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## Low-frequency electric microfield calculations by iterative methods

B. Held and P. Pignolet

Laboratoire d'Electronique des Gaz et des Plasmas, I.U.R.S., Université de Pau, avenue de l'Université, 64000 Pau, France

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**Résumé.** — Dans cet article, une méthode itérative utilisant la règle du second moment est proposée pour le calcul de la composante basse fréquence du microchamp en un point chargé. Les résultats, en bon accord avec ceux de travaux récents, sont déduits d'une simulation numérique particulièrement simple. Cette méthode permet d'entreprendre des calculs pour des mélanges d'ions avec des temps de calcul non prohibitifs.

**Abstract.** — An iterative method using the second moment rule is proposed for the calculation of the low-frequency component of the microfield at a charged point. The results, in good agreement with other recent works, are deduced from a useful and simple numerical simulation. This method permits extensive calculations for ionic mixtures without prohibitive calculation times.

### 1. Introduction.

During the last few years, because of the Stark broadening diagnostic of stripped ions immersed in ionic perturbers, many papers have been devoted to the microfield calculations [1] (and references given there), [2-15].

The density and temperature effects are in general introduced into the microfield, using the correlation function  $g(y)$ . In the past,  $g(y)$  was deduced from the Debye-Hückel potential with or without linearization [1]. Recent studies improve this method, introducing a more accurate function  $g(y)$  [6] or propose an all-order resummation of the Baranger-Mozer series [9-15].

In a previous paper [16] hereafter referred to as I, we proposed a general semi-empirical expression for the correlation function  $g(y)$  in the one-component and the two-ionic component plasma cases.

The purpose of this paper is to present an iterative method for the microfield calculations, taking advantage of correlation functions deduced from I.

The calculations are performed at a charged point ( $Z_a e$ ) for the low frequency component of the microfield  $H(\beta)$ , using the second moment rule as a constraint for the resummation of the Baranger-Mozer series from the second order term to infinity.

This numerical simulation permits extensive calcu-

lations for ionic mixtures without prohibitive calculation time.

In section 2, the formalism is presented for the microfield and the second moment rule in the case of two-component plasma.

Section 3 is devoted to applications of the formalism where useful expressions are given for the parameters, the correlation functions, the low frequency component of the microfield and the second moment rule used as the convergent criterion for the computational method.

The results are presented in section 4 and compared with other theories and finally, section 5 gives general conclusions.

### 2. Formalism.

**2.1 GENERAL FORMALISM.** — We consider a plasma with two ionic components (a, b). If  $N$  is the total number of ions ( $N_a, N_b$ ) and  $\mathbf{E}$  the total microfield at the origin  $O$ , it is convenient to consider the Fourier transform of the probability distribution  $W(\mathbf{E})$  [1]:

$$F(\mathbf{k}) = \int \exp(i\mathbf{k} \cdot \mathbf{E}) W(\mathbf{E}) d^3E. \quad (1)$$

Introducing the probability of occurrence of a

given configuration of the  $N$  particles, it is possible, by a cluster expansion method [17-18], to express  $F(\mathbf{k})$  with a development of integral functions of correlation functions  $g(\mathbf{r})$  [1].

Finally, the probability distribution  $W(\mathbf{E})$  is obtained by inverting the Fourier transform :

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

The main difficulties which appear with this method are the knowledge of the correlation function  $g(\mathbf{r})$  and the resummation over all the orders for the development of  $F(\mathbf{k})$  : these points are particularly important for increasing values of the plasma parameter, i.e. for increasing values of electronic density or highly stripped ions (fusion applications).

In I, we introduced a general semi-empirical expression for the correlation function. We take advantage of these results, introducing accurate  $g(\mathbf{r})$  functions in the general formalism. The first order terms of  $F(\mathbf{k})$  are calculated classically [1] and we introduce a corrective function to serve as a substitute for the resummation over all the other orders. Assuming that this correction is proportional to the first order terms, the coefficient of proportionality is determined by an iterative method using the second moment rule (Sect. 3).

**2.2 SECOND MOMENT RULE.** — The second moment rule is a useful constraint for the microfield calculations [19-22]. If  $V$  is the total potential energy of the system and  $Z_a e$  the charge of the central ion, the second moment can be written in the form [19] :

$$\langle \mathbf{E} \cdot \mathbf{E} \rangle = \frac{k_B T}{(Z_a e)^2} \langle \nabla_0^2 V \rangle \quad (3)$$

where  $\nabla_0$  is the gradient with respect to the position of the central ionic charge.

Using the non-linearized Poisson-Boltzmann equation, it is possible to introduce the correlation function in the second moment rule expression :

$$\begin{aligned} \langle \mathbf{E} \cdot \mathbf{E} \rangle &\simeq 4 \pi k_B T \frac{\bar{n}_e}{Z_a} \times \\ &\times \left\{ \bar{n}_a \int \left[ \exp \left( \frac{u_{aa}(r)}{k_B T Z_a} \right) - 1 \right] g_{aa}(r) d^3r \right. \\ &\left. + \bar{n}_b \int \left[ \exp \left( \frac{u_{ab}(r)}{k_B T Z_a} \right) - 1 \right] g_{ab}(r) d^3r \right\} \quad (4) \end{aligned}$$

where  $\bar{n}_e$ ,  $\bar{n}_a$ , and  $\bar{n}_b$  are the mean values for the electronic and ionic densities,  $u_{aa}(r)$  and  $u_{ab}(r)$  being the two-body potential functions.

In first approximation, we assume that the two-body potential functions  $u_{aa}(r)$  and  $u_{ab}(r)$  are given by the Debye-Hückel screened potential, this non-

linear formulation (4) taking care of more coupling effects. Finally, the second moment rule can be explicitly expressed using the appropriate correlation function  $g(r)$ .

### 3. General results.

**3.1 PARAMETERS.** — Assuming that the plasma is composed of two ionic components (a, b) and an electronic one, the description of this plasma can be given by four parameters [1] :

— *Correlation* :

$$v = \frac{r_e}{\lambda_{D_e}} \quad (5)$$

where  $r_e$  is the mean inter-electronic length and  $\lambda_{D_e}$  the Debye length for the electrons (Appendix A) ;

— *Proportion* :

$$p = \frac{C_b}{C_a + C_b} \quad (6)$$

where  $C_a(C_b)$  is the concentration of ions ;

— *Number of charges on ions a and b* :  $Z_a, Z_b$ .

Under these conditions, the two-ionic plasma parameter  $\Gamma$  [16] can be written (Appendix A) :

$$\Gamma = \frac{\bar{Z}^2}{\bar{Z}^{1/3}} \Gamma_e \quad (7)$$

where  $\bar{Z}$  is the average ionic charge,  $\bar{Z}$  the root mean square ionic charge (Appendix A) and  $\Gamma_e$  the electronic plasma parameter :

$$\Gamma_e = \frac{2(2\pi)^{1/2}}{15} \cdot v^2. \quad (8)$$

**3.2 CORRELATION FUNCTION.** — In I, the correlation function  $g(\mathbf{r})$  is deduced from a semi-empirical method, using physical and numerical constraints. These results, in good agreement with Monte-Carlo simulations, are introduced in the general formalism, the general expressions for a two-ionic component plasma being given by [16] :

$$g_{aa}(y) = \exp \left[ -\frac{\Gamma_{aa}}{y} + H_{aa}(y) \right] \quad (9)$$

$$g_{ab}(y) = \exp \left[ -\frac{\Gamma_{ab}}{y} + H_{ab}(y) \right] \quad (10)$$

with

$$\Gamma_{aa} = \frac{Z_a^2}{\bar{Z}^{1/3}} \Gamma_e \quad (11)$$

$$\Gamma_{ab} = \frac{Z_a Z_b}{\bar{Z}^{1/3}} \Gamma_e \quad (12)$$

The screening potentials  $H_{aa}(y)$  and  $H_{ab}(y)$  are deduced from the screening potentials at the origin [16]:

$$H_{aa}(y) = \frac{H_{aa}(0)}{\frac{H_{aa}(0)}{\Gamma_{aa}} y + f(y)} \quad (13)$$

$$H_{ab}(y) = \frac{H_{ab}(0)}{\frac{H_{ab}(0)}{\Gamma_{ab}} y + f(y)} \quad (14)$$

where  $y$  is the reduced length (Appendix A) and  $f(y)$  the oscillating function:

$$f(y) = e^{-A'y} \left[ \frac{\sin B'w}{B'w} - C'w \cos w \right] \quad (15)$$

with

$$w = \frac{2\pi}{d} y \quad (16)$$

the screening potentials at the origin  $H_{ij}(0)$ , the plasma screening length  $d$  and the parameters  $A'(\Gamma)$ ,  $B'(\Gamma)$ ,  $C'(\Gamma)$  being defined in I.

**3.3 MICROFIELD.** — General expressions for the microfield are deduced from the general formalism introducing:

— the reduced microfield:

$$\beta = \frac{E}{E_0} \quad (17)$$

with

$$E_0 = \frac{e}{r_c^2} \quad (18)$$

— a new variable for the expression of  $F(k)$ :

$$a = u^{1/2} v \quad (19)$$

with

$$u = kE_0 \quad (k = |\mathbf{k}|). \quad (20)$$

With this notation, if  $H(\beta)$  is the probability distribution of the scalar-microfield  $\beta$ , it is possible to write:

$$H(\beta) = 4\pi\beta^2 W(\beta) = \frac{2\beta}{\pi} \int_0^\infty uF(u) \sin(\beta u) du \quad (21)$$

where  $F(u)$  is given by:

$$F(u) = \exp\{-u^{3/2}[\Psi_1 + \text{high order terms}]\} \quad (22)$$

with

$$\Psi_1 = \Psi_1^{aa} + \Psi_1^{ab} \quad (23)$$

$\Psi_1^{aa}$  and  $\Psi_1^{ab}$  being given by [1]:

$$\Psi_1^{aa} = \frac{n_a}{n_c} \frac{15}{2(2\pi)^{1/2}} \frac{1}{a^3} \int_0^\infty [1 - j_0(U_a)] \times g_{aa}(x) x^2 dx \quad (24)$$

$$\Psi_1^{ab} = \frac{n_b}{n_c} \frac{15}{2(2\pi)^{1/2}} \frac{1}{a^3} \int_0^\infty [1 - j_0(U_b)] \times g_{ab}(x) x^2 dx \quad (25)$$

where  $j_0$  is the spherical Bessel function of order zero and

$$U_a = Z_a \frac{a^2}{x^2} (1+x) e^{-x} \quad (26)$$

$$U_b = Z_b \frac{a^2}{x^2} (1+x) e \quad (27)$$

$x$  being a reduced length defined in Appendix A.

The asymptotic behaviour of  $H(\beta)$  can be given with an analytical expression [1]:

$$H(\beta) = H_{aa}(\beta) + H_{ab}(\beta) \quad (28)$$

$$H_{aa}(\beta) = \frac{15}{4(2\pi)^{1/2}} \frac{n_a \rho_a^5}{n_c Z_a} \frac{e^{\rho_a v}}{\left(1 + \rho_a v + \frac{\rho_a^2 v^2}{2}\right)} g_{aa}(x) \times \exp\left[-\int_0^{\rho_a} \frac{15}{2(2\pi)^{1/2}} \frac{n_a}{n_c} g_{aa}(x) \rho_a'^2 d\rho_a'\right] \quad (29)$$

$$H_{ab}(\beta) = \frac{15}{4(2\pi)^{1/2}} \frac{n_b \rho_b^5}{n_c Z_b} \frac{e^{\rho_b v}}{\left(1 + \rho_b v + \frac{\rho_b^2 v^2}{2}\right)} g_{ab}(x) \times \exp\left[-\int_0^{\rho_b} \frac{15}{2(2\pi)^{1/2}} \frac{n_b}{n_c} g_{ab}(x) \rho_b'^2 d\rho_b'\right] \quad (30)$$

with

$$\beta = \frac{Z_a}{\rho_a^2} (1 + \rho_a v) e^{-\rho_a v} \quad \text{for a ions} \quad (31)$$

$$\beta = \frac{Z_b}{\rho_b^2} (1 + \rho_b v) e^{-\rho_b v} \quad \text{for b ions} \quad (32)$$

Finally, using parameters introduced in section 3.1, we find (Appendix A) :

$$u^{3/2} \Psi_1^{aa} = \frac{15}{2(2\pi)^{1/2}} \cdot (1-p) \int_0^\infty [1 - j_0(U_a)] g_{aa}(y) y^2 dy \quad (33)$$

$$u^{3/2} \Psi_1^{ab} = \frac{15}{2(2\pi)^{1/2}} \cdot p \int_0^\infty [1 - j_0(U_b)] g_{ab}(y) y^2 dy \quad (34)$$

and the asymptotic form (for high values of  $\beta$ ) :

$$H(\beta) \approx \frac{15}{4(2\pi)^{1/2}} \cdot \frac{1}{\bar{Z}} \cdot \frac{1}{\beta^{5/2}} \cdot [(1-p) Z_a^{3/2} g_{aa}(y_a) + p Z_b^{3/2} g_{ab}(y_b)] \quad (35)$$

where  $y_a$  and  $y_b$  are given in Appendix A as :

$$y_a \approx \frac{Z_a^{1/2}}{\bar{Z}^{1/3}} \cdot \frac{1}{\beta^{1/2}} \quad (36)$$

$$y_b \approx \frac{Z_b^{1/2}}{\bar{Z}^{1/3}} \cdot \frac{1}{\beta^{1/2}} \quad (37)$$

**3.4 SECOND MOMENT RULE.** — The second moment rule can be expressed using the definition of the reduced microfield and the parameters (Appendix A). For a two-component plasma :

$$\begin{aligned} \langle \beta^2 \rangle_r \approx & \left[ \frac{15}{2(2\pi)^{1/2}} \right]^3 \cdot \frac{1}{v^5 Z_a} \cdot \left\{ \frac{(1-p)}{\bar{Z}} \right. \\ & \times \int_0^\infty \left[ \exp\left(\frac{u_{aa}(x)}{k_B T Z_a}\right) - 1 \right] \cdot g_{aa}(x) x^2 dx + \frac{p}{\bar{Z}} \\ & \left. \times \int_0^\infty \left[ \exp\left(\frac{u_{ab}(x)}{k_B T Z_a}\right) - 1 \right] g_{ab}(x) x^2 dx \right\} \end{aligned} \quad (38)$$

the one-component plasma result being obtained in the limit  $p = 0$ .

Taking, for the two-body potential function  $u(r)$  the screened Debye-Hückel potential :

$$u_{aa}(r) = Z_a^2 e^2 \frac{e^{-r/\lambda_{Dc}}}{r} \quad (39)$$

$$u_{ab}(r) = Z_a Z_b e^2 \frac{e^{-r/\lambda_{Dc}}}{r} \quad (40)$$

it is easy to see that :

$$\frac{u_{aa}(x)}{k_B T Z_a} = Z_a \Lambda_e \frac{e^{-x}}{x} \quad (41)$$

$$\frac{u_{ab}(x)}{k_B T Z_a} = Z_b \Lambda_e \frac{e^{-x}}{x} \quad (42)$$

with

$$\Lambda_e = \frac{2(2\pi)^{1/2}}{15} \cdot v^3 \quad (43)$$

It is of interest to note that, for a one-component plasma without correlation ( $\Lambda_c \rightarrow 0$ ), the limit is given by [19] :

$$\langle \beta^2 \rangle_r = \left[ \frac{15}{2(2\pi)^{1/2}} \right]^2 \cdot \frac{1}{v^2} \cdot \frac{1}{Z_a} \quad (44)$$

**3.5 ITERATIVE METHOD FOR THE MICROFIELD CALCULATIONS.** — The microfield calculation is performed using the general formalism results for the first order terms in the development of  $F(u)$  (Eqs. (33) and (34)). The higher order terms are calculated with the second moment rule assuming that (22) :

$$F(u) = \exp[-u^{3/2}(\Psi_1 - k\Psi_1)] \quad (45)$$

where  $k\Psi_1$  is the corrective term.

In practice, the microfield is calculated in four steps :

— calculation of the correlation function  $g(y)$  with a semi-empirical method [16] : the first order terms  $\Psi_1$  (23) to (25) and the second moment rule  $\langle \beta^2 \rangle_r$  (38) are deduced from  $g(y)$

— for  $k = 0$ , determination of the microfield distribution  $H(\beta)$  (Appendix A)

— verification of the conditions of normalization :

$$\int_0^\infty H(\beta) d\beta = 1 \quad (46)$$

— calculation of the second moment :

$$\langle \beta^2 \rangle_c = \int_0^\infty \beta^2 H(\beta) d\beta \quad (47)$$

and comparison with the second moment rule.

After an incrementation on  $k$ , the last three steps are still performed and so on, until the convergence is reached. Finally, the final  $k_0$  value is determined by a linear interpolation using the last two values of  $k$ .

**4. Applications.**

In tables I and II, the results for the test of convergence are presented for a one-component and a two-component plasma for various values of the plasma

parameter  $\Gamma$  (7); the second moment rule  $\langle \beta^2 \rangle_r$  (38) is compared with the second moment  $\langle \beta^2 \rangle_c(N)$  calculated from the microfield distribution,  $N$  being the number of iteration on  $k$ .

Table I. — Comparison between the second moment rule  $\langle \beta^2 \rangle_r$  and the second moment  $\langle \beta^2 \rangle_c(N)$  calculated for several values of  $k(N)$  (one component plasma).

$v$	$p$	$Z_a$	$Z_b$	$\Gamma$	$\langle \beta^2 \rangle_r$	0	1	2	3	4	5	$N$
						0.0	0.1	0.2	0.3	0.4	0.5	
0.173	1	1	1	0.01	298.55	300.37	299.23	297.47	296.16	294.78	292.84	$\langle \beta^2 \rangle_c(N)$
0.2	1	9	9	0.52	24.37	34.79	31.06	29.19	26.97	24.72	22.31	
0.4	1	35	35	20.03	1.01	2.50	2.12	1.86	1.51	1.27	0.80	

Table II. — Comparison between the second moment rule  $\langle \beta^2 \rangle_r$  and the second moment  $\langle \beta^2 \rangle_c(N)$  calculated for several values of  $k(N)$  (two-component plasma).

$v$	$p$	$Z_a$	$Z_b$	$\Gamma$	$\langle \beta^2 \rangle_r$	0	1	2	3	4	5	$N$
						0.0	0.1	0.2	0.3	0.4	0.5	
0.2	0.5	9	1	0.32	24.29	30.41	28.70	26.56	24.38	22.43	20.25	$\langle \beta^2 \rangle_c(N)$
0.8	0.5	9	1	5.13	0.97	1.30	1.17	0.89	0.73	0.60	0.47	
0.6	0.5	17	1	8.39	0.95	2.20	1.81	1.63	1.23	1.04	0.66	

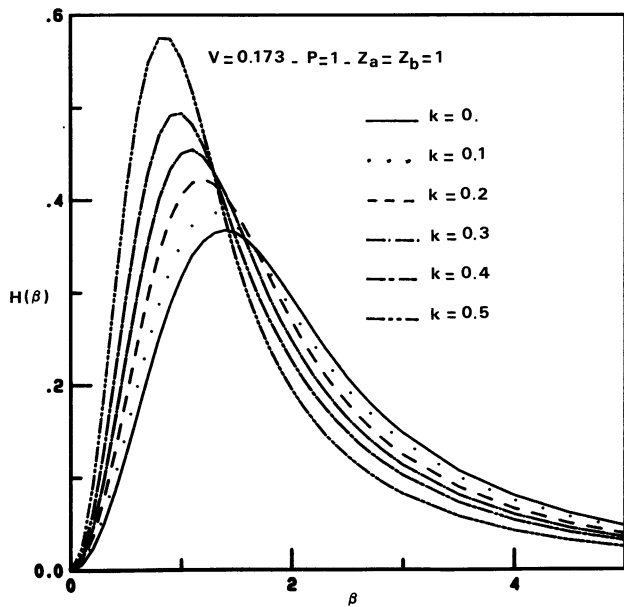


Fig. 1. — Microfield distributions of  $H(\beta)$  for a one-component plasma (test of convergence for various values of  $k$ ) with  $v = 0.173$ ,  $p = 1$ ,  $Z_a = Z_b = 1$  and  $\Gamma = 0.01$ .

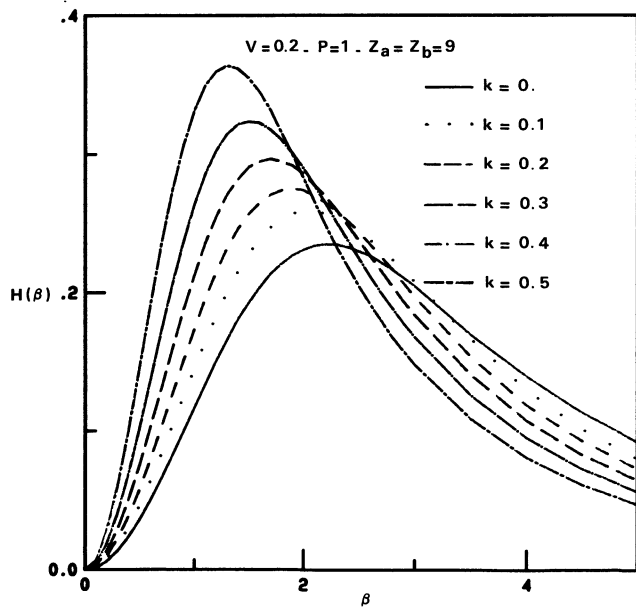


Fig. 2. — Same as figure 1 with  $v = 0.2$ ,  $p = 1$ ,  $Z_a = Z_b = 9$  and  $\Gamma = 0.52$ .

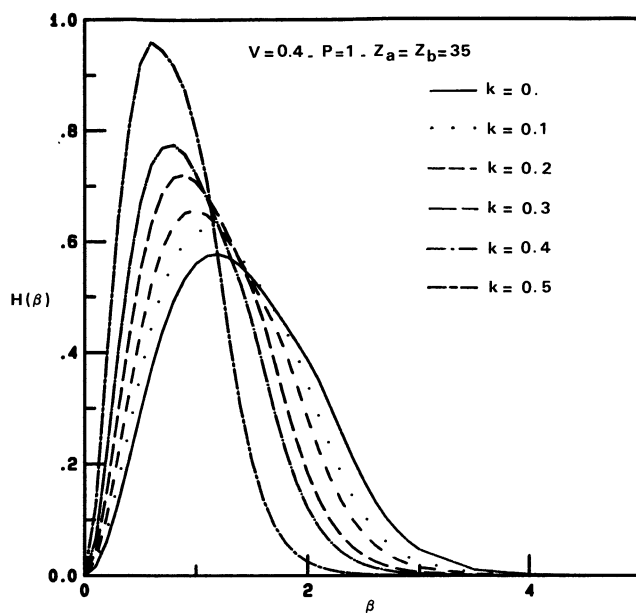


Fig. 3. — Same as figure 1 with  $v = 0.4$ ,  $p = 1$ ,  $Z_a = Z_b = 35$  and  $\Gamma = 20.03$ .

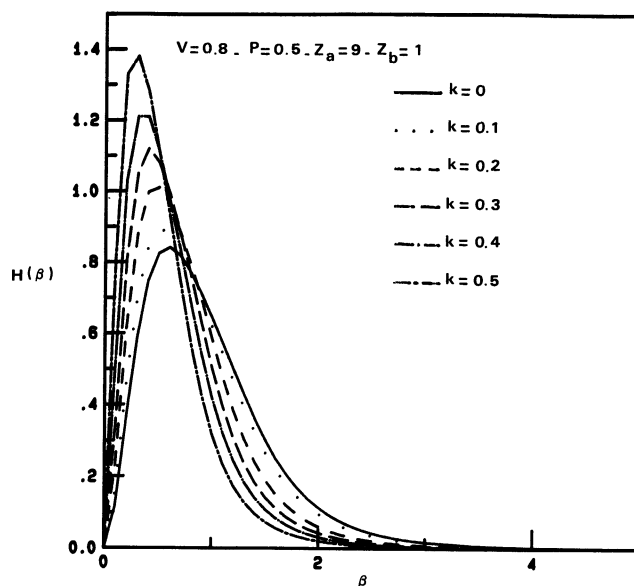


Fig. 5. — Same as figure 4 with  $v = 0.8$ ,  $p = 0.5$ ,  $Z_a = 9$ ,  $Z_b = 1$  and  $\Gamma = 5.13$ .

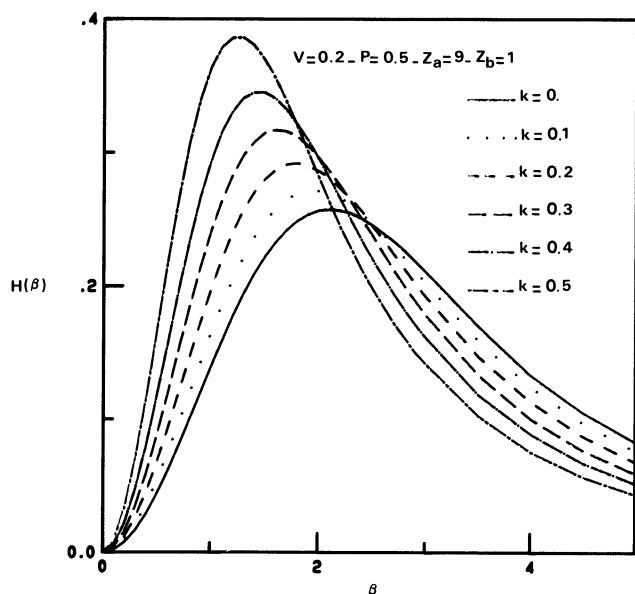


Fig. 4. — Microfield distributions of  $H(\beta)$  for a two-component plasma (test of convergence for various values of  $k$ ) with  $v = 0.2$ ,  $p = 0.5$ ,  $Z_a = 9$ ,  $Z_b = 1$  and  $\Gamma = 0.32$ .

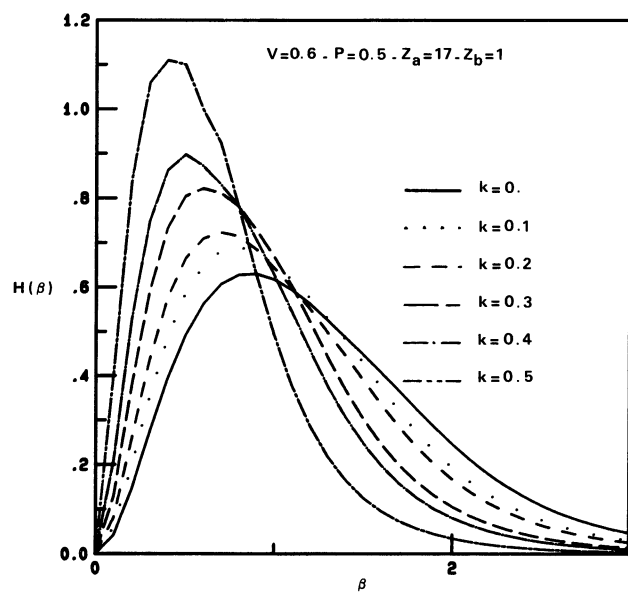


Fig. 6. — Same as figure 4 with  $v = 0.6$ ,  $p = 0.5$ ,  $Z_a = 17$ ,  $Z_b = 1$  and  $\Gamma = 8.39$ .

The corresponding microfield distributions  $H(\beta)$  are plotted in figures 1 to 3 for a one-component plasma and in figures 4 to 6 for a two-component plasma.

For increasing values of  $k$ , the microfield  $H(\beta)$  is shifted towards smaller values of the reduced microfield  $\beta$  with a pinch effect on the distribution and on enhancement of the maximum.

Comparing  $\langle \beta^2 \rangle_r$  and  $\langle \beta^2 \rangle_c(N)$  (Tab. I and II), it is easy to determine the convergent  $k_0$  values

(Appendix A) and to deduce the final microfields distribution  $H(\beta)$ . These results (Fig. 7 to 12) are compared with the more recent results given by other theories using the Debye-Hückel screened potential approximation [2-8]: next-nearest-neighbour (NNN) approximation, Hooper (H) or Tighe-Hooper (TH) calculations, adjustable parameter exponential (APEX) approximation, Monte Carlo (MC) simulations.

In figures 7 and 10, we note a very good agreement

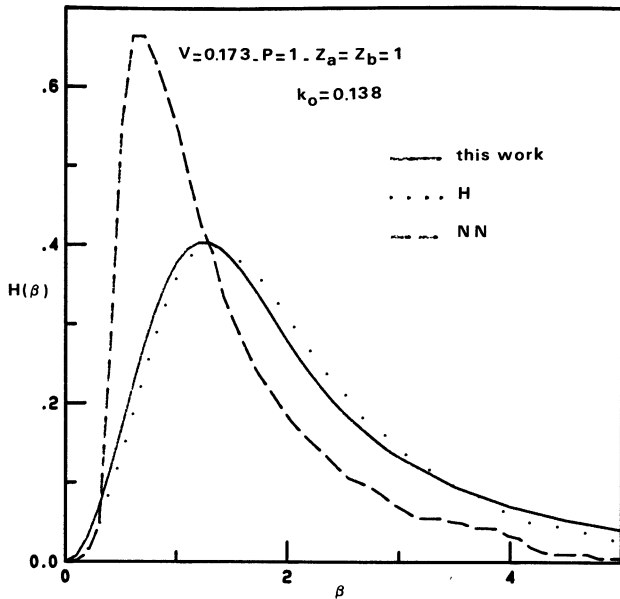


Fig. 7. — Definitive microfield distributions of  $H(\beta)$  for a one-component plasma compared with the results of Iglesias *et al.* [2-8] with  $k_0 = 0.138$ ,  $v = 0.173$ ,  $p = 1$ ,  $Z_a = Z_b = 1$  and  $\Gamma = 0.01$ .

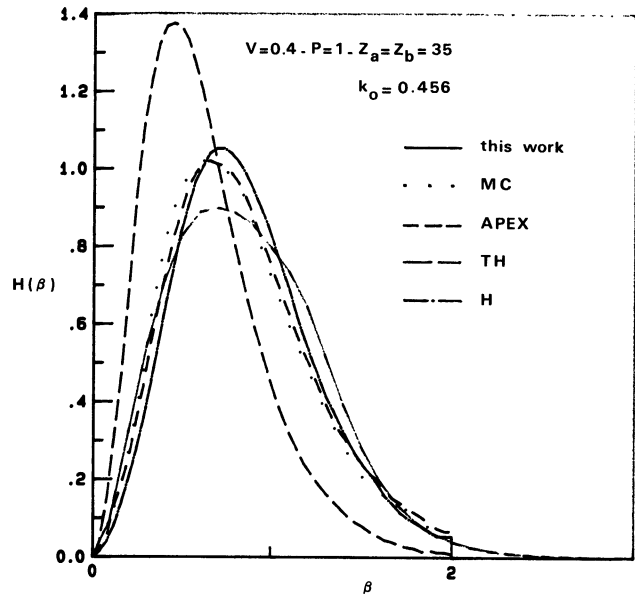


Fig. 9. — Same as figure 7 with  $k_0 = 0.456$ ,  $v = 0.4$ ,  $p = 1$ ,  $Z_a = Z_b = 35$  and  $\Gamma = 20.03$ .

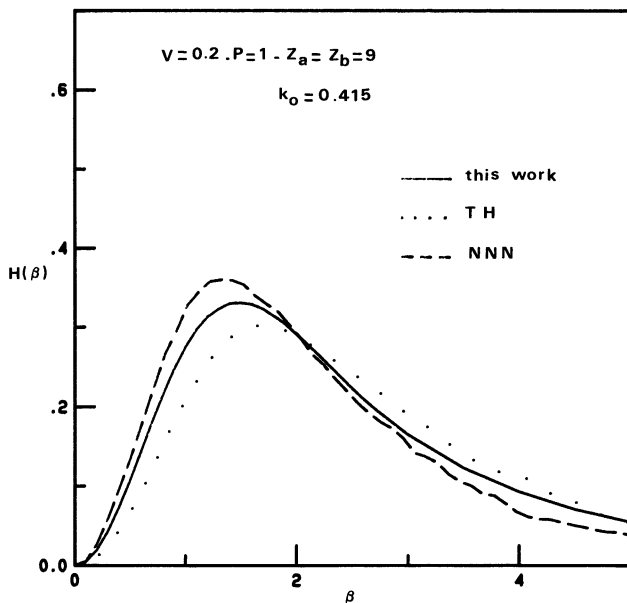


Fig. 8. — Same as figure 7 with  $k_0 = 0.415$ ,  $v = 0.2$ ,  $p = 1$ ,  $Z_a = Z_b = 9$  and  $\Gamma = 0.52$ .

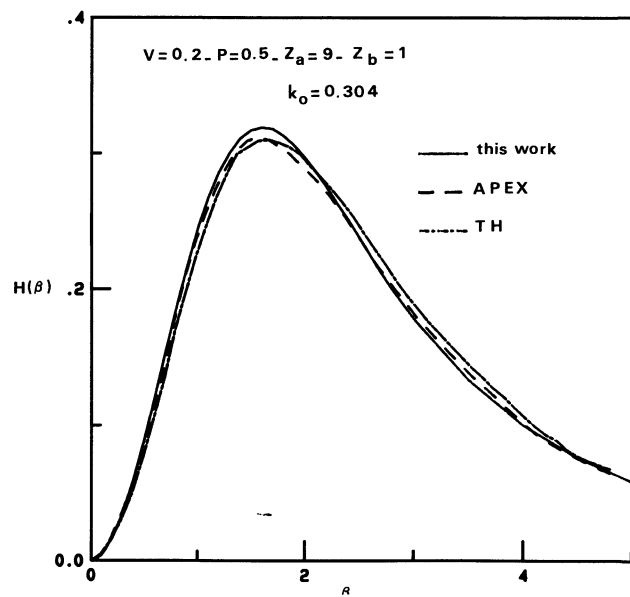


Fig. 10. — Definitive microfield distributions of  $H(\beta)$  for a two-component plasma compared with the results of Iglesias *et al.* [2-8] with  $k_0 = 0.304$ ,  $v = 0.2$ ,  $p = 0.5$ ,  $Z_a = 9$ ,  $Z_b = 1$  and  $\Gamma = 0.32$ .

with H and APEX. In the other cases, the discrepancy is in general small, our results being inside the dispersion given by NNN, TH, APEX or MC.

**5. Conclusion.**

In this paper, a general iterative method for the microfield calculations has been presented in view of

applications to the Stark diagnostic of highly stripped ions.

The results are in good agreement with APEX and the calculation times are very short compared with Monte-Carlo simulations or more usual theories [1].

With this iterative method, it is possible to consider extensive applications, taking care of the kinetic-collectif plasma limit ( $\Gamma = 1$  for  $Z_a =$

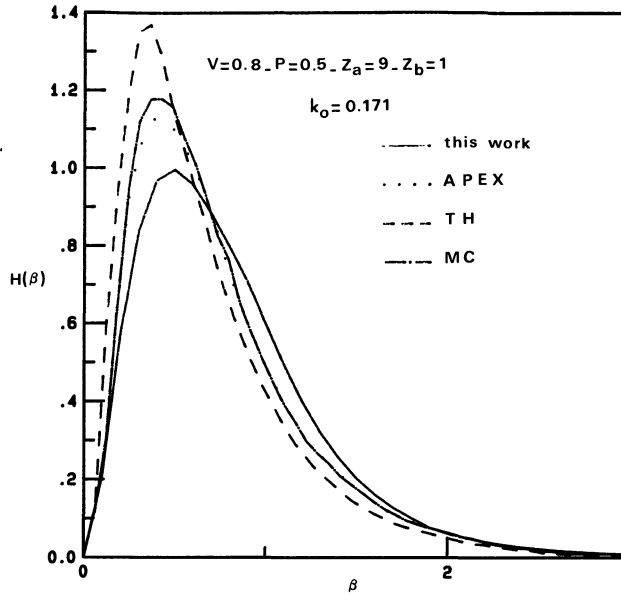


Fig. 11. — Same as figure 10 with  $k_0 = 0.171$ ,  $v = 0.8$ ,  $p = 0.5$ ,  $Z_a = 9$ ,  $Z_b = 1$  and  $\Gamma = 5.13$ .

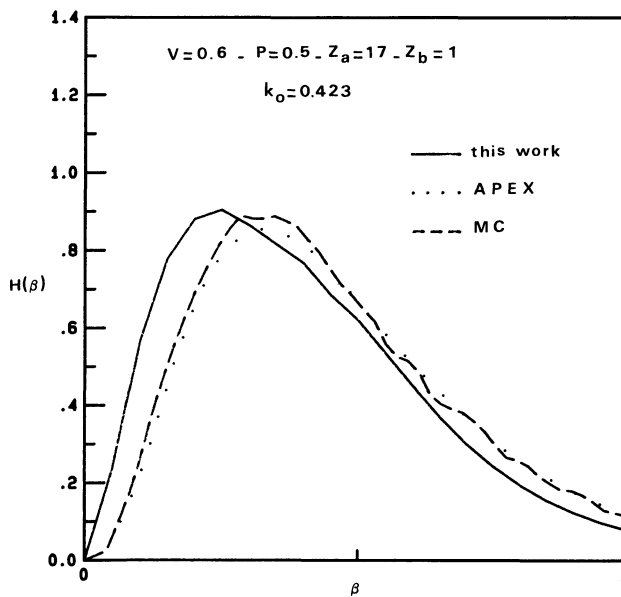


Fig. 12. — Same as figure 10 with  $k_0 = 0.423$ ,  $v = 0.6$ ,  $p = 0.5$ ,  $Z_a = 17$ ,  $Z_b = 1$  and  $\Gamma = 8.39$ .

$Z_b = 1$ , i.e.  $v = 1.732$ ) and the Holtmark limit ( $v = 0$ ).

Finally, it is of interest to note that the accuracy of these numerical results could certainly be improved by introducing the electronic degeneracy in the electronic screening function [23-26] or using effective two-body potential function solution of the non-linearized Poisson-Boltzmann equation.

Other cases were studied for different values of the parameters  $v$ ,  $p$ ,  $Z_a$ ,  $Z_b$  and these results are available on request.

## Appendix A. General results.

1. PARAMETERS. — We consider a two-ionic component plasma with a neutralizing background.

The electronic plasma parameter  $\Gamma_e$  is defined by :

$$\Gamma_e = \frac{e^2}{k_B T} \cdot \frac{1}{r_e} \quad (\text{A.1})$$

where  $r_e$  is the inter-electronic length :

$$\frac{4}{15} (2\pi)^{3/2} r_e^3 n_e = 1. \quad (\text{A.2})$$

Introducing the average ionic charge  $\bar{Z}$  [16] :

$$\bar{Z} = Z_a + p(Z_b - Z_a) \quad (\text{A.3})$$

the root mean square ionic charge  $\tilde{Z}$  :

$$\tilde{Z}^2 = Z_a^2 + p(Z_b^2 - Z_a^2) \quad (\text{A.4})$$

and the electronic Debye length :

$$\lambda_{D_e}^2 = \frac{k_B T}{4\pi n_e e^2} \quad (\text{A.5})$$

the two-ionic plasma parameter  $\Gamma$  can be written [16] :

$$\Gamma = \frac{\tilde{Z}^2}{\bar{Z}^{1/3}} \cdot \Gamma_e. \quad (\text{A.6})$$

In order to express the microfield and the second moment rule explicitly, it is interesting to introduce the relation for the concentrations and the conditions of neutrality :

$$C_e + C_a + C_b = 1 \quad (\text{A.7})$$

$$-C_e + Z_a C_a + Z_b C_b = 0. \quad (\text{A.8})$$

In these conditions, we obtain the rates [1] :

$$\frac{n_a}{n_e} = \frac{1-p}{\bar{Z}} \quad (\text{A.9})$$

$$\frac{n_b}{n_e} = \frac{p}{\bar{Z}}. \quad (\text{A.10})$$

Finally, for the correlation function applications, it is useful to define two reduced lengths  $x$  and  $y$  :

$$x = \frac{r}{\lambda_{D_e}} \quad (\text{A.11})$$

$$y = \frac{r}{r_i} \quad (\text{A.12})$$

where  $r$  is the position of the charge particle, and  $r_i$  the inter-ionic length :

$$\frac{4}{15} (2\pi)^{3/2} r_i^3 n_i = 1 \quad (\text{A.13})$$



with

$$n_i = n_a + n_b \quad (\text{A.14})$$

the relation between  $x$  and  $y$  being given by :

$$\frac{x}{y} = \bar{Z}^{1/3} \cdot v. \quad (\text{A.15})$$

2. MICROFIELD. — The asymptotic behaviour of the microfield at a charged point (ion a) is given by [1] :

$$H_{aa}(\beta) d\beta = \frac{15}{2(2\pi)^{1/2}} \frac{n_a}{n_e} g_{aa}(x) \rho^2 d\rho \times \exp \left[ - \int_0^\rho \frac{15}{2(2\pi)^{1/2}} \frac{n_a}{n_e} g_{aa}(x) \rho'^2 d\rho' \right] \quad (\text{A.16})$$

$$H_{ab}(\beta) d\beta = \frac{15}{2(2\pi)^{1/2}} \frac{n_b}{n_e} g_{ab}(x) \rho^2 d\rho \times \exp \left[ - \int_0^\rho \frac{15}{2(2\pi)^{1/2}} \frac{n_b}{n_e} g_{ab}(x) \rho'^2 d\rho' \right] \quad (\text{A.17})$$

with

$$H(\beta) = H_{aa}(\beta) + H_{ab}(\beta) \quad (\text{A.18})$$

and the notation

$$\rho = \frac{r}{r_e}. \quad (\text{A.19})$$

For the ionic part of the microfield,  $\rho$  and  $\beta$  are connected by equations (31) and (32).

Using the definitions for  $x$  and  $y$ , it is easy to show that

$$\rho = \frac{x}{v} = y \bar{Z}^{1/3}. \quad (\text{A.20})$$

For high values of  $\beta$ , the exponential integral term vanishes and the asymptotic expression becomes fairly simple :

$$H(\beta) \approx \frac{15}{4(2\pi)^{1/2}} \cdot \frac{1}{\bar{Z}} \cdot \frac{1}{\beta^{5/2}} \cdot [(1-p) \times \times Z_a^{3/2} \cdot g_{aa}(y_a) + p \cdot Z_b^{3/2} \cdot g_{ab}(y_b)] \quad (\text{A.21})$$

where

$$y_k \approx \frac{Z_k^{1/2}}{\bar{Z}^{1/3}} \cdot \frac{1}{\beta^{1/2}} \quad (\text{A.22})$$

with  $k = a$  or  $b$ .

3. SECOND MOMENT RULE. — It is possible to give explicit expressions for the second moment rule, using the reduced microfield and the parameters.

For a one-component plasma :

$$\langle \beta^2 \rangle \approx 4 \pi k_B T n_e^2 \frac{1}{\bar{Z} Z_a E_0^2} \times \int \left[ \exp \left( \frac{u(r)}{k_B T Z_a} \right) - 1 \right] g(r) d^3r \quad (\text{A.23})$$

it is easy to show that :

$$4 \pi k_B T \frac{n_e^2}{E_0^2} = \left[ \frac{15}{2(2\pi)^{1/2}} \right]^2 \cdot \frac{n_e}{v^2} \quad (\text{A.24})$$

and we find :

$$\langle \beta^2 \rangle \approx \left[ \frac{15}{2(2\pi)^{1/2}} \right]^2 \cdot \frac{n_e}{v^2} \cdot \frac{1}{\bar{Z} Z_a} \times \int \left[ \exp \left( \frac{u(r)}{k_B T Z_a} \right) - 1 \right] g(r) d^3r. \quad (\text{A.25})$$

Noticing that :

$$4 \pi n_e \lambda_{D_e}^3 = \frac{1}{\Lambda_e} \quad (\text{A.26})$$

with

$$\Lambda_e = \frac{2(2\pi)^{1/2}}{15} v^3 \quad (\text{A.27})$$

the second moment rule becomes, using the reduced length  $x$  :

$$\langle \beta^2 \rangle \approx \left[ \frac{15}{2(2\pi)^{1/2}} \right]^3 \cdot \frac{1}{v^5 \bar{Z} Z_a} \times \int_0^\infty \left[ \exp \left( \frac{u(x)}{k_B T Z_a} \right) - 1 \right] g(x) x^2 dx. \quad (\text{A.28})$$

For a two-component plasma :

$$\langle \beta^2 \rangle \approx \left[ \frac{15}{2(2\pi)^{1/2}} \right]^3 \cdot \frac{1}{v^5 Z_a} \cdot \left\{ \frac{(1-p)}{\bar{Z}} \times \times \int_0^\infty \left[ \exp \left( \frac{u_{aa}(x)}{k_B T Z_a} \right) - 1 \right] g_{aa}(x) x^2 dx + \frac{p}{\bar{Z}} \times \int_0^\infty \left[ \exp \left( \frac{u_{ab}(x)}{k_B T Z_a} \right) - 1 \right] g_{ab}(x) x^2 dx \right\}. \quad (\text{A.29})$$

4. CONVERGENT METHOD. — For the microfield calculations, we consider three regions. For small values of the reduced microfield  $\beta$ ,  $H(\beta)$  is computed starting from the general formalism (21), (24), (25), (45) and using the Krylov-Skoblya approximations for the Fourier transform [27]. These calculations are performed until numerical noise appears, criterium on the slope stops the numerical procedure. For large values of  $\beta$ , the microfield is easily deduced from the asymptotic development (28) to (30) and (35). In the intermediate region, we use an appropriate function for the interpolation of  $H(\beta)$ . This function is introduced from the general asymptotic development, assuming that :

$$H(\beta) = A \frac{e^{-B/\beta^{1/2} - C\beta^{1/2}}}{\beta^D}. \quad (\text{A.30})$$

The four parameters are deduced from constraints on the value of  $H(\beta)$  and the first derivative of this term for the last computed point ( $H_1 = H(\beta_1)$ ,

$H'_1 = \frac{dH}{d\beta} / \beta = \beta_1$ ) and the first asymptotic point ( $H_2 = H(\beta_2)$ ,  $H'_2 = \frac{dH}{d\beta} / \beta = \beta_2$ ).

$$C = \frac{\left[ \frac{H'_1}{H_1} \beta_1^{3/2} - \frac{H'_2}{H_2} \beta_2^{3/2} \right] \left[ \ln \frac{H_1}{H_2} + 2 \frac{H'_1}{H_1} \beta_1^{3/2} \left( \frac{1}{\beta_1^{1/2}} - \frac{1}{\beta_2^{1/2}} \right) \right]}{\left[ \beta_1^{1/2} - \beta_2^{1/2} \right] \left[ \ln \frac{\beta_1}{\beta_2} + 2 \beta_1^{1/2} \left( \frac{1}{\beta_1^{1/2}} - \frac{1}{\beta_2^{1/2}} \right) \right]} \quad (\text{A.31})$$

$$D = - \frac{\left[ \beta_1 \left( \frac{1}{\beta_1^{1/2}} - \frac{1}{\beta_2^{1/2}} \right) + (\beta_1^{1/2} - \beta_2^{1/2}) \right] \left[ \ln \frac{\beta_1}{\beta_2} + 2 \beta_1^{1/2} \left( \frac{1}{\beta_1^{1/2}} - \frac{1}{\beta_2^{1/2}} \right) \right]}{\left[ \beta_1 \left( \frac{1}{\beta_1^{1/2}} - \frac{1}{\beta_2^{1/2}} \right) + (\beta_1^{1/2} - \beta_2^{1/2}) \right] + \left[ \ln \frac{H_1}{H_2} + 2 \frac{H'_1}{H_1} \beta_1^{3/2} \left( \frac{1}{\beta_1^{1/2}} - \frac{1}{\beta_2^{1/2}} \right) \right]} \quad (\text{A.32})$$

$$B = - C \beta_1 - 2 D \beta_1^{1/2} - 2 \frac{H'_1}{H_1} \beta_1^{3/2} \quad (\text{A.33})$$

$$A = \beta_1^D H_1 e^{-B/\beta_1^{1/2} + C\beta_1^{1/2}} \quad (\text{A.34})$$

The numerical values of  $H(\beta)$  can be adjusted after verification of the conditions of normalization :

$$\int_0^\infty H(\beta) d\beta = 1. \quad (\text{A.35})$$

Noticing that (45) :

$$F(u) = [\exp(-u^{3/2} \Psi_1)]^{1-k} \quad (\text{A.36})$$

the microfield distribution calculation is performed for every iterative value of  $k$ .

$N$  being the iteration number,  $\langle \beta^2 \rangle_r$  the second moment rule (38),  $\langle \beta^2 \rangle_c(N)$  the calculation of the

second moment (47) from the  $N$ -th  $H(\beta)$  microfield distribution, the discrepancy  $\Delta(N)$  can be written :

$$\Delta(N) = \langle \beta^2 \rangle_r - \langle \beta^2 \rangle_c(N). \quad (\text{A.37})$$

Assuming that :

$$\Delta(N) = a' k(N) + b' \quad (\text{A.38})$$

the definitive  $k_0$  value is calculated when the convergence is reached.

$k(N)$  being the  $N$ -th value of  $k$ ,  $k_0$  is given by :

$$k_0 = - \frac{k(N-1) \Delta(N) - k(N) \Delta(N-1)}{\Delta(N-1) - \Delta(N)} \quad (\text{A.39})$$

where  $(N-1)$  and  $N$  are the last two iterations before and after the convergence.

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