JOURNAL OF COMPUTATIONAL PHYSICS 59, 96–107 (1985)

Solution of a Nonlinear Integral Equation Arising in Particle Transport Theory

V. C. BOFFI

Nuclear Engineering Laboratory, University of Bologna, Via dei Colli 16, Bologna 40136, Italy

G. SPIGA*

Laboratory for Transport Theory and Mathematical Physics, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061

AND

J. R. THOMAS, JR.

Nuclear Engineering Group, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061

Received December 27, 1983; revised June 12, 1984

Iterative schemes for the solution of a nonlinear integral equation arising in particle transport theory are illustrated, and their convergence is studied in the frame of the Lebesgue space L_1. Numerical results are then reported for some specializations of practical interest of the physical parameters entering the considered transport equation. © 1985 Academic Press, Inc.

1. INTRODUCTION

In a recent paper [1], dealing with stationary transport of test particles (t.p.) interacting between themselves and with an infinite homogeneous background of field particles (fp), the following nonlinear integral equation was derived, in the absence of scattering collisions, for the isotropic tp distribution function $f(v)$ as a function of the speed v:

$$\hat{n}\hat{g}_R(v)f(v)+f(v)\int_0^\infty K(v,v')f(v')\,dv'=Q_0S(v). \tag{1}$$

* Permanent address: Nuclear Engineering Laboratory, University of Bologna, Via dei Colli 16, Bologna 40136, Italy.

0021-9991/85 $3.00

In Eq. (1) $\hat{n}$ is the fixed fp density and Q_0 denotes the intensity of the external source, and

$$K(v, v') = \frac{1}{2vv'} \int_{|v-v'|}^{v+v'} u g_R(u)\, du, \qquad \int_0^\infty S(v)\, dv = 1, \tag{2}$$

where $\hat{g}_R$ and g_R stand for the tp – fp and tp – tp removal microscopic collision frequencies, respectively. The L_1-norm of the nonnegative function f provides the unknown tp density

$$n = \int_0^\infty f(v)\, dv = \| f \|. \tag{3}$$

Because of their physical meaning, the parameters $\hat{n}$ and Q_0 are positive, and the functions $\hat{g}_R$, g_R, and S are nonnegative for $v \in (0, \infty)$. It is assumed, here and in the sequel, that $S(v)/\hat{g}_R(v) \in L_1(0, \infty)$, in agreement with Ref. [1].

A natural field of application of Eq. (1) concerns certain annihilation problems occurring in radiation and positron physics [2, 3]. From a mathematical point of view it can be rewritten as an equation of Hammerstein type [4]

$$\psi(v) = \int_0^\infty K(v, v')\, \phi[v', \psi(v')]\, dv', \qquad \phi(v, u) = \frac{Q_0 S(v)}{\hat{n}\hat{g}_R(v) + u}, \tag{4}$$

where $f(v) = \phi[v, \psi(v)]$, but with a function ϕ which is not continuous with respect to u. A more important feature of Eq. (1) is its resemblance to the somewhat simpler H-equation of Chandrasekhar

$$H(\mu) - \mu H(\mu) \int_0^1 \frac{\psi(\mu')}{\mu + \mu'} H(\mu')\, d\mu' = 1, \tag{5}$$

which has been widely studied in neutron transport and astrophysics [5, 6], and for which accurate numerical results have been recently given [7]. The main differences between the two equations are the lack of analyticity properties in the kernel K for the class of nonlinear integral equations described by Eqs. (1) and (2), and the opposite sign in front of the quadratic term, that implies a different trend in the sign of solutions, as is shown in the next section. In another study [9], iterative schemes for a related equation arising in the study of inhomogeneous atmospheres are put on a rigorous footing. We consider here an iterative scheme not available for the equation studied in [9], however, because of the complicated form of that equation.

It is known that [1], by a straightforward application of the contraction mapping principle, and under certain regularity assumptions and restrictions on the various parameters, Eq. (1) admits a solution in the space L_1, which is unique in a suitable ball of L_1, and can be proved to be nonnegative. In this paper we shall construct this solution numerically by iteration, with the aim of providing accurate numerical results for some cases of physical interest. After considering briefly some simple specializations in which all solutions can be found explicitly, and discussing the iterative schemes suggested by Eq. (1) itself (equivalent to those recently proposed [8] and exploited [7] for the solution of the H-equation), we come to the description of the computational method and of the obtained numerical results.

2. Analytically Solvable Cases

In this section we shall examine two cases for which an explicit analytical solution to Eq. (1) can be easily obtained. The first one refers to a monochromatic source

$$S(v) = \delta(v - v_0), \qquad v_0 > 0 \tag{6}$$

where δ is the Dirac delta function. It is easily found that all solutions have the form $f(v) = n\delta(v - v_0)$, as is clear on physical grounds, where the density n follows from the second order algebraic equation

$$K(v_0, v_0)\, n^2 + \hat{n}\hat{g}_R(v_0)\, n - Q_0 = 0, \tag{7}$$

which always has two real roots, one positive (smaller in modulus) and one negative. There are thus two solutions, but only the positive one has a physical meaning. It may be recalled that the situation is different in the case of the H-equation for which two real solutions exist, both positive, only one of which has the proper behavior when analytically continued to the complex plane [6].

Another simple situation for which an analytical solution can be devised is that in which the microscopic collision frequencies are constant: $\hat{g}_R(v) = \hat{C}$ and $g_R(v) = C$. The contraction mapping principle would guarantee [1] existence and uniqueness of the solution to Eq. (1) with norm less than $\hat{n}\hat{C}/2C$, provided the condition

$$Q_0 < \hat{n}^2\hat{C}^2/4C \tag{8}$$

is fulfilled. Anyway Eq. (1) implies directly

$$f(v) = \frac{Q_0}{\hat{n}\hat{C} + Cn}\, S(v), \tag{9}$$

showing that the spectrum remains unchanged with respect to the source shape function $S(v)$ (removal effects are equally effective at all speeds), and yielding by integration the continuity equation for n

$$Cn^2 + \hat{n}\hat{C}n - Q_0 = 0. \tag{10}$$

This equation also admits one positive and one negative root, namely

$$n^{\pm}=\frac{-\hbar\hat{C}\pm[\hbar^2\hat{C}^2+4CQ_0]^{1/2}}{2C}, \tag{11}$$

to be used in $f(v)=nS(v)$ to get the two L_1 solutions to Eq. (1) for this case. The unique nonnegative solution f^+ (the only physical one) has smaller norm, actually less than $\hbar\hat{C}/2C$, but the solutions f^+ and f^- exist regardless of condition (8).

3. Iterative Schemes

The same conditions that guarantee existence and uniqueness of a solution in a suitable ball of L_1 via contraction mapping are also sufficient conditions for the convergence of the iterative procedure

$$\begin{aligned} f_{k+1}(v)&=\frac{1}{\hbar\hat{g}_R(v)}\left[Q_0S(v)-f_k(v)\int_0^\infty K(v,v')f_k(v')\,dv'\right],\\ f_0(v)&=Q_0S(v)/\hbar\hat{g}_R(v), \end{aligned} \tag{12}$$

in the sense that the sequence of approximate solutions f_k converges in the L_1-norm to the unique solution in such a ball. Of course, this is not necessarily the most effective solution technique. Another iterative procedure suggested by Eq. (1) is

$$f_{k+1}(v)=\frac{Q_0S(v)}{\hbar\hat{g}_R(v)+\int_0^\infty K(v,v')f_k(v')\,dv'},\quad f_0(v)=Q_0S(v)/\hbar\hat{g}_R(v), \tag{13}$$

which has the great advantage of preserving positivity at any step, starting from a nonnegative initial guess. The two schemes corresponding to Eqs. (12) and (13) have been considered also for the solution of Chandrasekhar's H-equation, in which case Eq. (12) is not subject to any condition for convergence and Eq. (13) always converges faster [8]. For the present problem it is reasonable to expect similarly that Eq. (13) should again be preferred, and that it could allow us to relax the unphysical restriction on Q_0 associated with Eq. (12).

To obtain more insight, let us examine briefly the two iteration schemes applied to the simple case $\hat{g}_R(v)=\hat{C}$, $g_R(v)=C$, whose solution has been explicitly determined in the previous section. Setting

$$\rho=\frac{\hbar\hat{C}}{Q_0}n,\qquad x=CQ_0/\hbar^2\hat{C}^2, \tag{14}$$

one ends up with the algebraic iterative schemes

$$\rho_{k+1}=1-x\rho_k^2,\qquad \rho_0=1 \tag{15a}$$

and

$$\rho_{k+1} = 1/(1 + x\rho_k), \qquad \rho_0 = 1, \tag{15b}$$

respectively. The exact physical solution is

$$\rho = \frac{(1+4x)^{1/2} - 1}{2x}. \tag{16}$$

Since only positive values of x are considered, the numerical sequence obtained from (15a) is found to converge (again by contraction mapping) when $x < \frac{1}{4}$. In general the ρ_k are polynomials in x of increasing order; the convergence is alternating, with two monotone subsequences converging to the limit from above and below. There is numerical evidence of convergence even for $x \geqslant \frac{1}{4}$, but it becomes slower and slower with increasing x, until a breakdown occurs at about $x = \frac{3}{4}$, when the monotone subsequences no longer converge to the same limit. If x is increased to unity, we get a sequence oscillating between 0 and 1. For x increasing beyond 1, there appears to be more and more subsequences converging to different, even negative limits, until the ρ_k just appear as random numbers; eventually the sequence divergences for $x > 2$. In turn, the iteration procedure (15b) yields instead the ρ_k as rational functions of x, which can be expressed in the continued fraction notation [10] as

$$\rho_k = \frac{1}{x}\underbrace{\left(\frac{x}{1+}\,\frac{x}{1+}\cdots\right)}_{k \text{ times}} = \frac{B_k}{B_{k+1}}. \tag{17}$$

The positive numbers B_k are uniquely determined by

$$B_k = B_{k-1} + xB_{k-2}, \qquad B_{-1} = 0,\ B_0 = 1. \tag{18}$$

The behaviour of this second sequence ρ_k has been tested numerically for several x in the interval $(0, \infty)$. A slight decrease of convergence rate as x increases has been noted, as expected, but no breakdown occurs. The convergence turns out to be always much faster than for the first (polynomial) sequence.

We can actually prove that the sequence ρ_k of Eq. (15b) converges for $k \to \infty$, to the appropriate solution (16) for any $x > 0$. For B_k, in fact, the following recursion formula

$$B_k = \tfrac{1}{2}B_{k-1} + [(x + \tfrac{1}{4})\, B_{k-1}^2 + (-1)^k\, x^{k+1}]^{1/2} \tag{19a}$$

holds for $k = 0$, and can be proved by induction for $k > 0$. Using in fact Eq. (18) yields first

$$B_k^2 - B_{k+1}B_{k-1} = (-1)^{k-1}\, x^{k+1}. \tag{19b}$$

We then evaluate B_{k+1} from Eq. (18), eliminate B_{k-1} by using Eq. (19b), and solve the resulting quadratic equation for B_{k+1}, selecting the only positive root, to find just the recursion relation (19a) for the index $k+1$. This implies in particular that Eq. (19b) is valid for any value of k, and a consequence of (19b) is

$$\frac{B_{k+2}}{B_{k+3}} - \frac{B_k}{B_{k+1}} = \frac{B_{k+1}^2 - B_{k+2}B_k}{B_{k+1}B_{k+3}} = (-1)^k \frac{x^{k+2}}{B_{k+1}B_{k+3}}, \tag{19c}$$

where the sign of the r.h.s. depends thus only on the value of k. Therefore the subsequence $\rho_{2k} = B_{2k}/B_{2k+1}$ is monotonically increasing, while the subsequence $\rho_{2k+1} = B_{2k+1}/B_{2k+2}$ is monotonically decreasing and both must have a nonnegative limit, L_e and L_0, respectively. Equation (18) implies also

$$\frac{B_k}{B_{k-1}} = 1 + x\frac{B_{k-2}}{B_{k-1}}, \tag{20a}$$

and, in the limit for $k \to \infty$, with k even, and, respectively, odd, we get

$$L_0^{-1} = 1 + xL_e, \qquad L_e^{-1} = 1 + xL_0, \tag{20b}$$

and finally, from the difference, $L_0 = L_e$. The subsequences have a common limit L satisfying

$$xL^2 + L - 1 = 0, \tag{20c}$$

so that, since $L > 0$, the limit L is just equal to ρ, as given by Eq. (16). It may be noted that the limit always lies between the two successive approximations ρ_k and ρ_{k+1}.

4. Convergence in the General Case

The analysis of the previous section gives good evidence that Eq. (13) should be preferred to Eq. (12) to get accurate numerical solutions of Eq. (1). Another point to be taken into account is that, in the case of Eq. (13), if some approximation f_k has been found which is too small on the average, the iterate arising from it will be on the average too large, and vice versa [7].

Even though we do not know in general the number of solutions to Eq. (1), or if they exist at all, and in particular we do not know the number of physical ones, nevertheless the convergence of the iterative scheme of Eq. (13) can be guaranteed under suitable assumptions. More precisely, let us suppose that there is a nonnegative solution $f(v)$ to Eq. (1). Consider then

$$\gamma(v) = 1 - \frac{\hat{n}\hat{g}_R(v)}{Q_0 S(v)} f(v) = 1 - \frac{f(v)}{f_0(v)}, \tag{21}$$

for which we have, in view of Eq. (1), $0 \leqslant \gamma(v) \leqslant 1$ for any v. Suppose further that

$$\gamma_0 = \sup_{v \in (0,\infty)} \gamma(v) < 1. \tag{22}$$

Then the sequence $f_k(v)$, defined by Eq. (13), converges pointwise to $f(v)$.

To prove this, we first remark that Eq. (22) implies

$$(1+p) f(v) < f_0(v) < (1+q) f(v), \tag{23}$$

where p and q are real numbers with $-1 < p < 0 < q < \infty$. Inserting Eq. (23) into the right hand side of Eq. (13) yields now, on account of Eq. (1),

$$\left[1 - \frac{q\gamma(v)}{1+q\gamma(v)}\right] f(v) \leqslant f_1(v) \leqslant \left[1 - \frac{p\gamma(v)}{1+p\gamma(v)}\right] f(v), \tag{24a}$$

and in particular

$$\left(1 - \frac{q\gamma_0}{1+q\gamma_0}\right) f(v) \leqslant f_1(v) \leqslant \left(1 - \frac{p\gamma_0}{1+p\gamma_0}\right) f(v). \tag{24b}$$

The same procedure is then repeated for the higher order approximations $f_2, f_3, \ldots$, to verify that the upper and lower limits for the general $f_k(v)$ both converge to $f(v)$ when $k \to \infty$. This is actually the case, due to Eq. (22); the details are omitted here since the proof is, from now on, a straightforward extension of the one given in Ref. [8] for the H-equation.

Of the existence of one physical nonnegative solution we have numerical evidence in all considered cases.

5. Numerical Methods and Results

We have constructed numerical solutions of Eq. (1) using the iterative schemes of both Eqs. (12) and (13) for several different cases of interest. We used a Maxwellian source

$$S(v) = 4\pi^{-1/2} \beta^{3/2} v^2 e^{-\beta v^2}, \tag{25a}$$

with

$$\beta = m/2k_B T. \tag{25b}$$

The integral in the equation was approximated by Gauss quadrature, and we thus solved for $f(v)$ at the speed points specified by the chosen quadrature scheme. With this approximation Eq. (13) may be written

$$f_{k+1}(v_l) = Q_0 S(v_l) \left[\hat{n} \hat{g}_R(v_l) + \sum_{m=1}^{N} K(v_l, v_m) f_k(v_m)\, w_m \right]^{-1}, \qquad l = 1, 2, \ldots, N \tag{26}$$

where the v_l are the nodes in the N-point quadrature scheme, and w_m the corresponding weights.

Note that during each iteration, for each successive l we know $f_{k+1}(v_m)$ for $1 \leqslant m \leqslant l-1$, thus we can use these most recent values for f on the right hand side of Eq. (26); i.e., we rewrite Eq. (26) in the form

$$\begin{aligned} f_{k+1}(v_l) = Q_0 S(v_l) \Bigg[& \hat{n}\hat{g}_R(v_l) + \sum_{m=1}^{l-1} K(v_l, v_m) f_{k+1}(v_m)\, w_m \\ & + \sum_{m=l}^{N} K(v_l, v_m) f_k(v_m)\, w_m \Bigg]^{-1}, \qquad l = 1, 2, ..., N. \end{aligned} \tag{27}$$

This progressive "updating" of the solution within each iteration has a very positive effect on the convergence rate, and in some cases produces convergence when it is not obtainable otherwise.

Solutions were obtained for a wide variety of removal microscopic collision frequencies of the general form

$$\hat{g}_R(v) = \hat{C} v^r, \qquad g_R(v) = C v^s, \qquad r, s = -3, -2, ..., 1, 2. \tag{28}$$

With the iterative scheme of Eq. (13), convergence was always achieved, typically in 15 iterations or less, when we required agreement to 12 significant figures between successive iterates at each speed point. As expected on the basis of the discussion in Section 4, the convergence is not monotone, but oscillating, and there are two subsequences of functions, one converging from above and one from below to the exact solution, with no overlapping between successive approximations. The same trend was found for the numerical sequence (15b).

The iterative scheme of Eq. (12) was not nearly so well behaved. Without updating, convergence was achieved only for small values of Q_0 slightly beyond the limit given in Ref. [1] by contraction mapping. Updating can produce convergence also for some larger value of Q_0, and accelerates convergence, but typically 80 or 100 iterations are required, instead of the 10 or 12 which are typical for Eq. (27). The scheme of Eq. (13) instead always converges, for any Q_0, and in relatively few iterations (25 or less for Q_0 as large as 10^3 times the contraction mapping limit).

In Tables I through V we give results of our calculations for different values of the exponents r and s in Eq. (28), for which we used various combinations of -1, 0, and 1. The values 0 and 1 correspond to the case of constant collision frequency and constant cross section, respectively. The parameters $\hat{n}$, $\hat{C}$, C, Q_0, and β have been taken to be unity in all cases. Each table shows the converged values of the distribution function f and of its ratio to the shape S of the external source versus the speed v, at some selected points

$$v_j = \frac{j}{20-j}, \qquad j = 1, 2, ..., 19. \tag{29}$$

TABLE I

$\hat{g}_R(v) = 1$ and $g_R(v) = 1$: $n = 0.618034$

j	f	f/S
1	0.385290(−02)	0.618034
2	0.170079(−01)	0.618034
3	0.421034(−01)	0.618034
4	0.818906(−01)	0.618034
5	0.138676	0.618034
6	0.213194	0.618034
7	0.302613	0.618034
8	0.397462	0.618034
9	0.478047	0.618034
10	0.513101	0.618034
11	0.467775	0.618034
12	0.330763	0.618034
13	0.152868	0.618034
14	0.328064(−01)	0.618034
15	0.154914(−02)	0.618034
16	0.251134(−05)	0.618034
17	0.507545(−12)	0.618034
18	0.750118(−33)	0.618034
19	0.0	—

TABLE II

$\hat{g}_R(v) = v$ and $g_R(v) = v$: $n = 0.591837$

j	f	f/S
1	0.996453(−02)	0.159839(+01)
2	0.402240(−01)	0.146166(+01)
3	0.908653(−01)	0.133381(+01)
4	0.160804	0.121360(+01)
5	0.246782	0.109983(+01)
6	0.341954	0.991300
7	0.434258	0.886897
8	0.505301	0.785719
9	0.531620	0.687294
10	0.491360	0.591846
11	0.378812	0.500494
12	0.222160	0.415108
13	0.835148(−01)	0.337645
14	0.142889(−01)	0.269187
15	0.524875(−03)	0.209401
16	0.638168(−06)	0.157051
17	0.910407(−13)	0.110860
18	0.847180(−34)	0.698006(−01)
19	0.0	—

TABLE III

$\hat{g}_R(v) = v^{-1}$ and $g_R(v) = v^{-1}$: $n = 0.708964$

j	f	f/S
1	0.317222(−03)	0.508849(−01)
2	0.285116(−02)	0.103606
3	0.107828(−01)	0.158280
4	0.284974(−01)	0.215072
5	0.615367(−01)	0.274250
6	0.116002	0.336281
7	0.196838	0.402007
8	0.304150	0.472940
9	0.426778	0.551751
10	0.533878	0.643060
11	0.571145	0.754608
12	0.481023	0.898795
13	0.270632	0.109415(+01)
14	0.725404(−01)	0.136658(+01)
15	0.440024(−02)	0.175549(+01)
16	0.951087(−05)	0.234060(+01)
17	0.272306(−11)	0.331585(+01)
18	0.639185(−32)	0.526635(+01)
19	0.0	—

TABLE IV

$\hat{g}_R(v) = 1$ and $g_R(v) = v$: $n = 0.566873$

j	f	f/S
1	0.385392(−02)	0.618198
2	0.170122(−01)	0.618191
3	0.421117(−01)	0.618155
4	0.818899(−01)	0.618029
5	0.138595	0.617674
6	0.212771	0.616808
7	0.301071	0.614886
8	0.392884	0.610916
9	0.466597	0.603230
10	0.489268	0.589327
11	0.428520	0.566169
12	0.284393	0.531390
13	0.119992	0.485121
14	0.228433(−01)	0.430341
15	0.928132(−03)	0.370282
16	0.124359(−05)	0.306045
17	0.194960(−12)	0.237401
18	0.198909(−33)	0.163885
19	0.0	—

TABLE V

$\hat{g}_R(v) = v$ and $g_R(v) = 1$: $n = 0.618307$

j	f	f/S
1	0.929163(−02)	0.149045(+01)
2	0.377278(−01)	0.137096(+01)
3	0.857155(−01)	0.125821(+01)
4	0.152598	0.115167(+01)
5	0.235784	0.105082(+01)
6	0.329509	0.955221
7	0.423280	0.864477
8	0.500482	0.778226
9	0.538464	0.696142
10	0.513014	0.617930
11	0.411227	0.543322
12	0.252648	0.472075
13	0.999191(−01)	0.403967
14	0.179839(−01)	0.338795
15	0.692742(−03)	0.276372
16	0.879854(−06)	0.216530
17	0.130665(−12)	0.159110
18	0.126188(−33)	0.103968
19	0.0	—

Note that the right hand side of Eq. (1) vanishes at $v = 0$, so that both nonnegative terms in the l.h.s. must also vanish at $v = 0$. Since $K(v, v')$ tends to $g_R(v')$ for $v \to 0$, we have in particular $f(0) = 0$, and f/S is at least $O(1)$ for $v \to 0$. The total density n is given in the table caption. When $r = s = 0$, the ratio f/S is of course constant, and the total density n coincides with the result of Eq. (16), namely $(5^{1/2} - 1)/2$.

For each case, successively higher order quadrature sets were used until the computed results failed to change by more than ± 1 digit in the last significant figure shown in the tables. Thus we have confidence in the tabulated results to the number of significant figures given. In all tables convergence was achieved within 13 iterations and with no more than 400 quadrature points.

Acknowledgments

The authors thank Dr. C. V. M. van der Mee for discussions and for calling their attention to Ref. [7]. One of the authors (G. S.) gratefully acknowledges research opportunities and kind hospitality offered to him by the Department of Physics and the Laboratory for Transport Theory and Mathematical Physics of the Virginia Polytechnic Institute and State University during Fall 1983. Another author (J.R.T.) acknowledges partial support from the U. S. National Science Foundation. The paper was also supported in part by Department of Energy Contract DE-AS05-80ER10711.

REFERENCES

1. V. C. BOFFI AND G. SPIGA, *J. Math. Phys.* **24** (1983), 1625.
2. M. HAISSINSKY, "The Chemical and Biological Action of Radiation," Academic Press, London/New York, 1961.
3. E. SEGRE, "Nuclei and Particles: An Introduction to Nuclear and Subnuclear Physics," Benjamin, New York, 1964.
4. F. G. TRICOMI, "Integral Equations," Interscience, New York, 1957.
5. I. W. BUSBRIDGE, "The Mathematics of Radiative Transfer," Cambridge Univ. Press, Cambridge, 1960.
6. R. L. BOWDEN AND P. F. ZWEIFEL, *Astrophys. J.* **210** (1976), 178.
7. P. B. BOSMA AND W. A. DE ROOIJ, *Astron. Astrophys.* **126** (1983), 283.
8. C. T. KELLEY, *J. Math. Phys.* **21** (1980), 403.
9. C. T. KELLEY, *J. Integral Eqs.* **4** (1982), 221.
10. M. ABRAMOWITZ AND I. A. STEGUN, "Handbook of Mathematical Functions," Dover, New York, 1965.