ON THE NUMERICAL STUDY OF THE LOW DENSITY PLASMA SHEATH EQUATIONS IN THE PLASMA LIMIT

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Abstract.

The cylindrical low density plasma sheath in the plasma limit for three ionization source functions is formulated and is discussed numerically. The three functions are: (1) the function proportional to electron density, (2) a constant function, and (3) the function proportional to the inverse radius except in a range near the center of the cylinder. We apply two iteration schemes to the formulated equations and consider the convergence of the iterations. Comparisons are made between the two processes and the numerical results.

I. Introduction.

The classic paper of Tonks and Langmuir [9] analyzed the low-pressure discharge for plane, cylindrical and spherical geometries. The ion mean free path is assumed to be large compared to the transverse dimensions of the discharge tube and hence the positive ions fall freely to the tube walls in the self-consistent field. The electron density is assumed to have a simple Boltzmann dependence and a function which describes the spatial variation of ion-electron pair generation must be assumed. With Poisson's equation, these assumptions lead to what Tonks and Langmuir termed the complete plasma-sheath equation, and they obtained solutions in the form of a power series for the plasma limit, i.e. they assumed exact charge neutrality everywhere. Harrison and Thompson [3] analytically solved the plasma equation in plane geometry. Solutions of the complete plasma-sheath equations have been obtained in plane geometry by Self [8] and in cylindrical geometry by Parker [6]. Parker considered only the case where the ionization source function is proportional to electron density.

In this report we shall present a numerical study of the cylindrical low density plasma sheath in the plasma limit for three ionization source functions: (1) the ionization function proportional to electron density¹; (2) a constant function²; (3) a function which is proportional to the inverse radius except for small radii where it is constant. The lattermost case has application to low density

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¹⁾ This case was considered by Parker and is applicable to a positive column.

²⁾ This case has application to beam generated plasmas.

cylindrical screen cathode discharges [2].

Let us consider the low density plasma sheath in cylindrical geometry. We assume the ions to be in free fall to the walls and the electrons to have a Boltzmann distribution. Thus,

(1-1)
$$n_i(r) = \frac{1}{r} \int_0^r \frac{S(\rho)\rho d\rho}{\sqrt{(2e/m_i)[V(\rho) - V(r)]}},$$

(1-2)
$$n_e(r) = n_0 \exp \left[e V(r)/kT \right]$$

where S is the ionization source function, e is the electron charge, m_i is the ion mass, k is Boltzmann's constant, T is the electron temperature and n_0 is the electron density at r=0 where the potential is chosen to be zero (i.e. V(0)=0). In the plasma limit the ion and electron densities are equal everywhere. Thus,

(1-3)
$$\frac{1}{r} \int_{0}^{r} \frac{S(\rho)\rho d\rho}{\sqrt{(2e/m_i)[V(\rho) - V(r)]}} = n_0 \exp(eV/kT)$$

Numerical solutions of the non-linear integral equation (1-3) for the three forms of S are described.

Case 1. The ionization source function is assumed to be proportional to the electron density,

$$S(r) = \alpha n_e(r)$$

which with the substitutions

$$\zeta = \frac{\alpha}{\sqrt{2kT/m_i}} r,$$
$$\eta = -\frac{eV}{kT}$$

reduces equation (1-3) to

(1-4)
$$\int_{0}^{\zeta} \frac{e^{-\eta(\sigma)}\sigma d\sigma}{\sqrt{\eta(\zeta)-\eta(\sigma)}} = \zeta e^{-\eta(\zeta)}$$

Solutions of (1-4) are desired for $0 \leq \zeta \leq \zeta_{\omega}$ and ζ_{ω} defines the location of the wall where the electron and ion fluxes must be equal. These quantities are

$$J_e = \frac{1}{2\sqrt{\pi}} n_0 e^{-\eta(\zeta_w)} \sqrt{\frac{2kT}{m_e}},$$
$$J_i = \frac{1}{r_w} \int_0^{r_w} S(\rho) \rho d\rho$$

where m_e is the electron mass. Therefore, the equation which determines ζ_{ω} is

(1-5)
$$\frac{1}{\zeta_{\omega}}e^{\eta(\zeta_{\omega})}\int_{0}^{\zeta_{\omega}}e^{-\eta(\sigma)}\sigma d\sigma = \sqrt{\frac{m_{i}}{4\pi m_{o}}}$$

Case 2. The source function is assumed to be constant, $S(r)=S_0$, which with the substitutions

$$\zeta = rac{S_0}{n_0 \sqrt{2kT/m_i}}r,$$

 $\eta = -rac{eV}{kT},$

reduces (1-3) to

(1-6)
$$\int_{0}^{\zeta} \frac{\sigma d\sigma}{\sqrt{\eta(\zeta) - \eta(\sigma)}} = \zeta e^{-\eta(\zeta)}$$

In this case the quantity ζ_{ω} is given by

(1-7)
$$\zeta_{\omega}e^{\eta(\zeta_{\omega})} = \sqrt{\frac{m_i}{\pi m_e}}.$$

Case 3. We assume the source function to be given by

(1-8)
$$S(r) = \begin{cases} S_0 & (r \leq a), \\ S_0 \frac{a}{r} & (r \geq a) \end{cases}$$

We use this function and the same substitutions as in Case 2 to reduce equation (1-3) to

(1-9a)
$$\int_{0}^{\zeta} \frac{\sigma d\sigma}{\sqrt{\eta(\zeta) - \eta(\sigma)}} = \zeta e^{-\eta(\zeta)}, \ \zeta \leq \zeta_{a},$$

(1-9b)
$$\int_{0}^{\zeta_{a}} \frac{\sigma d\sigma}{\sqrt{\eta(\zeta) - \eta(\sigma)}} + \zeta_{a} \int_{\zeta_{a}}^{\zeta} \frac{d\sigma}{\sqrt{\eta(\zeta) - \eta(\sigma)}} = \zeta e^{-\eta(\zeta)}, \quad \zeta \ge \zeta_{a}.$$

In this case the quantity $\zeta_{\omega} > \zeta_a$ is given by

$$\zeta_{\omega}\left(1-\frac{1}{2}\frac{\zeta_{a}}{\zeta_{\omega}}\right)e^{\eta(\zeta_{\omega})}=\sqrt{\frac{m_{i}}{4\pi m_{e}}}.$$

We will solve equations (1-4), (1-6) and (1-9) numerically by applying iteration schemes. One is Newton's Method and the other is the inverse treatment of the function $\eta(\zeta)$. A comparison of results using these two schemes will be presented.

II. Application of Newton's Method.

An approximate linear equation can be obtained if the function

(2-1)
$$P(x, f(x)) = \int_{a}^{x} \frac{e^{-f(z)}z}{\sqrt{f(x) - f(z)}} dz - xe^{-f(x)} = 0$$

is differential at a point $f_0(x)$ with a fixed x, this allows the function P(x, f(x)) to be expressed in the form

$$P(x, f(x)) = P(x, f_0(x)) + P'(x, f_0(x))(f(x) - f_0(x)) + d[f(x) - f_0(x)]$$

where

$$||d[f(x)-f_0(x)]|| = O[||f(x)-f_0(x)||^2]$$

and

$$P'(x, f_0(x)) = \left[\frac{\partial}{\partial f(x)} P(x, f(x))\right]_{f(x) = f_0(x)}^{3}$$

and where the norms are the infinite ones.

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As $||f(x)-f_0(x)|| \to 0$, that is, $f_0(x)$ is close to f(x) then $P(x, f_0(x)) + P'(x, f_0(x))$ $(f(x)-f_0(x)) \to 0$, $P(x, f(x)) \to 0$. If $[P'(x, f_0(x))]^{-1}$ exists, we have a unique solution

(2-2)
$$f_1(x) = f_0(x) - [P'(x, f_0(x))]^{-1} P(x, f_0(x)).$$

This procedure may be repeated with $f_0(x)$ replaced by $f_1(x)$ to obtain another approximation, $f_2(x)$, and so on. In order to see through the procedure, we shall consider that if f(y) might be perturbated as $f(y)=\hat{f}(y)+\Delta \hat{f}(y)+\Delta^2 \hat{f}(y)+\cdots$, then the equation (2-1) is

$$\int_{\alpha}^{x} \frac{ze^{-\hat{f}(z)-\Delta\hat{f}(z)-\Delta\hat{f}(z)-\cdots}dz}{(\hat{f}(x)+\Delta\hat{f}(x)+\Delta^{2}\hat{f}(x)+\cdots-\hat{f}(z)-\Delta\hat{f}(z)-\Delta^{2}\hat{f}(z)-\cdots)^{1/2}}$$

= $xe^{-\hat{f}(x)-\Delta\hat{f}(x)-\Delta\hat{f}(x)-\Delta\hat{f}(z)-\ldots}$

where $\Delta^i \hat{f}(y) = O(\varepsilon^i)$, ε is an order perturbation. Hereafter we shall use the original notation, f(x), instead of $\hat{f}(x)$. Suppose we only consider the quadratic perturbations for evaluation of the linear approximation on Newton's method, so that

³⁾ It is consistent with the derivative in the sense of Frecht.

$$e^{-f(x)-\Delta f(x)-\Delta^2 f(x)} = e^{-f(x)} \left(1 - f(x) + \frac{1}{2!} \Delta^2 f(x) - \cdots\right) (1 - \Delta^2 f(x) + \cdots)$$
$$= e^{-f(x)} \left(1 - \Delta f(x) + \frac{1}{2!} \Delta^2 f(x) - \Delta^2 f(x) + \cdots\right)$$
$$= e^{-f(x)} \left(1 - \Delta f(x) - \frac{1}{2} \Delta^2 f(x)\right)$$

and in the denominator of equation (2-3)

$$\left(1 + \frac{\Delta f(x) - \Delta f(z) + \Delta^2 f(x) - \Delta^2 f(z)}{f(x) - f(z)}\right)^{-1/2}$$

= $1 - \frac{1}{2} \frac{\Delta f(x) - \Delta f(z)}{f(x) - f(z)} - \frac{1}{2} \frac{\Delta^2 f(x) - \Delta^2 f(z)}{f(x) - f(z)} + \frac{3}{8} \left(\frac{\Delta f(x) - \Delta f(z)}{f(x) - f(z)}\right)^2.$

Since the equations are Volterra type of the second kind [5], in a numerical process, we may find the solution $f(x_i)$ at a fixed value x_i by using Newton's method and a set of known values of $f(x_j)$ at $0 \le x_j < x_i$. Simultaneously, we assume the f(z) $(0 \le z < x)$ has already been found, so that $\Delta f(z)$ and $\Delta^2 f(z)$ may be replaced with zero.

The equation (2-3) becomes

$$\int_{\alpha}^{x-0} \frac{ze^{-f(z)}}{\sqrt{f(x)-f(z)}} \left\{ 1 - \frac{1}{2} \frac{\Delta f(x)}{f(x)-f(z)} + \frac{3}{8} \left(\frac{\Delta f(x)}{f(x)-f(z)} \right)^2 - \frac{1}{2} \frac{\Delta^2 f(x)}{f(x)-f(z)} \right\} dz$$

$$= xe^{-f(x)} \left(1 - \Delta f(x) - \frac{1}{2} \Delta^2 f(x) \right).$$

We introduce new symbols

$$G_{0} = G_{0}(x, f(x)) = \int_{a}^{x} \frac{ze^{-f(z)}}{\sqrt{f(x) - f(z)}} dz - xe^{-f(x)},$$

$$G_{1} = G_{1}(x, f(x)) = -\frac{1}{2} \int_{a}^{x} \frac{ze^{-f(z)}}{(f(x) - f(z))^{3/2}} dz + xe^{-f(x)},$$

$$G_{2} = G_{2}(x, f(x)) = \frac{3}{4} \int_{a}^{x} \frac{ze^{-f(z)}}{(f(x) - f(z))^{5/2}} dz - xe^{-f(x)}.$$

Equation (2-4) may be written

(2-5)
$$\left(\frac{1}{2}G_2 + G_1\right) \varDelta^2 f(x) + G_1 \varDelta f(x) + G_0 = 0.$$

 $\Delta f(x)$ will be real values, if the discriminant $D \ge 0$. That is.

 $D = G_1^2 - 4\left(\frac{1}{2}G_2 + G_1\right)G_0 \ge 0,$

(2-6)

$$\frac{1}{4} \ge \frac{1}{2} \left| \frac{G_2}{G_1} \right| \left| \frac{G_0}{G_1} \right| + \left| \frac{G_0}{G_1} \right| \ge \left| \frac{1}{2} \frac{G_2 G_0}{G_1^2} + \frac{G_0}{G_1} \right|.$$

If we use $G_1 \Delta f(x) + G_0 = 0$ as an approximate equation instead of perturbated quadric equation (2-5), we have

$$f_{n+1}(x) = f_n(x) + \Delta f_n(x)$$

= $f_n(x) - [G_1(x, f_n(x))]^{-1}G_0(x, f_n(x))$

as in Newton's method.

We will now discuss the theorem on the convergence of Newton's method in a Banach space as formulated by Kantrovic [4], [7].

If $K \ge ||G_2(x, f(x))||$ for a fixed x in $||f(x)-f_0(x)|| \le \rho$

$$B_{0} \ge ||[G_{1}(x, f_{0}(x))]^{-1}||,$$

$$(2-7) \qquad \qquad \eta_{0} \ge ||f_{1}(x) - f_{0}(x))|| = ||[G_{1}(x, f_{0}(x))]^{-1}G_{0}(x, f_{0}(x))||,$$

$$\hat{\boldsymbol{h}}_{0} = \left(\frac{1}{2}KB_{0} + 1\right)\eta_{0} \le \frac{1}{4}.$$

Newton's method will converge to a solution f(x) of equation (2-1) in the closed ball $\overline{U}(f_0(x), \rho)$, where

(2-8)
$$\rho \ge \rho_0 = \min \left| \frac{-1 \pm \sqrt{1 - 4\eta_0((1/2)KB_0 + 1)}}{(1/2)KB_0 + 1} \right|.$$

We have used the abbreviations $G_{0,0}=G_0(x,f_0(x)), G_{1,0}=G_1(x,f_0(x)).$

From the Taylor expansion we obtain

$$||G_{1,1} - G_{1,0}|| \leq K ||f_1(x) - f_0(x)|| \leq K \eta_0$$

and from the Neumann series expansion of an inverse operator, we have

$$[G_{1,1}]^{-1} = \sum_{n=0}^{\infty} \{I - [G_{1,0}]^{-1} [G_{1,1}]\}^n [G_{1,0}]^{-1}$$

where

$$||I - [G_{1,0}]^{-1}[G_{1,1}]|| < 1$$

therefore,

$$||[G_{1,1}]^{-1}|| \leq \frac{||[G_{1,0}]^{-1}||}{1 - ||[G_{1,0}]^{-1}|| ||G_{1,1} - G_{1,0}||}$$

if $[G_{1,1}]^{-1}$ exists, therefore, using the above notations for B_0, η_0 and K,

$$||[G_{1,1}]^{-1}|| \leq \frac{B_0}{1 - B_0 K \eta_0} = \frac{B_0}{1 - h_0} = B_1$$

where $h_0 = B_0 K \eta_0$.

Multiplying both sides of the above Neumann series by $G_{0,1}$ we obtain

$$||[G_{1,1}]^{-1}G_{0,1}|| \leq \frac{1}{1-h_0} ||[G_{1,0}]^{-1}G_{0,1}||,$$

then our iterations process from $f_1(x)$ to $f_2(x)$ is

$$||f_2(x)-f_1(x)|| = ||[G_{1,1}]^{-1}G_{0,1}|| \le \frac{1}{1-h_0} ||[G_{1,0}]^{-1}|| ||G_{0,1}||.$$

Define

$$\begin{split} F(f(x)) &= f(x) - [G_{1,0}]^{-1}G_0(x,f(x)), \\ F'(f(x)) &= I - [G_{1,0}]^{-1}G_1(x,f(x)), \\ F''(f(x)) &= -[G_{1,0}]^{-1}G_2(x,f(x))) \end{split}$$

at $f(x)=f_1(x)$ by a fixed x,

$$\begin{split} [G_{1,0}]^{-1}G_{0,1} = & f_1(x) - F(f_1(x)) \\ = & - [F(f_1(x)) - F(f_0(x)) - F'(f_0(x))(f_1(x) - f_0(x))]. \end{split}$$

The norm of this is

$$\begin{split} ||[G_{1,0}]^{-1}G_{0,1}|| &= ||F(f_1(x)) - F(f_0(x)) - F'(f_0(x))(f_1(x) - f_0(x))|| \\ &\leq \sup_{\bar{f} \in [f_0(x), f_1(x)]} ||F''(\bar{f})|| \frac{||f_1(x) - f_0(x)||^2}{2} \end{split}$$

from

$$F(f_1(x)) = F(f_0(x)) + F'(f_0(x))(f_1(x) - f_0(x)) + F''(f_0(x) + \theta(f_1(x) - f_0(x))) \frac{(f_1(x) - f_0(x))^2}{2}$$

where $0 \leq \theta \leq 1$. From the above definition

$$||F''(f(x))|| \leq ||[G_{1,0}]^{-1}|| ||G_2(x, f(x))|| \leq B_0 K,$$

therefore

$$||[G_{1,0}]^{-1}|| ||G_{0,1}|| \leq \sup_{\bar{f} \in [f_0(x), f_1(x)]} ||F''(\bar{f})|| \frac{||f_1(x) - f_0(x)||^2}{2} \leq B_0 K \frac{\eta_0^2}{2}.$$

Finally in the iteration process from $f_1(x)$ to $f_2(x)$, the correction is less than η_1

(2-9)
$$||f_2(x)-f_1(x)|| \leq \frac{1}{1-h_0} \frac{h_0}{2} \eta_0 = \eta_1.$$

Now we investigate h_1 and \hat{h}_1 ,

$$(2-10a) h_1 = B_1 \eta_1 K = \left(\frac{B_0}{1-h_0}\right) \left(\frac{1}{1-h_0} \frac{h_0}{2} \eta_0\right) K = \frac{h_0^2}{2(1-h_0)^2},$$

$$\hat{h}_1 = \frac{1}{2} h_1 + \eta_1$$

$$(2-10b) = \frac{1}{4} \frac{h_0^2}{(1-h_0)^2} + \frac{1}{2} \frac{h_0}{1-h_0} \eta_0 = \frac{h_0}{2(1-h_0)^2} \left(\frac{h_0}{2} + \eta_0 - \eta_0 h_0\right)$$

$$\leq \frac{1}{2} \frac{1}{1/2 + 2\eta_0} (\hat{h}_0 - \eta_0 h_0) \leq \hat{h}_0 - \eta_0 h_0 \leq \hat{h}_0$$

since $h_0/(1-h_0) < 1$ and $1-h_0 \ge 1/2 + 2\eta_0$ from $1/2 - \hat{h}_0 \ge 1/4$. From equation (2-8)

$$\rho_0 = \frac{1 - \sqrt{1 - 4\hat{h}_0}}{2\hat{h}_0} \eta_0$$

similarly

$$\rho_1 = \frac{1 - \sqrt{1 - 4\hat{h}_1}}{2\hat{h}_1} \eta_1.$$

From equations (2-7), (2-9), and (2-10) since $h_0 = \sqrt{2h_1}/(1 + \sqrt{2h_1})$,

$$\begin{split} \eta_{0} &\geq 2\eta_{1}, \ 1 \geq \sqrt{2h_{1}} \geq h_{0} \ \text{and} \ \eta_{0} &= 2\eta_{1}(1-h_{0})/h_{0}, \\ \hat{h}_{0} &= \frac{1}{2}h_{0} + \eta_{0} = \frac{1}{2}\frac{2h_{1}}{\sqrt{2h_{1}}(1+\sqrt{2h_{1}})} + \frac{1}{\sqrt{2h_{1}}}2\eta_{1} \leq \frac{1}{h_{0}}(h_{1}+2\eta_{1}) = \frac{2\hat{h}_{1}}{h_{0}} \end{split}$$

and

$$ho_0 \!=\! rac{1\!-\!\sqrt{1\!-\!4\hat{m{h}}_0}}{2\hat{m{h}}_0} \eta_0 \!\geq\! rac{1\!-\!\sqrt{1\!-\!4\hat{m{h}}_1}}{\hat{m{h}}_0} \eta_1 \!\geq\! rac{1\!-\!\sqrt{1\!-\!4\hat{m{h}}_1}}{2\hat{m{h}}_1} \eta_1 h_0 \!=\!
ho_1.$$

When we choose the maximum values $\hat{h}_0 = 1/4$, $\hat{h}_1 = 1/4$, $\rho_0 = 2\eta_0$, $\eta_0 \ge 2\eta_1$, $2\eta_1 h_0 = \rho_1$ then $\bar{U}(f_1(x), \rho_1) \subset \bar{U}(f_0(x), \rho_0)$. It follows by mathematical induction that Newton's process generates an infinite sequence $\{f_n(x)\}$ by starting from $f_0(x)$ at which $h_0/2$ $+\eta_0 \le 1/4$ is satisfied, and by substituting $h_1 \rightarrow h_0$, $B_1 \rightarrow B_0$, $\eta_1 \rightarrow \eta_0$, and $\hat{h}_1 \rightarrow \hat{h}_0$ in previous equations. Hence, we find the sequences of numbers $\{h_n\}$, $\{B_n\}$, $\{\eta_n\}$ and $\{\hat{h}_n\}$

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$$h_{n} = \frac{1}{2} \frac{h_{n-1}^{2}}{(1-h_{n-1})^{2}},$$

$$B_{n} = \frac{1}{1-h_{n-1}} B_{n-1},$$

$$\eta_{n} = \frac{1}{2} \frac{h_{n-1}}{1-h_{n-1}} \eta_{n-1},$$

$$\hat{h}_{n} = \frac{1}{2} h_{n} + \eta_{n},$$

$$\rho_{n} = \frac{1-\sqrt{1-4\hat{h}_{n}}}{2\hat{h}_{n}} \eta_{n}(h_{0}h_{1}\cdots h_{n-1})$$

for $n=0, 1, 2, \dots, m$. We would like to show $\{f_n(x)\}$ is a Cauchy series. Let p>0be an integer, then $f_{n+p}(x) \subset \overline{U}(f_n(x), \rho_n)$,

$$||f_{n+p}(x)-f_n(x)|| \leq \rho_n = \frac{1-\sqrt{1-4\hat{h}_n}}{2\hat{h}_n} \eta_n(h_0h_1\cdots h_{n-1}) \leq 2\eta_n(h_0)^n.$$

In equation (2-11), h_i $(i=0, 1, 2, \dots, n)$ is less than one half,

(2-12)
$$\eta_{n} = \frac{1}{2} \frac{h_{n-1}}{1 - h_{n-1}} \eta_{n-1} \leq h_{n-1} \eta_{n-1} \leq h_{n-1} h_{n-2} \eta_{n-2} \leq \cdots$$
$$\leq h_{n-1} h_{n-2} h_{n-3} \cdots h_{0} \eta_{0} \leq h_{0}^{n} \eta_{0}.$$

as $n \to \infty$, $\rho_n \leq 2h_0^{2n} \eta_0 \to 0$, then the sequence $\{f_n(x)\}$ is a Cauchy series. The error estimation may be obtained from the fact that

 $\{f_{n+1}(x), f_{n+2}(x), f_{n+3}(x), \cdots\} \subset \overline{U}(f_n(x), \rho_n)$

and $||f^*(x)-f_n(x)|| \leq 2h_0^{2n}\eta_0$, where $f^*(x)$ is a fixpoint value.

We have mentioned only equation (1-4), but the arguments for establishing equation (1-6) and (1-9) are similar. We have proved the existence of the solution of Newton's method. The uniqueness and other theorems on the convergence of Newton's method may be found elsewhere [7], [1].

III. Inverse function of f(x).

When we take an inverse function of f(x) like

$$f(x) = u, \qquad g(u) = x,$$

$$f(z) = v, \qquad g(v) = z,$$

$$f(\alpha) = \beta, \qquad g(\beta) = \alpha$$

and dz = g'(v)dv.

Case 1, equation (2–1).

(2-1)
$$\int_{\alpha}^{x} \frac{e^{-f(z)}z}{\sqrt{f(x) - f(z)}} dz - x e^{-f(x)} = 0$$

becomes

(3-1)
$$\int_{\beta}^{u} \frac{e^{-v}g(v)g'(v)dv}{\sqrt{u-v}} - g(u)e^{-u} = 0.$$

Let $g(u)^2 = F(u)$, 2g(u)g'(u) = F'(u) and multiply equation (3-1) by the term $1/\sqrt{w-u}$ and integrate from β to w with respect to the variable u,

$$\int_{\beta}^{w} \frac{1}{\sqrt{w-u}} \int_{\beta}^{u} \frac{e^{-v}F'(v)dv}{\sqrt{u-v}} du - 2 \int_{\beta}^{w} \frac{\sqrt{F(u)}}{\sqrt{w-u}} e^{-u} du = 0.$$

Changing the order of integration

$$\int_{\beta}^{w} e^{-u} F'(v) \int_{\beta}^{w} \frac{du}{\sqrt{w-u}\sqrt{u-v}} dv - 2 \int_{\beta}^{w} \frac{\sqrt{F(u)}}{\sqrt{w-u}} e^{-u} du = 0.$$

The second integral in the first term of the above equation is π .

$$[F(v)e^{-v}]^w_{\beta} + \int_{\beta}^w F(v)e^{-v}dv - \frac{2}{\pi}\int_{\beta}^w \frac{\sqrt{F(u)}}{\sqrt{w-u}}e^{-u}du = 0.$$

The initial condition is $\alpha = 0$, $\beta = 0$, then $F(\beta) = 0$.

(3-2)
$$F(w) = e^{w} \left\{ \frac{2}{\pi} \int_{0}^{w} \frac{\sqrt{F(u)}}{\sqrt{w-u}} e^{-u} du - \int_{0}^{w} F(v) e^{-v} dv \right\}.$$

We will use equation (3-2) as an iteration scheme for equation (1-4) by using $F_{m+1}(w)$ in the left hand side and $F_m(u)$ in the right hand side.

For numerical calculation, we use the discretized value of F(u), $u=i\Delta w$, i=0,1,2...,n, where Δw is the length of increment, n is the number of subdivision of the distance zero to w. Suppose we are now at the n^{th} step or at a point $u=\Delta w \cdot n$. We may consider F(u); $0 \leq u \leq (n-1) \cdot \Delta w$ is a known value, then at m^{th} iteration with a fixed w,

$$F_{m+1}(w) - F_m(w)$$

$$= e^w \left\{ \frac{2}{\pi} \int_{w-4w}^w \frac{\sqrt{F_m(u)} - \sqrt{F_{m-1}(u)}}{\sqrt{w-u}} e^{-u} du - \int_{w-4w}^w F_m(v) e^{-v} - F_{m-1}(v) e^{-v} dv \right\}$$

$$= P\{F_m(w)\} - P\{F_{m-1}(w)\}$$

where

$$||P|| = \sup_{u \in D = [w - Aw, w]} \frac{||P\{F(u)\}||}{||F(u)||} \leq \sup_{D} e_{w} \int_{D} \left| \frac{2}{\pi} \frac{1}{\sqrt{F(u^{*})}} \sqrt{w - u} - 1 \right| e^{-u} du$$

$$(3-3) \qquad \leq \sup_{D} e^{w} \left[\frac{2}{\pi} \frac{1}{\sqrt{F(u^{*})}} \int_{D} \frac{e^{-u}}{\sqrt{w - u}} du + \int_{D} e^{-u} du \right]$$

$$= \sup_{D} e^{w} \left[\frac{4}{\pi} \frac{1}{\sqrt{F(u^{*})}} \left\{ \sqrt{\Delta w} e^{-w + Aw} - \int_{D} \sqrt{w - u} e^{-u} du \right\} + e^{-w} (e^{Aw} - 1) \right]$$

where $F(u^*) = \sup_{u \in D} F(u)^{4}$

$$||P|| \leq \left[\frac{4}{\pi} \frac{\sqrt{\Delta w}}{\sqrt{F(u^*)}} e^{dw} + e^{dw} - 1\right]$$

$$= \left\{\frac{4}{\pi} \sqrt{\frac{\Delta w}{F(u^*)}} + 1\right\} e^{dw} - 1 = \theta$$

then

$$(3-5) ||F_{m+1}(w) - F_m(w)|| = ||P\{F_m(w)\} - P\{F_{m-1}(w)\}|| \le \theta ||F_m(w) - F_{m-1}(w)||.$$

If 0 < 1 for $m=0, 1, 2, \cdots$ with a suitable starting $F_0(w)$, then the scheme converges in a ball $U(F_0(w), r)$.

The error is

$$||F_m(w) - F^*(w)|| \leq \theta^m r_0$$

from equation (3-5), where $r \ge r_0 = (1/(1-\theta))||F_1(w) - F_0(w)||$, $F^*(w)$ is the fixed point value. As we have mentioned above, we may take the same procedure for equations (1-6) and (1-9).

Case 2, equation (1-6).

$$\int_{\alpha}^{x} \frac{zdz}{\sqrt{f(x)-f(z)}} - xe^{-f(x)} = 0$$

becomes

(3-7)
$$F(w) = F(\beta) + \frac{2}{\pi} \int_{\beta}^{w} \frac{\sqrt{F(u)}}{\sqrt{w-u}} e^{-u} du.$$

With the initial conditions $\alpha=0$, $\beta=0$, and $F(\beta)=0$, we will use equation (3-7) as an iteration scheme of equation (1-6).

(3-8)

$$F_{m+1}(w) = \frac{2}{\pi} \int_{0}^{w-4w} \frac{\sqrt{F_m(u)}}{\sqrt{w-u}} e^{-u} du + \frac{2}{\pi} \int_{w-4w}^{w} \frac{\sqrt{F_m(u)}}{\sqrt{w-u}} e^{-u} du + P\{F_m(u)\},$$

⁴⁾ In general, u^* is a specific point which satisfies above the definition of norm P among a kind of norms ||F(u)||.

where $F(u^*) = \sup_{u \in D} F(u)$,

$$||F_{m+1}(w) - F_m(w)|| = ||P\{F_m(w)\} - P\{F_{m-1}(w)\}||$$

$$\leq ||P|| ||F_m(w) - F_{m-1}(w)|| \leq \theta ||F_m(w) - F_{m-1}(w)||.$$

If $\theta = (4/\pi)\sqrt{\Delta w/F(u^*)} e^{-w}e^{\omega} < 1$ for $m = 0, 1, 2, \cdots$ with a fixed w then the iteration scheme (3-8) will converge with same error as equation (3-6).

Case 3, equation (1-9).

(1-9b)
$$\int_0^\alpha \frac{zdz}{\sqrt{f(x)-f(z)}} + \alpha \int_\alpha^x \frac{dz}{\sqrt{f(x)-f(z)}} = xe^{-f(x)}, x \ge \alpha$$

becomes the following by the same process

(3-10)
$$\int_{0}^{\beta} \frac{g(v)g'(v)}{\sqrt{u-v}} dv + g(\beta) \int_{\beta}^{u} \frac{g(v)g'(v)}{\sqrt{u-v}} dv = g(u)e^{-u}, \ u \ge v.$$

The first term is

$$\begin{split} \int_{0}^{w} \int_{0}^{\beta} \frac{F'(v)}{\sqrt{w-u}\sqrt{u-v}} dv du &= \int_{0}^{w} \int_{0}^{u} \frac{F'(v)}{\sqrt{w-u}\sqrt{u-v}} dv du - \int_{\beta}^{w} \int_{\beta}^{u} \frac{F'(v)}{\sqrt{w-u}\sqrt{u-v}} dv du \\ &= \int_{0}^{w} \int_{v}^{w} \frac{F'(v)}{\sqrt{w-u}\sqrt{u-v}} du dv - \int_{\beta}^{w} \int_{v}^{w} \frac{F'(v)}{\sqrt{w-u}\sqrt{u-v}} du dv \\ &= \pi \int_{0}^{w} F'(v) dv - \pi \int_{\beta}^{w} F(v) dv \\ &= \pi F(\beta) - \pi F(0). \end{split}$$

The second term is

$$\sqrt{F(\beta)} \int_{0}^{w} \int_{\beta}^{u} \frac{F'(v)}{\sqrt{w-u}\sqrt{u-v}} \frac{dvdu}{\sqrt{F(v)}} = \sqrt{F(\beta)} \int_{\beta}^{w} \int_{v}^{w} \frac{F'(v)}{\sqrt{F(v)}} \frac{dudv}{\sqrt{w-u}\sqrt{u-v}}$$
$$= \sqrt{F(\beta)} \pi \int_{\beta}^{w} \frac{1}{\sqrt{F(v)}} d[F(v)] = 2\sqrt{F(\beta)} \pi [\sqrt{F(w)} - \sqrt{F(\beta)}], \ u \ge \beta$$

then equation (1-9b) is

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(3-11)
$$\sqrt{F(w)} = \frac{\sqrt{F(\beta)}}{2} + \frac{1}{\pi\sqrt{F(\beta)}} \int_0^w \frac{\sqrt{F(u)}}{\sqrt{w-u}} e^{-u} du, \ w \ge \beta,$$

(3-12)
$$g(w) = \frac{g(\beta)}{2} + \frac{1}{\pi g(\beta)} \int_0^w \frac{g(u)}{\sqrt{w-u}} e^{-u} du, \ w \ge \beta.$$

We will use equation (3-11) or (3-12) in the range $w \ge \beta$, and equation (3-8) in the range $w \le \beta$ as an iterational scheme for equation (1-9).

The norm of operator P as same as equation (3-3) or (3-9)

$$||P|| = \sup_{u \in D = [w - \Delta w, w]} \frac{||P\{g(u)\}||}{||g(u)||} \leq \sup_{D} \frac{e^{-w}}{\pi g(\beta)} \int_{D} \frac{e^{w-u}}{\sqrt{w-u}} du$$

$$(3-13) \qquad \leq \sup_{D} \frac{e^{-w}}{\pi g(\beta)} \int_{0}^{\Delta w} \frac{e^{t}}{\sqrt{t}} dt \leq \sup_{D} \frac{e^{-w}}{\pi g(\beta)} \int_{0}^{\Delta w} \frac{1}{\sqrt{t}} \left\{ \frac{e^{\Delta w} - 1}{\Delta w} t + 1 \right\} dt$$

$$= \frac{2}{3} \frac{e^{-w}}{\pi g(\beta)} \sqrt{\Delta w} [e^{\Delta w} + 2] = \theta.$$

The scheme will converge to the fixed point-value if $\theta < 1$ for $m=0, 1, 2, \cdots$ We may estimate equation (3-13) roughly as if $2/\pi \leq g(\beta)/\Delta w$, then $\theta \leq 1$. Equation (3-2), equation (3-7) and equation (3-11) define an integral operator of F(w) from C[0, w]into itself. Let us take $F_0(w)=1$ as a starting value of the iteration. The function e^{-u} in the interval $0 \leq u \leq w$ may be replaced by linear functions, one is the upper bound, the other is the lower bound, that is

$$\frac{e^{-w}-1}{w}u + b \le e^{-u} \le \frac{e^{-w}-1}{w}u + 1$$

where

$$b = \frac{1 - e^{-w}}{w} \left(1 + \ln \frac{w}{1 - e^{-w}} \right),$$

then the bounded range of $F_1(w)$ may be found after one iteration,

$$F_{1}^{L}(w) = \left(\frac{8}{3\pi}w^{1/2} + 1\right) + e^{w}\left(\frac{4}{3\pi}w^{1/2}(3b - 2) - 1\right)$$
$$\leq F(w) \leq \left(\frac{8}{3\pi}w^{1/2} + 1\right) + e^{w}\left(\frac{4}{3\pi}w^{1/2} - 1\right) = F_{1}^{u}(w)$$

from equation (3-2),

$$F_{1}^{L}(w) = \frac{4}{3\pi} w^{1/2} (2e^{-w} + (3b-2)) \le F(w) \le \frac{4}{3\pi} w^{1/2} (2e^{-w} + 1) = F_{1}^{u}(w)$$

using equation (3-7), in Case 3 the same results are obtained.

One may establish a relation between Δw and w by substituting $F_1^L(w)$ for

 $F(u^*)$ into equation (3-4) and equation (3-9) so that

(3-14a)
$$\Delta w < \frac{\pi^2}{16} \left(\frac{8}{3\pi} w^{1/2} + 1 + e^w \left(\frac{4}{3\pi} w^{1/2} (3b-2) - 1 \right) \right)$$

and

(3-14b)
$$\Delta w < \frac{\pi}{12} w^{1/2} (2 + e^w (3b - 2)).$$

Suppose w^* is satisfied when the right hand side of (3-14) equals zero, the relations are valid in a domain $0 \le w < w^*$.

We know F(u) on $0 \le u \le w$, in which w is less than w^* , is bounded because $\sup_{0 \le u \le w} F(u)$ indicates the position of a cylindrical wall.

Our iteration schemes will converge to a fixed point from the contraction mapping principle, such that by choosing Δw properly from (3-14) and starting with $F_0(u) = F_1^L$ or F_1^u , there is a convergent ball $\tilde{U}(F_0(u), r)$ for our integral operator P where $r \ge (1/(1-\theta))||P\{F_0(u)\} - F_0(u)||$.

IV. Numerical results.

Given the interval mesh Δx of numerical integration, the first I intervals are integrated with a fine mesh $\Delta x/100$, and the following $I \times 9$ are done with the other fine mesh $\Delta x/10$. The remaining intervals are done with Δx .

In order to avoid the singularity of the integrand, the last interval mesh uses a formula of integration by parts with linear interpolation of the unknown function.

If we assume that f(x) is increasing monotonously as x increases and the $f'(x) \neq 0$, $f'(x) < \infty$ at $x_1 > x > 0$ then $||G_2(x, f(x))||$ at a fixed $x_1 > x > 0$ is bounded, and if the condition equation (2-6) is satisfied, namely $G_{0,0}$ is enough to be smaller (the first approximation $f_0(x)$ is sufficiently close to the fixed point value), we may find a numerical solution at a fixed x.

The error and error propagation may be taken as

$$(4-1) \quad \text{error} = e_i + e_i + Ne_i + 2(N-1)(e_i + e_i)\Delta x + (N-1)Ne_i\Delta x + O(e_i\Delta x^2) + O((e_i + e_i)\Delta x^2)$$

where $e_l = (\Delta x^2/2) \max |f''(\zeta)|$ is an error of the linearization of last integration step with $x - \Delta x \leq \zeta \leq x$, e_t is a truncation error of the iteration schemes. e_i is a numerical integration formula error, Δx is an integration step seize and N is the number of the integration step.

For example, take $\Delta x=5\times 10^{-3}$, N=200, $e_l=10^{-6}$, $e_i=\Delta x^5$, and max $f''(\zeta)=20$, then, $\operatorname{error} \simeq 3e_l=7.5\times 10^{-4}<10^{-3}$ is a good indication of the accuracy of our results. See Table I, $\Delta x=0.0025$ and $\Delta x=0.005$, at the position near wall.

In the case of inverse treatment of f(x), the following numerical approximation of the integration was used.

$$F(N\Delta x) = \sum_{i=1}^{N-1} W_i \sqrt{F(i\Delta x)} + W_N \sqrt{F(N\Delta x)} = \text{const} + W_N \sqrt{F(N\Delta x)}$$

Where Δx , N are as before, the W_i are the weights for the numerical integration.

Equations θ , equation (3-4), equation (3-9), and equation (3-13) are always less than one where u^* is near zero because the solutions are expected as $w^{1/n}(n>1)$ near the origin, Δw can be chosen small enough so that θ is less than one. In the region far from zero of w, the term e^{-w} becomes very small and the θ will be smaller.

The inverse treatment has the following advantages from the numerical view point when compared with Newton's method:

- (1) less calculation during iteration,
- (2) faster convergence,
- (3) less error,

(4) we may find more accurate wall position since unknown functions F'(s)=0 $(f'(s)=\infty$ in Newton's method) where s is the wall position.

However Newton's method is a powerful one when we cannot apply the inverse treatment.

All the numerical integration was done by Simpson rule. By using the Atkin's extrapolation formula [1], we may estimate a more accurate wall position.

Case 1 0.77186, Case 2 0.58280.

The numerical results are presented in Table I, Table II, Figure 1, Figure 2, and Figure 3.

		Newton's Method $\epsilon t \leq 10^{-5}$		
	Parker's Results	DX=0.00	DX = 0.005	
x	f(x)	f(x)	f(x)	
0.	0.	0.	0.	
0.1	0.0100	0.01006	0.010125	
0.2	0.0407	0.04101	0.040872	
0.3	0.0935	0.09414	0.093850	
0.4	0.1719	0.17284	0.17238	
0.5	0.2821	0.28351	0.28283	
0.6	0.4378	0.43985	0.43881	
0.7	0.6787	0.68265	0.68058	
0.75	0.8901	0.89985	0.89433	
0.76	0.9598	0.97671	0.96650	
0.765		no sol'n	1.01718	
0.77	1.0790		no sol'n	
wall	0.772	_		

Table 1-A (Case 1)

DX=0.01		DX=0.005		DX = 0.0025	
x	f(x)	x	f(x)	x	f(x)
0.	0.	0.	0.	0.	0.
$0.09971 \\ 0.10342$	0.01 0.011	0.09937 0.10181	$\begin{array}{c} 0.01\\ 0.0105\end{array}$	$0.09962 \\ 0.10084$	$0.01 \\ 0.01025$
$0.19797 \\ 0.20037$	$\begin{array}{c} 0.04\\ 0.041\end{array}$	$0.19943 \\ 0.20066$	$\begin{array}{c} 0.0405\\ 0.0410\end{array}$	$\begin{array}{c} 0.19729 \\ 0.20329 \end{array}$	$\begin{array}{c} 0.04 \\ 0.0425 \end{array}$
$0.29897 \\ 0.30054$	$\begin{array}{c} 0.093 \\ 0.094 \end{array}$	$0.29307 \\ 0.300815$	0.090 0.095	$0.29775 \\ 0.30166$	$0.0925 \\ 0.0950$
$0.39570 \\ 0.40649$	0.17 0.18	$0.39699 \\ 0.40232$	$0.170 \\ 0.175$	$0.39756 \\ 0.40022$	$0.17 \\ 0.1725$
$0.49664 \\ 0.50424$	$\begin{array}{c} 0.28\\ 0.29\end{array}$	$0.49763 \\ 0.50143$	0.28 0.285	$0.49996 \\ 0.501924$	$0.2825 \\ 0.285$
0.59965	0.44	$0.59779 \\ 0.60053$	$\substack{0.435\\0.440}$	$0.59954 \\ 0.60092$	$\begin{array}{c} 0.4375\\ 0.440\end{array}$
$0.69861 \\ 0.70158$	$\begin{array}{c} 0.68\\ 0.69\end{array}$	$0.69797 \\ 0.69959$	$\begin{array}{c} 0.675\\ 0.68\end{array}$	$0.69922 \\ 0.70004$	$0.6775 \\ 0.68$
$0.74936 \\ 0.75081$	$\substack{0.9\\0.91}$	$0.74893 \\ 0.74968$	0.89 0.895	$0.74985 \\ 0.75030$	0.8925 0.895
0.75990	0.98	$0.75888 \\ 0.75941$	$0.960 \\ 0.965$	$0.75974 \\ 0.76008$	$0.9625 \\ 0.965$
0.77	no sol'n	$0.76883 \\ 0.768993$	$\begin{array}{c} 1.080\\ 1.085 \end{array}$	0.76999 0.77013	$1.0925 \\ 1.095$
* 0.76906	1.16	* 0.77051	1.150	* 0.77121	1.155

 $\begin{array}{c} {\rm Table \ 1-B} \quad ({\rm Case \ 1}) \\ {\rm Inverse \ Case \ $\epsilon t \leq 10^{-5}$ Where $*$ Indicates Wall Position} \end{array}$

Table 2-A (Case 2)

x	Newton's Method $f(x) \epsilon t \leq 10^{-5}$				
	DX=0.04	DX = 0.02	DX=0.01		
0.	0.	0.	0.		
0.1	0.010198	0.010166	0.01046		
0.2	0.042255	0.042165	0.04246		
0.3	0.10190	0.10284	0.10240		
0.4	0.20388	0.20649	0.20493		
0.48	0.35411	0.35050	0.34648		
0.50		0.040368	0.39829		
0.52	0.48291	0.47011	0.46221		
0.54	no sol'n	0.55865	0.54582		
0.56		0.69995	0.66987		
0.57		no sol'n	0.77239		
			no sol'n		

DX = 0.01		$DX\!\!=\!0.005$		DX = 0.0025	
x	f(x)	x	f(x)	x	f(x)
0.	0.	0.	0.	0.	0.
0.099315	0.01	0.099417	0.01	0.099305	0.01
0.19501	0.04	0.19519	0.04	0.19527	0.04
0.21681	0.05	0.21697	0.05	0.21703	0.05
0.29788	0.1	0.29798	0.1	0.29767	0.1
0.31061	0.11	0.31061	0.11		
0.39755	0.2	0.39721	0.2	0.39743	0.2
0.40434	0.21	0.40470	0.21		
0.45941	0.3	0.45971	0.3	0.45986	0.3
0.48254	0.35	0.48285	0.35	0.48297	0.35
0.50187	0.4	0.50208	0.4	0.50219	0.4
0.52084	0.46	0.52102	0.46	0.521102	0.46
0.52357	0.47	0.523791	0.47	0.52388	0.47
0.53139	0.5	0.53154	0.5	0.53162	0.5
0.54051	0.54	0.54065	0.54	0.54072	0.54
0.54459	0.56	0.54472	0.56	0.54479	0.56
0.55189	0.6	0.55200	0.6	0.55206	0.6
0.56091	0.66	0.56101	0.66	0.56106	0.66
0.56217	0.67	0.56231	0.67	0.56236	0.67
0.56581	0.7	0.56590	0.7	0.565951	0.7
0.57251	0.77	0.57263	0.77	0.57267	0.77
0.57481	0.8	0.57488	0.8	0.57493	0.8
0.58006	0.9	0.58012	0.9	0.58016	0.9
0.58242	1.0	0.58248	1.0	0.58251	1.0
0.58273	1.06	0.58279	1.06	0.58282	1.06
0.58255	1.1	0.58760	1.1	0.58264	1.1

Table 2–B (Case 2) Inverse Case $\varepsilon t \leq 10^{-5}$

A starting value of iterations at each step was chosen as a linear extrapolation, namely $f_0(x) = w \cdot f(x - \Delta x) + (1 - w) \cdot f(x - 2\Delta x)$ where w is a weight parameter.

In order to accelerate convergences of Newton's method an acceleration factor was used. If the whole terms of Equation (2-5) is using as an evalution of a perturbation term ε instead of only the linear term of the equation, several Newton's iteration steps will be replaced by one step of this evaluation with the calculation of $G_2(f(x), x)$.





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Added in $\mathsf{Proof.}$ After presenting the paper, we have applied the Newton's method for the equations to solve

$$\frac{1}{b} \frac{d^2 F(x)}{dx^2} - \int_0^x \frac{e^{-F(x)} dz}{(F(x) - F(z) - \gamma(x - z)^2)^{1/2}} - e^{-F(x)} = 0,$$

$$\frac{1}{b} \left[\frac{x d^2 F(x)}{dx^2} + \frac{dF(x)}{dx} \right] - \int_0^x \frac{z e^{-F(x)} dz}{(F(x) - F(z) - \gamma(x - z)^2)^{1/2}} - x e^{-F(x)} = 0$$

The mathematical proof and the numerical process for these equations are similar to those presented in this paper.