A classical description of the electrons in plasma

Saïd DOUIS* and Mohammed Tayeb MEFTAH
Laboratoire LRPPS, Faculté des Sciences et de la Technologie et des Sciences de la Matière, Université Kasdi Merbah Ouargla, Ouargla 30000 Algérie
* E-mail : fdouis@gmail.com

ملخص : في هذا العمل قمنا بحساب الكُمون الفِعْلي على إلكترون في بلازما. هذا الكمون المُتحَصَل عليه من حل مُعَادلة تكاملية غير خطية، هو نِتَاج ثلاث مُساهمات: الأولى هي طاقة التفاعل بين إلكترون البلازما وشحنة اختبار نَعْتَبرها كشَائِبَة. وقد أخذنا هذا التفاعل مساوي لِـ "كالب" ذو الحُجُبْ. الثانية هي طاقة التفاعل الكولومبي بين هذا الإلكترون السابق ذكرهُ وبقية إلكترونات البلازما، وقد حسبناها باستعمال توزيع ماكسويل بولتزمان. الثالثة والأخيرة هي طاقة التفاعل الكولومبي بين الإلكترون والأيونات المُتَوزعة بانتظام في البلازما. الكُمون الفِعْلي تُحصِلَ عليه، في المرحلة الأولى حَسبنا توزع الحقول الكهربائية المِجْهَرية النَاشِئة من الإلكترونات عند الشائبة. وفي المرحلة الثانية حسبنا دالة الارتباط الذاتي الزمني للحقول الكهربائية. النتائج المُتَحَصِل عليها قُورِنت مع التي أعطتها مُحَاكاة الديناميك الجُزيئي.

كلمات دالة : كَالبْ ذو الحُجُبْ، الارتباط الذاتي الزمني، الحقول الكهربائية المجهرية.

RÉSUMÉ : Dans ce travail, nous avons calculé le potentiel effectif sur un électron dans un plasma. Ce potentiel, qui s'obtient en résolvant une équation intégrale non linéaire, est une somme de trois contributions : la première est l'énergie d'interaction entre l'électron du plasma et une charge test considérée comme une impureté. Nous avons pris cette interaction égale à celle de "Kelbg" écranté. La seconde est l'énergie d'interaction coulombienne entre l'électron en question et les autres électrons du plasma, et nous la calculons en utilisant une distribution de Maxwell-Boltzmann. La troisième est l'énergie d'interaction coulombienne entre l'électron et les ions répartis uniformément dans le plasma. Le potentiel effectif, étant obtenu, en première étape, nous avons calculé la distribution du microchamp électrique crée par les électrons sur l'impureté. En seconde étape nous avons calculé la fonction d'autocorrélation temporelle du microchamp électrique. Les résultats obtenus sont comparés à ceux donnés par la simulation de la dynamique moléculaire.

MOTS-CLÉS : Kelbg écranté, autocorrélation temporelle, Microchamp Electrique.

ABSTRACT: In this work, we calculated the effective potential of an electron in a plasma. This potential, which is obtained by solving a non-linear integral equation, is a sum of three contributions: the first is the interaction energy between the electron plasma and a test charge regarded as an impurity. We have taken this interaction equal to screened "Kelbg". The second is the Coulomb interaction energy between the electron in question and the other electrons plasma, that we calculate using a Maxwell-Boltzmann distribution. The third is Coulomb interaction energy between the electron and ions plasma uniformly distributed. The effective potential, is obtained, in the first stage, we have calculated the distribution of electric microfield created by the electrons on the impurity. In the second stage we calculated the time autocorrelation function of the electric microfield. The results are compared with those given by molecular dynamics simulation.

KEYWORDS: Screened Kelbg, Time autocorrelation, Electrical Microfield.

1. Introduction

System comprised of charged particles are of fundamental interest for many fields of physics. The theory for the equilibrium distribution of fields and the nonlinear behavior of electric charges around an impurity charge of the same sign is a problem that has been studied for a long time due to its great importance in many techniques. Worth to mention that for fully ionized plasma composed of electrons and positive ions, the hypothesis of one component plasma (OCP) allows us to ignore the effects of ions movements to those of electrons because the ratio mass is about $m_e/m_i \approx 1/2000$. So the system is only composed of one kind of mobile charges (electrons), whereas the species of opposite charges (ions) are modeled by the continuous background which provides electrical neutrality. Coulomb forces between point charges are purely repulsive and do not approach very close to each other only rarely what ever the plasma conditions. Concerning the ion-electron interaction, it is clear that it requires a quantum mechanical description. In this case the Coulomb

potential is replaced by the screened Kelbg pseudo-potential finite and regularized at the origin [1-4] where the quantum effects are approximately taken into account. Furthermore, when we compute the effective potential $V(r)$, we consider that the electron interacts with the test charge and with the continuous background positive charge. In section 2 we construct the nonlinear integral equation governing the effective potential on which is centered all the subsequent results of this paper. We also solve this equation with the fixed point method (FPM) and the Runge-Kutta method (RKM). Section 3 is devoted to present the static properties of the electronic electric microfied on the impurity. This concern the distribution function of the electron microfield. The dynamics properties, that is to say, the time autocorrelation function of the electron microfield is presented in section 4. At the end we close this paper by a conclusion.

Before starting the second section, recall the relevant parameters for our study: the charge number Z of the impurity, the average distance between electrons $a=(3/4\pi n_e)^{1/3}$, the electron coupling constant $\Gamma = e^2/(k_B T a)$, the electron Louis De Broglie thermal length λ_T, the degree of quanticity $\eta = \lambda_T / a$ and the Debye length λ_D. The cases reviewed in this work are: the coupling parameter $\Gamma = 0.1$, the quanticity parameter $\eta = 0.177$, the dimensionless Debye length $\eta' = \lambda_D / a = 1.826$. These parameters correspond to the electron density $n_e = 2.5\times10^{22} cm^{-3}$ and to the temperature $T = 7.9\times10^5 K$. These parameters are found in a class of plasmas created by the laser or in some planets corresponding to the warm dense matter. The calculation are done for the charge number Z=2 and Z=8.

2. Integral equation for the effective energy potential

2. 2. Construction of integral equation for the effective energy potential

Let us consider a medium consisting of electrons and a continuous background of neutralizing positive electrical charges. At first, the distribution of the electrons is that of Maxwell-Boltzmann governing the equilibrium state of the electrons' system. If we place a positive ion of charge *Ze* (called test charge or impurity) at the coordinates origin: the system is disturbed and after a certain time *t*, it will reach a new equilibrium state described by a novel distribution of the electrons over the space around the charge *Ze*. The latter is determined through the potential energy of an electron located at a distance *r* from the test charge *Ze* when the system has reaches this novel equilibrium state. This potential energy is built as a sum of three contributions:

$$V(r) = V_{ie}(r) + V_{ee}(r) + V_{ef}(r) \tag{1}$$

where $V_{ie}(r)$ is the potential energy of ion-electron interaction (the ion is the test charge), $V_{ee}(r)$ is the interaction energy of the electron with all the other electrons and $V_{ef}(r)$ is the interaction energy of the electron with the continuous neutralizing background of ions. The ion-electron interaction is taken in a way that we can consider the quantum effects at short distances: we represent it here by screened Kelbg pseudo-potential [1,2,3,4]:

$$V_{ie}(r) = -\frac{Ze^2}{r}\left[1 - e^{-(r/\lambda_{ie})^2} + \sqrt{\pi}\,\frac{r}{\lambda_{ie}}\left(1 - erf\left(\frac{r}{\lambda_{ie}}\right)\right)\right] e^{-r/\lambda_D} \tag{2}$$

where: $\lambda_{ie} = \lambda_T = \hbar\sqrt{2 m_{ie} K_B T}$ is the de Broglie length of relative movement, $m_{ie} = m_e m_i / (m_e + m_i) \approx m_e$ (because in our case $m_e / m_i \approx 1/2000$), and $\lambda_D = \sqrt{K_B T / (4\pi n_e e^2)}$ is the Debye length.

And we consider that the Coulomb potential governing the electron-electron interaction and the interaction of the electron with the positive continuous background.

$$V_{ee}(r) = e^2 \iint f(\vec{r}, \vec{p}) \frac{1}{\left|\vec{r} - \vec{r}'\right|} d\vec{p}^{\,3} d\vec{r}'^{\,3} \tag{3}$$

where:

$$f(\vec{r},\vec{p}\,)=\frac{N}{\Omega}\left(\frac{m_e\beta}{2\pi}\right)^{3/2}e^{-\beta(\frac{\vec{p}^2}{2m}+V(r))} \tag{4}$$

is Maxwell-Boltzmann distribution, N is the total electrons number, Ω is the volume of the system and $\beta=1/K_BT$. Whereas the energy potential of the electron with the positive background neutralizing charge is given by:

$$V_{ef}(r)=-n_e e^2\int\frac{1}{\left|\vec{r}-\vec{r}'\right|}d\vec{r}'^3 \tag{5}$$

Therefore, the expression of the potential energy of an electron at the position r of the origin is:

$$V(r)=V_{ie}(r)+e^2\iint\frac{f(\vec{r}',\vec{p})}{\left|\vec{r}-\vec{r}'\right|}d\vec{p}^3d\vec{r}'^3-n_e e^2\int\frac{1}{\left|\vec{r}-\vec{r}'\right|}d\vec{r}'^3 \tag{6}$$

When we replace the equation (4) into (6), and we integrate on impulses, the equation becomes:

$$V(r)=V_{ie}(r)+n_e e^2\int\frac{(e^{-\beta V(r')}-1)}{\left|\vec{r}-\vec{r}'\right|}d\vec{r}'^3 \tag{7}$$

Using spherical coordinates and some basic calculations, the last integral equation is transformed into the following:

$$\begin{aligned}V(r)=&-\frac{Ze^2}{r}\left[1-e^{-(r/\lambda_{ie})^2}+\sqrt{\pi}\frac{r}{\lambda_{ie}}(1-erf(\frac{r}{\lambda_{ie}}))\right]e^{-r/\lambda_D}+\\&4\pi n_e e^2\int_0^\infty\frac{r'}{r}\left[\left(r+r'\right)-\left|r-r'\right|\right](e^{-\beta V(r')}-1)dr'\end{aligned} \tag{8}$$

In order to deal with an adimensional equation, put $Y(x)=-aV(r)/(Ze^2)$, $a=\left(4\pi n_e/3\right)^{-1/3}$, $x=r/a$, $\eta=\lambda_{ie}/a$, $\eta'=\lambda_D/a$ and. After that, we obtain the desired adimensional equation:

$$Y(x)=\frac{1}{x}\left[1-e^{-(x/\eta)^2}+\sqrt{\pi}\frac{x}{\eta}(1-erf(\frac{x}{\eta}))\right]e^{-x/\eta'}-\frac{3}{2Z}\int_0^\infty\frac{x'}{x}\left(x+x'-\left|x-x'\right|\right)\left(e^{Z\Gamma Y(x')}-1\right)dx' \tag{9}$$

This equation is a nonlinear integral equation, representing the dimensionless potential energy equation *Y (x)* of an electron at the distance *x* (dimensionless) from the impurity localized at the coordinate origin.

2.2. Numerical solution of the integral equation for the potential energy

We can solve the nonlinear integral equation (9) by the fixed point method FPM [5,6], starting with the initial function $Y_0(x)=Y_{ie}(x)$. We can also solve this integral equation by transforming it into a second order nonlinear differential equation and then we use the method of Runge-Kutta RKM [7] to solve it. The numerical solution of the nonlinear integral equations (9), in the case $\Gamma=0.1$, $\eta=0.4$, $\eta'=1.826$, $Z=8$ by the FPM gives the potential energy as shown in the figure 1.

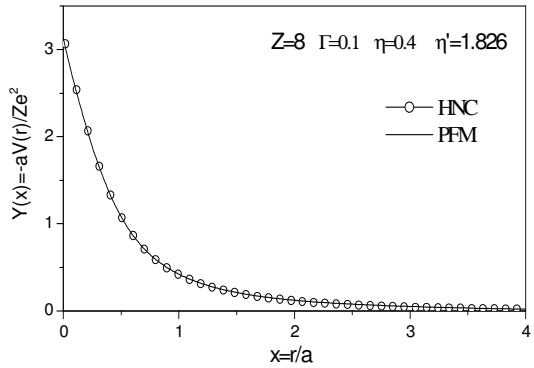

Figure 1 : Effective potential energy of the electron for Z=8, calculated with FPM and HNC.

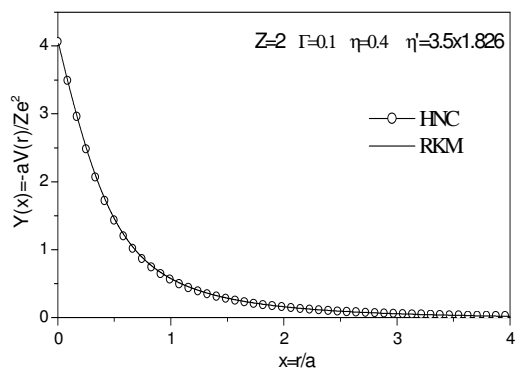

Figure 2 : Effective potential energy of the electron for Z=2, calculated with RKM and HNC.

The RKM allows us to solve, equivalently to the integral equation, the nonlinear differential equation. This way we have solved the equation:

$$Y'' + \frac{2}{x}Y' = \frac{3}{Z}\left(e^{Z\Gamma Y} - 1\right) - \frac{1}{x\left(\eta'\eta\right)^2} e^{-\frac{x}{\eta'}} \left[\left(2\eta'^2 + \eta^2\right) e^{-\frac{x^2}{\eta^2}} + \sqrt{\pi}\eta\left(2\eta' - x\right)\left(1 - \operatorname{erf}\left(\frac{x}{\eta}\right)\right) - \eta^2 \right] \tag{10}$$

with initial conditions:

$$\begin{cases} Y(0) = \lim\limits_{x\to 0} Y_{ie}(x) = \dfrac{\sqrt{\pi}}{\lambda} \\ Y'(0) = \lim\limits_{x\to 0} Y'_{ie}(x) = \dfrac{1}{\eta^2} - \dfrac{1}{\eta}\left(\dfrac{2}{\eta} + \dfrac{\sqrt{\pi}}{\lambda}\right) \end{cases} \tag{11}$$

In figure 2 we present the RKM and HNC solution for the case $\Gamma = 0.1$, $\eta = 0.4$, $\eta' = 6.4$ and $Z = 2$. Agreement between theory (FPM and RKM) and HNC (Hypernetted-chain approximation) [8,9] is quite good in general.

As expected we have also found that the RKM (differential equation) is faster than the fixed point method (integral equation). The drawback of the RKM is that it is very sensitive to the initial conditions. Conversely, the FPM, despite that it requires much time for computation, it has more guarantees that the result converge towards an exact solution. Another drawback of the FPM is that

it is adaptable only for the shielded initial potential. Mathematically the integral equation (9) admits finite solutions at short distance. This rapid convergence towards the solution is guaranteed by the screening effect. Physically, this may be interpreted by the following reasoning: a non bounded electron interacts with a neighborhood of some mean inter-electron distance a. This neighborhood contains electrons that are distributed with a density $n_e(r)$ around a single impurity of positive electric charge. This means that the impurities are distributed in plasma with a mean constant density such that the neighborhood of each electron contains only a single impurity. What has just been said suggests that numerical integration of the integral equation or the equation differential must be truncated to the size of this neighborhood.

3. Electrical Microfield Distribution

The probability to measure an electrical microfield at the impurity ion equal to ε is given in the Baranger-Mozer approximation [10] by:

$$P(\varepsilon)=\frac{2\varepsilon}{\pi}\int_0^\infty T(\lambda)\sin(\varepsilon\lambda)\lambda d\lambda \tag{12}$$

where:

$$T(\lambda)=e^{G(\lambda)} \tag{13}$$

And

$$G(\lambda)=4\pi\int_0^\infty r^2 e^{-\beta V(r)}\left[\frac{\sin(\lambda\varepsilon(r))}{\lambda\varepsilon(r)}-1\right]dr \tag{14}$$

or after the dimensionless of (12) and (14) we find:

$$\bar{P}(\bar{\varepsilon})=\varepsilon_0 P(\varepsilon)=\frac{2}{\pi}\int_0^\infty(\lambda\bar{\varepsilon})\sin(\lambda\bar{\varepsilon})e^{G(\lambda/\varepsilon_0)}d\lambda \tag{15}$$

and

$$\bar{G}(\lambda)=G(\lambda/\varepsilon_0)=3\int_0^\infty x^2 e^{Z\Gamma Y(x)}\left(\frac{1}{\lambda Y_{ie}'(x)}\sin\left(\lambda Y_{ie}'(x)\right)-1\right)dx \tag{16}$$

such that: $\varepsilon_0=e/a^2$, $Y_{ie}'(x)=\partial Y_{ie}(x)/\partial x$ and $Y_{ie}(x)=\frac{1}{x}\left[1-e^{-(x/\eta)^2}+\sqrt{\pi}\frac{x}{\eta}(1-erf(\frac{x}{\eta}))\right]e^{-x/\eta'}$.

In figure.3 we present the electric microfield distribution $\bar{P}(\bar{\varepsilon})$ for *Z=8*. This figure shows the good agreement of the theoretical (Baranger-Mose approximation) with the MD simulation. Mention here we can see that the distribution $P(\varepsilon)$ goes to zero as follow: when ε becomes large enough (mathematically going to infinity), the first term in the integrand (14) goes to zero then $G(\lambda)$ goes to $-\infty$ and both (13) and (12) goes to zero when ε becomes too large. For further details of the behavior and more detailed calculations and simulations of the electron microfield distribution $P(\varepsilon)$ on positive charge in plasmas, we can find them in [11,12].

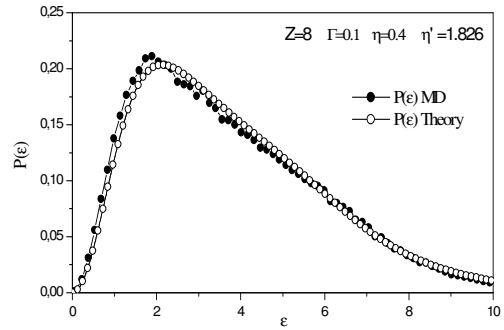

Figure 3 : Electric field distribution of the electrons for Z=8.

4. The microfield autocorrelation function

The total electric microfield due to the electrons on the impurity centered at the coordinates origin is given by:

$$\vec{E} = \sum_{k=1}^{N_e} \vec{e}_{ie}(r_k) \tag{17}$$

where is the individual electric field due to a plasma electron on the impurity. then the dimensionless electric field auto-correlation function is given by [10]:

$$\begin{aligned} C_{EE}(t) &= \frac{a^4}{e^2}\left\langle \vec{E}(t)\cdot\vec{E}\right\rangle \\ &= \frac{a^4}{e^2}\int d\vec{r}_1 d\vec{v}_1 ....d\vec{r}_N d\vec{v}_N \vec{E}\cdot\vec{E}(-t)\rho_e = \frac{a^4}{e^2}\int d\vec{r}_1 d\vec{v}_1 \vec{e}(r_1) N \int d\vec{r}_2 d\vec{v}_2 ....d\vec{r}_N d\vec{v}_N \vec{E}(-t)\rho_e \\ &= \frac{a^4}{e^2}\int d\vec{r}_1 d\vec{v}_1 \vec{e}(r_1)\Psi(\vec{r}_1,\vec{v}_1,t) \end{aligned} \tag{18}$$

where ρ_e is the equilibrium canonical ensemble density matrix and $e(r_\alpha)$ is the single particle field. The integrations over degrees of freedom *2...N* in the second equality define a reduced function $\Psi(r_1, v_1, t)$, which is the first member of a set of such functions.

$$\Psi(\vec{r}_1,\vec{v}_1....\vec{r}_s,\vec{v}_s,t) = N^s \int d\vec{r}_{s+1} d\vec{v}_{s+1} ....d\vec{r}_N d\vec{v}_N \vec{E}(-t)\rho_e \tag{19}$$

it is straightforward to verify that these functions satisfy the BBGKY hierarchy [9].

$$\begin{aligned} &(\partial_t + \vec{v}\cdot\vec{\nabla}_r - \frac{1}{m_e}\{\vec{\nabla}_r(V_{ie}(r)+V_{ef}(r))\}\cdot\vec{\nabla}_v)\Psi(\vec{r},\vec{v},t) \\ &= \frac{1}{m_e}\int d\vec{r}_1 d\vec{v}_1 (\vec{\nabla}_r V_{ee}(\vec{r}-\vec{r}_1))\cdot\vec{\nabla}_v \Psi^{(2)}(\vec{r},\vec{v};\vec{r}_1,\vec{v}_1,t) \end{aligned} \tag{20}$$

where m_e is the electron mass at the rest and. Recognizing this linear relationship, the basic approximation for weak coupling among the electrons is to neglect all of their correlations at all times.

$$\Psi^{(2)}(\vec{r}_1,\vec{v}_1,\vec{r}_2,\vec{v}_2,t) \to f(\vec{r}_2,\vec{v}_2)\Psi(\vec{r}_1,\vec{v}_1,t) + f(\vec{r}_1,\vec{v}_1)\Psi(\vec{r}_2,\vec{v}_2,t) \tag{21}$$

where $f(\vec{r},\vec{v})$ is the Maxwell-Boltzmann distribution given by the equation (4).

Use of (21) in first hierarchy equation (20) gives directly the kinetic equation

$$\left(\partial_t + L\right)\Psi(\vec{r},\vec{v},t) = \frac{1}{m_e} f(\vec{r},\vec{v})\vec{v}.\vec{\nabla}_r \int d\vec{r}_2 V_{ee}\left(\vec{r}-\vec{r}_2\right)\int d\vec{v}_2 \Psi(\vec{r}_2,\vec{v}_2,t) \tag{22}$$

where:

$$L = \vec{v}.\vec{\nabla}_r - \frac{1}{m_e}(\vec{\nabla}_r V(r)).\vec{\nabla}_v \tag{23}$$

We limit ourselves to the solution of the homogeneous equation of (22) which is given by:

$$\Psi(\vec{r},\vec{v},t) = f(\vec{r},\vec{v})\vec{e}_{mf}(\vec{r}(t)) \tag{24}$$

where:

$$\vec{e}_{mf}(\vec{r}) = \frac{1}{Ze}\vec{\nabla}V(r) \tag{25}$$

Replace (25) in (22) we find:

$$C_{EE}(t) = \frac{a^4}{e^2}\int f(\vec{r},\vec{v})\vec{e}(r)\cdot\vec{e}_{mf}(r(t))d\vec{r}d\vec{v} \tag{26}$$

where $\vec{r}(t)$ is the time-dependent position vector. We get it at all time t, we have solved numerically (using the Verlet algorithm) the movement equation $d\vec{P}/dt = -e.\vec{e}_{mf}(r)$.

Figure.4 shows the numerical resolution, with the Monte Carlo method of equation (26) for the case Z=8, Γ=0.1, η=0.4, η′=1.826. The agreement between the molecular dynamics MD and the theory is quite good and provides a way to interpret the results of the MD simulation. The initial position and velocity of an electron are sampled from the equilibrium distribution $f(\vec{r},\vec{v})$ which favors electrons close to the ion and hence large fields. Since the force on the electron is also large, its initial acceleration will be large. This is the source of the short decay time. For less energetic electrons, the trajectories are bound and there is continual correlation and anti-correlation as the correlation function decays in magnitude due to phase averaging.

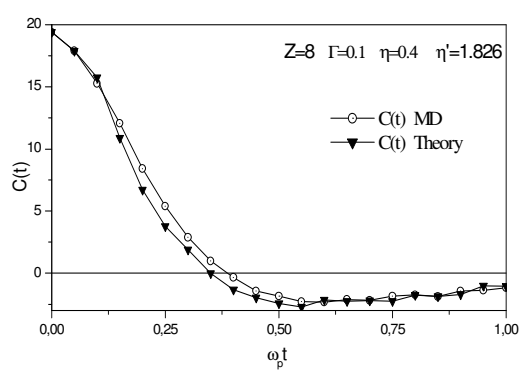

Figure 4 : Electric field time auto-correlation function for Z=8

5. Conclusion

In this work we have established a nonlinear integral equation describing the effective interaction between an electron and a plasma, the ions are represented by a continuous positive background assuring the electric neutrality of the system. We have used this effective potential to derive, theoretically and by the molecular dynamics:-the electric microfield distribution of the total electric field due of all the electrons on an impurity charge embedded at the coordinates origin in the plasma, - to find the classical trajectories of the electrons around the impurity. This allows us to compute the time autocorrelation function for the total electric microfield on the impurity. Agreement between theory and simulation of MD is quite good in general.

References

[1] K. Wünsch, P. Hilse, M. Schlanges and D.O. Gericke ; Phys. Rev. E, **77**, 056404 (2008).
[2] S. P. Sadykova, W. Ebeling, I. Valuev and I. M. Sokolov1 ; 36th EPS Conference on Plasma Phys. Sofia, June 29 - July 3, 2009 ECA Vol. **33** E, P-5.076 (2009).
[3] A.V. Filinov, M. Bonitz and W. Ebeling; J. Phys. A: Math. Gen., **36** 5957-5962 (2003)
[4] I. Morozov, H. Reinholz, G. Rpke, A. Wierling and G. Zwicknagel ; Phys. Rev. E, **71**, 066408 (2005).
[5] S. D. Conte and Carl de Boor ; Elementary Numerical Analysis-An Algorithmic Approach, P362, McGraw-Hill Book Company, (1980).
[6] R. Ansorge, Th. Meis and W. Tornig ; Iterative Solution of Nonlinear Systems of Equation, Proceedings of a Meeting held at Oberwolfach, Germany, (1982).
[7] S. T. Karris ; Numerical Analysis using MATLAB and Excel, Orchard Publications (2007).
[8] H. B. Nersisyan, C. Toepffer and G. Zwicknagel; Phys. Rev. E, **72**, 036403 (2005).
[9] K. Wünsch, P. Hilse, M. Schlanges and D.O. Gericke; Phys. Rev. E, **77**, 056404 (2008).
[10] B. Talin, A. Calisti, J. W. Dufty and I. V. Pogorelov; Phys. Rev. E, **77**, 036410 (2008).
[11] N. G. Van Kampen and B. U. Felderhof; Theoretical Methods in plasma physics (North-Holland Publishing Amsterdam), Chap 8 170 (1967).
[12] S. Alexiou; Phys. Rev. A, **49** 106 (1994).