasma at the position of a typical atom. In all experiments, in which the hydrogen lines profiles were investigated (see e.g. [15] including an extensive list of references), the plasma parameter (see Eq. (4)) was $\Gamma \le 0.25$. Plasmas consisted of singly charged ions (and — at the very most — doubly charged ions) and electrons. For such Debye plasmas the approximation proposed by Mozer and Baranger in [16] is accurate enough for calculation of the microfield distribution function $W_a(\beta)$ as well as the quadrupole $E^{(2)}_{ij}$ and the octupole $E^{(3)}_{ijk}$ inhomogeneity tensors.

In experiment [17], for electron density $N_e \sim 10^{19}$ cm^{-3}, the plasma consisted of almost solely He^{++} ions. We again calculated the inhomogeneity quadrupole tensor $E^{(2)}_{ij}$, because (i) there are no numerical values of the tensor for such plasma as that in the experiment [17], and (ii) numerical results of the tensor for singly ionized plasma published in [7, 9b], are differ slightly from one another.

2 Emitter-plasma interaction

The Hamiltonian of a typical emitter immersed in plasma can be described as follows:

$$H = H_0 + U_{ae} + U_{ee} + U_{ai} + U_{ii} + U_{ie}, \qquad (1)$$

where U is the Coulomb interaction indexed by a for the emitter, i for ions, and e for electrons. The interaction between the neutrals, i.e., atoms, is neglected. Interaction U varies with time. The relaxation time measure of the ionic microfield component in plasma is $\tau_i \approx F_i/\dot{F}_i \approx v_i/R_i$, where v_i is the mean thermal velocity of ions, while R_i is

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the mean distance between them, resulting from the relationship $(4\pi/3)R_i^3 N_i = 1$, where N_i is ions density. Similarly, for the electronic microfield component the relaxation time is $\tau_e \approx v_e/R_e$. These times fulfill the following relation

$$\tau_e \ll \Delta t \ll \tau_i, \tag{2}$$

which allows us, via the Poisson equation,

$$\nabla^2\phi_\alpha(\mathbf{r}) = -4\pi e N_e(1-\exp(e\phi_\alpha(\boldsymbol{r})/kT)) - 4\pi Z_\alpha e\delta(\mathbf{r}-\mathbf{R}_\alpha) \tag{3}$$

to calculate the potential (averaged in time Δt) produced at the point $\mathbf{r}$ by the statistical α-th ion at position $\mathbf{R}_\alpha$ in the *sea* of free electrons. If the plasma parameter Γ satisfies the relation, e.g. [18],

$$\Gamma = \langle e\phi_\alpha(\mathbf{r})\rangle/k_B T = \frac{1}{3}Z_\alpha^{5/3}a^2 \ll 1, \tag{4}$$

where k_B is the Boltzmann constant, T is temperature, $Z_\alpha e$ is the electric charge of the perturbing ion, $a = R_0/D$ is the screening parameter with $D = \sqrt{kT/(4\pi e^2 N_e)}$ the electronic Debye length, and R_0 — the distance defined by the relationship $(4/15)(2\pi)^{3/2}R_0^3 N_e = 1$ (see, e.g., [16]), we obtain the Debye potential:

$$\phi_\alpha(\mathbf{r}) = \frac{Z_\alpha e}{|\mathbf{r}-\mathbf{R}_\alpha|}\exp(-|\mathbf{r}-\mathbf{R}_\alpha|/D). \tag{5}$$

In the case of strongly coupled plasmas, i.e. when the plasma parameter does not fulfill the relation given by equation (4), the potential $\phi_\alpha(\mathbf{r})$ resulting from equation (3), is an even shorter-range potential than the Debye one.

In this way, for weakly-coupled plasmas ($\Gamma \ll 1$), the sum

$$U_{ai}^{eff} = U_{ai} + U_{ie}, \tag{6}$$

is well approximated by the effective interaction emitter-ions, when the Debye-screened potential for ions is used:

$$\phi(\mathbf{r}) = \sum_\alpha \frac{Z_\alpha e}{|\mathbf{r}-\mathbf{R}_\alpha|}\exp(-|\mathbf{r}-\mathbf{R}_\alpha|/D). \tag{7}$$

In our paper [19] we showed that the sum of the interactions

$$U_{ae}^{eff} = U_{ae} + U_{ee}, \tag{8}$$

is well approximated by the effective interaction described by the Coulomb potential for electrons cut-off at the distance equal to the electronic Debye length. Then the Hamiltonian can be written as follows

$$H = H_0 + U_{ae}^{eff} + U_{ai}^{eff}, \tag{9}$$

with the assumption that the ion-ion correlation (caused by the U_{ii} interaction) is included in the statistics of quantity U_{ai}^{eff}.

2.1 The multipole expansion

The multipole expansion of the potential produced by (pseudo) ions in the neighbourhood of point $\mathbf{r} = \mathbf{0}$ is given by

$$\phi(\mathbf{r}) = \phi - \mathbf{r}\cdot\mathbf{E} - \frac{1}{6}\sum_{ij} c_{ij}E_{ij}^{(2)} - \frac{1}{30}\sum_{ijk} c_{ijk}E_{ijk}^{(3)} + \frac{1}{6}r^2\nabla\cdot\mathbf{E} + \frac{1}{10}r^2\mathbf{r}\cdot\nabla(\nabla\cdot\mathbf{E}) + \cdots \tag{10}$$

The first four terms are the monopole, dipole, quadrupole, and the octupole ones, respectively. The fifth term is connected with the quadrupole term and the sixth term — with the octupole term. The quantities: $c_{ij} = 3x_i x_j - r^2\delta_{ij}$ and $c_{ijk} = 5x_i x_j x_k - r^2(x_i\delta_{jk} + x_j\delta_{ik} + x_k\delta_{ij})$ are the quadrupole and the octupole tensors, whereas:

- the electric potential

$$\phi = \phi(\mathbf{0}) = \sum_\alpha Z_\alpha e\exp(-R_\alpha/D)/R_\alpha, \tag{11}$$

- the electric field

$$\mathbf{E} = -\nabla\phi(\mathbf{r})|_{\mathbf{r}=0} = \sum_\alpha Z_\alpha e(1+R_\alpha/D)\exp(-R_\alpha/D)\mathbf{R}_\alpha/R_\alpha^3, \tag{12}$$

- the symmetrical ($E_{ij}^{(2)} = E_{ji}^{(2)}$) and of traceless ($\mathrm{Tr}\{E_{ij}^{(2)}\} = 0$) inhomogeneous electric field quadrupole tensor

$$E_{ij}^{(2)} = \left.\left(\frac{\partial E_i(\mathbf{r})}{\partial x_j} - \frac{1}{3}\delta_{ij}\nabla\cdot\mathbf{E}\right)\right|_{\mathbf{r}=0}, \tag{13}$$

- the symmetrical

$$\left(E_{ijk}^{(3)} = E_{jik}^{(3)} = E_{kji}^{(3)} = E_{kij}^{(3)} = E_{jki}^{(3)} = E_{ikj}^{(3)}\right)$$

and of "traceless" ($\sum_{ij} E_{ijk}^{(3)}\delta_{ij} = 0$ for $k = 1,2,3$) inhomogeneous electric field octupole tensor

$$E_{ijk}^{(3)} = \left.\left(\frac{\partial^2 E_i(\mathbf{r})}{\partial x_j\partial x_k} - \frac{1}{5}\left[\frac{\partial}{\partial x_i}\nabla\cdot\mathbf{E}(\mathbf{r})\delta_{jk} + \frac{\partial}{\partial x_j}\nabla\cdot\mathbf{E}(\mathbf{r})\delta_{ik} + \frac{\partial}{\partial x_k}\nabla\cdot\mathbf{E}(\mathbf{r})\delta_{ij}\right]\right)\right|_{\mathbf{r}=0}, \tag{14}$$

- the divergence of the electric field

$$\nabla\cdot\mathbf{E} = \nabla\cdot\mathbf{E}(\mathbf{r})|_{\mathbf{r}=0} = -\frac{\phi(\mathbf{0})}{D^2} + 4\pi\sum_\alpha Z_\alpha e\delta(\mathbf{R}_\alpha), \tag{15}$$

- and the gradient of the divergence of the electric field

$$\nabla(\nabla\cdot\mathbf{E}) = \nabla(\nabla\cdot\mathbf{E}(\mathbf{r}))|_{\mathbf{r}=0}, \tag{16}$$

are calculated in point $\mathbf{r} = \mathbf{0}$. From the symmetry property it follows results that the quadrupole tensor has five independent components: E_{xx}, E_{xy}, E_{xz}, E_{yz}, E_{zz}, whereas the octupole tensor has seven independent components: E_{xxy}, E_{xxz}, E_{xyy}, E_{xyz}, E_{xzz}, E_{yzz}, E_{zzz}.

The divergence $\nabla \cdot \mathbf{E}$ requires a supplementary comment. In paper [7], in the multipole expansion, the term proportional to the divergence was neglected as a small one in comparison with the quadrupole term. Justification of such a treatment of this term was given by calculation in [20]. In paper [20], we showed that divergence $\nabla \cdot \mathbf{E}(\beta)$, as a function of the field strength in reduced scale $\beta = F/F_0$ (where F_0 is the so-called Holtsmark field), is piecewise positive or negative in such a way that the mean value of the divergence $\int_0^\infty \nabla \cdot \mathbf{E}(\beta) W_a(\beta) d\beta = 0$, is equal to zero. This result is not surprising, because the total charge of plasma is equal to zero. On the contrary, in paper [6] it was emphasized that the term proportional to the divergence has a significant influence on the line shapes formed in plasma. Such disagreement in estimation of the importance of that term is caused by the fact that in [6] only the electronic component of the divergence was calculated, whereas the ionic contribution was omitted. Such an incomplete calculation was presented in [9] as well as in all the earlier papers of the authors cited in it. Similarly, an incomplete calculation was performed in paper [13], corrected (by introduction of an additional term, taken ad hoc, by no means resulting from the multipole expansion) in order to get the mean value of charge density equal to zero. After such a correction results [13] are formally correct. We would like to notice that all the calculations mentioned above were performed for the exactly neutral point. Actually, even the neutral emitter interacting with free electrons causes some modification of the distribution of electron sea charge density. In our opinion, at the point $\mathbf{r} = \mathbf{0}$ and in its near neighbourhood this density is equal to zero, because the (free electron)–(atomic nucleus) distance cannot be arbitrarily small. (About interactions in plasma at small interparticle distance — see e.g. [21]). Then, of course, the divergence of the microfield is equal to zero also, $\nabla \cdot \mathbf{E} = 0$. Ions also cannot locate by themselves arbitrarily close to the point $\mathbf{r} = \mathbf{0}$. For example, the approach of an ion to the atom down to a distance smaller than about $3n^2 a_0$ (double the Bohr radius) causes ionization of the atom, so it stops being the neutral emitter. This ionization effect can be taken into account by introduction of a critical maximum value β_c for the distribution $W_a(\beta)$. However, in the case of electrons it is difficult to precisely determine the reference volume at point $\mathbf{r} = \mathbf{0}$, i.e. volume free from the electric charge. We can estimate the influence of this volume on the resultant value of the plasma-emitter interaction energy. Let us assume that the emitter is located in a cavity of the spherical shape and of the radius R_s, at the center in point $\mathbf{r} = \mathbf{0}$; inside the sphere the density of plasma electric charge equals zero. We consider only such cases when the nearest ion-emitter distance is greater than R_s (wide ionization problem). Then, we can calculate the resultant potential $\phi'(\mathbf{r})$as a difference between the potential $\phi(\mathbf{r})$ and the potential $\phi^s(\mathbf{r})$ produced by the sphere of radius R_s and of density equal to the electron sea charge density:

$$\phi'(\mathbf{r}) = \phi(\mathbf{r}) - \phi^s(\mathbf{r}). \tag{17}$$

The potential $\phi^s(\mathbf{r})$ produced by the sphere can be calculated from the Poisson-Laplace equation

$$\nabla^2 \phi^s(\mathbf{r}) = \begin{cases} \phi(\mathbf{r})/D^2, & \text{for} \quad r < R_s, \\ 0, & \text{for} \quad r \geq R_s. \end{cases} \tag{18}$$

First of all, we are interested in the strength of the electric field in the vicinity of the point $\mathbf{r} = \mathbf{0}$, which is convenient to calculate using — in the above equation — the multipole expansion for the potential $\phi(\mathbf{r})$ given by equation (10). In such a case the potential satisfying the above Poisson-Laplace equation is as follows

$$\phi^s(\mathbf{r}) = -\frac{1}{2}s^2\phi + \frac{1}{6}s^2\mathbf{r}\cdot\mathbf{E} + \frac{1}{10}s^2\sum_{ij} c_{ij}E_{ij}^{(2)} + \frac{1}{6}r^2\nabla\cdot\mathbf{E} + \frac{1}{10}r^2\mathbf{r}\cdot\nabla(\nabla\cdot\mathbf{E}) + \cdots, \tag{19}$$

where $s \equiv R_s/D$. Finally, the multipole expansion of the emitter-perturbing (*pseudo*) ions interaction is given by

$$\begin{aligned} U_{ai}^{eff} &= (Z-1)e\left(1+\frac{1}{2}s^2\right)\phi - \left(1+\frac{1}{6}s^2\right)\mathbf{d}\cdot\mathbf{E} \\ &\quad - \frac{1}{6}\left(1+\frac{1}{10}s^2\right)\sum_{ij} Q_{ij}E_{ij}^{(2)} \\ &\quad - \frac{1}{30}\left(1+\frac{1}{14}s^2\right)\sum_{ijk} O_{ijk}E_{ijk}^{(3)} + \cdots \end{aligned} \tag{20}$$

The quantities: $\mathbf{d} = -e\mathbf{r}$ is the dipole moment, $Q_{ij} = -ec_{ij}$ and $O_{ijk} = -ec_{ijk}$ are the quadrupole and the octupole moment tensors of the emitter; whereas Ze is a charge of the emitter. So, using symmetry of the quadrupole Q_{ij} and for the octupole O_{ijk} tensors, which are the same as corresponding symmetry of the inhomogeneous electric field quadrupole $E_{ij}^{(2)}$ and octupole $E_{ijk}^{(3)}$ tensors, the sums in equation (20) can be written as follows:

$$\begin{aligned} \sum_{ij} Q_{ij}E_{ij}^{(2)} &= (2Q_{xx}+Q_{zz})E_{xx}^{(2)} + (Q_{xx}+2Q_{zz})E_{zz}^{(2)} \\ &\quad + 2Q_{xy}E_{xy}^{(2)} + 2Q_{xz}E_{xz}^{(2)} + 2Q_{yz}E_{yz}^{(2)}, \end{aligned} \tag{21}$$

and

$$\begin{aligned} \sum_{ijk} O_{ijk}E_{ijk}^{(3)} &= (4O_{xxy}+O_{yzz})E_{xxy}^{(3)} \\ &\quad + (6O_{xxz}+3O_{zzz})E_{xxz}^{(3)} + (4O_{xyy}+O_{xzz})E_{xyy}^{(3)} \\ &\quad + (O_{xyy}+O_{xzz})E_{xzz}^{(3)} + 6O_{xyz}E_{xyz}^{(3)} \\ &\quad + (O_{xxy}+Q_{yzz})E_{yzz}^{(3)} + (4O_{zzz}+3O_{xxz})E_{zzz}^{(3)}. \end{aligned} \tag{22}$$

Moreover, we want to observe that the interaction (Eq. (20)) contains no terms proportional to the divergence of the electric microfield strength, in contrast with equation (10). The significance of the new terms proportional to s^2 is very small. We are not able to precise define the value of R_s, but even if we assume that the radius of the sphere not containing a free plasma charge (reference volume) equals the classical atom radius $R_s = 3/2n^2a_0$, then the resulting contribution of that reference volume to the resulting interaction energy U_{ai}^{eff} is negligible as well anyway.

3 Distribution functions of microfield inhomogeneity tensors

In order to describe mathematical formulas in a compact form it is convenient to introduce, similarly as in reference [7], a formal vector $\mathbf{G}$, which represents the independent components of the inhomogeneity microfield tensor. For the description of the quadrupole inhomogeneity tensor we have introduced a five-dimensional vector

$$\mathbf{G}^{(2)} = \{G_n^{(2)}\} \equiv \{E_{xx}, E_{xy}, E_{xz}, E_{yz}, E_{zz}\}, \tag{23}$$

however for the octupole inhomogeneity tensor a seven-dimensional vector is needed

$$\mathbf{G}^{(3)} = \left\{G_n^{(3)}\right\} \equiv \{E_{xxy}, E_{xxz}, E_{xyy}, E_{xyz}, E_{xzz}, E_{yzz}, E_{zzz}\}. \tag{24}$$

(Any tensor $\mathbf{G}^{(t)}$ can be described similarly.) Then the joint probability distribution function for the microfield strength $\mathbf{E}$ and the microfield inhomogeneity tensor is given by [7]

$$W(\mathbf{E},\mathbf{G}) = \frac{1}{(2\pi)^{3+m}}\int d^3k\ d^m\sigma \times \exp\{-i\left[\mathbf{k}\cdot\mathbf{E} + \sigma\cdot\mathbf{G}\right]\}F(\mathbf{k},\sigma), \tag{25}$$

where $m \equiv n_{max}$ is the dimension of the vector $\mathbf{G}$. In the case of the plasma containing ions of one kind only (i.e. $q_\alpha = Z_pe = const$) with density N_p, the Fourier transform has the form

$$F(\mathbf{k},\sigma) = \exp\left\{\sum_{l=1}^{\infty}\frac{N_p^l}{l!}h_l(\mathbf{k},\sigma)\right\}. \tag{26}$$

The function $h_l(\mathbf{k},\sigma)$ corresponds to the increasing orders in the cluster expansion method [22,16]. The general expression for a function of lth order is

$$h_l(\mathbf{k},\sigma) = \int \varphi_1\varphi_2\cdots\varphi_l \times g_l(\mathbf{R}_1,\mathbf{R}_2,\cdots,\mathbf{R}_l)dR_1dR_2\cdots,dR_l, \tag{27}$$

with

$$\varphi_\alpha = \exp\left[i(\mathbf{k}\cdot\mathbf{E}_\alpha + \sigma\cdot\mathbf{G}_\alpha)\right] - 1, \tag{28}$$

where g_l is the l-body correlation function depending on the configuration of l ions located at $\mathbf{R}_1, \mathbf{R}_2, \cdots, \mathbf{R}_l$.

For calculations of the line profiles, the average of the microfield inhomogeneity tensor $\langle\mathbf{G}\rangle_\mathbf{E}$ alone is sufficient [3–11,13], because contributions of the quadrupole, octupole and higher order terms to the line profile, are considerably lesser than the contribution from the dipole term. They are defined by

$$\langle G_n\rangle_\mathbf{E} \equiv \int d^mGG_nW(\mathbf{E},\mathbf{G})/W(\mathbf{E}) \tag{29}$$

and can be calculated [4] from

$$W(\mathbf{E})\langle G_n\rangle_\mathbf{E} = -\frac{i}{8\pi^3}\int d^3k\exp(-\mathbf{k}\cdot\mathbf{E})\left[\partial F(\mathbf{k},\sigma)/\partial\sigma_n\right]_{\sigma=\mathbf{0}}. \tag{30}$$

For small $|\sigma_n|$, the Fourier transform has the series expansion

$$F(\mathbf{k},\sigma) \simeq F^{(0)}(\mathbf{k},\sigma) + \sum_{n=1}^{m}F_n^{(1)}(\mathbf{k})\sigma_n, \tag{31}$$

where

$$F_n^{(1)}(\mathbf{k}) = F^{(0)}(\mathbf{k})\sum_{l=1}^{\infty}\frac{N_p^l}{l!}h_{l,n}(\mathbf{k}) \tag{32}$$

with

$$h_{l,n}(\mathbf{k}) = \left[\partial h_l(\mathbf{k},\sigma)/\partial\sigma_n\right]_{\sigma=\mathbf{0}}. \tag{33}$$

The function $F^{(0)}(\mathbf{k})$ is the Fourier transform of the microfield distribution function $W(\mathbf{E})$ given by

$$F^{(0)}(\mathbf{k}) = \exp\left\{\sum_{l=1}^{\infty}\frac{N_p^l}{l!}h_l^{(0)}(\mathbf{k})\right\} \tag{34}$$

with $h_l^{(0)}(\mathbf{k}) \equiv h_l(\mathbf{k},\mathbf{0})$, whereas the microfield distribution function is:

$$W(\mathbf{E}) = \frac{1}{(2\pi)^3}\int d^3k\exp(-i\mathbf{k}\cdot\mathbf{E})F^{(0)}(\mathbf{k}). \tag{35}$$

In reference [23] it was showed 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 (26), (32), and (34) the expansions can be limited to the first two terms only. Then the derivate of the Fourier transform can be written

$$\left[\partial F(\mathbf{k},\sigma)/\partial\sigma_n\right]_{\sigma=\mathbf{0}} = \left[N_ph_{1,n}(\mathbf{k}) + \frac{1}{2}N_p^2h_{2,n}(\mathbf{k})\right]F^{(0)}(\mathbf{k}) \tag{36}$$

with

$$F^{(0)}(\mathbf{k}) = \exp\left[N_ph_1^{(0)}(\mathbf{k}) + \frac{1}{2}N_p^2h_2^{(0)}(\mathbf{k})\right]. \tag{37}$$

The functions $h(\mathbf{k})$ resulting from equation (27) can be written as follows:

- one-body functions

$$h_1^{(0)}(\mathbf{k}) = \int g_1(\mathbf{R}_1)\left[\exp(i\mathbf{k}\cdot\mathbf{E}_1) - 1\right]d^3R_1 \tag{38}$$

and

$$h_{1,n}(\mathbf{k}) = i\int g_1(\mathbf{R}_1)G_{1,n}\exp(i\mathbf{k}\cdot\mathbf{E}_1)d^3R_1; \tag{39}$$

– two-body functions

$$h_2^{(0)}(\mathbf{k}) = \int g_2(\mathbf{R}_1,\mathbf{R}_2)\,[\exp(i\mathbf{k}\cdot\mathbf{E}_1)-1] \times [\exp(i\mathbf{k}\cdot\mathbf{E}_2)-1]\,d^3R_1d^3R_2 \quad (40)$$

and

$$h_{2,n}(\mathbf{k}) = i\int d^3R_1d^3R_2g_2(\mathbf{R}_1,\mathbf{R}_2)G_{1,n}\exp(i\mathbf{k}\cdot\mathbf{E}_1) \times [\exp(i\mathbf{k}\cdot\mathbf{E}_2)-1]G_{2,n}\exp(i\mathbf{k}\cdot\mathbf{E}_2) \times [\exp(i\mathbf{k}\cdot\mathbf{E}_1)-1]\,. \quad (41)$$

In the case of the quasi-neutral plasma consisting of atoms, ions with charge Z_pe and the density N_p and electrons of density N_e, the one-body correlation function at a neutral point (for a H-atom) is $g_1 = 1$, whereas the two-body correlation function is given by the expression, cf. [7,16,24],

$$g_2 = -\frac{2(2\pi)^{1/2}}{15}Z_p^2a^3\frac{\exp(-|\mathbf{R}_1-\mathbf{R}_2|/D_p)}{|\mathbf{R}_1-\mathbf{R}_2|/D}, \quad (42)$$

where $D_p = D/\sqrt{1+Z_p}$ is the plasma Debye length.

In spherical coordinates (R, θ, and φ), the ionic microfield strength $\mathbf{E}_\alpha$ and the components of the inhomogeneity tensors $G_{\alpha,n}^{(t)}$, can be written as follows:

$$\mathbf{E}_\alpha = -E(R_\alpha)\mathbf{R}_\alpha/R_\alpha, \quad (43)$$

$$G_{\alpha,n}^{(t)} = -G^{(t)}(R_\alpha)A_n^{(t)}(\theta_\alpha,\varphi_\alpha). \quad (44)$$

The quantity $E(R_\alpha)$ is the radial contribution to the field given by equation (12). The radial contribution to the quadrupole inhomogeneity tensor described by equation (13) is

$$G^{(2)}(R_\alpha) = \frac{Z_pe}{R_\alpha^3}\left[1+R_\alpha/D+(R_\alpha/D)^2/3\right]\exp(-R_\alpha/D), \quad (45)$$

while the five components depending on angles are as follows:

$$A_{xx}^{(2)} = \frac{\sqrt{6}}{2}(C_2^2+C_{-2}^2)-C_0^2, \quad A_{xy}^{(2)} = -i\frac{\sqrt{6}}{2}(C_2^2-C_{-2}^2),$$
$$A_{xz}^{(2)} = -\frac{\sqrt{6}}{2}(C_1^2-C_{-1}^2), \quad A_{yz}^{(2)} = i\frac{\sqrt{6}}{2}(C_1^2+C_{-1}^2),$$
$$A_{zz}^{(2)} = 2C_0^2, \quad (46)$$

where $C_m^l(\theta,\varphi) = \sqrt{4\pi/(2l+1)}Y_{lm}(\theta,\varphi)$. The radial contribution to the octupole inhomogeneity tensor described by equation (14) is

$$G^{(3)}(R_\alpha) = \frac{Z_pe}{R_\alpha^4}\left[1+3R_\alpha/D+6(R_\alpha/D)^2+(R_\alpha/D)^2/5\right] \times \exp(-R_\alpha/D), \quad (47)$$

while the seven components depending on angles are as follows:

$$A_{xxy}^{(3)} = -i\frac{\sqrt{3}}{6}[C_1^3+C_{-1}^3-\sqrt{15}(C_3^3+C_{-3}^3)],$$
$$A_{xxz}^{(3)} = \frac{\sqrt{30}}{6}(C_2^3+C_{-2}^3)-C_0^3,$$
$$A_{xyy}^{(3)} = \frac{\sqrt{3}}{6}[C_1^3-C_{-1}^3+\sqrt{15}(C_3^3-C_{-3}^3)],$$
$$A_{xyz}^{(3)} = -i\frac{\sqrt{30}}{6}(C_2^3-C_{-2}^3),$$
$$A_{xzz}^{(3)} = -\frac{\sqrt{12}}{3}(C_1^3-C_{-1}^3),$$
$$A_{yzz}^{(3)} = i\frac{\sqrt{12}}{3}(C_1^3+C_{-1}^3),$$
$$A_{zzz}^{(3)} = 2C_0^3. \quad (48)$$

Applying a similar calculation technique as in [16,24] for calculation of the microfield distribution function, and as in our earlier papers [7,25] for calculations of the average microfield gradients — we have introduced also the auxiliary functions $\Psi(v)$. Then, the contributions of one-body and two-body clusters in equations (38)–(41), using the auxiliary functions, can be written:

$$N_ph_1^{(0)} = -x^{3/2}\Psi_1^{(0)}(v),$$
$$\frac{1}{2}N_p^2h_2^{(0)} = x^{3/2}\Psi_2^{(0)}(v),$$
$$N_ph_{1,n}^{(2)} = -i\frac{5}{(32\pi)^{1/2}}\frac{E_0}{R_0}\Psi_{1,n}^{(2)}(v)A_n^{(2)}(\theta_k,\varphi_k),$$
$$\frac{1}{2}N_p^2h_{2,n}^{(2)} = -i\frac{5}{(32\pi)^{1/2}}\frac{E_0}{R_0}\Psi_{2,n}^{(2)}(v)A_n^{(2)}(\theta_k,\varphi_k),$$
$$N_ph_{1,n}^{(3)} = \frac{15}{28}\frac{E_0}{R_0^2}\Psi_{1,n}^{(3)}(v)A_n^{(3)}(\theta_k,\varphi_k),$$
$$\frac{1}{2}N_p^2h_{2,n}^{(3)} = \frac{15}{28}\frac{E_0}{R_0^2}\Psi_{2,n}^{(3)}(v)A_n^{(3)}(\theta_k,\varphi_k). \quad (49)$$

The new variables are defined as follows: $v = ax^{1/2}$ and $x = kE_0$, whereas the angles θ_k and φ_k describe the direction of $\mathbf{k}$ vector in the coordinate system xyz. The one-body auxiliary dipole function

$$\Psi_1^{(0)}(v) = \frac{15}{(8\pi)^{1/2}}Z_p^{-1}\int_0^\infty dyy^2[1-j_0(\epsilon)], \quad (50)$$

and the two-body auxiliary dipole function

$$\Psi_2^{(0)}(v) = -\frac{15}{(8\pi)^{1/2}}\sqrt{1+Z_p}v^3\sum_{l=0}^\infty(-1)^l(2l+1) \times \int_{y_1=0}^\infty dy_1y_1^2\int_{y_2=0}^{y_1}dy_2y_2^2 \times[j_l(\epsilon_1)-\delta_{l,0}][j_l(\epsilon_2)-\delta_{l,0}]f_l\rangle(u_1)f_l\langle(u_2) \quad (51)$$

are analogous (for $Z_p = 1$ — the same ones) as in papers [16,24]. The function $j_l(\epsilon)$ is the *Spherical Bessel Function* of order l. The next new variables are defined as follows:

$$y = (ke)^{-1/2}R \text{ and } u = \sqrt{1+Z_p}vy, \text{ and}$$
$$\epsilon(v,y) = kE(R) = Z_py^{-2}(1+vy)\exp(-vy)\,; \quad (52)$$

and functions $f_l\rangle(u)$ and, $f_l\langle(u)$, defined according to [24], are given by

$$f_l\rangle(u) = (-1)^l u^l \left(\frac{d}{udu}\right)^l \left(\frac{e^{-u}}{u}\right), \quad (53)$$

and

$$f_l\langle(u) = i^{-l} j_l(iu) = u^l \left(\frac{d}{udu}\right)^l \left(\frac{\sinh u}{u}\right). \quad (54)$$

For the quadrupole auxiliary functions we have derived the expressions

$$\Psi_1^{(2)}(v) = 6\int_0^\infty dyy^2\gamma^{(2)}(v,y)j_2(\epsilon) \quad (55)$$

and

$$\Psi_2^{(2)}(v) = 12Z_p\sqrt{1+Z_p}v^3 I_p^{(2)}(v), \quad (56)$$

however for the octupole auxiliary functions we have derived the expressions

$$\Psi_1^{(3)}(v) = \frac{14}{(2\pi)^{1/2}}\int_0^\infty dyy^2\gamma^{(3)}(v,y)j_3(\epsilon) \quad (57)$$

and

$$\Psi_2^{(3)}(v) = \frac{28}{(2\pi)^{1/2}} Z_p\sqrt{1+Z_p}v^3 I_p^{(3)}(v); \quad (58)$$

where

$$\begin{aligned} I_p^{(t)}(v) = &\int_{y_1=0}^\infty dy_1 y_1^2 \int_{y_2=0}^{y_1} dy_2 y_2^2 \gamma^{(t)}(v,y_1) \\ &\times \left\{ \frac{i}{2t+1}\sum_{l=0}^\infty (i)^l(2l+1)j_l(\epsilon_2) f_l\rangle(u_1) f_l\langle(u_2) \right. \\ &\times \left[\sum_{l'=0}^\infty (i)^{l'}(2l'+1)j_{l'}(\epsilon_1)\left(C_{l0,l'0}^{t0}\right)^2\right] \\ &\left. + (-i)^{t+1} j_t(\epsilon_1) f_0\rangle(u_1) f_0\langle(u_2)\right\}, \quad (59) \end{aligned}$$

whereas

$$\begin{aligned} \gamma^{(2)}(v,y) &= (Z_p e)^{-1}(vD)^3 G^{(2)}(R) \\ &= y^{-3}\left[1+vy+(vy)^2/3\right]\exp(-vy), \quad (60) \end{aligned}$$

and

$$\begin{aligned} \gamma^{(3)}(v,y) &= (Z_p e)^{-1}(vD)^3 G^{(3)}(R) \\ &= y^{-4}\left[1+3vy+6(vy)^2+(vy)^3/5\right]\exp(-vy), \quad (61) \end{aligned}$$

while $C_{l0,l'0}^{t0}$ is the Clebsch–Gordan coefficient.

Finally, the average of the microfield inhomogeneity tensors given by equation (29) are as follows:

– for the quadrupole

$$\langle E_{ij}^{(2)}\rangle_{\mathbf{E}} = \frac{5}{(32\pi)^{1/2}}\frac{E_0}{R_0} B_a^{(2)}(\beta) A_{ij}^{(2)}(\theta_E,\varphi_E), \quad (62)$$

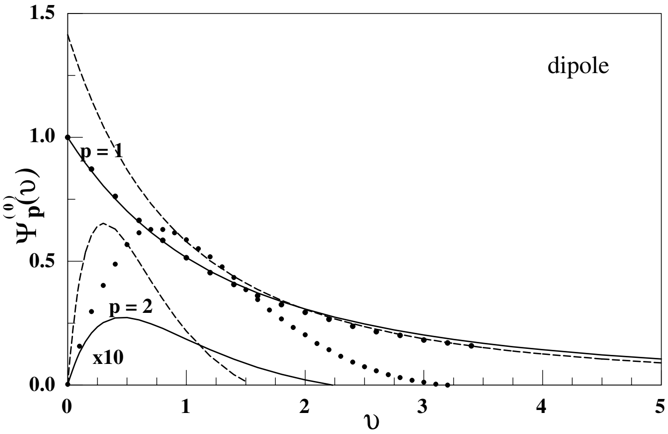

Fig. 1. The one-body $\Psi_{p=1}^{(0)}$ and the two-body $10\Psi_{p=2}^{(0)}$ auxiliary dipole functions at a neutral emitter ($Z_e = 0$) versus the quantity v. The solid lines are obtained for the singly charged perturbers ($Z_p = 1$), while the dashed lines are obtained for doubly charged perturbers ($Z_p = 2$). The points represent original Mozer-Baranger's [16] results.

– for the octupole

$$\langle E_{ijk}^{(3)}\rangle_{\mathbf{E}} = \frac{15}{28}\frac{E_0}{R_0^2} B_a^{(3)}(\beta) A_{ijk}^{(3)}(\theta_E,\varphi_E), \quad (63)$$

where

$$\begin{aligned} B_a^{(t)}(\beta) = &\frac{2}{\pi}\beta^2/W_a(\beta) \\ &\times \int_0^\infty dxx^2\left[\Psi_1^{(t)}(ax^{1/2}) + \Psi_2^{(t)}(ax^{1/2})\right] \\ &\times \exp\left\{-x^{3/2}\left[\Psi_1^{(0)}(ax^{1/2}) - \Psi_2^{(0)}(ax^{1/2})\right] j_t(\beta x)\right\}; \quad (64) \end{aligned}$$

whereas the microfield distribution function is

$$\begin{aligned} W_a(\beta) = &\frac{2}{\pi}\beta^2\int_0^\infty dxx^2 \\ &\times \exp\left\{-x^{3/2}\left[\Psi_1^{(0)}(ax^{1/2}) - \Psi_2^{(0)}(ax^{1/2})\right]\right\} j_0(\beta x). \quad (65) \end{aligned}$$

In a particular case, in the coordinate system $x'y'z'$ with $\mathbf{E}||0z'$, the effective atom-(plasma) ions interaction is given by the expression:

$$\begin{aligned} U_{ai}^{eff} \simeq &-\mathbf{d}\cdot\mathbf{E} - \frac{5}{(32\pi)^{1/2}}\frac{eE_0}{2R_0} B_a^{(2)}(\beta)(3z'^2 - r'^2) \\ &- \frac{15}{28}\frac{eE_0}{6R_0^2} B_a^{(3)}(\beta) z'(5z'^2 - r'^2) + ... \quad (66) \end{aligned}$$

4 Numerical results

Figures 1, 2, and 3 present the one-body and the two-body, the dipole, the quadrupole, and the octupole auxiliary functions. These results show that ordinates of the

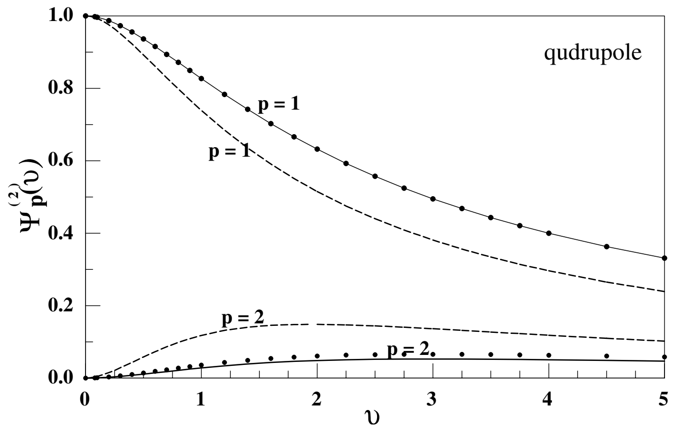

Fig. 2. The one-body $\Psi^{(2)}_{p=1}$ and the two-body $\Psi^{(2)}_{p=2}$ auxiliary quadrupole functions at a neutral emitter versus the quantity v. The lines have the same meaning as in Figure 1. The points represent our earlier results [7].

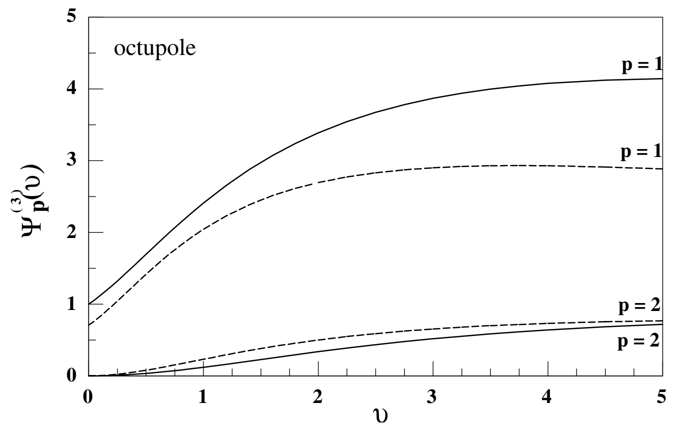

Fig. 3. The one-body $\Psi^{(3)}_{p=1}$ and the two-body $\Psi^{(3)}_{p=2}$ auxiliary octupole functions at a neutral emitter versus the quantity v. The lines have the same meaning as in Figure 1.

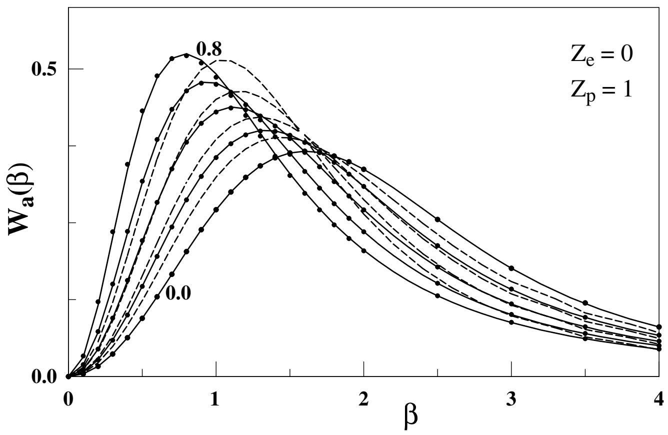

Fig. 4. The electric microfield distribution function $W_a(\beta)$ at a neutral emitter in the case of singly charged perturbers as a function of the reduced electric field β, for several values of the screening parameter $a = 0.0, 0.2, 0.4, 0.6$, and 0.8. The solid lines represent our results, the points represent Hooper's results [26], whereas the dashed lines represent Mozer-Baranger's [16] results.

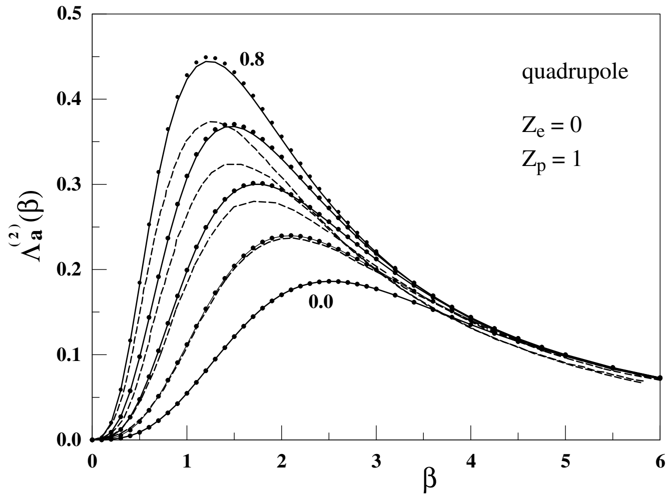

Fig. 5. The quadrupole function $\Lambda^{(2)}_a(\beta)$ at a neutral emitter in the case of singly charged perturbers as a function of the reduced electric field β, for several values of the screening parameter $a = 0.0, 0.2, 0.4, 0.6$, and 0.8. The solid lines show results obtained in this paper, while the points represent our earlier results [7]. The dashed lines indicate the results [9b].

two-body function are much lesser than the corresponding values of the one-body function $\Psi^{(t)}_2 \ll \Psi^{(t)}_1$ in any case. Such a relation confirms the assumption accepted by us for Debye plasma, that inclusion of two terms only in the Mayer-Mayer group expansion (Eqs. (36) and (37)) is accurate enough for calculation of the distribution function $W_a(\beta)$ and inhomogeneity tensors $B^{(t)}_a(\beta)$. The most important argument supporting the opinion is presented in Figure 4, where we find an excellent agreement between our results and Hooper's ones [26], which are not limited by such approximation. We conclude that the discrepancy between Hooper's function $W_a(\beta)$ [26] and original Mozer-Baranger [16] — for the first time reported in reference [26] — are not caused by differences between models but by numerical inaccuracies (especially for the function $\Psi^{(0)}_2$, see Fig. 1) in reference [16].

In Figure 5, the quadrupole function $\Lambda^{(2)}_a(\beta) = W_a(\beta)B^{(2)}_a(\beta)/\beta$ is presented. This function is more suitable for a graphical presentation than the quadrupole inhomogeneity tensor $B^{(2)}_a(\beta)$. (Function $\Lambda^{(2)}_a(\beta)$ was defined by Demura and Sholin in Ref. [3]). Some minimal differences between our currently obtained values and our earlier results [7] are caused by a slightly worse numerical accuracy in [7]. In that paper a smaller number of terms in sum equation (59) were taken into account, moreover the terms were ordered in a different way. The disagreement between our results and those from [9b] is far bigger. It increases when the screening parameter a increases up to 15% for $a = 0.8$. Authors in [9b] suggest that a reason for the discrepancy of their results with [7] is the difference in the two-body quadrupole auxiliary function $\Psi^{(2)}_2$, caused by applying (in [7]) the series expansion of the

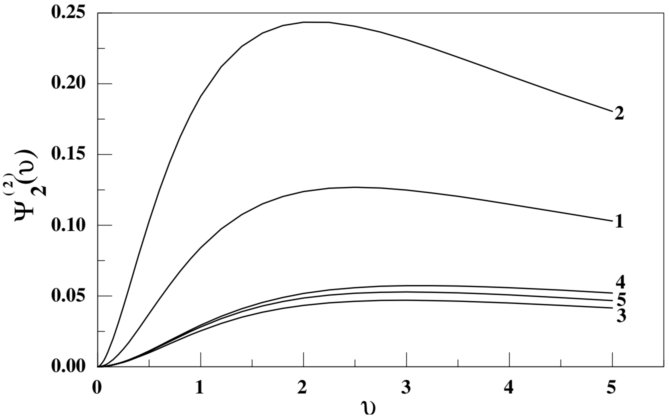

Fig. 6. The two-body quadrupole auxiliary function $\Psi^{(2)}_{p=2}$ versus the quantity v. The numbers near the lines describe the number of terms taken into account in equation (59).

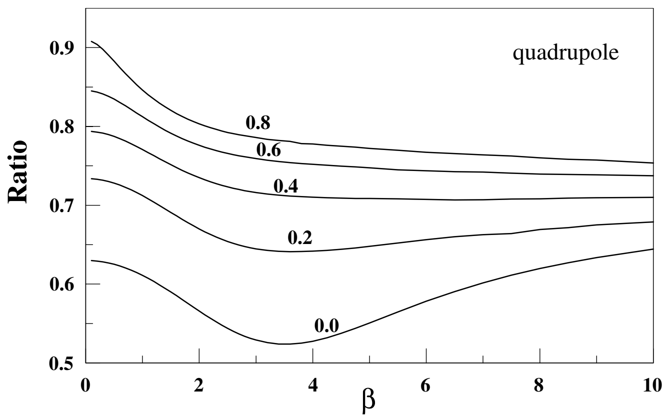

Fig. 7. Ratio of the quadrupole function $B_a^{(2)}(\beta, Z_p = 2)$ at a neutral emitter in the case of doubly charged perturbers and the quadrupole function $B_a^{(2)}(\beta, Z_p = 1)$ at a neutral emitter in the case of singly charged perturbers as a function of the reduced electric field β, for several values of the screening parameter $a = 0.0, 0.2, 0.4, 0.6$, and 0.8.

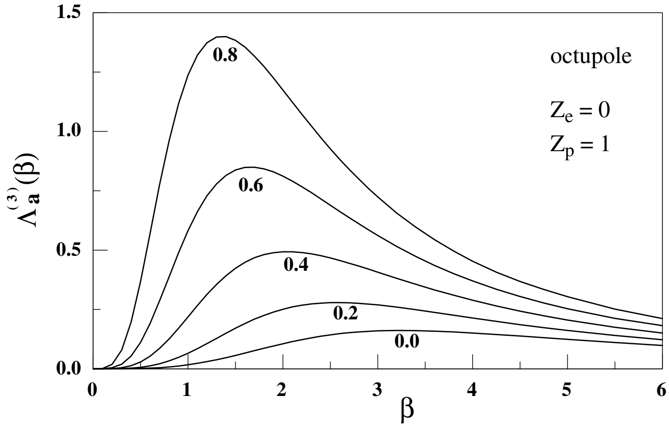

Fig. 8. The octupole function $\Lambda_a^{(3)}(\beta)$ at a neutral emitter in the case of singly charged perturbers as a function of the reduced electric field β, for several values of the screening parameter $a = 0.0, 0.2, 0.4, 0.6$, and 0.8.

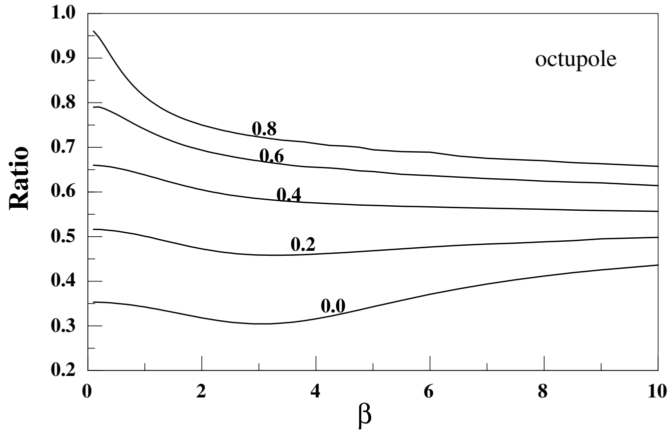

Fig. 9. Ratio of the octupole function $B_a^{(3)}(\beta, Z_p = 2)$ at a neutral emitter in the case of doubly charged perturbers and the octupole function $B_a^{(3)}(\beta, Z_p = 1)$ at a neutral emitter in the case of singly charged perturbers as a function of the reduced electric field β, for several values of the screening parameter $a = 0.0, 0.2, 0.4, 0.6$, and 0.8.

two-body correlation function (Eq. (42)). The results of checking of the series convergence of function $\Psi_2^{(2)}$ presented in Figure 6 contradict this opinion. The first five terms in sum equation (59) are sufficient to stabilize function $\Psi_2^{(2)}$. Moreover, we note that function $\Lambda_a^{(2)}(\beta)$ very weakly depends on $\Psi_2^{(2)}$. Even changing the sign of the last function does not destroy the 15% discrepancy. Function $\Lambda_a^{(2)}(\beta)$ depends much more on the two-body dipole auxiliary function $\Psi_2^{(0)}$. In our opinion, the considered discrepancies can be caused by differences in function $\Psi_2^{(0)}$ from [9b] and that from [7].

Figure 7 shows the perturber's charge effect for the quadrupole inhomogeneity tensor of the ion microfield. For two quasi-neutral plasmas of identical temperatures and of identical electron concentrations, but of different charges of the ion-perturber $Z_p e$ — the quadrupole inhomogeneity tensor of the ion microfield is the smaller if the Z_p is larger. This happens because for quasi-neutral plasmas the ion density decreases simultaneously. Figures 8 and 9 present the ion octupole inhomogeneity tensors. The octupole function $\Lambda_a^{(3)}(\beta)$ is defined analogously to the quadrupole function $\Lambda_a^{(2)}(\beta)$. The interpretation is also similar.

From a comparison of quadrupole function $\Lambda_a^{(2)}(\beta)$ (in Fig. 5) with octupole function $\Lambda_a^{(3)}(\beta)$ (in Fig. 8) it follows results that the importance of screening characteristic of plasma and correlations effects, represented by the screening parameter a, increases with the increasing order of the inhomogeneity tensor t. Thus, one can expect that in strongly-coupled plasmas the importance of the ion microfield inhomogeneity is relatively larger than in Debye's plasmas. In the case of strongly-coupled plasmas such calculation could be also performed using the Mayer-Mayer cluster expansion if the higher order correction to the pair correlation are included as in reference [27].

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